

**Cross sections for collisions of electrons, positive and negative ions,
and neutral atoms and molecules with H₂ and surfaces
for modeling low pressure discharges in H₂**

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Referencing:

A.V. Phelps, private communication, <http://www.lxcat.laplace.univ-tlse.fr>.

*This paper is obtained using automatic conversion from original Wolfram
Mathematica® file. Some references, figures, tables or comments can be missing.*

Cross sections for collisions of electrons, positive and negative ions, and neutral atoms and molecules with H₂ and surfaces for modeling low pressure discharges in H₂.

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Abstract

We report a compilation of cross sections that have been used² to model the collisional kinetics of low-pressure discharges in H₂. Processes that are considered include momentum transfer, H_α excitation, ionization, and charged pair formation in collisions of H⁺, H₂⁺, H₃⁺, H, H₂, and H⁻ with H₂; collisions of ions and atoms with surfaces resulting in electron and ion induced secondary electrons, particle reflection, atom excitation, and negative ion formation. The emphasis is on heavy particle collisions with a minimal set of electron cross sections, including electron momentum transfer, excitation, and ionization collisions with H₂ and e + H₃⁺ recombination. The compilation includes a section reviewing data sources for each major category. The recommendations are expressed as analytic formulas. This compilation is expected to be refined from time to time. As part of the Plasma Data Exchange Project, the compilation will be made available at <http://www.icecat.laplace.univ-tlse.fr/>.

The notes are Adobe PDF©translations of Mathematica 7©notebooks (available on request) and so contain many lines of commands not relevant to the data compilation. File size: 8Mb and 400+ pages.

² A. V. Phelps, Phys. Rev. E 79, 066401 (2009); Plasma Sources Sci. Technol. 20, 043001 (2011); GEC11 Poster QRP1.00066

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Outline of notes

1. H^+ collisions with H_2 .
2. H_2^+ collisions with H_2 .
3. H_3^+ collisions with H_2
4. H^- collisions with H_2
5. H collisions with H_2 .
6. H_2 collisions with H_2 .
7. Surface effects
 - (a) Ion induced electron emission
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 - (c) Secondary and backscattered electrons
 - (d) Atom excitation at surface
 - (e) Negative ion production at surface
8. Electron collisions
 - (a) Electron beam cross sections
 - (b) Electron swarm coefficients
 - (c) Electron - H_3^+ recombination
9. Summary of analytical expressions for angle integrated cross sections.

Appendix: Differential cross sections for $H^+ + H_2$ elastic collisions

.....

Please inform the author of the errors you find at avp@jila.colorado.edu.

1 H+ collisions with
H2

Collisions of H+ with H2: cross sections

Setup notebook environment

```
In[151]:= a = 1.;
```

```
In[152]:= ClearAll["Global`*"];
```

```
In[153]:= Remove["Global`*"];
```

```
In[154]:= startclock = SessionTime[];
```

```
In[155]:= Off[General::spell];
```

```
In[156]:= Off[General::spell1];
```



```
In[157]:= SetDirectory["c:\\users\\avp\\documents\\Mathbook\\Hydrogen\\H2HpCollisions"]
```

```
Out[157]= c:\\users\\avp\\documents\\Mathbook\\Hydrogen\\H2HpCollisions
```

```
In[158]:= plotColorsLines = {
  (*1-red*) {Hue[0.0], Thickness[0.007], Dashing[{}]},
  (*2-orange*) {Hue[0.1], Thickness[0.007], Dashing[{}]},
  (*3-green*) {Hue[0.3], Thickness[0.007], Dashing[{}]},
  (*4-cyan*) {Hue[0.5], Thickness[0.007], Dashing[{}]},
  (*5-dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{}]},
  (*6-purple*) {Hue[0.8], Thickness[0.007], Dashing[{}]},
  (*7-black*) {Thickness[0.007], Dashing[{}]},
  (*8-dash red*) {Hue[0.0], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*9-dash orange*) {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*10-dash green*) {Hue[0.3], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*11-dash cyan*) {Hue[0.5], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*12-dash dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*13-dash purple*) {Hue[0.8], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*14-dash black*) {Thickness[0.007], Dashing[{0.02, 0.02}]}];

In[159]:= plotColorsPoints = {
  (*1-red*) {Hue[0.0], PointSize[0.02]},
  (*2-orange*) {Hue[0.1], PointSize[0.02]},
  (*3-green*) {Hue[0.3], PointSize[0.02]},
  (*4-cyan*) {Hue[0.5], PointSize[0.02]},
  (*5-dk blue*) {Hue[0.7], PointSize[0.02]},
  (*6-purple*) {Hue[0.8], PointSize[0.02]},
  (*7-yellow*) {Hue[0.2], PointSize[0.02]},
  (*8-black*) {PointSize[0.02]}
};
```

- This procedure imports a graph read by the HP scanner. It then allows me to read off points and prepare an output file of the points read.

One way to scan and import the image to be analyzed is to:

- 1) enlarge image as much as possible with copier if it can be done without distortion
- 2) use the HP Deskscan II to Preview the image
- 3) select the portion of the image to be analyzed
- 4) use Final to make a *.bmp file of the image
- 5) start the desired Mathematica notebook
- 6) in Mathematica use Import[*.bmp] to place the image in the notebook.
- 7) use Show to display the image

To read the points from the graph

- 1) enlarge the graph as much as possible while keeping all of image on screen.
 - 2) click on the figure to get the frame. This activates the cursor for the next step.
 - 3) holding ^cntrl down, move mouse pointer to first point and control-click on the desired data point.
- If one then moves to the desired points in succession keeping ^cntrl down, the final list will be in the correct list format.
- 4) with ^cntrl still down, select Copy from the Edit menu
 - 5) select the text insertion point and click on Paste from the Edit menu
 - 6) note that it seems to work better if one uses only two points for the xscale and two for the yscale
 - 7) after reading points, reduce the size of the image and make the Import and Show cells not evaluated to avoid reimporting and/or losing the image later.

H+ + H2 cross sections

Total Q for elastic and inelastic scattering of H+ by H2 from Krstic and Schultz (1999), Fig. 1a

```
Import ["KrsticH2Hp.bmp"];
Show[%];
```

- Record of desired data points and representative points for both axes.

The total elastic cross section curve Qt gives

```
In[160]:= qtdata ={{307.155, 1881.63}, {343.353, 1877.61},
  {367.486, 1877.61}, {385.585, 1869.57},
  {403.685, 1857.5}, {421.784, 1847.44},
  {435.861, 1839.4}, {445.916, 1839.4},
  {462.005, 1837.39}, {474.071, 1837.39},
  {488.148, 1825.32}, {502.225, 1815.27},
  {516.303, 1811.25}, {532.391, 1809.24},
  {552.501, 1803.2}, {574.623, 1791.14},
  {600.766, 1783.09}, {624.899, 1775.05},
  {649.031, 1769.01}, {669.142, 1764.99},
  {681.208, 1758.96}, {705.34, 1746.89},
  {749.583, 1736.84}, {791.815, 1722.76},
  {821.98, 1714.72}, {858.179, 1698.63},
  {870.245, 1696.62}, {890.356, 1698.63},
  {912.477, 1690.58}, {946.665, 1682.54},
  {1002.97, 1668.46}, {1039.17, 1658.41},
  {1091.46, 1646.34}, {1139.72, 1634.27},
  {1190, 1624.22}, {1222.18, 1614.16},
  {1274.46, 1604.11}, {1294.57, 1600.09}};

In[161]:= xscaledata ={{305.144, 1475.4}, {1294.57, 1469.37}};

In[162]:= xscalegraph = Log[10,{0.1,100.}];

In[163]:= yscaledata ={{303.133, 1521.66}, {309.166, 1923.86}};

In[164]:= yscalegraph =Log[10, {100.0,1000.0}];
```

- Determine relation of screen scale to graph scale for logarithmic x axis and linear y axes

```
In[165]:= analyzeDigitizedData :=
Block[{xscaledata1,xscaledata2,xfit,yscaledata1,yscaledata2,yfit,data1,
xdata,xdatagraph,ydata,ydatagraph,xdataout,ydataout},
xscaledata1 = Flatten[Take[Transpose[xscaledata],1]];
xscaledata2 = Transpose[{xscaledata1,xscalegraph}];
xfit = Fit[xscaledata2,{1,x},x];
yscaledata1 = Flatten[Take[Transpose[yscaledata],-1]];
yscaledata2 = Transpose[{yscaledata1,yscalegraph}];
yfit = Fit[yscaledata2,{1,y},y];
data1 = Transpose[qtdata];
xdata = Take[data1,1];
xdatagraph = Flatten[(xfit /. x ->xdata)];
ydata = Take[data1,-1];
ydatagraph = Flatten[(yfit /. y ->ydata)];
xdataout = Power[10, xdatagraph];
ydataout = Power[10, ydatagraph];
dataout = Transpose[{xdataout,ydataout}];
]
```

```
In[166]:= analyzeDigitizedData
```

```
In[167]:= data1Plot = ListLogLogPlot[dataout, PlotRange -> {{0.1, 100.}, {100., 1000.}},
PlotLabel -> {"Total Q (10^-20 m^2) versus Erel (eV)"},
ImageSize -> 432, PlotStyle -> PointSize[0.02]];
```

Note that this data is plotted versus COM energy.

We change the energy scale to LAB

```
In[168]:= dataout1=Map[#{1.5, (.529)^2}&,dataout,{1}];
```

```
In[169]:= H2HpTotalQKrsticPlot = ListLogLogPlot [
Map[#{1.5, (.529)^2} &, dataout, {1}], PlotRange -> {{0.1, 1000.}, {0.1, 1000.}},
PlotLabel -> {"Total Q (10^-20 m^2) versus Elab (eV)"},
ImageSize -> 432, PlotStyle -> {Hue[0.3], Thickness[0.007]};
```

```
In[170]:= dataout1 // TableForm
```

```
Out[170]/TableForm=
  0.152121 219.742
  0.195859 214.743
  0.231801 214.743
  0.263023 205.083
  0.298451 191.39
  0.33865 180.678
  0.373623 172.551
  0.400793 172.551
  0.448439 170.576
  0.487852 170.576
  0.538233 159.187
  0.593817 150.287
  0.655146 146.868
  0.733024 145.187
  0.843515 140.253
  0.984392 130.896
  1.1815 125.
  1.39832 119.377
  1.65492 115.32
  1.90439 112.696
  2.07176 108.872
  2.45194 101.603
  3.33932 95.9221
  4.48443 88.4935
  5.53566 84.5126
  7.12733 77.0755
  7.75375 76.1937
  8.92257 77.0755
  10.4127 73.604
  13.2197 70.2929
  19.5858 64.8491
  25.2175 61.2232
  36.3287 57.1355
  50.8835 53.3208
  72.2817 50.3395
  90.49 47.5222
  130.352 44.8651
  150. 43.8444
```

Export data to file.

```
In[171]:= dataout1 = Map[ToString[SetPrecision[#, 4.2], FormatType -> FortranForm] &, dataout1, {2}];
```

```
In[172]:= dataout2 = TableForm[dataout1, TableHeadings -> {None,
  {"%LAB energy (eV)", "Qt (10^-20 m^2)"},
  TableSpacing -> {0,1}];
```

```

SetOptions[$Output,PageWidth->120];
outputfile := "c:\\Mathbook\\hydrogen\\h2hpcollisions\\KrsticTheory.dat";
stream1 = OpenWrite[outputfile,PageWidth -> Infinity];
WriteString[stream1, "%",
  StringForm["Totalcross section for fast H+ + H2"],
  "\n",
  ToString[dataout2]];
Close[stream1];
SetOptions[$Output,PageWidth->53];

```

■ Polarization potential scattering

```

In[173]:= mroma = 1. * 2. / (1. + 2.);
mr = mroma * 1.661 * 10^-27;
qe = 1.602 * 10^-19;
ng = 2.69 * 10^25; (*m^-3*)
alphaMcDaniel = 0.808 * 10^-30; (*m^3 from McDaniel (1993)*)
epsilon0 = 0.808 * 10^-12;
ao = 0.529 * 10^-10; (*m*)
me = 9.11 * 10^-31; (*kgm*)
ry = 27.211 / 2; (*eV*)

```

From Lieberman and Lichtenberg (1994), Eq. (3.3.17). Their alphaR is given in terms of McDaniel and Mason's alpha by

```

In[182]:= alphaau = alphaMcDaniel / ao^3

```

```

Out[182]= 5.45814

```

```

In[183]:= kLLieberman = 8.99 * 10^-16 * (alphaau / mroma)^0.5

```

```

Out[183]= 2.57233 × 10^-15

```

■ Langevin cross section

```

In[184]:= langevinQ = 2 * Pi * ao^2 * (13.6 / enrel * alphaau)^0.5 /. enrel -> 2 * enlab / 3

```

```

Out[184]= 1.85536 × 10^-19  $\left(\frac{1}{\text{enlab}}\right)^{0.5}$ 

```

■ Total cross section

For a polarization potential

```

In[185]:= n = 4;

```

The Landau-Lifshitz formula for gammaLL is

```

In[186]:= fn = Pi / 4;

```

```

In[187]:= gammaLL = N[Pi^2 * (2 fn)^(2 / (n - 1)) * Csc[Pi / (n - 1)] / Gamma[2 / (n - 1)]]

```

```

Out[187]= 11.3726

```

Note that the gammaLL formula is different than that given in Massey, Burhop, and Gilbody (1971) or in McDaniel, Mitchell, and Rudd (1993), but gives numbers in exact agreement with Massey et al Table 16.2.

```
In[188]:= qttotal = gammaLL * ao^2 * alphaau^(2/3) * (mr / me / 4 * ry / enrel)^(1/3) /.
enrel -> 2 * enlab / 3 // PowerExpand
```

```
Out[188]= 
$$\frac{1.8126 \times 10^{-18}}{\text{enlab}^{1/3}}$$

```

```
In[189]:= langevinQPlot = LogLogPlot [
  {Evaluate[10^20 * langevinQ], Evaluate[10^20 * qttotal]}, {enlab, 0.005, 10 000},
  PlotRange -> {{0.01, 10 000}, {0.01, 200}}, ImageSize -> 432,
  PlotStyle -> {{Hue[1], Thickness[0.007]}},
  {Hue[1], Dashing[{0.05, 0.05}], Thickness[0.007]}}, DisplayFunction -> Identity];
```

■ Download cross sections from H+ - H2 elastic scattering model from ORNL web site

```
!! h2hpkrstic.txt
```

```
In[190]:= krsticHpH2Table = Transpose[Drop[Drop[Import["h2hpkrstic.txt", "Table"], 4], -1]];
```

```
In[191]:= Dimensions [%]
```

```
Out[191]= {8, 10}
```

```
In[192]:= H2HpElasticTotalQKrsticPlot = ListLogLogPlot[Transpose[[krsticHpH2Table[[1]]*1.5, 10^20*krsticHpH2],
PlotRange -> {{0.1,1000.},{0.1,1000.}}, PlotLabel→{"Total Q (10^-20 m^2) versus Erel (eV)",
Joined -> True, PlotStyle -> {Hue[0.1],Thickness[0.007]}, ImageSize -> 432, DisplayFunction -> Identity];
```

```
In[193]:= H2HpKrsticLangevinPlot = ListLogLogPlot[Transpose[[krsticHpH2Table[[1]]*1.5, 10^20*krsticHpH2Table],
PlotRange -> {{0.1,1000.},{0.1,1000.}}, PlotLabel→{"Total Q (10^-20 m^2) versus Erel (eV)",
Joined -> True, PlotStyle -> {Hue[0.8],Thickness[0.015]}, ImageSize -> 432, DisplayFunction -> Identity];
```

Note conversion to LAB energy

```
In[194]:= Show[H2HpTotalQKrsticPlot, H2HpKrsticLangevinPlot, H2HpElasticTotalQKrsticPlot,
langevinQPlot, PlotLabel → {"H+ + H2: Total Q (10^-20 m^2) versus Elab (eV)"},
ImageSize -> 432, DisplayFunction → $DisplayFunction];
```

■ The total vibrational excitation cross section

```
In[195]:= interpDataout = Interpolation[ToExpression[dataout]]
```

```
Out[195]= InterpolatingFunction [{{0.101414, 100.}}, <>]
```

```

In[196]:= vibrationalExcitation = Table[{krsticHpH2Table[[1, j]] * 1.5,
      (interpDataout[krsticHpH2Table[[1, j]]] - krsticHpH2Table[[2, j]])},
      {j, 5, Length[krsticHpH2Table[[1]]]}]

Out[196]= {{2.9925, 3.73438}, {7.518, 5.26887}, {15., 26.102},
      {29.925, 32.6681}, {75.18, 34.0248}, {150., 24.474}}

In[197]:= H2HpKrsticVibExcitationPlot = ListLogLogPlot[Map[#{1.5, (.529)^2}&, vibrationalExcitation, {1}],
      PlotRange -> {{0.1, 100.}, {0.1, 1000.}}, PlotLabel -> {"Total Q (10^-20 m^2) versus Elab (eV)"},
      Joined -> True, PlotStyle -> {Hue[0.8], Thickness[0.015]}, ImageSize -> 432, DisplayFunction -> Identity];

```

Diffusion Q for elastic and inelastic scattering of H+ by H2 from Krstic and Schultz (1999), Fig. 1b

- Record of desired data points and representative points for both axes.

The total elastic cross section curve Qd gives

```

In[198]:= qtdata = {{305.144, 1415.07}, {345.364, 1409.04},
      {389.607, 1405.02}, {431.839, 1398.98},
      {486.137, 1394.96}, {560.546, 1386.92},
      {604.788, 1380.88}, {642.998, 1374.85},
      {671.153, 1374.85}, {711.373, 1362.78},
      {743.55, 1350.72}, {765.671, 1338.65},
      {803.881, 1318.54}, {842.091, 1300.44},
      {884.323, 1276.31}, {936.61, 1248.16},
      {1004.98, 1213.97}, {1047.22, 1195.87},
      {1089.45, 1173.75}, {1137.71, 1145.59},
      {1177.93, 1125.48}, {1210.11, 1105.37},
      {1254.35, 1075.21}, {1290.55, 1055.1}};

In[199]:= xscaledata = {{303.133, 986.721}, {1290.55, 980.688}};

In[200]:= xscalegraph = Log[10, {0.1, 100.}];

In[201]:= yscaledata = {{303.133, 1041.02}, {305.144, 1382.9}};

In[202]:= yscalegraph = Log[10, {0.1, 100.}];

In[203]:= analyzeDigitizedData

In[204]:= Map[#{1.5, (.529)^2}&, dataout, {1}];

In[205]:= H2HpDiffKrsticPlot = ListLogLogPlot[Map[#{1.5, (.529)^2}&, dataout, {1}],
      PlotRange -> {{0.1, 1000.}, {0.0099, 1000.}}, PlotLabel -> {"Diffusion Q (10^-20 m^2) versus Elab (eV)"},
      Join ImageSize -> 432, PlotStyle -> {Hue[.5], Thickness[0.007]}(*, DisplayFunction -> Identity*);

```

```
In[206]:= dataout // TableForm
```

```
Out[206]/TableForm=  
0.101417 191.554  
0.134372 169.582  
0.183117 156.352  
0.246059 138.389  
0.359756 127.593  
0.605452 108.461  
0.825082 96.0007  
1.07792 84.9887  
1.31259 84.9887  
1.73911 66.5958  
2.17815 52.194  
2.54271 40.8984  
3.32191 27.2421  
4.33989 18.8979  
5.83162 11.6057  
8.40715 6.57136  
13.5635 3.29335  
18.2267 2.2846  
24.4913 1.46119  
34.3271 0.827185  
45.4815 0.550982  
56.9646 0.367005  
77.6276 0.199534  
100. 0.132908
```

We changed the energy scale to LAB

Export data to file.

```
In[207]:= dataout = Map[ToString[SetPrecision[#, 4.2], FormatType -> FortranForm] &, dataout, {2}];
```



```
In[208]:= dataout2 = TableForm[dataout,TableHeadings -> {None,
{"%rel energy (eV)", "elQd (10^-20 m^2)"},
TableSpacing -> {0,1}]
```

```
Out[208]/TableForm=
```

%rel energy (eV)	elQd (10 ⁻²⁰ m ²)
0.10142	191.6
0.13437	169.6
0.1831	156.35
0.2461	138.39
0.3598	127.59
0.6055	108.46
0.8251	96.
1.0779	84.99
1.3126	84.99
1.739	66.6
2.178	52.19
2.543	40.9
3.322	27.24
4.34	18.9
5.832	11.606
8.407	6.571
13.564	3.293
18.23	2.285
24.49	1.4612
34.33	0.8272
45.48	0.551
56.96	0.367
77.63	0.1995
100.	0.13291

```
SetOptions[$Output,PageWidth->120];
outputfile := "c:\\mathbook\\hydrogen\\h2hpcollisions\\KrsticElasticQm.dat";
stream1 = OpenWrite[outputfile,PageWidth -> Infinity];
WriteString[stream1, "%",
StringForm["Cross section for H+ + H2 -> H+ + H2"],
"\n",
ToString[dataout2]];
Close[stream1];
SetOptions[$Output,PageWidth->53];
```

Diffusion Q for elastic and inelastic scattering of H+ by H2 by Bachmann and Reiter copied from Krstic and Schultz (1999), Fig. 1b

- Record of desired data points and representative points for both axes.

The total elastic cross section curve Q_t gives

```
In[209]:= qtdata ={{419.773, 1407.03}, {560.546, 1394.96},
{671.153, 1384.91}, {727.462, 1368.82},
{749.583, 1362.78}, {840.08, 1324.57},
{960.742, 1286.37}, {1049.23, 1268.27},
{1081.4, 1262.23}, {1200.06, 1242.12},
{1282.51, 1226.03}};
```

```
In[210]:= xscaledata ={{301.122, 984.71}, {1290.55, 982.699}};
```

```
In[211]:= xscalegraph = Log[10,{0.1,100.}];
```

```
In[212]:= yscaledata ={{303.133, 1041.02}, {305.144, 1382.9}};
```

```
In[213]:= yscalegraph =Log[10,{0.1,100.}];
```

```
In[214]:= analyzeDigitizedData
```

```
In[215]:= H2HpDiffBachmannPlot = ListLogLogPlot[Map[##{1.5, (.529)^2}&, dataout, {1}], PlotRange -> {{0.1, 100.}, {0
PlotLabel->{" Diffusion Q (10^-20 m^2) versus Elab (eV)"}, Joined -> True,
ImageSize -> 432, PlotStyle -> {Hue[0.7], Thickness[0.007]}, DisplayFunction -> Identity];
```

```
In[216]:= dataout // TableForm
```

```
Out[216]/TableForm=
0.228958 162.832
0.611769 127.593
1.3242 104.145
1.96194 75.2398
2.28959 66.5958
4.30676 30.7719
10.0001 14.2216
18.5483 9.86554
23.2191 8.73212
53.1654 5.8164
94.5415 4.20208
```

Export data to file.

```
In[217]:= dataout = Map[ToString[SetPrecision[#, 4.2], FormatType -> FortranForm] &, dataout, {2}];
```

```
In[218]:= dataout2 = TableForm[dataout, TableHeadings -> {None,
{"%lab energy(eV)", "elQd(10^-20 m^2)"},
TableSpacing -> {0, 1}]
```

```
Out[218]/TableForm=
%lab energy (eV)  elQd(10^-20 m^2)
0.229            162.8
0.6118          127.59
1.3242          104.14
1.962           75.24
2.29            66.6
4.307           30.77
10.             14.222
18.55          9.866
23.22          8.732
53.17          5.816
94.54          4.202
```

```
SetOptions[$Output, PageWidth->120];
outputfile := "c:\\Mathbook\\Hydrogen\\H2HpCollisions\\ElasticQmBachman.txt";
stream1 = OpenWrite[outputfile, PageWidth -> Infinity];
WriteString[stream1, "%",
StringForm["Cross section for H+ + H2 -> H+ + H2
"],
"\n",
ToString[dataout2]];
Close[stream1];
SetOptions[$Output, PageWidth->53];
```

- Summary of H+ - H2 diffusion cross sections
- Download H+ - H2 elastic scattering from ORNL web site

```
!! H2Hpkrstic.txt
```

```
In[219]:= Import["h2hpkrstic.txt", "CSV"]//TableForm
```

```
Out[219]//TableForm=
```

Krstic and Schulz

Cross Section for H+ + H2

Energy (CM) (eV)	Elastic (a.u.)	Elastic (m ²)	Elastic (a.u.)	Momentum Transfer (m ²)	Momentum Transfer (a.u.)	Momentum Transfer (m ²)	Momentum Transfer (m ²)	Viscosity
0.1000	7.784520E+02	2.241964E-18	1.926340E+02	5.547913E-19	1.226790E+02	3		
0.1995	6.758570E+02	1.946487E-18	1.470050E+02	4.233785E-19	8.974590E+01	2		
0.5012	5.239360E+02	1.508950E-18	1.127690E+02	3.247779E-19	6.665490E+01	1		
1.0000	4.209960E+02	1.212480E-18	8.202520E+01	2.362349E-19	5.336660E+01	1		
1.9950	3.388640E+02	9.759378E-19	5.031730E+01	1.449152E-19	4.289050E+01	1		
5.0120	2.677590E+02	7.711534E-19	1.044350E+01	3.007757E-20	1.809340E+01	5		
10.0000	2.215300E+02	6.380126E-19	2.470400E+00	7.114821E-21	4.021700E+00			
19.9500	1.782010E+02	5.132239E-19	8.039740E-01	2.315468E-21	1.118240E+00			
50.1200	1.445910E+02	4.164261E-19	1.157880E-01	3.334727E-22	2.078540E-01			
100.00	1.322020E+02	3.807455E-19	3.232590E-02	9.309950E-23	6.313280E-02	1		

This does not include vibrational excitation.

```
In[220]:= krsticH2HpTable = Transpose[Drop[Drop[Import["h2hpkrstic.txt", "Table"], 4], -1]];
```

Dimensions [%]

```
In[221]:= H2HpElasticDiffQKrsticPlot = ListLogLogPlot[Transpose[{krsticH2HpTable[[1]]*1.5, 10^20*krsticH2HpTable[[1]]}, {0.1, 1000.}, {0.0099, 1000.}], PlotLabel->{"Total Q (10^-20 m^2) versus Elab (eV)"}, Joined -> True, PlotStyle -> {Hue[0.1], Thickness[0.007]}, ImageSize -> 432, DisplayFunction -> Identity];
```

```
In[222]:= H2HpKrsticLangevinPlot = ListLogLogPlot[Transpose[{krsticH2HpTable[[1]]*1.5, 10^20*krsticH2HpTable[[1]]}, {0.1, 1000.}, {0.0099, 1000.}], PlotLabel->{"Total Q (10^-20 m^2) versus Elab (eV)"}, Joined -> True, PlotStyle -> {Hue[0.8], Thickness[0.015]}, ImageSize -> 432, DisplayFunction -> Identity];
```

```
In[223]:= Show[H2HpElasticDiffQKrsticPlot , H2HpDiffKrsticPlot , H2HpKrsticLangevinPlot ,
  H2HpKrsticVibExcitationPlot , H2HpDiffBachmannPlot , langevinQPlot ,
  PlotLabel -> {"H+ + H2: Total Q (10^-20 m^2) versus Elab (eV)"},
  ImageSize -> 432, DisplayFunction -> $DisplayFunction];
```

I am amazed (and skeptical) that the total vibrational excitation cross section is so large compared to elastic diffusion scattering.

Viscosity Q for elastic and inelastic scattering of H+ by H2 from Krstic and Schultz (1999), Fig. 1c

- Record of desired data points and representative points for both axes.

The total elastic cross section curve Q_v gives

```
In[224]:= qtdata ={{303.133, 920.356}, {351.398, 910.301},
  {393.629, 904.268}, {417.762, 900.246},
  {451.95, 896.224}, {494.181, 890.191},
  {524.347, 886.169}, {552.501, 880.136},
  {596.744, 876.114}, {626.91, 874.103},
  {657.075, 870.08}, {701.318, 870.08},
  {741.539, 868.069}, {765.671, 866.058},
  {803.881, 853.992}, {846.113, 831.871},
  {886.334, 809.749}, {940.632, 779.584},
  {980.852, 755.451}, {1027.11, 731.319},
  {1057.27, 713.219}, {1101.51, 689.087},
  {1137.71, 664.955}, {1175.92, 644.844},
  {1216.14, 618.701}, {1254.35, 592.557},
  {1288.54, 568.425}};

In[225]:= xscaledata ={{299.111, 496.027}, {1288.54, 489.994}};

In[226]:= xscalegraph = Log[10,{0.1,100.}];

In[227]:= yscaledata ={{299.111, 520.16}, {301.122, 910.301}};

In[228]:= yscalegraph = Log[10,{0.1,100.}];

In[229]:= analyzeDigitizedData
```

Changed to lab energy

```
In[230]:= H2HpViscKrsticPlot = ListLogLogPlot[Map[##{1.5, (.529)^2}&.dataout,{1}], PlotRange -> {{0.1,1000.},{0.00
  PlotLabel->{"Viscosityl Q (10^-20 m^2) versus Erel (eV)"}, Joined -> True,
  ImageSize -> 432, PlotStyle ->{ Hue[0.5],Thickness[0.007]}, DisplayFunction -> Identity];
```

```
In[231]:= dataout // TableForm
```

```
Out[231]/TableForm=
```

0.102848	119.486
0.144058	100.
0.193457	89.8688
0.228958	83.6916
0.29068	77.9389
0.390357	70.0428
0.481867	65.2283
0.586532	58.6199
0.798801	54.5906
0.98606	52.6811
1.21721	49.0591
1.65772	49.0591
2.19515	47.343
2.59797	45.687
3.39226	36.8986
4.55552	24.9408
6.03241	16.8579
8.81302	9.88207
11.6701	6.4458
16.1187	4.20449
19.8965	3.05163
27.0966	1.99053
34.888	1.29839
45.5544	0.909413
60.3225	0.572445
78.7652	0.360329
100.	0.235036

Export data to file.

```
In[232]:= dataout = Map[ToString[SetPrecision[#, 4.2], FormatType -> FortranForm] &, dataout, {2}];
```

```
In[233]:= dataout2 = TableForm[dataout,TableHeadings -> {None,
  {"%lab energy(eV)", "Qv(10^-20 m^2)"},
  TableSpacing -> {0,1}]
```

```
Out[233]/TableForm=
```

%lab energy (eV)	Qv (10 ⁻²⁰ m ²)
0.10285	119.49
0.14406	100.
0.1935	89.87
0.229	83.69
0.2907	77.94
0.3904	70.04
0.4819	65.23
0.5865	58.62
0.7988	54.59
0.9861	52.68
1.2172	49.06
1.658	49.06
2.195	47.34
2.598	45.69
3.392	36.9
4.556	24.94
6.032	16.86
8.813	9.882
11.67	6.446
16.12	4.204
19.9	3.052
27.1	1.991
34.89	1.2984
45.55	0.9094
60.32	0.5724
78.77	0.3603
100.	0.235

```
SetOptions[$Output,PageWidth->120];
outputfile := "c:\\mathbook\\hydrogen\\h2hpcollisions\\h2hpkrsticViscosity.dat";
stream1 = OpenWrite[outputfile,PageWidth -> Infinity];
WriteString[stream1, "%",
  StringForm["Cross section for H+ + H2 -> H+ +H2"],
  "\n",
  ToString[dataout2]];
Close[stream1];
SetOptions[$Output,PageWidth->53];
```

Viscosity Q for elastic and inelastic scattering of H+ by H2 by Bachmann and Reiter from Krstic and Schultz (1999), Fig. 1c

- Record of desired data points and representative points for both axes.

The total elastic cross section curve Qv gives

```
In[234]:= qtdata ={{367.486, 922.367}, {474.071, 912.312},
  {663.108, 888.18}, {705.34, 880.136},
  {783.771, 874.103}, {832.036, 858.014},
  {910.466, 821.816}, {1015.04, 787.628},
  {1069.34, 773.551}, {1288.54, 723.275}};
```

```
In[235]:= xscaledata ={{299.111, 494.016}, {1288.54, 489.994}};
```

```
In[236]:= xscalegraph = Log[10,{0.1,100.}];
```

```
In[237]:= yscaledata ={{299.111, 520.16}, {303.133, 908.29}};
```

```
In[238]:= yscalegraph = Log[10,{0.1,100.}];
```

```
In[239]:= analyzeDigitizedData
```

```
In[240]:= dataout // TableForm
```

```
Out[240]/TableForm=
  0.161182 128.471
  0.339225 107.421
  1.26957  69.9137
  1.70493  60.5881
  2.94791  54.4197
  4.12911  40.8694
  7.13937  21.4591
  14.8161  11.6777
  21.6458  9.08976
  100.     3.71493
```

```
In[241]:= H2HpViscBachmannPlot = ListLogLogPlot[Map[#^{1.5, (.529)^2} &, dataout, {1}], PlotRange -> {{0.1, 110.}, {0.1, 1000.}}, {0.1, 1000.}, {0.1, 1000.}], PlotLabel -> {"Viscosity Q (10^-20 m^2) versus Erel (eV)"}, Joined -> True, ImageSize -> 432, PlotStyle -> {Hue[0.3], Thickness[0.007]}, DisplayFunction -> Identity];
```

- Summary of H+ - H2 viscosity cross sections
- Download H+ - H2 elastic scattering from ORNL web site

```
!! H2Hpkrstic.txt
```

```
In[242]:= H2HpElasticViscQKrsticPlot = ListLogLogPlot[Transpose[{{krsticH2HpTable[[1]]*1.5, 10^20*krsticH2HpT}, {krsticH2HpTable[[2]]*1.5, 10^20*krsticH2HpT}], PlotRange -> {{0.1, 100.}, {0.1, 1000.}}, PlotLabel -> {"Total Q (10^-20 m^2) versus Elab (eV)"}, Joined -> True, PlotStyle -> {Hue[0.1], Thickness[0.007]}, ImageSize -> 432, DisplayFunction -> Identity];
```

```
In[243]:= Show[{H2HpViscKrsticPlot, H2HpViscKrsticPlot, H2HpViscBachmannPlot, langevinQPlot, H2HpElasticViscQKrsticPlot}, PlotLabel -> {"H+ + H2: Total Q (10^-20 m^2) versus Elab (eV)"}, ImageSize -> 432, DisplayFunction -> $DisplayFunction];
```

Export data to file.

```
In[244]:= dataout = Map[ToString[SetPrecision[#, 4.2], FormatType -> FortranForm] &, dataout, {2}];
```

```
In[245]:= dataout2 = TableForm[dataout,TableHeadings -> {None,
{"%rel energy(eV)", "Qt(10^-20 m^2)"},
TableSpacing -> {0,1}]
```

```
Out[245]/TableForm=
```

%rel energy (eV)	Qt (10 ⁻²⁰ m ²)
0.1612	128.47
0.3392	107.42
1.2696	69.91
1.705	60.59
2.948	54.42
4.129	40.87
7.139	21.46
14.816	11.678
21.65	9.09
100.	3.715

```
SetOptions[$Output,PageWidth->120];
outputfile := "c:\\Mathbook\\Hydrogen\\h2hpcollisions\\H2HpNackmannViscosity.dat";
stream1 = OpenWrite[outputfile,PageWidth -> Infinity];
WriteString[stream1, "%",
StringForm["Cross section for H+ + H2 -> H+ + H2"],
"\n",
ToString[dataout2]];
Close[stream1];
SetOptions[$Output,PageWidth->53];
```

- Summary of H+ - H2 total cross sections
- Download H+ - H2 elastic scattering from ORNL web site

```
In[93]:= !! H2Hpkrstic.txt
```

```
In[246]:= Import["H2Hpkrstic.txt", "CSV"] // TableForm
```

```
Out[246]/TableForm=
```

Krstic and Schulz
Cross Section for H+ + H2

Energy (CM) (eV)	Elastic (a.u.)	Elastic (m ²)	Momentum Transfer (a.u.)	Momentum Transfer (m ²)	Viscosity	
0.1000	7.784520E+02	2.241964E-18	1.926340E+02	5.547913E-19	1.226790E+02	3
0.1995	6.758570E+02	1.946487E-18	1.470050E+02	4.233785E-19	8.974590E+01	2
0.5012	5.239360E+02	1.508950E-18	1.127690E+02	3.247779E-19	6.665490E+01	1
1.0000	4.209960E+02	1.212480E-18	8.202520E+01	2.362349E-19	5.336660E+01	1
1.9950	3.388640E+02	9.759378E-19	5.031730E+01	1.449152E-19	4.289050E+01	1
5.0120	2.677590E+02	7.711534E-19	1.044350E+01	3.007757E-20	1.809340E+01	5
10.0000	2.215300E+02	6.380126E-19	2.470400E+00	7.114821E-21	4.021700E+00	
19.9500	1.782010E+02	5.132239E-19	8.039740E-01	2.315468E-21	1.118240E+00	
50.1200	1.445910E+02	4.164261E-19	1.157880E-01	3.334727E-22	2.078540E-01	
100.00	1.322020E+02	3.807455E-19	3.232590E-02	9.309950E-23	6.313280E-02	1

This does not include vibrational excitation.

```
In[247]:= krsticH2HpTable = Transpose[Drop[Drop[Import["H2Hpkrstic.txt", "Table"], 4], -1]];
```



```
In[248]:= Dimensions [%]
```

```
Out[248]= {8, 10}
```

```
In[249]:= H2HTotalQKrsticPlot = ListLogLogPlot[Transpose[{{krsticH2HpTable[[1]]*1.5, 10^20*krsticH2HpTable[[3]
PlotRange -> {{0.1,100.},{0.1,1000.}}, PlotLabel->{"Total Q (10^-20 m^2) versus Elab (eV)"},
Joined -> True, PlotStyle -> {Hue[0.1],Thickness[0.007]}, ImageSize -> 432(*, DisplayFunction -> Identity*
```

■ Energy loss function

```
In[250]:= inelasticLossFcn=Import["H2HpQ&L85.txt", "CSV"]//TableForm
```

```
Out[250]//TableForm=
```

LAB EN EV	L (TOT)
0.15	7.79755555555556
0.3	7.637861111111111
0.75	8.688472222222222
1.5	10.205364444444444
2.25	10.901903333333333
3	11.405407777777778
4.5	10.816516666666667
6	10.560483333333333
7.5	9.875855555555556
10.5	9.353022222222222
13.5	8.664625
15	8.534555555555556
17.55	8.4451
18.75	8.331263888888889
22.5	8.369975
25.5	8.368502777777778
30	8.608534444444445
37.5	8.642186666666667
45	8.459170833333334
60	8.196738888888889
75	7.795025972222222
105	7.491611111111111
150	7.2718
225	7.0772
300	7.4392
450	8.5542
750	10.9943
1050	13.6993
1500	17.0563
2250	22.2915
3000	26.9516
4500	35.63164
7500	50.11488
10500	62.82228
15000	78.28824

```
In[251]:= inelasticLossFcn=Drop[Import["H2HpQ&L85.txt", "Table"], 5];
```

```
In[252]:= inelasticLossFcnPlot=ListLogLogPlot[inelasticLossFcn, PlotRange->{{.1, 10000}, {1, 100}}, PlotSt
```

```
In[253]:= fitInelasticLossFcn=8*(1+(enLab/450)^4)^(1/6) (*10^-20 eV m^2*)
```

$$\text{Out[253]} = 8 \left(1 + \frac{\text{enLab}^4}{41\,006\,250\,000} \right)^{1/6}$$

This was changed on about 9/16/06 to pass through the energy loss function data for rotational and vibrational excitation as in Phelps (1990) and to drop the elastic recoil contribution.

This needs to be redone using the lower vibrational cross sections!!!

```
In[254]:= fit2InelasticLossFcn =1.2*10^-20*enLab^0.45*(1+(enLab/350)^4)^0.02;
```

```
In[255]:= fitInelasticLossFcnPlot=LogLogPlot[{fitInelasticLossFcn,10^20*fit2InelasticLossFcn}, {enLab,
PlotRange->{{1,10000},{1,100}}, PlotStyle->plotColorsLines];
```

```
In[256]:= Show[fitInelasticLossFcnPlot,inelasticLossFcnPlot, ImageSize->400, DisplayFunction->$Display
```

Check energy scale

- H+ - H2 -> H2+ + fast H - charge transfer

- From my 1988 cross section set

```
In[257]:= Import["hph2q88b.txt", "CSV"] // TableForm
```

```
Out[257]/TableForm=
```

H+ + H2 cross sections		recalc	10/02/06	10:27	L'			
Q's in 10^-20 m2		-----Energy bal.-----						
Process	H2+			V=0-2	V=0-3	+fast H	Ly ALPH	Bal AL
	J=0-2	J=1-3	V=0-1					
	4.40E-02	7.30E-02	5.16E-01	1.00E+00	1.50E+00	1.80E+00	1.50E+01	1.5
Lab En.								
1.00E-01	1.30E+01	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-0
1.33E-01	2.00E+01	5.00E+00	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-0
1.78E-01	2.10E+01	1.17E+01	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-0
2.37E-01	2.14E+01	1.23E+01	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-0
3.16E-01	2.25E+01	1.28E+01	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-0
4.22E-01	2.65E+01	1.42E+01	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-0
5.62E-01	2.80E+01	1.64E+01	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-0
7.50E-01	2.90E+01	1.85E+01	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-0
1.00E+00	2.90E+01	1.98E+01	3.90E-02	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-0
1.33E+00	2.87E+01	2.00E+01	8.80E-02	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-0
1.78E+00	2.73E+01	1.90E+01	1.73E-01	2.30E-02	1.00E-05	1.00E-05	1.00E-05	1.00E-0

2.37E+00	2.52E+01	1.78E+01	2.96E-01	6.60E-02	1.20E-02	1.00E-05	1.00E-0
3.16E+00	2.25E+01	1.57E+01	5.10E-01	1.33E-01	4.30E-02	5.90E-01	1.00E-0
4.22E+00	1.98E+01	1.33E+01	7.90E-01	2.13E-01	9.00E-02	7.50E-01	1.00E-0
5.62E+00	1.64E+01	1.09E+01	1.22E+00	3.25E-01	1.43E-01	7.10E-01	1.00E-0
7.50E+00	1.32E+01	8.60E+00	1.78E+00	5.00E-01	2.40E-01	6.15E-01	1.00E-0
1.00E+01	9.80E+00	6.60E+00	2.65E+00	7.20E-01	2.90E-01	5.40E-01	1.00E-0
1.33E+01	7.20E+00	4.80E+00	3.60E+00	1.03E+00	3.95E-01	4.80E-01	1.00E-0
1.78E+01	4.80E+00	3.10E+00	4.60E+00	1.45E+00	5.10E-01	4.35E-01	1.00E-0
2.37E+01	2.85E+00	1.93E+00	5.45E+00	1.86E+00	6.30E-01	3.97E-01	1.00E-0
3.16E+01	1.60E+00	1.08E+00	6.00E+00	2.20E+00	7.30E-01	3.65E-01	1.00E-0
4.22E+01	8.00E-01	5.50E-01	6.30E+00	2.30E+00	7.50E-01	3.40E-01	1.00E-0
5.62E+01	3.60E-01	2.45E-01	6.35E+00	2.20E+00	7.00E-01	3.33E-01	1.00E-0
7.50E+01	1.50E-01	9.50E-02	6.30E+00	1.98E+00	5.40E-01	3.40E-01	7.70E-0
1.00E+02	5.80E-02	3.40E-02	6.10E+00	1.73E+00	4.70E-01	3.70E-01	1.25E-0
1.33E+02	2.10E-02	1.20E-02	5.75E+00	1.45E+00	3.80E-01	4.30E-01	3.00E-0
1.78E+02	8.50E-03	4.60E-03	5.40E+00	1.20E+00	2.90E-01	5.40E-01	7.40E-0
2.37E+02	3.10E-03	1.70E-03	4.90E+00	9.30E-01	2.20E-01	7.30E-01	1.55E-0
3.16E+02	1.10E-03	1.00E-05	4.30E+00	7.10E-01	1.63E-01	1.03E+00	2.90E-0
4.22E+02	1.00E-05	1.00E-05	3.70E+00	5.30E-01	1.18E-01	1.54E+00	5.30E-0
5.62E+02	1.00E-05	1.00E-05	3.15E+00	3.90E-01	8.30E-02	2.30E+00	8.90E-0
7.50E+02	1.00E-05	1.00E-05	2.60E+00	2.75E-01	5.00E-02	3.35E+00	1.37E-0
1.00E+03	1.00E-05	1.00E-05	2.15E+00	1.98E-01	4.00E-02	4.50E+00	1.80E-0
1.33E+03	1.00E-05	1.00E-05	1.72E+00	1.42E-01	2.70E-02	5.70E+00	2.07E-0
1.78E+03	1.00E-05	1.00E-05	1.36E+00	9.80E-02	1.80E-02	6.80E+00	2.24E-0
2.37E+03	1.00E-05	1.00E-05	1.06E+00	6.80E-02	1.20E-02	7.60E+00	2.43E-0
3.16E+03	1.00E-05	1.00E-05	8.10E-01	4.70E-02	1.00E-05	8.20E+00	2.85E-0
4.22E+03	1.00E-05	1.00E-05	6.10E-01	3.23E-02	1.00E-05	8.40E+00	3.65E-0
5.62E+03	1.00E-05	1.00E-05	4.55E-01	2.17E-02	1.00E-05	8.40E+00	4.50E-0
7.50E+03	1.00E-05	1.00E-05	3.25E-01	1.44E-02	1.00E-05	8.30E+00	5.40E-0
1.00E+04	1.00E-05	1.00E-05	2.35E-01	9.50E-03	1.00E-05	8.10E+00	6.50E-0

Note: No Q's or L's for H2+ or H2 excitation or dissociation to gnd. state H atoms.

Qm from thermal mobility:

Ko = 1.60E+01 cm²/V.s at NTP

un = 4.30E+20 V-1s-1cm-1

= 4.30E+22 V-1s-1m-1

Mr = 6.67E-01 au

num/n = e/unMr = 3.36E-15 m³/s

If Q varies as 1/v then: If Q is constant then:

QmE^{0.5} = 1.92E-19 Qm = 8.19E-19 m²

In[258]:= Drop[Drop[Import["hph2q88b.txt", "Table"], 6], -11];

In[259]:= h2HpChgTranQPlot = ListLogLogPlot[Table[{{%[[j,1]],%[[j,7]]},{j,Length[%]}],
PlotRange -> {{0.1,10⁶},{1,100.}}, PlotLabel->{"Total Q (10⁻²⁰ m²) versus LAB energy (eV)"},
PlotStyle -> {Hue[0.1],PointSize[0.02]}, ImageSize -> 432, DisplayFunction -> Identity];

In[260]:= h2HpChgTranFit=UnitStep[w1-2.7]*((4.5 10⁻²⁰*(2*w1/(1000+w1))^{1.7}/((w1/25000)+1)+
(5.5*10⁻²¹/((w1+0.04)/10)^{0.5}))+1.*10⁻³⁰);

```
In[261]:= Import["ORNL6086H2HpChEx.txt", "Table"] // TableForm
```

```
Out[261]//TableForm=
```

2.6206	3.5049	4.6875	6.2692	8.3845	11.214
2.1389×10^{-17}	3.9569×10^{-17}	4.1797×10^{-17}	3.2819×10^{-17}	2.3025×10^{-17}	1.629×10^{-17}

```
In[262]:= Import["ORNL6086H2HpChEx.txt", "Table"];
```

```
In[263]:= redbookChargeTransH2Hp = Transpose[{{%[[1]], %[4] / 10^4 * 10^20}}];
```

```
In[264]:= redbookChargeTransH2HpPlot = ListLogLogPlot[redbookChargeTransH2Hp,
PlotRange -> {{1, 10^6}, {0.01, 10}}, PlotLabel -> {"Total Q (10^-20 m^2) versus LAB energy (eV)"},
PlotStyle -> plotColorsPoints[[1]]];
```

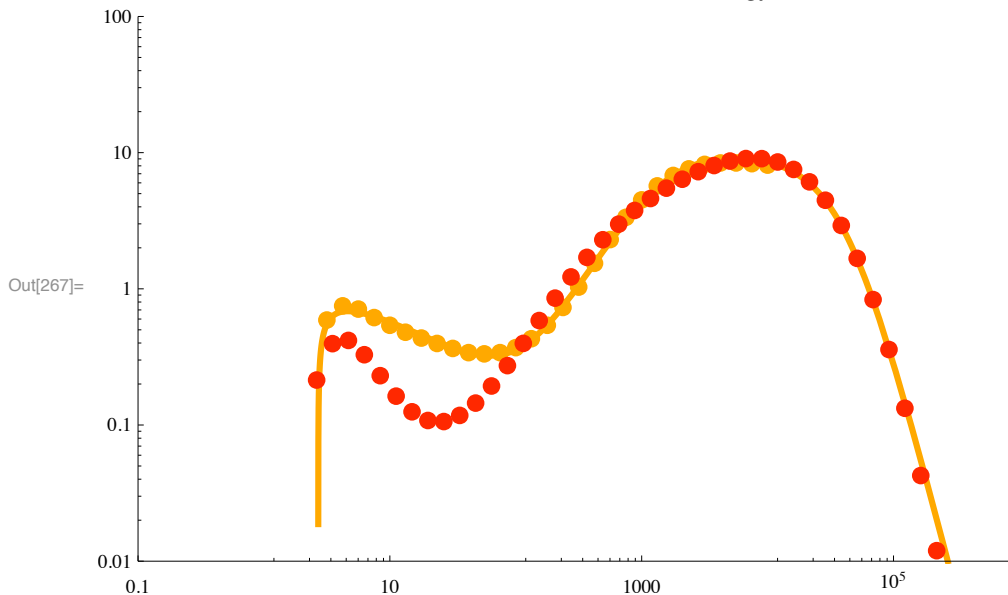
I do not like the way this cross section approaches threshold and so have fitted the tabular data with the following.

```
In[265]:= h2HpChgTranFit = 2.* 10^-20*UnitStep[w1-2.7]/(1+1/(w1-2.7))^0.5/(1+(w1/110)^0.5*(1+(w1/110)^2.1)
(1+(w1/42000)^2)^1.75;
```

```
In[266]:= h2HpChgTranFitPlot = LogLogPlot[10^20*h2HpChgTranFit, {w1, 1, 10^6}, PlotRange -> {{0.1, 10^6}, {0.01, 10}},
PlotStyle -> {Hue[0.1], Thickness[0.007]}, ImageSize -> 432];
```

```
In[267]:= Show[h2HpChgTranFitPlot,h2HpChgTranQPlot,redbookChargeTransH2HpPlot, PlotLabel->{"Total Q (10^20 m^2) versus LAB energy (eV)"}
ImageSize -> 432, DisplayFunction->$DisplayFunction]
```

{Total Q (10²⁰ m²) versus LAB energy (eV)}



■ Summary of H+ - H2 total cross sections

■ Download H+ - H2 elastic scattering from ORNL web site

```
In[268]:= !! h2hpkrstic.txt
```

```
Out[268]= h2hpkrstic.txt
```

```
In[269]:= krsticHpH2Table = Transpose[Drop[Drop[Import["h2hpkrstic.txt", "Table"], 4], -1]];
```

```
In[270]:= Dimensions [%]
```

```
Out[270]= {8, 10}
```

```
In[271]:= H2HTotalQKrsticPlot = ListLogLogPlot[Transpose[{{krsticHpH2Table[[1]]*1.5, 10^20*krsticHpH2Table[[3]]}
PlotRange -> {{0.1,1000.},{0.0099,1000.}}, PlotLabel->{"Total Q (10^-20 m^2) versus Erel (eV)"},
Joined -> True, PlotStyle -> {Hue[0.1],Thickness[0.007]}, ImageSize -> 432, DisplayFunction -> Identity];
```

```
In[272]:= H2HpKrsticQdPlot = ListLogLogPlot[Transpose[{{krsticHpH2Table[[1]]*1.5, 10^20*krsticHpH2Table[[5]]}
PlotRange -> {{0.1,1000.},{0.0099,1000.}}, PlotLabel->{"Total Q (10^-20 m^2) versus Erel (eV)"},
Joined -> True, PlotStyle -> {Hue[0.8],Thickness[0.007]}, ImageSize -> 432, DisplayFunction -> Identity];
```


7.50E-01	2.90E+01	1.85E+01	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-05
1.00E+00	2.90E+01	1.98E+01	3.90E-02	1.00E-05	1.00E-05	1.00E-05	1.00E-05
1.33E+00	2.87E+01	2.00E+01	8.80E-02	1.00E-05	1.00E-05	1.00E-05	1.00E-05
1.78E+00	2.73E+01	1.90E+01	1.73E-01	2.30E-02	1.00E-05	1.00E-05	1.00E-05
2.37E+00	2.52E+01	1.78E+01	2.96E-01	6.60E-02	1.20E-02	1.00E-05	1.00E-05
3.16E+00	2.25E+01	1.57E+01	5.10E-01	1.33E-01	4.30E-02	5.90E-01	1.00E-05
4.22E+00	1.98E+01	1.33E+01	7.90E-01	2.13E-01	9.00E-02	7.50E-01	1.00E-05
5.62E+00	1.64E+01	1.09E+01	1.22E+00	3.25E-01	1.43E-01	7.10E-01	1.00E-05
7.50E+00	1.32E+01	8.60E+00	1.78E+00	5.00E-01	2.40E-01	6.15E-01	1.00E-05
1.00E+01	9.80E+00	6.60E+00	2.65E+00	7.20E-01	2.90E-01	5.40E-01	1.00E-05
1.33E+01	7.20E+00	4.80E+00	3.60E+00	1.03E+00	3.95E-01	4.80E-01	1.00E-05
1.78E+01	4.80E+00	3.10E+00	4.60E+00	1.45E+00	5.10E-01	4.35E-01	1.00E-05
2.37E+01	2.85E+00	1.93E+00	5.45E+00	1.86E+00	6.30E-01	3.97E-01	1.00E-05
3.16E+01	1.60E+00	1.08E+00	6.00E+00	2.20E+00	7.30E-01	3.65E-01	1.00E-05
4.22E+01	8.00E-01	5.50E-01	6.30E+00	2.30E+00	7.50E-01	3.40E-01	1.00E-05
5.62E+01	3.60E-01	2.45E-01	6.35E+00	2.20E+00	7.00E-01	3.33E-01	1.00E-05
7.50E+01	1.50E-01	9.50E-02	6.30E+00	1.98E+00	5.40E-01	3.40E-01	7.70E-05
1.00E+02	5.80E-02	3.40E-02	6.10E+00	1.73E+00	4.70E-01	3.70E-01	1.25E-05
1.33E+02	2.10E-02	1.20E-02	5.75E+00	1.45E+00	3.80E-01	4.30E-01	3.00E-05
1.78E+02	8.50E-03	4.60E-03	5.40E+00	1.20E+00	2.90E-01	5.40E-01	7.40E-05
2.37E+02	3.10E-03	1.70E-03	4.90E+00	9.30E-01	2.20E-01	7.30E-01	1.55E-05
3.16E+02	1.10E-03	1.00E-05	4.30E+00	7.10E-01	1.63E-01	1.03E+00	2.90E-05
4.22E+02	1.00E-05	1.00E-05	3.70E+00	5.30E-01	1.18E-01	1.54E+00	5.30E-05
5.62E+02	1.00E-05	1.00E-05	3.15E+00	3.90E-01	8.30E-02	2.30E+00	8.90E-05
7.50E+02	1.00E-05	1.00E-05	2.60E+00	2.75E-01	5.00E-02	3.35E+00	1.37E-05
1.00E+03	1.00E-05	1.00E-05	2.15E+00	1.98E-01	4.00E-02	4.50E+00	1.80E-05
1.33E+03	1.00E-05	1.00E-05	1.72E+00	1.42E-01	2.70E-02	5.70E+00	2.07E-05
1.78E+03	1.00E-05	1.00E-05	1.36E+00	9.80E-02	1.80E-02	6.80E+00	2.24E-05
2.37E+03	1.00E-05	1.00E-05	1.06E+00	6.80E-02	1.20E-02	7.60E+00	2.43E-05
3.16E+03	1.00E-05	1.00E-05	8.10E-01	4.70E-02	1.00E-05	8.20E+00	2.85E-05
4.22E+03	1.00E-05	1.00E-05	6.10E-01	3.23E-02	1.00E-05	8.40E+00	3.65E-05
5.62E+03	1.00E-05	1.00E-05	4.55E-01	2.17E-02	1.00E-05	8.40E+00	4.50E-05
7.50E+03	1.00E-05	1.00E-05	3.25E-01	1.44E-02	1.00E-05	8.30E+00	5.40E-05
1.00E+04	1.00E-05	1.00E-05	2.35E-01	9.50E-03	1.00E-05	8.10E+00	6.50E-05

Note: No Q's or L's for H2+ or H2 excitation or dissociation to gnd. state H atoms.

Qm from thermal mobility:

Ko = 1.60E+01 cm²/V.s at NTP

un = 4.30E+20 V-1s-1cm-1

= 4.30E+22 V-1s-1m-1

Mr = 6.67E-01 au

num/n = e/unMr = 3.36E-15 m³/s

If Q varies as 1/v then:

If Q is constant then:

QmE^{0.5} = 1.92E-19

Qm = 8.19E-19 m²

```
In[275]:= Drop[Drop[Import["hph2q88b.txt", "Table"], 6], -11];
```

```
In[276]:= Table[{{%[[j, 1]], %[[j, 9]]}, {j, Length[%]}}];
```

```
In[277]:= h2HpAlpha90Plot = ListLogLogPlot[Table[{{%[[j, 1]], %[[j, 9]]}, {j, Length[%]}}], PlotRange -> {{10, 10^4}, {10^-20, 10^2}}, PlotLabel -> {"Total Q (10^-20 m^2) versus LAB energy (eV)", PlotStyle -> {Hue[0.1], PointSize[0.02]}}];
```

■ From ORNL 6086

```
In[278]:= Import["ORNL6086H2HpAlpha.txt", "CSV"] // TableForm
```

```
Out[278]//TableForm=
```

Energy in eV (TargetFrame)		Cross section in cm2		Cross sections cm2 vs eV/amu (Target
5.0397E+02	2.4232E-19	5.0000E+02	2.4232E-19	
5.7763E+02	3.8605E-19	5.7308E+02	3.8605E-19	
6.6206E+02	5.4749E-19	6.5685E+02	5.4749E-19	
7.5883E+02	7.1849E-19	7.5285E+02	7.1849E-19	
8.6974E+02	8.9600E-19	8.6289E+02	8.9600E-19	
9.9687E+02	1.0804E-18	9.8902E+02	1.0804E-18	
1.1426E+03	1.2731E-18	1.1336E+03	1.2731E-18	
1.3096E+03	1.4749E-18	1.2993E+03	1.4749E-18	
1.5010E+03	1.6853E-18	1.4892E+03	1.6853E-18	
1.7204E+03	1.9018E-18	1.7068E+03	1.9018E-18	
1.9718E+03	2.1204E-18	1.9563E+03	2.1204E-18	
2.2601E+03	2.3366E-18	2.2422E+03	2.3366E-18	
2.5904E+03	2.5465E-18	2.5700E+03	2.5465E-18	
2.9690E+03	2.7476E-18	2.9456E+03	2.7476E-18	
3.4030E+03	2.9398E-18	3.3762E+03	2.9398E-18	
3.9004E+03	3.1258E-18	3.8696E+03	3.1258E-18	
4.4705E+03	3.3110E-18	4.4352E+03	3.3110E-18	
5.1239E+03	3.5034E-18	5.0835E+03	3.5034E-18	
5.8728E+03	3.7124E-18	5.8266E+03	3.7124E-18	
6.7312E+03	3.9488E-18	6.6782E+03	3.9488E-18	
7.7151E+03	4.2234E-18	7.6543E+03	4.2234E-18	
8.8427E+03	4.5465E-18	8.7731E+03	4.5465E-18	
1.0135E+04	4.9262E-18	1.0055E+04	4.9262E-18	
1.1617E+04	5.3670E-18	1.1525E+04	5.3670E-18	
1.3315E+04	5.8667E-18	1.3210E+04	5.8667E-18	
1.5261E+04	6.4133E-18	1.5140E+04	6.4133E-18	
1.7491E+04	6.9808E-18	1.7353E+04	6.9808E-18	
2.0048E+04	7.5262E-18	1.9890E+04	7.5262E-18	
2.2978E+04	7.9890E-18	2.2797E+04	7.9890E-18	
2.6337E+04	8.2957E-18	2.6129E+04	8.2957E-18	
3.0186E+04	8.3706E-18	2.9948E+04	8.3706E-18	
3.4598E+04	8.1545E-18	3.4326E+04	8.1545E-18	
3.9655E+04	7.6239E-18	3.9343E+04	7.6239E-18	
4.5451E+04	6.8060E-18	4.5093E+04	6.8060E-18	
5.2095E+04	5.7794E-18	5.1684E+04	5.7794E-18	
5.9709E+04	4.6573E-18	5.9239E+04	4.6573E-18	
6.8436E+04	3.5597E-18	6.7897E+04	3.5597E-18	
7.8439E+04	2.5843E-18	7.7821E+04	2.5843E-18	
8.9904E+04	1.7880E-18	8.9196E+04	1.7880E-18	
1.0304E+05	1.1849E-18	1.0223E+05	1.1849E-18	
1.1811E+05	7.5717E-19	1.1718E+05	7.5717E-19	
1.3537E+05	4.7000E-19	1.3430E+05	4.7000E-19	
1.5516E+05	2.8551E-19	1.5393E+05	2.8551E-19	
1.7783E+05	1.7079E-19	1.7643E+05	1.7079E-19	
2.0383E+05	1.0094E-19	2.0222E+05	1.0094E-19	
2.3362E+05	5.8864E-20	2.3178E+05	5.8864E-20	
2.6777E+05	3.3570E-20	2.6566E+05	3.3570E-20	
3.0690E+05	1.8368E-20	3.0448E+05	1.8368E-20	
3.5176E+05	9.3269E-21	3.4899E+05	9.3269E-21	
4.0318E+05	4.1738E-21	4.0000E+05	4.1738E-21	


```
In[279]:= Drop[Import["ORNL6086H2HpAlpha.txt", "Table"], 1];
```

```
In[280]:= ornl6086HpAlpha = Table[{%[[j, 1]], %[j, 2]] / 10^4 * 10^20}, {j, Length[%]}];
```

```
In[281]:= ornl6086HpAlphaPlot = ListLogLogPlot[ornl6086HpAlpha, PlotRange -> {{10, 10^6}, {0.0001, 1}},
  PlotLabel -> {"Total Q (10^-20 m^2) versus LAB energy (eV)", PlotStyle -> plotColorsPoints[[1]]];
```

From H2XSectPubNegIon051710_7.nb

```
In[282]:= q1haOld[w1_] :=
  6. * 10^-28 * UnitStep[w1 - 50] (w1 - 50)^2 / (1 + (w1 / 700)^4)^0.5 * (1 + (w1 / 3000)^4)^0.25;
```

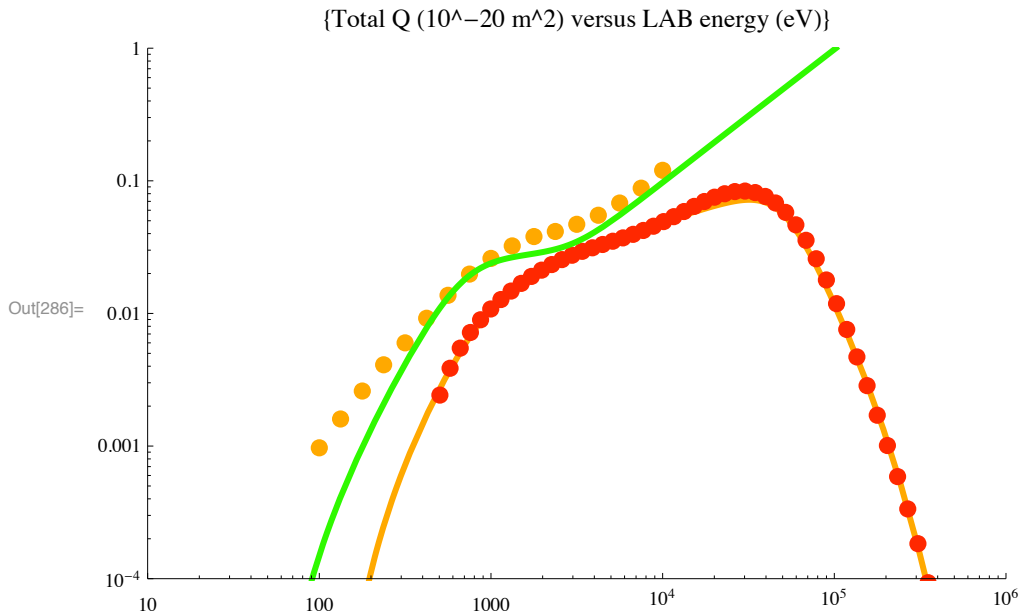
```
In[283]:= h2HpAlphaOldFitPlot = LogLogPlot[10^20 * q1haOld[w1], {w1, 10, 10^6}, PlotRange -> {{10, 10^6}, {0.0001, 1}},
  PlotStyle -> {Hue[0.3], Thickness[0.007]}];
```

In order to fit the ORNL 6086 recommendation, we need to reduce q1ha and shift it to higher energies.

```
In[284]:= q1haNew[w1_] := 2. * 10^-28 * UnitStep[w1 - 125] (w1 - 125)^2 / (1 + (w1 / 1000)^3.2)^0.5 *
  (1 + (w1 / 50000)^4)^0.25 / (1 + (w1 / 50000)^4.3 + (w1 / 100000)^7.5);
```

```
In[285]:= h2HpAlphaNewFitPlot = LogLogPlot[10^20 * q1haNew[w1], {w1, 10, 10^6}, PlotRange -> {{10, 10^6}, {0.0001, 1}},
  PlotStyle -> {Hue[0.1], Thickness[0.007]}];
```

```
In[286]:= Show[h2HpAlphaNewFitPlot,orn16086HpAlphaPlot,h2HpAlpha90Plot,h2HpAlphaOldFitPlot,
PlotLabel->{"Total Q (10^-20 m^2) versus LAB energy (eV)"},
ImageSize -> 432, DisplayFunction->$DisplayFunction]
```



■ H- formation - Barnett Red Book

```
In[287]:= Import["barnett.txt", "CSV"] // TableForm
```

```
Out[287]//TableForm=
  5.0E-02  2.7E-17  1E-30  1E030
  1.0E-01  4.1E-17  1E-30  1E-30
  2.0E-01  7.3E-17  1.2E-20  1E-30
  5.0E-01  2.3E-16  4.4E-20  1E-30
  1.0E+00  5.2E-16  1.2E-19  1E-30
  2.0E+00  8.5E-16  3.8E-19  4.5E-18
  5.0E+00  8.6E-16  1.6E-18  2.1E-17
  1.0E+01  8.5E-16  4.7E-18  2.2E-17
  2.0E+01  6.0E-16  1.0E-17  1.9E-17
  4.0E+01  2.6E-16  2.5E-18  9.5E-18
  6.0E+01  1.1E-16  2.2E-19  5.3E-18
  1.0E+02  2.8E-17  1.0E-20  2.1E-18
  2.0E+02  1.8E-18  1.2E-22  1.4E-19
  4.0E+02  5.7E-20  1.3E-24  6.0E-21
  6.0E+02  7.2E-21  2.4E-26  1E-30
  1.0E+03  4.6E-22  2.6E-28  1E-30
  2.0E+03  1.2E-23  1E-30  1E-30
  3.0E+03  2.4E-24  1E-30  1E-30
Barnett Red Book
Energy      Cross Sections
 (keV)      (cm2)
CY 10      Q1-1 I      CF 0-1
H .L +H --U 0      H-L +H -I.-H      HO+H
```

```
In[288]:= Drop[Import["barnett.txt", "Table"], -5];
```

```
In[289]:= barnettH2HpData = Table[{{%[[j, 1]] * 1000, %[[j, 3]] * 10^-4}, {j, Length[%]}};
```

```
In[290]:= barnettH2HpPlot = ListLogLogPlot [%,  
          PlotRange -> {{10, 1.01 * 10^6}, {10^-29, 10^-21}}, PlotStyle -> plotColorsPoints [[3]]];
```

Newer RedBook

```
In[291]:= Import ["RedBookVol1Pa30.txt", "CSV"] // TableForm
```

Out[291]//TableForm=

2.0E+02	1.96E+07	1.17E-20
4.0E+02	2.78E+07	2.22E-20
7.0E+02	3.68E+07	4.82E-20
1.0E+03	4.39E+07	8.94E-20
2.0E+03	6.21E+07	2.80E-19
4.0E+03	8.79E+07	8.64E-19
7.0E+03	1.16E+08	2.09E-18
1.0E+04	1.39E+08	3.63E-18
2.0E+04	1.96E+08	8.89E-18
4.0E+04	2.78E+08	2.21E-18
7.0E+04	3.68E+08	2.42E-19
1.0E+05	4.39E+00	3.15E-20
2.0E+05	6.21E+08	1.84E-22
4.0E+05	8.78E+08	7.22E-25
7.0E+05	1.16E+09	6.64E-27
1.0E+06	1.39E+09	2.70E-28

<http://www-cfadc.phy.ornl.gov/redbooks/one/a/1a30.html>

Double Electron Capture Cross Sections for H+ + H2

(eV/amu) (cm/s) (cm^2)

```
In[292]:= barnettH2HpNewData = Table[{{#[[j, 1]], #[[j, 3]] / 10 000}, {j, Length[#]}} &[  
          Drop[Import ["RedBookVol1Pa30.txt", "Table"], -4]]];
```

```
In[293]:= barnettH2HpNewPlot = ListLogLogPlot [%,  
          PlotRange -> {{10, 1.01 * 10^6}, {10^-29, 10^-21}}, PlotStyle -> plotColorsPoints [[4]]];
```

Salazar (2010?) data

```
In[294]:= Import["salazar10fig8.dat", "CSV"] // TableForm
```

```
Out[294]/TableForm=
```

```
1.48735E+02    1.02485E-24
1.98734E+02    1.27815E-24
2.57591E+02    1.45297E-24
4.03824E+02    2.56552E-24
4.70247E+02    3.38855E-24
6.98688E+02    6.87310E-24
9.99078E+02    1.52910E-23
2.02758E+03    6.89902E-23
2.83516E+03    1.08463E-22
4.08699E+03    1.80696E-22
4.94478E+03    2.27899E-22
6.07360E+03    3.22710E-22
```

```
Salazar-Zapeda
```

```
Nuc. Instr. Methods in Ohys. Res. B 268
```

```
1558 (2010)
```

```
In[295]:= Drop[Import["salazar10fig8.dat", "Table"], -1];
```

```
In[296]:= salazarH2HpData = Table[{{j, 1}}, {{j, 2}}, {j, Length[%]}];
```

```
In[297]:= salazarH2HpPlot = ListLogLogPlot[%,
  PlotRange -> {{10, 1.01 * 10^6}, {10^-29, 10^-21}}, PlotStyle -> plotColorsPoints[[5]]];
```

Note that the portion of the fit below the lowest value (200 eV) listed by the newer Barnett et al. Redbook table is my guess as to the threshold behavior.

```
In[298]:= fith2HpPair[w1_] =
```

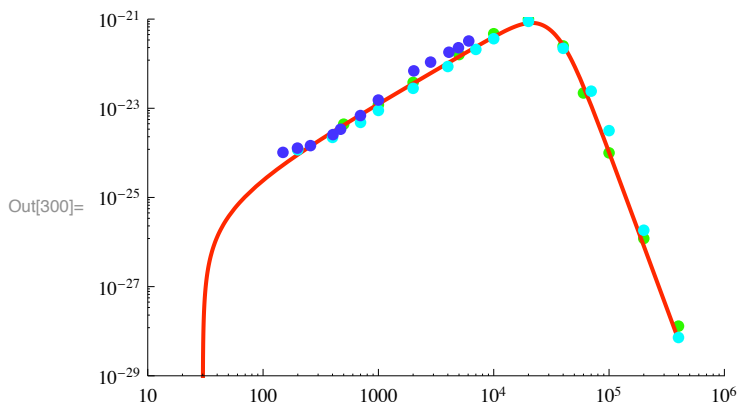
```
1.3 * 10^-23 * ((w1 - 30) / 1000.)^1.5 / (1 + (w1 / 25 000.)^4 + (w1 / 33 000.)^8.5) UnitStep[w1 - 30]
```

```
Out[298]= 
$$\frac{4.11096 \times 10^{-28} (-30 + w1)^{1.5} \text{UnitStep}[-30 + w1]}{1 + 2.56 \times 10^{-18} w1^4 + 3.9141 \times 10^{-39} w1^{8.5}}$$

```

```
In[299]:= fith2HpPairPlot = LogLogPlot[%, {w1, 10, 4. * 10^5}, PlotStyle -> plotColorsLines[[1]]];
```

```
In[300]:= Show[barnettH2HpPlot, fith2HpPairPlot, barnettH2HpNewPlot, salazarH2HpPlot]
```



Cross sections for H2+ + H2 collisions

Setup notebook environment

```

In[1]:= a = 1;

In[2]:= ClearAll["Global`*"];

In[3]:= Remove["Global`*"];

In[4]:= startclock = SessionTime[];

In[5]:= Off[General::spell];

In[6]:= Off[General::spell1];

In[7]:= today = StringForm["`"/`"/` ``:``:``", Date][[2]],
          Date][[3]], Date][[1]], Date][[4]], Date][[5]], Date][[6]]
Out[7]:= 12/10/2010 20:58:58.9291957`9.522905344594703

In[8]:= SetDirectory["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\h2h2pcollisions "]
Out[8]:= c:\\users\\avp\\documents\\Mathbook\\hydrogen\\h2h2pcollisions

In[9]:= plotColorsLines = {
  (*1-red*) {Hue[0.0], Thickness[0.007], Dashing[{}]},
  (*2-orange*) {Hue[0.1], Thickness[0.007], Dashing[{}]},
  (*3-green*) {Hue[0.3], Thickness[0.007], Dashing[{}]},
  (*4-cyan*) {Hue[0.5], Thickness[0.007], Dashing[{}]},
  (*5-dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{}]},
  (*6-purple*) {Hue[0.8], Thickness[0.007], Dashing[{}]},
  (*7-black*) {Thickness[0.007], Dashing[{}]},
  (*8-dash red*) {Hue[0.0], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*9-dash orange*) {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*10-dash green*) {Hue[0.3], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*11-dash cyan*) {Hue[0.5], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*12-dash dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*13-dash purple*) {Hue[0.8], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*14-dash black*) {Thickness[0.007], Dashing[{0.02, 0.02}]}];

In[10]:= plotColorsPoints = {
  (*1-red*) {Hue[0.0], PointSize[0.02]},
  (*2-orange*) {Hue[0.1], PointSize[0.02]},
  (*3-green*) {Hue[0.3], PointSize[0.02]},
  (*4-cyan*) {Hue[0.5], PointSize[0.02]},
  (*5-dk blue*) {Hue[0.7], PointSize[0.02]},
  (*6-purple*) {Hue[0.8], PointSize[0.02]},
  (*7-black*) {PointSize[0.02]},
  (*8-dash red*) {Hue[0.0], PointSize[0.02]},
  (*9-dash orange*) {Hue[0.1], PointSize[0.02]},
  (*10-dash green*) {Hue[0.3], PointSize[0.02]},
  (*11-dash cyan*) {Hue[0.5], PointSize[0.02]},
  (*12-dash dk blue*) {Hue[0.7], PointSize[0.02]},
  (*13-dash purple*) {Hue[0.8], PointSize[0.02]},
  (*14-dash black*) {PointSize[0.02]}];

```

Charge transfer collisions between H2+ and H2

From Phelps, J. Phys. Chem. Ref. Data 19, 653 (1990)

```
In[11]:= Import["h2h2pchargeTransferQ.txt", "CSV"] // TableForm
```

```
Out[11]/TableForm=
```

```
"H2+ + H2 cross sections from Phelps, J. Phys. Chem. Ref. Data 19, 653 (1990)"
```

```
eV      slow H2+
```

eV	slow H2+
0.1	0.28
0.1334	0.34
0.1778	0.43
0.237	0.49
0.316	0.6
0.422	0.75
0.562	0.95
0.75	1.19
1	1.53
1.334	2.03
1.778	2.6
2.37	4.1
3.16	5.9
4.22	8.5
5.62	10.4
7.5	11
10	10.8
13.34	10.6
17.78	10.2
23.7	9.9
31.6	9.6
42.2	9.2
56.2	8.9
75	8.6
100	8.4
133.4	8.2
177.8	7.9
237	7.7
316	7.4
421	7.2
562	7.1
750	6.8
1000	6.4
1334	6.2
1778	5.9
2371	5.9
3162	5.9
4217	6.1
5623	6.4
7499	6.8
10000	7

```
In[12]:= h2h2pCTData = Drop[Import["h2h2pchargeTransferQ.txt", "Table"], 5];
```

```

In[13]:= h2h2pCTDataPlot =ListLogLogPlot[h2h2pCTData, PlotStyle->plotColorsPoints[[1]],
PlotRange->{{0.1,10^5},{.1,100}}];

In[14]:= h2h2pCTFit=1.45*enlab^0.8*(1+(enlab/1.9)^4.5)^(1/4)/(1+(enlab/4.5)^4.1)^(1/2)*(1+(enlab/2500

In[15]:= h2h2pCTFitPlot=LogLogPlot[h2h2pCTFit,{enlab,0.1,10000},PlotStyle->plotColorsPoints[[1]],
PlotRange->{{0.1,10000},{.1,100}}];

```

According to Rothwell et al, J. Chem. Phys. 61, 3851 (1974) the cross sections given above are significantly too large for energies ~500 eV.

```

In[16]:= Import["rothwell174fig1.dat","CSV"]//TableForm

```

Out[16]//TableForm=

4.84523E+01	1.00976E-19
9.72971E+01	7.65378E-20
1.95268E+02	5.53915E-20
3.00311E+02	5.51545E-20
3.94678E+02	5.33984E-20
4.92201E+02	5.13356E-20
5.94192E+02	5.49538E-20
6.95818E+02	5.25826E-20
7.88474E+02	5.79872E-20
1.46242E+03	6.70540E-20
1.94007E+03	7.15836E-20

```

In[17]:= Import["rothwell174fig1.dat","Table"];

```

```

In[18]:= Table[{{%[[j,1]],%[[j,2]]*10^20},{j,Length[%]}}];

```

```

In[19]:= rothwellh2h2pCTPlot =ListLogLogPlot[%, PlotStyle->plotColorsPoints[[6]], PlotRange->{{0.1,10

```

RedBook Vol. 11

```
In[20]:= Import["RedbookVol1pA58.txt", "CSV"]//TableForm
```

```
Out[20]//TableForm=
```

1.0000E-01	2.1320E-15	1.0000E-01	2.1320E-15
1.2829E-01	1.9317E-15	1.2829E-01	1.9317E-15
1.6458E-01	1.7785E-15	1.6458E-01	1.7785E-15
2.1113E-01	1.6579E-15	2.1113E-01	1.6579E-15
2.7086E-01	1.5612E-15	2.7086E-01	1.5612E-15
3.4747E-01	1.4831E-15	3.4747E-01	1.4831E-15
4.4577E-01	1.4201E-15	4.4577E-01	1.4201E-15
5.7186E-01	1.3700E-15	5.7186E-01	1.3700E-15
7.3362E-01	1.3311E-15	7.3362E-01	1.3311E-15
9.4115E-01	1.3017E-15	9.4115E-01	1.3017E-15
1.2074E+00	1.2807E-15	1.2074E+00	1.2807E-15
1.5489E+00	1.2665E-15	1.5489E+00	1.2665E-15
1.9871E+00	1.2577E-15	1.9871E+00	1.2577E-15
2.5492E+00	1.2527E-15	2.5492E+00	1.2527E-15
3.2702E+00	1.2496E-15	3.2702E+00	1.2496E-15
4.1953E+00	1.2466E-15	4.1953E+00	1.2466E-15
5.3821E+00	1.2417E-15	5.3821E+00	1.2417E-15
6.9045E+00	1.2332E-15	6.9045E+00	1.2332E-15
8.8576E+00	1.2192E-15	8.8576E+00	1.2192E-15
1.1363E+01	1.1984E-15	1.1363E+01	1.1984E-15
1.4578E+01	1.1699E-15	1.4578E+01	1.1699E-15
1.8701E+01	1.1335E-15	1.8701E+01	1.1335E-15
2.3991E+01	1.0894E-15	2.3991E+01	1.0894E-15
3.0778E+01	1.0386E-15	3.0778E+01	1.0386E-15
3.9484E+01	9.8241E-16	3.9484E+01	9.8241E-16
5.0653E+01	9.2277E-16	5.0653E+01	9.2277E-16
6.4982E+01	8.6164E-16	6.4982E+01	8.6164E-16
8.3364E+01	8.0099E-16	8.3364E+01	8.0099E-16
1.0694E+02	7.4265E-16	1.0694E+02	7.4265E-16
1.3720E+02	6.8818E-16	1.3720E+02	6.8818E-16
1.7601E+02	6.3878E-16	1.7601E+02	6.3878E-16
2.2579E+02	5.9534E-16	2.2579E+02	5.9534E-16
2.8967E+02	5.5840E-16	2.8967E+02	5.5840E-16
3.7161E+02	5.2830E-16	3.7161E+02	5.2830E-16
4.7672E+02	5.0515E-16	4.7672E+02	5.0515E-16
6.1158E+02	4.8896E-16	6.1158E+02	4.8896E-16
7.8458E+02	4.7966E-16	7.8458E+02	4.7966E-16
1.0065E+03	4.7713E-16	1.0065E+03	4.7713E-16
1.2912E+03	4.8115E-16	1.2912E+03	4.8115E-16
1.6565E+03	4.9139E-16	1.6565E+03	4.9139E-16
2.1251E+03	5.0724E-16	2.1251E+03	5.0724E-16
2.7262E+03	5.2768E-16	2.7262E+03	5.2768E-16
3.4974E+03	5.5101E-16	3.4974E+03	5.5101E-16
4.4867E+03	5.7469E-16	4.4867E+03	5.7469E-16
5.7558E+03	5.9508E-16	5.7558E+03	5.9508E-16
7.3840E+03	6.0760E-16	7.3840E+03	6.0760E-16
9.4728E+03	6.0709E-16	9.4728E+03	6.0709E-16
1.2152E+04	5.8877E-16	1.2152E+04	5.8877E-16
1.5590E+04	5.4962E-16	1.5590E+04	5.4962E-16
2.0000E+04	4.8979E-16	2.0000E+04	4.8979E-16

```
In[21]:= Import["RedbookVol1pA58.txt", "Table"];
```

```
In[22]:= redbookv1pA58Data=Table[{{%[[j,1]],%[[j,2]]/1000*10^20},{j,Length[%]}}];
```

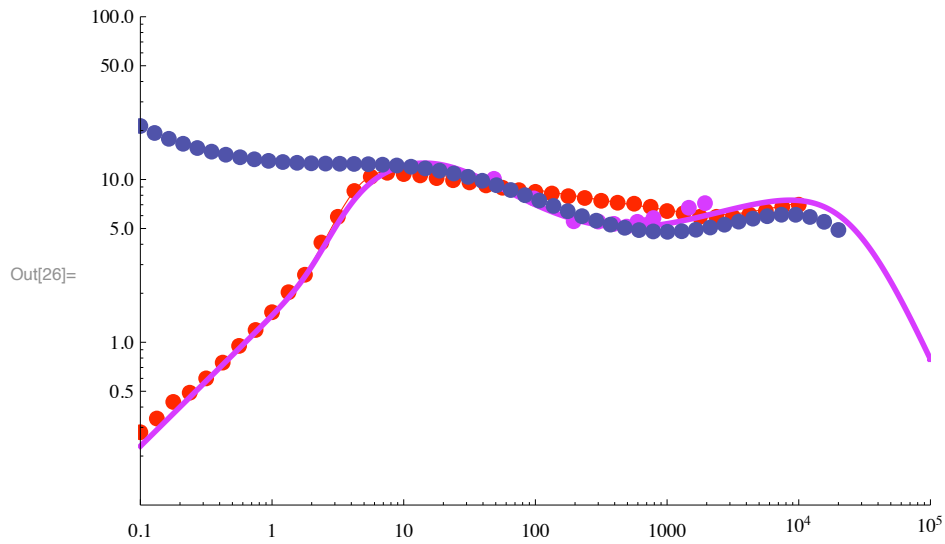


```
In[23]:= redbookvlpA58Plot =ListLogLogPlot[%, PlotStyle->plotColorsPoints[[7]], PlotRange->{{0.1,10^5
```

```
In[24]:= h2h2pRothwellFit=1.45*enlab^0.8*(1+(enlab/1.9)^4.5)^(1/4)/(1+(enlab/4.)^3.1)^(1/2)*  
(1+(enlab/16)^2)^-.5*(1+(enlab/400))^1.3/(1+(enlab/2000))^0.5/(1+(enlab/25000)^2);
```

```
In[25]:= h2h2pRothwellFitPlot=LogLogPlot[h2h2pRothwellFit,{enlab,0.1,100000},PlotStyle->plotColorsLin  
PlotRange->{{0.1,10^5},{.1,100}}, PlotPoints->10000];
```

```
In[26]:= Show[h2h2pCTDataPlot, h2h2pCTFitPlot, rothwellh2h2pCTPlot, h2h2pRothwellFitPlot, redbookv1pA58
```



The RedBook values are much too large at low energies.

■ Proton transfer collisions between H2+ and H2 to form H3+

```
In[27]:= Import["h2h2pToH3p.txt", "CSV"] // TableForm
```

```
Out[27]//TableForm=
```

```
"H2+ + H2 cross sections from Phelps, J. Phys. Chem. Ref. Data 19, 653 (1990)"
```

```
eV      H3+ + H
```

0.1	78
0.1334	68
0.1778	59
0.237	51
0.316	44
0.422	38
0.562	32.5
0.75	27
1	22.7
1.334	18.7
1.778	15.3
2.37	11.8
3.16	8.4
4.22	5.4
5.62	2.9
7.5	1.3
10	0.42
13.34	0.093
17.78	0.015

```
In[28]:= h2h2pToH3pData = Drop[Import["h2h2pToH3p.txt", "Table"], 5];
```

```
In[29]:= h2h2pToH3pDataPlot = ListLogLogPlot[h2h2pToH3pData, PlotStyle->plotColorsPoints[[3]], PlotRan
```

```
In[30]:= h2h2pToH3pFit=25.2*enlab^-0.5/(1+(enlab/13)^1+(enlab/4)^3.)^(0.9);
```

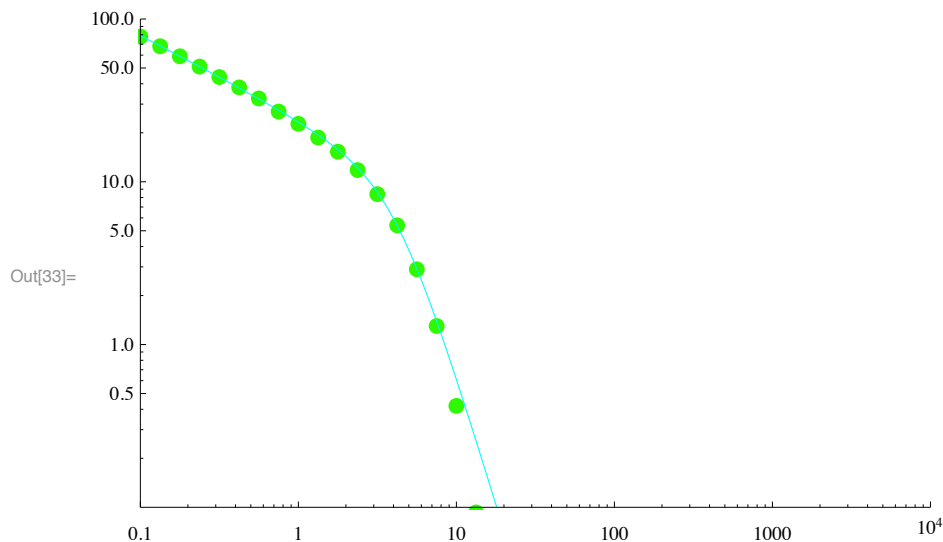
At low energies this corresponds to a constant collision frequency of

```
In[31]:= nuon=25.2*10^-20/enlab^0.5*Sqrt[2*qe*enlab/mH3]/.{qe->1.602*10^-19,mH3->3*1.673*10^-27} (*n
```

```
Out[31]= 2.01344 × 10-15
```

```
In[32]:= h2h2pToH3pFitPlot=LogLogPlot[h2h2pToH3pFit,{enlab,0.1,10000},PlotStyle->plotColorsPoints[[4],
PlotRange->{{0.1,10000},{.1,100}},PlotPoints->10000,DisplayFunction->Identity];
```

```
In[33]:= Show[h2h2pToH3pDataPlot, h2h2pToH3pFitPlot,ImageSize->400]
```



■ Product energy distribution

In our model we neglect any internal energy of the product H3+ and H atoms. Some relevant references and arguments are:

The proton transfer reaction occurs with significant probability only for energies below about 10 eV. See Neynaber and Trujillo, Phys.Rev.167, 63 (1968). As a result, the simultaneous production of excited H atoms with $n \geq 3$ and H3+ ions is not observed. See Gentry and Ringer, J.Chem.Phys.67, 5398 (1977). See also papers by Carrington et al.

The energy of the product H atoms is expected to be low and spread over a range of energies as the result of simultaneous excitation of rotational and vibrational states of the product H3+ ion. This follows from the statement that most of the reaction exothermicity goes into internal excitation of the products in Gentry et al, Rev. Sci. Instrum. 46, 367 (1975). Collisional relaxation of the internal energy of H3+ by H2 has been measured by Kim et al, Int. J. Mass Spectrom. and Ion Phys. 15, 223 (1974).

■ Dissociation collisions between H2+ and H2 to form H+ + H + H2

We currently have no information as to whether this cross section is for the production of fast H+ or slow H+. The difference may not be important in the formation of fast H because of the rapid loss and low flux of H2+. Presumably this is from JPCRD (1990)

```
In[34]:= Import["h2h2pToHp.txt", "CSV"] // TableForm
```

```
Out[34]/TableForm=
```

```
"H2+ + H2 cross sections from Phelps, J. Phys. Chem. Ref. Data 19, 653 (1990)"
```

eV	H+ + H	Ly alpha	Halp	e
5.62	0.33			
7.5	0.83			
10	0.85			
13.34	0.78			
17.78	0.72			
23.7	0.68			
31.6	0.67			
42.2	0.69			
56.2	0.7			
75	0.74			
100	0.78			
133.4	0.82			
177.8	0.86			
237	0.91			
316	0.95			
421	1.01			
562	1.08			
750	1.15			
1000	1.24			
1334	1.34			
1778	1.48			
2371	1.62			
3162	1.82			
4217	1.98			
5623	2.2			
7499	2.38			
10000	2.44			

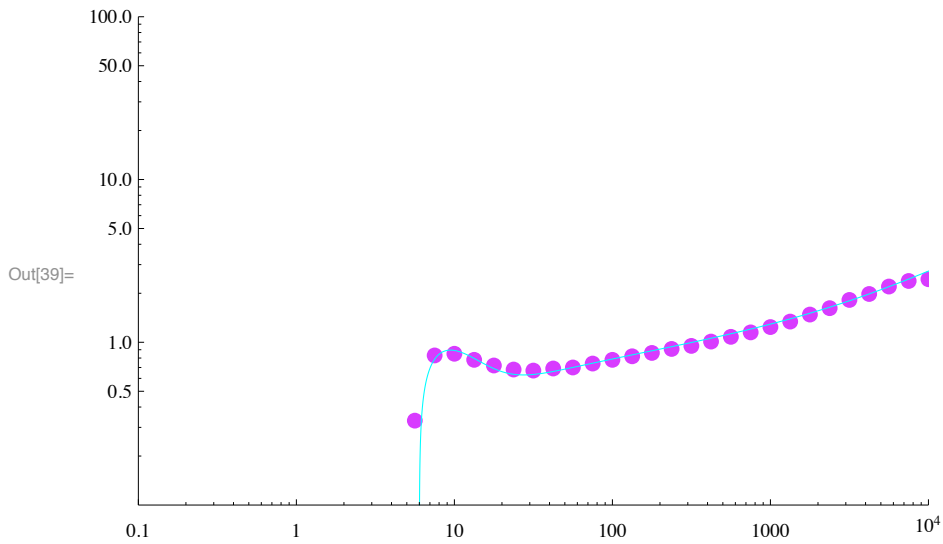
```
In[35]:= h2h2pToHpData = Drop[Import["h2h2pToHp.txt", "Table"], 4];
```

```
In[36]:= h2h2pToHpDataPlot = ListLogLogPlot[h2h2pToHpData, PlotStyle->plotColorsPoints[[6]],
PlotRange->{{0.1, 10000}, {0.1, 100}}];
```

```
In[37]:= h2h2pToHpFit=UnitStep[enlab-6]*(enlab-6)^0.5/(1+(enlab/6.5)^4)^(0.44)*
(1+(enlab/20)^4+(enlab/50)^4.9)^(0.355) + 1.*10^-30;
```

```
In[38]:= h2h2pToHpFitPlot=LogLogPlot[h2h2pToHpFit, {enlab, 0.1, 10000}, PlotStyle->plotColorsPoints[[4]],
PlotRange->{{0.1, 10000}, {0.1, 100}}, PlotPoints->10000, DisplayFunction->Identity];
```

```
In[39]:= Show[h2h2pToHpDataPlot, h2h2pToHpFitPlot, ImageSize->400]
```



- E/N required to accelerate H2+ rapidly enough to avoid H3+ formation at low energies.

We want the low energy limit of the reaction cross section

```
In[40]:= h2h2pToH3pPhelps[w2_] := 25.2*10^-20*(enlab+0.04)^-0.5/(1+(enlab/13)^1+(enlab/4)^3.)^(0.9)/.e
```

Consider

```
In[41]:= q2s3Limit=Limit[w2^0.5*25.2*10^-20*(enlab)^-0.5/(1+(enlab/13)^1+(enlab/4)^3.)^(0.9)/.enlab->
```

Out[41]= 2.52×10^{-19}

The corresponding collision frequency is

```
In[42]:= nu2s3onLimit=q2s3Limit/Sqrt[w2]*v2 /.v2->Sqrt[2*qe*w2/mH2]/.{qe->1.602*10^-19,mH2->2.016*1.66
```

Out[42]= 2.465×10^{-15}

This corresponds to $2.47\text{E-}9$ cm³/s, which seems a little high.

The energy gained by the H2+ during the time between reaction collisions is $s^*E = 1/2*a*t^2*E = 1/2*E/mH2*E/(n*nu2s3onLimit)^2$, where we replace t by the reciprocal of the reaction frequency $nu2s3onLimit*n$

```
In[43]:= Solve[enLimit==(1/2*qe*field/mH2)*field/(n*nu2s3onLimit)^2/.{qe->1.602*10^-19,mH2->2.016*1.6
```

Out[43]= $\left\{ \left\{ \text{field} \rightarrow -5.04 \times 10^{-19} \sqrt{\text{enLimit} \ n} \right\}, \left\{ \text{field} \rightarrow 5.04 \times 10^{-19} \sqrt{\text{enLimit} \ n} \right\} \right\}$

```
In[44]:= eonLimit=(field/.%[[2]])/n /.enLimit->10
```

```
Out[44]= 1.59379 × 10-18
```

This is only 1.59 kTd, i.e., in the middle of the E/N covered in our drift tube experiments. This derivation of a critical E/N does not take into account the fact that with each charge transfer collision there is a certain probability, even if small, that the low energy H2+ will form H3+ before it reaches the energy of the drop in reaction cross section. This will smear the transition and could lead to significant H3+ formation at E/N above the critical value.

An interesting question is whether this transition appears in our one-dimensional ion energy distribution and the associated matrix solution of the ion transport equations.

■ Continuous energy loss function for H2+ in H2

```
In[45]:= Import["H2H2p88ELoss.txt", "CSV"] // TableForm
```

Out[45]//TableForm=

```

H2+ + H2 cross sections
Q's in 10^-20 m2
Lab En.      Qm      L(inela)
0.1      0.56      0
0.133352143216332      0.68      0
0.177827941003892      0.8      0
0.237137370566166      0.98      0
0.316227766016838      1.2      0
0.421696503428582      1.5      0
0.562341325190349      1.9      0
0.749894209332456      2.38      0
1      3.06      0
1.33352143216332      4.06      0
1.77827941003892      5.6      0
2.37137370566166      8.2      0.00735
3.16227766016838      11.8      0.0171
4.21696503428582      17      0.0357
5.62341325190349      20.8      0.0675
7.49894209332456      22      0.12
10      21.6      0.189
13.3352143216332      21.2      0.255
17.7827941003892      20.4      0.336
23.7137370566166      19.8      0.408
31.6227766016838      19.2      0.448552979163724
42.1696503428582      18.4      0.469613637511624
56.2341325190349      17.8      0.48610678809479
74.9894209332456      17.2      0.526579684051313
100      16.8      0.593816421032121
133.352143216332      16.4      0.677790220042746
177.827941003892      15.8      0.995298532890543
237.137370566166      15.4      1.49967547444974
316.227766016838      14.8      2.31422731055353
421.696503428582      14.4      3.58037221685212
562.341325190349      14.2      5.20802535505166
749.894209332456      13.6      7.78026993284872
1000      12.8      10.5894555750806
1333.52143216332      12.4      14.0069678187948
1778.27941003892      11.8      18.1278336415004
2371.37370566166      11.8      23.5367887986285
3162.27766016838      11.8      30.1302445929499
4216.96503428582      12.2      38.8150816145138
5623.41325190349      12.8      50.333404953496
7498.94209332456      13.6      64.6871515220935
10000      14      85.74995371439

```

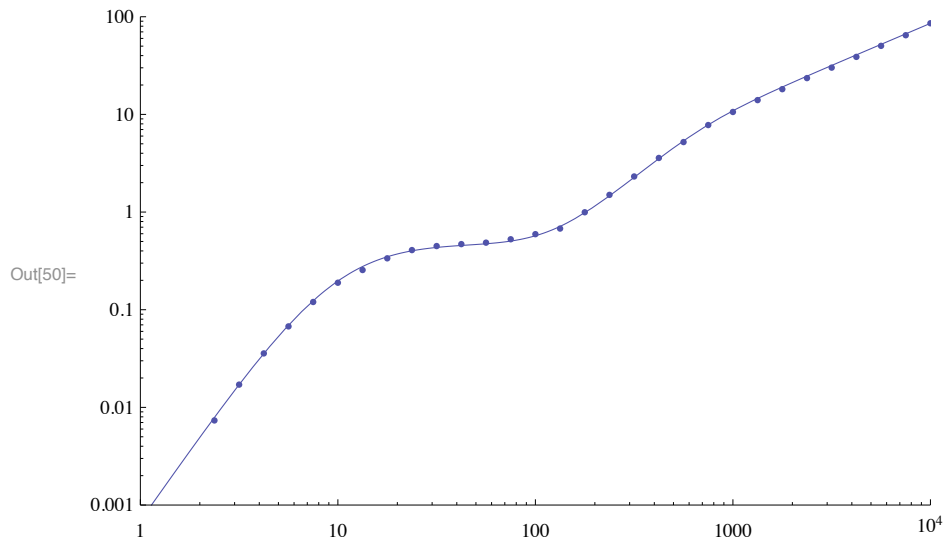
In[46]:= **Drop[Import["H2H2p88ELoss.txt", "Table"], 3];**

In[47]:= **energyLossDataPlot=ListLogLogPlot[Drop[Table[{{[[j, 1]], %[[j, 3]]}, {j, Length[%]}], 11], ImageSize PlotRange->{{1, 10000}, {.001, 100}}];**

In[48]:= **energyLossFit[enLab_]=0.0007*enLab^2.9/(1+(enLab/10)^2)^1.5*(1+(enLab/120)^3)^0.6/(1+(enLab/**

10000)^0.6);
energyLossFitPlot=LogLogPlot[energyLossFit[enLab], {enLab, 1, 10000}, PlotRange->{{1, 10000}, {.00

```
In[50]:= Show[energyLossFitPlot, energyLossDataPlot, ImageSize->400]
```



I suspect that one needs to add a term that slowly increases with energy at energies below a few eV to represent the effects of rotational excitation.

■ Halpha excitation

From H2H2PCROSSSECTIONS.xls and Phelps, J. Phys. Chem. Ref. Data 19, 653 (1990).


```
In[51]:= Import["H2H2pExcitation.txt", "CSV"] // TableForm
```

```
Out[51]/TableForm=
```

Elab (eV)	Lyalpha	Halp	ionization
177.8	0.013	1.00E-09	0.017
237	0.033	1.00E-09	0.024
316	0.068	1.00E-09	0.0335
421	0.12	1.00E-09	0.047
562	0.183	1.00E-09	0.064
750	0.255	0.0133	0.091
1000	0.325	0.0233	0.124
1334	0.39	0.034	0.17
1778	0.44	0.049	0.23
2371	0.5	0.064	0.31
3162	0.55	0.081	0.41
4217	0.58	0.099	0.55
5623	0.62	0.119	0.73
7499	0.64	0.138	0.95
10000	0.72	0.157	1.27

```
In[52]:= Drop[Import["H2H2pExcitation.txt", "Table"], 1];
```

```
In[53]:= Table[{{%[[j,1]],%[[j,3]]},{j,Length[%]}}];
```

```
In[54]:= h2H2pExcitationPhelpsPlot = ListLogLogPlot[%, PlotRange -> {{.1, 10 000}, {10^-3, 1.01}},
  ImageSize -> 400, PlotStyle -> plotColorsPoints[[1]], GridLines -> Automatic, PlotLabel ->
  "Cross section for H2+ + H2 -> Halp (10^-20 m^2) vs laboratory energy (eV)"];
```

A fit to this data is

```
In[55]:= fac=10^20;
```

```
In[56]:= q2ha[w2_] := 0.7*10^-26*UnitStep[w2-20]*(w2-20)^1.5/(1+(w2/2000.)^4)^.22+1.*10^-30
```

```
In[57]:= fitH2H2pHalpPlot =
  LogLogPlot[fac * q2ha[w2], {w2, 20, 10 000}, PlotRange -> {{.1, 10 000}, {10^-3, 1.01}},
  ImageSize -> 400, PlotStyle -> plotColorsLines, GridLines -> Automatic, PlotLabel ->
  "Cross section for H2+ + H2 -> Halp (10^-20 m^2) vs laboratory energy (eV)"];
```

Below 1 keV, the following is a fit to data scaled from the Lyman alpha excitation and then shifted to higher energies. From H+ + H2.

```
In[58]:= q2ha[w2_] := 4.*10^-28*UnitStep[w2-100](w2-100)^2/(1+(w2/1050)^4)^0.2/(1+(w2/4000))^1.1+ 1.*
```

```
In[59]:= hAlphaH2pFitPlot = LogLogPlot[{fac * q2ha[w1]}, {w1, .1, 10 000},
  PlotRange -> {{.099, 10 000}, {fac * 0.99 * 10^-24, fac * 1.01 * 10^-20}},
  PlotStyle -> plotColorsLines[[5]], ImageSize -> 400, GridLines -> Automatic,
  PlotLabel -> "Cross sections for H+ + H2 (10^-20 m^2) vs LAB energy (eV)"];
```

We need to plot the scaled results of Hess and of Lyman alpha

```
In[60]:= Import["h2h2phalphahessfig7.dat", "CSV"]//TableForm
```

```
Out[60]//TableForm=
```

4.92533E+02	5.45844E-20
5.45293E+02	7.06149E-20
5.93608E+02	8.52942E-20
7.04044E+02	9.95845E-20
8.93127E+02	1.61070E-19
1.04137E+03	1.84848E-19
1.32316E+03	1.94775E-19
1.76933E+03	2.19843E-19
2.28706E+03	2.27728E-19
2.95477E+03	2.70565E-19

```
In[61]:= Import["h2h2phalphahessfig7.dat", "Table"]; (*eV, cm^2*)
```

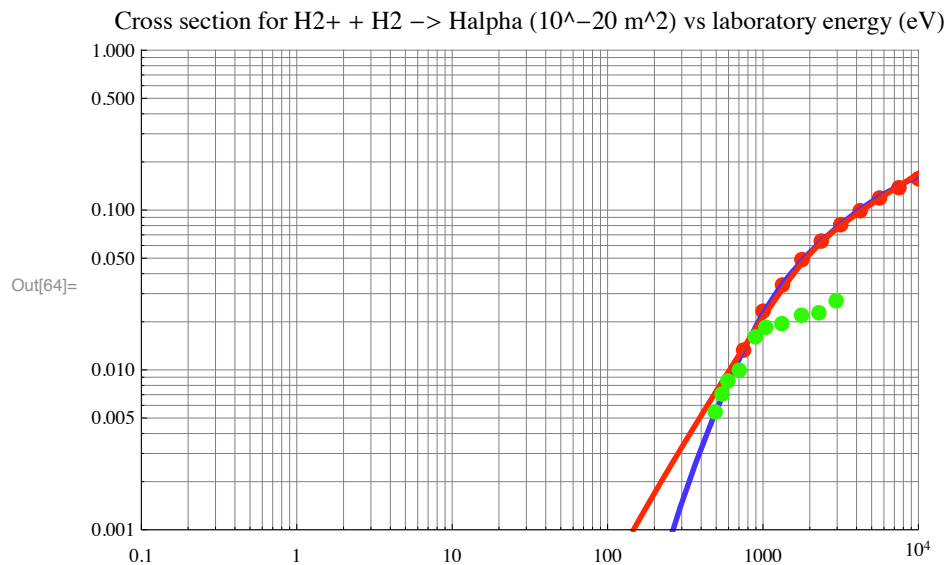
These cross sections are multiplied by 10 to get them to approximately match my 1990 values at energies above 1000 eV.

```
In[62]:= Table[{%[[j,1]],10*10^16*%[[j,2]]},{j,Length[%]}]; (*eV, 10^-20 m^2*)
```

```
In[63]:= h2H2pExcitationHessPlot = ListLogLogPlot[%, PlotRange -> {{.1, 10000}, {10^-3, 1.01}},
ImageSize -> 600, PlotStyle -> plotColorsPoints[[3]], GridLines -> Automatic, PlotLabel ->
"Cross section for H2+ + H2 -> Halpha (10^-20 m^2) vs laboratory energy (eV)"];

```

```
In[64]:= Show[h2H2pExcitationPhelpsPlot, hAlphaH2pFitPlot, fitH2H2pAlphaPlot, h2H2pExcitationHessPlot]
```



■ Ionization

From Phelps (1990)

```
In[65]:= Import["H2H2pExcitation.txt", "CSV"] // TableForm
```

```
Out[65]/TableForm=
```

Elab (eV)	Lyalpha	Halp	ionization
177.8	0.013	1.00E-09	0.017
237	0.033	1.00E-09	0.024
316	0.068	1.00E-09	0.0335
421	0.12	1.00E-09	0.047
562	0.183	1.00E-09	0.064
750	0.255	0.0133	0.091
1000	0.325	0.0233	0.124
1334	0.39	0.034	0.17
1778	0.44	0.049	0.23
2371	0.5	0.064	0.31
3162	0.55	0.081	0.41
4217	0.58	0.099	0.55
5623	0.62	0.119	0.73
7499	0.64	0.138	0.95
10000	0.72	0.157	1.27

```
In[66]:= Drop[Import["H2H2pExcitation.txt", "Table"], 1];
```

```
In[67]:= Table[{{%[[j,1]],%[[j,4]]},{j,Length[%]}}];
```

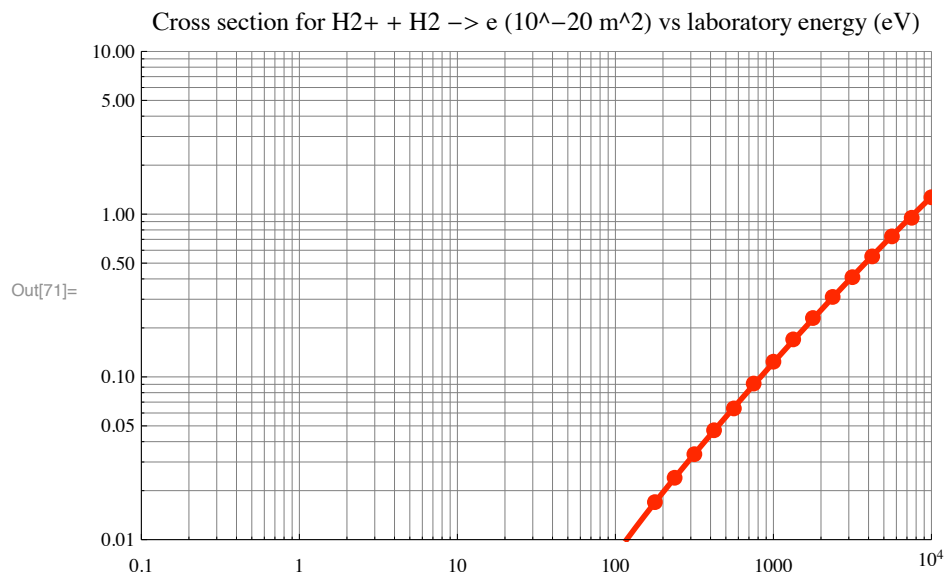
```
In[68]:= h2H2pIonizationPhelpsPlot = ListLogLogPlot[%, PlotRange -> {{.1, 10 000}, {10^-2, 10.01}},
  ImageSize -> 400, PlotStyle -> plotColorsPoints[[1]], GridLines -> Automatic,
  PlotLabel -> "Cross section for H2+ + H2 -> e (10^-20 m^2) vs laboratory energy (eV)"];
```

A fit to this data is

```
In[69]:= q2i[w2_] := 6.5*10^-25*UnitStep[w2-20]*(w2-20)^1.1/(1+w2/8000)^0.3
```

```
In[70]:= fitH2H2pIonizPlot =
  LogLogPlot[fac * q2i[w2], {w2, 20, 10 000}, PlotRange -> {{.1, 10 000}, {10^-2, 10.01}},
  ImageSize -> 400, PlotStyle -> plotColorsLines, GridLines -> Automatic, PlotLabel ->
  "Cross section for H2+ + H2 -> Halp (10^-20 m^2) vs laboratory energy (eV)"];
```

```
In[71]:= Show[h2H2pIonizationPhelpsPlot, fitH2H2pIonizPlot]
```



Negative ion formation

It should be kept in mind that nearly all of the H⁻ cross section measurements were designed to collect H⁻ only from the near forward direction so that the experiment does not measure H⁻ production in large angle scattering characteristic of target ionization. Only van Zyl et al measure all energy H⁻.

From Fig. 6 of Williams and Dunbar, Phys. Rev 149, 62 (1966)

```
In[72]:= Import["williamsdunbar66fig6.dat", "CSV"] // TableForm
```

```
Out[72]//TableForm=
```

2.84992E+03	7.74234E-24
3.84718E+03	1.18351E-23
4.92201E+03	1.86504E-23
6.39094E+03	2.10484E-23
8.69111E+03	2.68186E-23
9.53498E+03	3.74408E-23
1.50067E+04	5.63568E-23
2.10492E+04	8.29360E-23
3.02116E+04	1.20208E-22
3.86324E+04	1.39848E-22
4.78766E+04	1.12189E-22
5.36930E+04	8.47145E-23

```
In[73]:= williamsDunbarData = Import["williamsdunbar66fig6.dat", "Table"];
```

```
In[74]:= alvarezData1 = Import["alvarez76fig7.dat", "Table"];
```

From Fig. 7 of Alvarez et al, Phys. Rev. A 14, 602 (1976).

```
In[75]:= alvarezData =
  Table[{mh2 * (#[[j, 1]] / 100)^2 / (2 * qe) /. {qe -> 1.602 * 10^-19, mh2 -> 2 * 1.673 * 10^-27},
    #[[j, 2]]}, {j, Length[#]}] &[%];
```

Note that a factor of ~ 4 in magnitude would bring these two data set into moderately good agreement in the energy region of overlap.

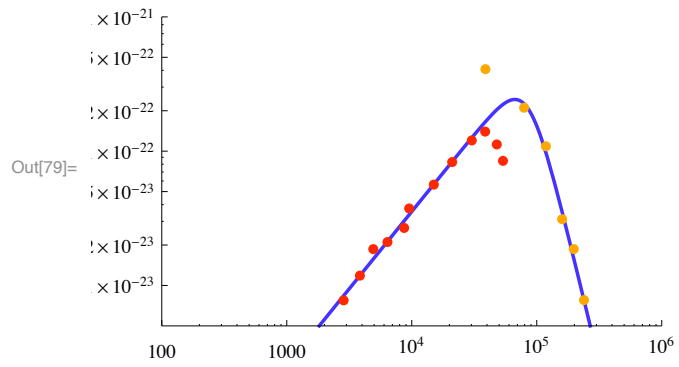
```
In[76]:= exptDataPlot = ListLogLogPlot[{williamsDunbarData, alvarezData},
  PlotRange -> {{100, 1. * 10^6}, {5 * 10^-24, 10^-21}}, PlotStyle -> plotColorsPoints];
```

```
In[77]:= fitExpt = 1.6 * 10^-23 * (en / 5000)^1.15 / (1 + (en / 85000)^5);
```

```
In[78]:= fitExptPlot = LogLogPlot[fitExpt, {en, 1000, 10^6},
  PlotStyle -> plotColorsLines[[5]], PlotRange -> {{100, 10^6}, {5 * 10^-24, 1 * 10^-21}}];
```

```
In[79]:= Show[fitExptPlot, exptDataPlot,
  PlotLabel -> "Cross section for H2+ + H2 -> H- (m^2) vs laboratory energy (eV)"]
```

Cross section for H2+ + H2 -> H- (m²) vs laboratory energy (eV)



```
In[80]:= Quit[]
```

3 H3+ collisions
with H2

H3+ + H2 cross sections

Setup notebook environment

```
In[1]:= a = 1;

In[2]:= ClearAll["Global`*"];

In[3]:= Remove["Global`*"];

In[4]:= startclock = SessionTime[];

In[5]:= Off[General::spell];

In[6]:= Off[General::spell1];

In[7]:= today = StringForm["`"/`"/` ``:``:``", Date][[2]],
          Date][[3]], Date][[1]], Date][[4]], Date][[5]], N[Date][[6]], 2]]

Out[7]:= 7/9/2011 13:31:30.1809488`2.

In[8]:= plotColorsLines = {
  (*1-red*) {Hue[0.0], Thickness[0.007], Dashing[{}]},
  (*2-orange*) {Hue[0.1], Thickness[0.007], Dashing[{}]},
  (*3-green*) {Hue[0.3], Thickness[0.007], Dashing[{}]},
  (*4-cyan*) {Hue[0.5], Thickness[0.007], Dashing[{}]},
  (*5-dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{}]},
  (*6*) {Magenta, Thickness[0.007], Dashing[{}]},
  (*7-yellow*) {Hue[0.2], Thickness[0.007], Dashing[{}]},
  (*8-pink*) {Hue[0.9], Thickness[0.007], Dashing[{}]},
  (*9-black*) {Thickness[0.007], Dashing[{}]},
  (*10-dash red*) {Hue[0.0], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*11-dash orange*) {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*12-dash green*) {Hue[0.3], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*13-dash cyan*) {Hue[0.5], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*14-dash dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*15-dash*) {Magenta, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*16-dash yellow*) {Hue[0.2], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*17-dash pink*) {Hue[0.9], Thickness[0.007], Dashing[{0.02, 0.02}]},
  (*18-dash black*) {Thickness[0.007], Dashing[{0.02, 0.02}]}
};
```

```
In[9]:= plotColorsPoints = {  
  (*1-red*) {Hue[0.0], PointSize[0.02]},  
  (*2-orange*) {Hue[0.1], PointSize[0.02]},  
  (*3-green*) {Hue[0.3], PointSize[0.02]},  
  (*4-cyan*) {Hue[0.5], PointSize[0.02]},  
  (*5-dk blue*) {Hue[0.7], PointSize[0.02]},  
  (*6*) {Magenta, PointSize[0.02]},  
  (*7-yellow*) {Hue[0.2], PointSize[0.02]},  
  (*9-pink*) {Hue[0.9], PointSize[0.02]},  
  (*8-black*) {PointSize[0.02]}  
};
```

A. V. Phelps, JILA
8/19/01

We wish to assemble a set of $H_3^+ + H_2$ cross sections that is consistent with as many experiments as possible. We especially wish to fit Peko and Champion (1997). There is a large spread in the high energy (> 1 keV) dissociation data of Federenko (1954), McClure (1963), and Williams and Dunbar (1966). Our cross sections for ionization, Balmer alpha excitation, and Lyman alpha excitation remain unchanged from those recommended in Phelps (1990). We also include data for momentum transfer from mobility measurements of Miller et al (1968). The total scattering of Simons et al (1943) is much smaller than theory as expected because of their large detector angle. Note that we are unable to reconcile the observations of fast H and H_2 production by McClure and Williams and Dunbar with the claim by Volger and Meierjohann (1978) that the production of 2 fast H + fast H^+ (or 3 fast H) is negligible at 10 keV compared to the production of fast H + fast H_2 .

A surprising thing to me about the experimental data was that measurements of the angular distributions of the products for $H_3^+ + D_2$ show that for energies above a few tenths of an eV the velocities of the high energy products CM are almost always in the forward direction and that significant large angle scattering in occurs only for energies well below 1 eV. This seems to mean that the reactions occur at large range such that the incident projectile is only slightly deflected. More specific angular distributions are cited for the individual cross sections.

One cannot hope to obtain a really good set of $H_3^+ + H_2$ cross sections until experiments (or theories) become available for state selected H_3^+ projectiles. Published experiments show up to 50% changes in cross sections as the conditions are changed in the gas discharge sources of H_3^+ . The changes are attributed to changes in the degree of vibrational relaxation of the H_3^+ following its initial production in an excited state from $H_2^+ + H_2$ collisions. Generally, the $H_3^+ + H_2$ cross sections are larger for conditions expected to yield greater populations of vibrationally excited H_3^+ , but the data is extremely qualitative. A similar problem appears to arise from rotational excitation in electron- H_3^+ recombination experiments.

Here we have attempted to assemble cross sections appropriate to H_3^+ ions that are thermally relaxed, e.g., the ~ 1.5 eV of internal energy resulting from the $H_2^+ + H_2 \rightarrow H_3^{+*} + H$ reaction has been dissipated in collisions with ambient temperature H_2 . It would be very desirable to assemble cross sections for collisions of H_3^+ with known degrees of internal energy with H_2 of known internal energy, but there is little hope of doing so in the foreseeable future.

One may wonder why a review of this topic is needed so soon after publication of the review of cross sections for collisions of hydrogenic species by Tabata and Shirai, Atomic Data and Nuclear Data Tables 76, 1 (2000). We undertook this compilation in order to provide a) cross sections with threshold behaviors consistent with the proposed processes, b) a set of cross sections that are consistent with the fact that Peko and Champion (1997) made only five independent measurements (not eight), and c) a cross section set consistent with the expected low energy behavior as modeled by Simko et al (1997).

We take a lead from Simko et al, Phys. Rev E 56, 5908 (1997) and consider the cross sections below the dissociation threshold at 4.4 eV to be made up of two components.

a) The low energy component, which Simko et al call elastic scattering, results in elastic scattering and/or rotational excitation. Based on the differential scattering experiments of Vestal et al (1976) one is tempted to assume that this process results in elastic isotropic scattering in CM with the Langevin cross section. Another possibility is to ignore Vestal et al and assume that proton transfer dominates, results in rotational excitation, and causes 180 deg scattering in CM. A reason for doing this is the low mobility of H3+ in H2 at low E/N compared to Langevin. Probably a mixture of processes is best.

b) The higher energy component, which Simko et al label as proton transfer scattering, is patched on to the proton transfer data of Peko and Champion at ~ 3 eV. In a modification of the model of Simko et al, we propose that all of this proton transfer results in vibrational excitation. It has an absolute threshold equal to the energy of the lowest vibrational mode of H3+, e.g., $\Delta E = 0.31$ eV. If the proton transfer model of the collision is valid, the actual threshold will be $9/5 \cdot \Delta E = 0.56$ eV. This process differs from the usual vibrational excitation collision in that the collision results in 180 deg scattering in CM.

```
In[10]:= SetDirectory["c:\users\avp\documents\Mathbook\hydrogen\h2h3pcollisions"]
```

```
Out[10]= c:\users\avp\documents\Mathbook\hydrogen\h2h3pcollisions
```

Note: Double click on the arrows to open the various sections.

- Procedure for importing, digitizing and exporting a graph read by the HP scanner.

Cross section for scattering by polarization potential for reference only.

These cross sections for scattering by a polarization potential are not part of our recommended set and are shown for reference only.

```
In[11]:= mramu = 3 * 2 / (3 + 2);
mr = mramu * 1.661 * 10^-27;
qe = 1.602 * 10^-19;
ng = 2.69 * 10^25; (*m^-3*)
alphaMcDaniel = 0.808 * 10^-30; (*m^3 from McDaniel (1993)*)
ao = 0.529 * 10^-10; (*m*)
me = 9.11 * 10^-31; (*kgm*)
ry = 27.211 / 2; (*eV*)
fac = 10^20;
```

```
In[20]:= alphaau = alphaMcDaniel / ao^3
```

```
Out[20]= 5.45814
```

■ Langevin cross section

```
In[21]:= langevinQ = 2 * Pi * ao^2 * (13.6 / enrel * alphaau)^0.5
```

```
Out[21]= 1.5149 × 10-19  $\left(\frac{1}{\text{enrel}}\right)^{0.5}$ 
```

■ Total cross section

For a polarization potential

```
In[22]:= n = 4;
```

The Landau-Lifshitz formula for gammaLL is

```
In[23]:= fn = Pi / 4;
```

```
In[24]:= gammaLL = N[Pi^2 * (2 fn)^(2 / (n - 1)) * Csc[Pi / (n - 1)] / Gamma[2 / (n - 1)]]
```

```
Out[24]= 11.3726
```

Note that this formula is different than that given in Massey, Burhop, and Gilbody (1971) or in McDaniel, Mitchell, and Rudd (1993), but gives numbers in exact agreement with Massey et al Table 16.2.

```
In[25]:= qtotal = gammaLL * ao^2 * alphaau^(2 / 3) * (mr / me / 4 * ry / enrel)^(1 / 3) // PowerExpand
```

```
Out[25]=  $\frac{1.92618 \times 10^{-18}}{\text{enrel}^{1/3}}$ 
```

```
In[26]:= langevinQPlot = LogLogPlot [
  {Evaluate[10^20 * langevinQ], Evaluate[10^20 * qtotal]}, {enrel, 0.005, 10000},
  PlotRange -> {{0.01, 10000}, {0.01, 200}}, ImageSize -> 432, PlotStyle ->
  {{Hue[1], Thickness[0.007]}, {Hue[1], Dashing[{0.05, 0.05]}, Thickness[0.007]}}];
```

Here the Langevin is solid red, while the total cross section is dashed red. Again, These are not part of our recommended set of cross sections.

fast H3+ + H2 -> fast H+ + fast H2 + slow H2 by CID of H3+ meas. by P&C, McClure, Williams&Dunbar

This cross section at relative energies from 3 to 115 eV is that obtained by a Peko and Champion (1997) using a retarding analysis of the ions produced in a H3+ + H2 collision. According to the collision induced dissociation (CID) model of P&C, the fast H+ are produced with an axial energy of approximately 1/3 of the energy of the incident ion. This argument seems to require that there is little scattering in angle. We force our fit to pass through the fast H+ results of Williams and Dunbar (1966) rather than those of McClure (1963) in order to keep down the total destruction of H3+. Another possibility would be to make this cross section to pass through McClure's 50% larger cross section for fast H2 production. We ignore the fast H+ results of Lange et al (1977) as being much too small to be consistent with those of Peko et al (1997). Prokofev et al (1978) agree with Peko and Champion for D3+ + H2 at 3 to 40 eV. The threshold for this reaction is 4.4 eV.

This collision process is most easily visualized as a two step process, i.e., the excitation of the H3+ and then its dissociation. The collision process appears to be one in which the H3+ projectile and thermal H2 target are not significantly deflected during excitation of the H3+. The H3+ losses kinetic energy because of its excitation to a dissociating state, e.g., roughly 10 eV. Then the H+ and H2 fragments probably fly apart more or less isotropically with a few eV energy. Assuming that the H3+ retains its kinetic energy, the final laboratory energy of the fast H+ is roughly 1/3 of the laboratory energy of the incident H3+. Similarly, the final laboratory energy of the fast H2 is approximately 2/3 of the laboratory energy of the incident H3+.

- **Cross section from Peko and Champion (1997), Fig.2(a) reaction (1)**

```
Import ["Peko97Fig2.bmp"];
Show[%];
Quit[]
```

- **Record of desired data points and representative points for both axes.**

- **Subroutine for analyzing digitized data and its application to Peko and Champion data**

```
In[32]:= analyzeDigitizedData :=
Block[{xscaledata1, xscaledata2, xfit, yscaledata1, yscaledata2, yfit,
  data1, xdata, xdatagraph, ydata, ydatagraph, xdataout, ydataout},
  xscaledata1 = Flatten[Take[Transpose[xscaledata], 1]];
  xscaledata2 = Transpose[{xscaledata1, xscalegraph}];
  xfit = Fit[xscaledata2, {1, x}, x];
  yscaledata1 = Flatten[Take[Transpose[yscaledata], -1]];
  yscaledata2 = Transpose[{yscaledata1, yscalegraph}];
  yfit = Fit[yscaledata2, {1, y}, y];
  data1 = Transpose[qtdata];
  xdata = Take[data1, 1];
  xdatagraph = Flatten[(xfit /. x → xdata)];
  ydata = Take[data1, -1];
  ydatagraph = Flatten[(yfit /. y → ydata)];
  xdataout = Power[10, xdatagraph];
  ydataout = ydatagraph;
  dataout = Transpose[{xdataout, ydataout}];]
```

```
In[33]:= analyzeDigitizedData
```

```
In[34]:= dataout // TableForm
```

```
Out[34]/TableForm=
```

```
6.10294 0.296943
10.3878 0.393015
14.3671 1.18776
18.6228 1.44104
22.9185 1.68561
27.1284 1.58952
31.2893 1.68561
35.1641 1.58952
41.6237 1.53712
62.2285 1.33624
82.7812 0.838429
103.206 1.0393
122.165 0.9869
162.513 0.890828
```

```
In[35]:= ListLogLinearPlot [dataout ,
  PlotRange -> {{2., 200.}, {0.0, 2.0}}, PlotStyle -> PointSize[0.02], PlotLabel ->
  {"Cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432];
```

```
In[36]:= data1Plot = ListLogLogPlot[dataout, PlotRange -> {{0.02,100000},{0.01,200.0}},
  PlotStyle->PointSize[0.02]];
```

■ Data from Fig. 10 of McClure (1963) for fast H+ production as read in 1985

```
In[37]:= mcClureDatafHp = {{2000., 0.44}, {2800., 0.64}, {4000., 0.92}, {6000., 1.25},
  {8000., 1.45}, {12 000., 1.75}, {20 000., 2.}, {28 000., 3.1}, {40 000., 3.1}};
```

```
In[38]:= mcClureDatafHp // TableForm
```

```
Out[38]/TableForm=
```

```
2000. 0.44
2800. 0.64
4000. 0.92
6000. 1.25
8000. 1.45
12 000. 1.75
20 000. 2.
28 000. 3.1
40 000. 3.1
```

```
In[39]:= mcClurefHpPlot = ListLogLogPlot[mcClureDatafHp, PlotRange -> {{0.02,100000},{0.01,200.0}},
  PlotStyle->{Hue[0.5],PointSize[0.02]},ImageSize -> 432];
```

■ Fast H2+ production from ORNL Rept. 8086

```
In[40]:= Import["Redbookvol1pg48.txt", "CSV"] // TableForm
```

```
Out[40]//TableForm=
```

Energy (eV/amu)	Velocity {cm/s}	Cross (cm ²)	Section
4.0E+01	6.84E+06	6.00E-18	
7.0E+01	1.16E+07	6.91E-18	
1.0E+02	1.39E+07	7.61E-18	
2.0E+02	1.96E+07	8.89E-18	
4.0E+02	2.78E+07	1.19E-17	
7.0E+02	3.68E+07	1.78E-17	
1.0E+03	4.39E+07	2.49E-17	
1.5E+03	5.38E+07	3.99E-17	
2.0E+03	6.21E+07	5.41E-17	
4.0E+03	8.79E+07	9.80E-17	
7.0E+03	1.16E+08	1.42E-16	
1.0E+04	1.39E+08	1.77E-16	
2.0E+04	1.96E+08	2.14E-16	
4.0E+04	2.78E+08	2.33E-16	
7.0E+04	3.68E+08	2.39E-16	
1.0E+05	4.39E+08	2.28E-16	
2.0E+05	6.21E+08	1.74E-16	
4.0E+05	8.78E+08	1.08E-16	
6.0E+05	1.08E+09	7.15E-17	

```
In[41]:= Drop[Import["Redbookvol1pg48.txt", "Table"], 2];
```

```
In[42]:= ornlq3f1Plot = ListLogLogPlot[Table[{{%[[j, 1]], %[j, 3]} * 10^16}, {j, Length[%]}],
  PlotRange -> {{0.02, 100 000}, {0.01, 200.0}}, PlotStyle -> plotColorsPoints[{{7}}];
```

■ Data from higher source pressure points of Fig. 8 of Williams and Dunbar (1966) for fast H+ production

```
In[43]:= williamsfHp = {{2000., 0.11}, {3000., 0.165}, {5000., 0.28},
  {7000., 0.4}, {10 000., 0.55}, {14 000., 0.8}, {20 000., 1.15}, {25 000., 1.3}};
```

```
In[44]:= williamsfHp // TableForm
```

```
Out[44]//TableForm=
```

2000.	0.11
3000.	0.165
5000.	0.28
7000.	0.4
10 000.	0.55
14 000.	0.8
20 000.	1.15
25 000.	1.3

Scale to CM energy

```
In[45]:= williamsfHp1 =
  Table[{{williamsfHp[[j, 1]] * 2 / 5, williamsfHp[[j, 2]]}, {j, 1, Length[williamsfHp]}];
```

```
In[46]:= williamsfHpPlot = ListLogLogPlot[williamsfHp1, PlotRange -> {{0.02,100000},{0.01,200.0}},
PlotStyle-> {Hue[0.8], PointSize[0.02]}, ImageSize -> 432];
```

■ Fit to data and compare

Fit to McClure at high energies

```
fastHpFit = UnitStep[enrel - 4.4] * 11 / Sqrt[enrel] / (1 + (12 / (enrel - 4.4)) ^ 2) *
(1 + (enrel / 1870) ^ 3.0) / (1 + (enrel / 4000) ^ 2.5) + 1. * 10^-30;
```

Fit to Williams at high energies

```
In[47]:= fastHpFit = UnitStep[enrel - 4.4] *
11 / Sqrt[enrel] / (1 + (12 / (enrel - 4.4)) ^ 2) /
(1 + (enrel / 300) ^ 3) *
(1 + (enrel / 550) ^ 4.5) / (1 + (enrel / 40 000) ^ 2)
```

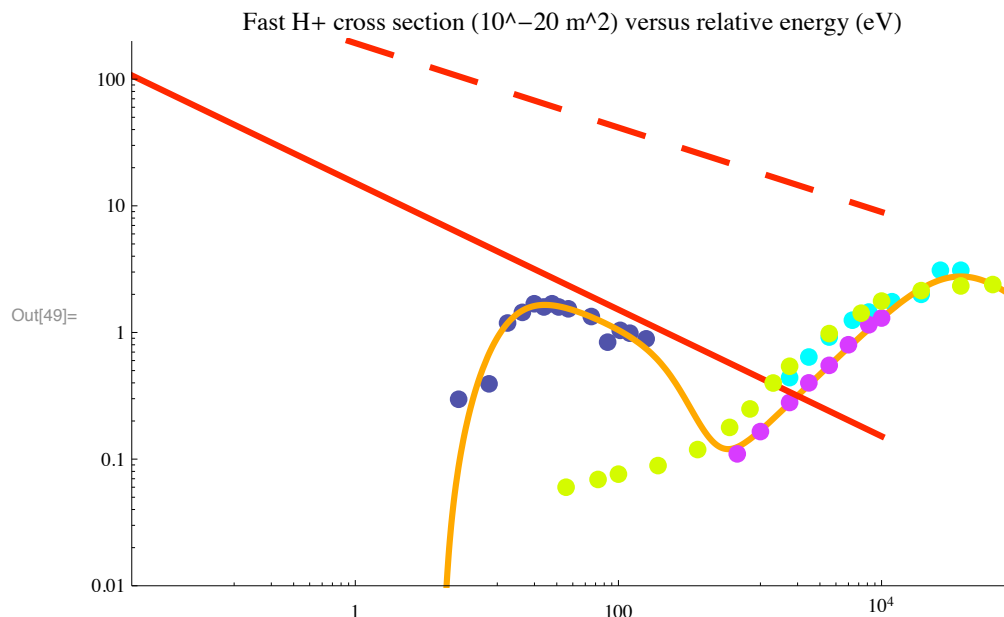
```
Out[47]= 
$$\frac{11 \left(1 + 4.65981 \times 10^{-13} \text{enrel}^{4.5}\right) \text{UnitStep}[-4.4 + \text{enrel}]}{\left(1 + \frac{144}{(-4.4 + \text{enrel})^2}\right) \sqrt{\text{enrel}} \left(1 + \frac{\text{enrel}^2}{1600000000}\right) \left(1 + \frac{\text{enrel}^3}{27000000}\right)}$$

```

7/9/11 This was modified at high energies based on ORNL 8086 Vol. 1, page G-48

```
In[48]:= fastHpPlot = LogLogPlot[fastHpFit, {enrel, 0.01, 100 000},
PlotStyle -> {Hue[0.1], Thickness[0.007]}, PlotRange -> {{0.01, 10 000}, {0.01, 200}}];
```

```
In[49]:= Show[data1Plot, mcClurefHpPlot, fastHpPlot,
williamsfHpPlot, langevinQPlot, ornlq3f1Plot, PlotLabel ->
"Fast H+ cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]
```



Heim and Stori, J. Appl. Phys. 72, 3330 (1992) disagree with this result and say that the fast H₃⁺ cross section is small on the ~2E-20 m² scale at energies from 40 to 150 eV.

Estimate of angular momentum quantum number, etc.

In order to get some feel for the probability that the the proton transfer collision will succeed in exciting rotational levels of the product H3+, Leone suggested that I estimate the angular momentum quantum number and spacing of the rotational levels for H3+. The lower rotational energy levels are shown in Fig. 2 of McCall, Phil. Trans. Roy. Soc. Lond. 358, 2385 (2000). The lowest levels, $J = 1 \rightarrow J=2$, are separated by roughly $80 \text{ cm}^{-1} = 0.01 \text{ eV}$. We estimate the internuclear separation from the collision cross section $r_a = \text{Sqrt}[Q/\text{Pi}] \sim \text{Sqrt}[1\text{E-}20/\text{Pi}] \sim 5\text{e-}11 \text{ m} \sim 1 \text{ au}$. The angular momentum of a collision at maximum radius is $m r^* v_{\text{rel}}/r_a$ and must equal $J \hbar$. At 1 eV

```
In[50]:= enrell = 1.;
```

```
In[51]:= Sqrt[2 * qe * enrell / mr]
```

```
Out[51]= 12 678.6
```

```
In[52]:= j = mr * vrel * ra / hbar /. {vrel -> Sqrt[2 * qe * enrell / mr], ra -> ao, hbar -> 1.054 * 10^-34}
```

```
Out[52]= 12.6834
```

The rigid rotator energy levels for this j are at

```
In[53]:= levelEnergy = j (j + 1) * 0.08 / 4
```

```
Out[53]= 3.47106
```

This energy is large compared to the energy that proton transfer theory says is transferred, i.e., $4/9 = 0.44 \text{ eV}$. The energy level spacing is

```
In[54]:= rotEnergyChange = (2 j + 2) * 0.08 / 4
```

```
Out[54]= 0.547337
```

This energy is comparable with the energy that proton transfer theory says is transferred, i.e., $4/9=0.44 \text{ eV}$, but the lower level needs to be occupied for a transition to take place.

fast H3+ + H2 -> fast H2+ + fast H + slow H2 by CID of H3+ meas. by McClure & Williams

This cross section is that obtained by a Peko et al (1997) using a retarding analysis of the ions produced in a H3+ + H2 collision and represents the middle energy group, i.e., those ions with an axial energy of approximately 2/3 of the energy of the incident ion. This argument seems to assume that there is little scattering in angle. We force our fit to pass through the fast H2+ results of McClure (1963). An alternative would be to make our cross section to pass through McClure's very large cross section for fast H production, as would be appropriate if McClure missed some of the fast H2+. We ignore the fast H2+ results of Lange et al (1977) as being much too small to be consistent with those of Peko et al (1997).

It may help to think of this as a two step process. The first step is an excitation process in which the H3+ projectile and thermal H2 target are not significantly deflected. During excitation of the H3+ to a dissociating state, the H3+ losses roughly 10 eV. In the second step, the H+ and H2 fragments fly apart more or less isotropically with a few eV energy. The kinetics model should show that the axial component of the final laboratory energy of the fast H2+ is approximately 2/3 of the laboratory energy of the incident H3+. Similarly, the final laboratory energy of the fast H is roughly 1/3 of the laboratory energy of the incident H3+.

- Cross section from Peko et al (1997), Fig.2a reaction (2)
- Digitize Peko and Champion.

The cross section curve gives

```

In[55]:= qtdata ={{483.921, 984.252}, {513.368, 941.215},
  {538.284, 877.792}, {558.67, 875.527},
  {565.465, 850.61}, {590.382, 812.103},
  {597.177, 798.513}, {622.093, 773.596},
  {644.744, 773.596}, {660.6, 798.513},
  {671.926, 771.331}, {710.433, 787.187},
  {742.144, 787.187}, {748.94, 775.861},
  {782.917, 775.861}, {791.977, 771.331},
  {832.749, 798.513}, {830.484, 787.187},
  {864.461, 784.922}, {912.028, 773.596}};

In[56]:= xscaledata ={{141.888, 698.847}, {948.27, 698.847}};

In[57]:= xscalegraph = Log[10,{2.,200.}];

In[58]:= yscaledata ={{144.153, 698.847}, {146.419, 1217.56}};

In[59]:= yscalegraph = {0.0,2.0};

In[60]:= analyzeDigitizedData

In[61]:= ListLogLinearPlot[dataout, PlotRange -> {{2.,200.},{0.0,2.0}},
  PlotLabel -> {"Cross section (10^-20 m^2) versus relative energy (eV)"}, ImageSize -> 432];

In[62]:= dataout // TableForm

Out[62]/TableForm=
  14.1041  1.10044
  16.6871  0.934497
  19.2388  0.689958
  21.6142  0.681224
  22.4694  0.585152
  25.9054  0.436681
  26.9305  0.384282
  31.0485  0.288209
  35.3363  0.288209
  38.6854  0.384282
  41.2703  0.279476
  51.4213  0.340612
  61.6302  0.340612
  64.0691  0.296943
  77.7892  0.296943
  81.92    0.279476
  103.398  0.384282
  102.069  0.340612
  123.927  0.331879
  162.608  0.288209

In[63]:= pekofH2pPlot = ListLogLogPlot[dataout, PlotRange -> {{0.01,100000},{0.01,200.0}},
  PlotLabel -> {"Cross section (10^-20 m^2) versus relative energy (eV)"},
  PlotStyle->PointSize[0.02]];

```


Data from McClure (1963) for fast H2+ production as read in 1985

```
In[64]:= mcClureDatafH2p = {{2000., 0.69}, {2800., 0.85}, {4000., 0.97}, {6000., 1.10},
      {8000., 1.20}, {12 000., 1.23}, {20 000., 1.18}, {28 000., 1.09}, {40 000., 0.93}};
```

```
In[65]:= mcClureDatafH2p // TableForm
```

```
Out[65]/TableForm=
```

```
2000.  0.69
2800.  0.85
4000.  0.97
6000.  1.1
8000.  1.2
12 000. 1.23
20 000. 1.18
28 000. 1.09
40 000. 0.93
```

```
In[66]:= mcClurefH2pPlot = ListLogLogPlot[mcClureDatafH2p, PlotRange -> {{0.02,100000},{0.01,200.0}},
      PlotStyle->{Hue[0.7],PointSize[0.02]},ImageSize -> 432  ];
```

- **Data from higher source pressure points of Fig. 8 of Williams and Dunbar (1966) for fast H2+ production**

```
In[67]:= williamsfH2p = {{2000., 0.2}, {3000., 0.28}, {5000., 0.45},
      {7000., 0.6}, {10 000., 0.83}, {14 000., 1.05}, {20 000., 1.3}, {25 000., 1.35}};
```

```
In[68]:= williamsfH2p // TableForm
```

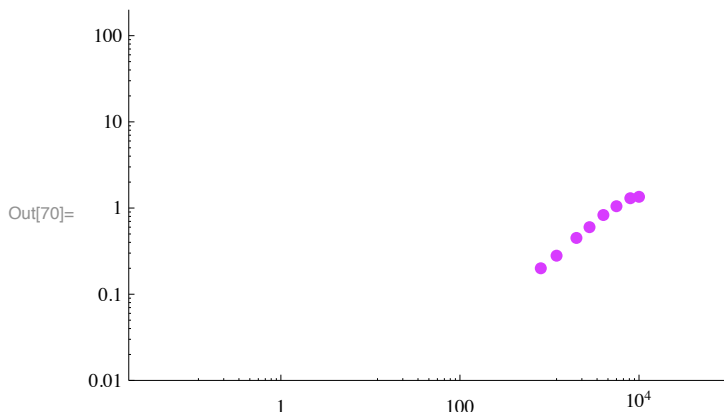
```
Out[68]/TableForm=
```

```
2000.  0.2
3000.  0.28
5000.  0.45
7000.  0.6
10 000. 0.83
14 000. 1.05
20 000. 1.3
25 000. 1.35
```

Scale to CM energy

```
In[69]:= williamsfH2p1 =
      Table[{williamsfH2p[[j, 1]] * 2 / 5, williamsfH2p[[j, 2]]}, {j, 1, Length[williamsfH2p]}];
```

```
In[70]:= williamsfH2pPlot = ListLogLogPlot[williamsfH2p1, PlotRange -> {{0.02,100000},{0.01,200.0}},
PlotStyle-> {Hue[0.8], PointSize[0.02]}]
```



■ Fast H2+ production from ORNL Rept. 8086

```
In[71]:= Import["Redbookvol1pg50.txt", "CSV"] // TableForm
```

Out[71]/TableForm=

Energy (eV/amu)	Cross (cm ²)	Section
1.1E+02	1.34E-17	
2.0E+02	1.99E-17	
4.0E+02	2.93E-17	
7.0E+02	4.17E-17	
1.0E+03	5.09E-17	
1.5E+03	6.53E-17	
2.0E+03	7.96E-17	
4.0E+03	1.18E-16	
7.0E+03	1.29E-16	
1.09+04	1.29E-16	
2.0E+04	1.18E-16	
4.0E+04	9.62E-17	
7.0E+04	7.75E-17	
1.0E+05	6.62E-17	
2.0E+05	4.69E-17	
4.0E+05	2.86E-17	
6.0E+05	2.03E-17	

```
In[72]:= Drop[Import["Redbookvol1pg50.txt", "Table"], 2];
```

```
In[73]:= ornlq3f2Plot = ListLogLogPlot[Table[{{%[[j, 1]], %[j, 2]] * 10^16}, {j, Length[%]}],
PlotRange -> {{0.02, 100 000}, {0.01, 200.0}}, PlotStyle -> plotColorsPoints[{{7}}]]];
```

■ Fit and compare

Fit to McClure

```
In[74]:= fastH2pFit = 1.3 * UnitStep[enrel - 6.2] *
enrel^0.6 / (1 + (25 / (enrel - 6.2)^1.1)) / (1 + (enrel / 16)^6)^1.0 *
(1 + (enrel / 27)^6)^0.9 / (1 + (enrel / 500)^2)^0.4 / (1 + (enrel / 70 000)) + 1. * 10^-30;
```

Fit to Williams and Dunbar

```

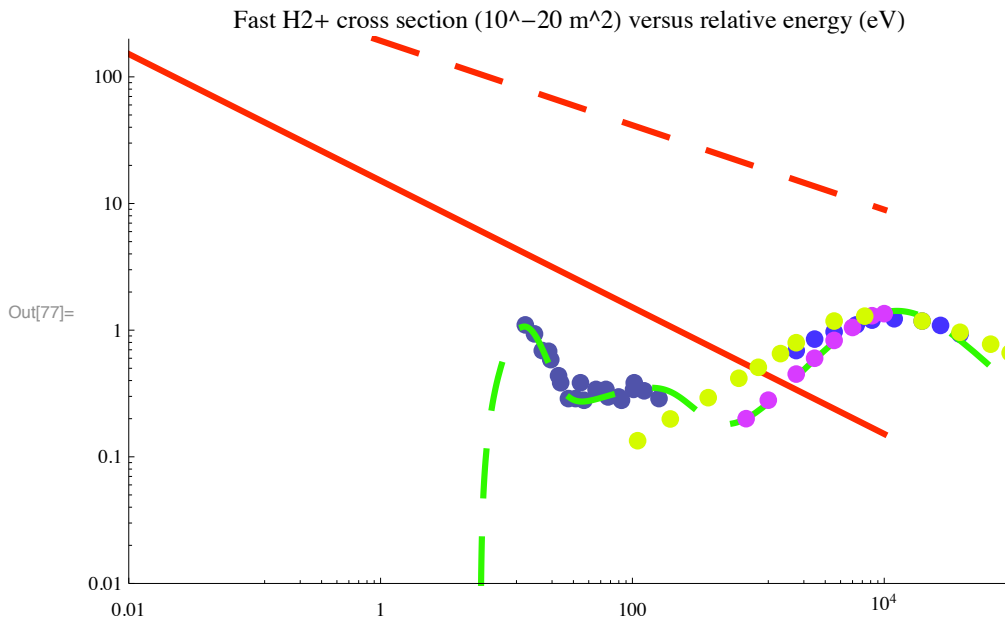
In[75]:= fastH2pFit = 1.3 * UnitStep[enrel - 6.2] *
          enrel ^ 0.6 / (1 + (25 / (enrel - 6.2) ^ 1.1)) /
          (1 + (enrel / 15) ^ 5.5) ^ 1.0 *
          (1 + (enrel / 27) ^ 5.5) ^ 0.9 / (1 + (enrel / 210) ^ 4.5) ^ 0.4 *
          (1 + (enrel / 480) ^ 2.8) / (1 + (enrel / 12 000) ^ 2)

Out[75]= 
$$\frac{1.3 \text{enrel}^{0.6} (1 + 3.10831 \times 10^{-8} \text{enrel}^{2.8}) (1 + 1.34122 \times 10^{-8} \text{enrel}^{5.5})^{0.9} \text{UnitStep}[-6.2 + \text{enrel}]}{\left(1 + \frac{25}{(-6.2 + \text{enrel})^{1.1}}\right) \left(1 + \frac{\text{enrel}^2}{144\,000\,000}\right) (1 + 3.54824 \times 10^{-11} \text{enrel}^{4.5})^{0.4} (1 + 3.40015 \times 10^{-7} \text{enrel}^{5.5})^1}$$


In[76]:= fastH2pFitPlot = LogLogPlot[fastH2pFit, {enrel, 2.5, 100 000},
          PlotStyle -> {Hue[0.3], Thickness[0.007], Dashing[{0.05, 0.05]}},
          PlotRange -> {{0.01, 100 000}, {0.01, 200}}];

```

```
In[77]:= Show[pekofH2pPlot, mcClurefH2pPlot, fastH2pFitPlot,
  williamsfH2pPlot, langevinQPlot, ornlq3f2Plot, PlotLabel ->
  "Fast H2+ cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]
```



Heim and Stori, J. Appl. Phys. 72, 3330 (1992) agree with this result, but say that the fast H+ cross section is small on the $\sim 10^{-20} \text{ m}^2$ scale at energies from 40 to 150 eV.

■ Fast H and H2+ production from Simko et al (1997)

```
In[78]:= Import["simkoqdissoch2p.dat", "CSV"] // TableForm
```

Out[78]/TableForm=

1.09356E+01	5.04725E-22
1.30913E+01	9.18811E-22
1.56700E+01	1.55653E-21
2.00515E+01	2.22913E-21
2.74343E+01	2.97037E-21
4.58849E+01	3.26586E-21
8.58237E+01	3.67704E-21
1.22718E+02	3.50227E-21
1.96191E+02	3.03002E-21
2.74329E+02	2.88612E-21
4.01266E+02	3.33006E-21
5.74039E+02	4.12902E-21
7.50892E+02	4.88087E-21
1.05046E+03	6.05221E-21

```
In[79]:= simkoDataF2=Import["simkoqdissoch2p.dat", "Table"];
```

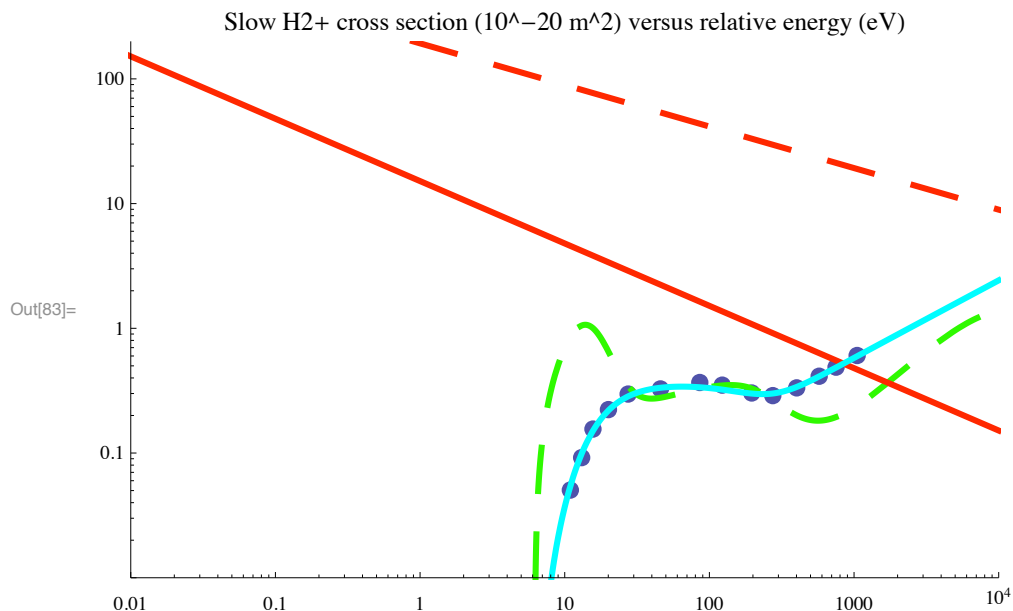
```
In[80]:= simkoF2DataPlot = ListLogLogPlot[Table[{{%[[j,1]],%[[j,2]]*fac},{j,Length[%]}], PlotRange -> {{0.01,10000}
  PlotLabel -> {"Cross section (10^-20 m^2) versus relative energy (eV)"}, ImageSize -> 432,
  PlotStyle->PointSize[0.02]]];
```

```
In[81]:= simkoF2Fit= 0.37*UnitStep[enre1-6.2]/(1+(130/(enre1-6.2)^2))/(1+(enre1/150)^2)^0.27*(1+(enre1
```

```

In[82]:= simkoF2FitPlot = LogLogPlot[simkoF2Fit, {enrel, 0.01, 10000},
    PlotStyle -> {Hue[0.5], Thickness[0.007]}, PlotRange -> {{0.01, 10000}, {0.01, 200}}];
In[83]:= Show[simkoF2DataPlot, fastH2pFitPlot, langevinQPlot, simkoF2FitPlot, PlotLabel ->
    "Slow H2+ cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]

```



fast H3+ + H2 -> **sum of slow ions** = INC = slow H3+* + slow H+ + slow H2+

This cross section is that obtained by a Peko and Champion (1997) using a retarding analysis of the ions produced in a H3+ + H2 collision and represents the slowest group, i.e., those ions with an axial energy of much less than that of the incident ion. This interpretation seems to make no specific assumption as to the scattering in angle. In the next three sections we discuss how P&C divide this component into three reactions based on a crossed beam experiment that collects only slow ions and analyzes them by mass into H3+, H2+, and H+. P&C claim that the "spectator" model of proton transfer leads to conversion of up to 5/9 of the CM energy (2/9 of the LAB energy for a cold target H2) into internal energy of the H3+. This could be an efficient means of vibrational excitation (and deexcitation) of the H3+ and is observed by P&C to lead to dissociation at CM collision energies above about 6 eV.

Measurements of the differential cross sections for H3+ + D2 -> D2H+* + H2 by Vestal et al (1976) show that this proton transfer process produces D2H+* with velocities near 180 deg in CM, but with kinetic energies somewhat higher than predicted by the spectator stripping model. The higher than expected energy of the product ion is attributed to initial internal energy of the projectile H3+. The "spectator stripping" model is described, for example, in Sec. 1.4 of Levine and Bernstein, "Molecular Reaction Dynamics" (Oxford Univ. Press, Oxford, 1974). See Peko and Champion (1997) for a statement as to its significance

for $H3^+ + H2$.

A model of the internal energy distribution for the $H3^+$ produced in the $H2^+ + H2$ relaxation is discussed by Anicich and Futrell, *Int. J. Mass. Spectrom. and Ion Processes* 55, 189 (1983). They find approximate agreement with a statistical distribution of $H3^+$ in the excited states. These considerations could serve as a guide to the internal energy distribution in the $H3^+$ produced in the reaction of fast $H3^+$ with $H2$. These authors also consider the relaxation of this energy in collisions with $H2$ and seem to assume 60% of the maximum rate (Langevin?) for the lowest excited state. I do not understand! The most recent reference on $H2^+ + H2$ that I have found is Pollard et al, *J. Chem. Phys.* 95, 4877 (1991). The most interesting new result appears to be that much of the translational energy ends up as rotational energy of the $H3^+$, whereas most of the reaction energy is found in vibration. The recoil energy is $\sim 30\%$ of the available energy.

Angular distributions, etc. will be discussed with the individual processes.

- **Total proton transfer cross section from Peko et al (1997), Fig.2b reactions (3), (4a), and (4b)**
- **Record of desired data points and representative points for both axes.**

```
Import ["PekoFig3.bmp"];
Show [%];
```

The cross section curve Q gives

```
In[84]:= qtdata ={{236.308, 585.552}, {275.794, 567.605},
  {308.1, 520.94}, {333.227, 443.764},
  {338.611, 404.279}, {358.354, 379.152},
  {378.096, 354.025}, {390.66, 337.872},
  {406.813, 318.129}, {424.761, 296.592},
  {433.735, 285.823}, {464.246, 260.696},
  {518.09, 223.006}, {552.191, 210.442},
  {571.933, 206.853}, {604.239, 203.263},
  {631.161, 201.468}, {647.314, 201.468},
  {670.647, 203.263}, {744.233, 210.442},
  {796.282, 215.827}, {837.562, 223.006},
  {869.868, 230.185}};

In[85]:= xscaledata ={{141.185, 149.419}, {947.044, 149.419}};

In[86]:= xscalegraph = Log[10,{2.,200.}];

In[87]:= yscaledata ={{142.979, 149.419}, {144.774, 594.526}};

In[88]:= yscalegraph = {0.0,5.0};

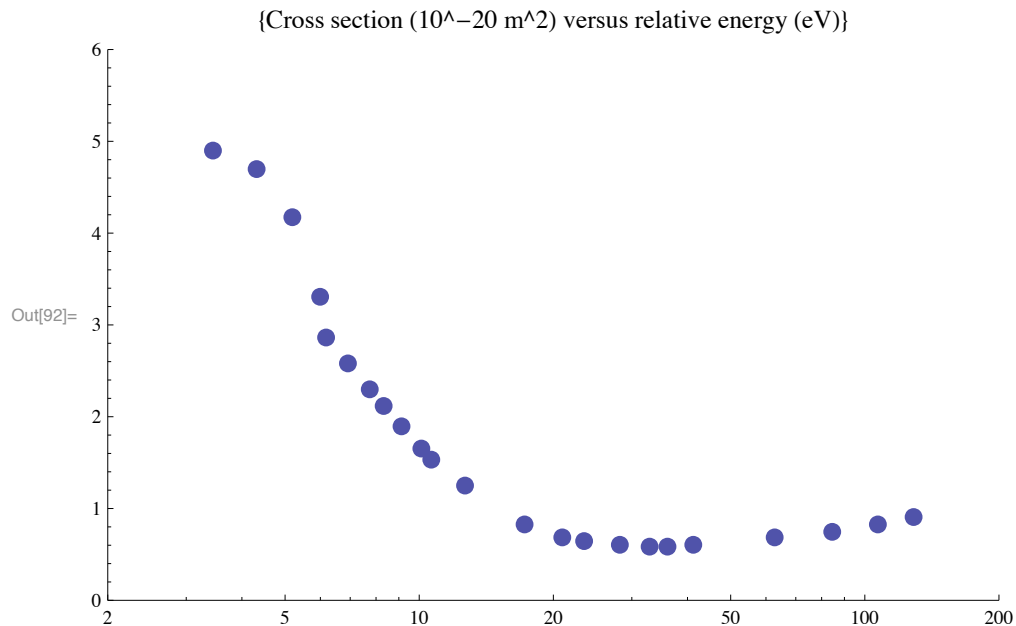
In[89]:= analyzeDigitizedData

In[90]:= data3Plot1 =ListLogLinearPlot[dataout, PlotStyle -> PointSize[0.02],
  PlotRange -> {{2.,200.},{0.0,6.0}},PlotLabel -> {"Cross section ( $10^{-20} \text{ m}^2$ ) versus relative energy (eV)}]
```

In[91]:= **dataout // TableForm**

```
Out[91]/TableForm=
  3.44436  4.89919
  4.31624  4.69759
  5.19139  4.17339
  5.993    3.30645
  6.18026  2.86291
  6.91839  2.58065
  7.74464  2.29839
  8.32114  2.11694
  9.12582  1.89516
  10.1115  1.65323
  10.6436  1.53226
  12.671   1.25
  17.2362  0.826621
  20.9447  0.685487
  23.4461  0.645171
  28.2     0.604843
  32.89    0.58468
  36.0706  0.58468
  41.2156  0.604843
  62.7609  0.685487
  84.5017  0.745978
  106.983  0.826621
  128.675  0.907265
```

In[92]:= **Show[data3Plot1, PlotLabel -> {"Cross section (10⁻²⁰ m²) versus relative energy (eV)"}, ImageSize -> 432]**



Note that this data is plotted versus CM energy.

In[93]:= **dataPTPlot2 = ListLogLogPlot[dataout, PlotRange -> {{0.01,10000},{0.01,200.0}}, PlotLabel -> {"Cross section (10⁻²⁰ m²) versus relative energy (eV)"}, PlotStyle->PointSize[0.02]];**

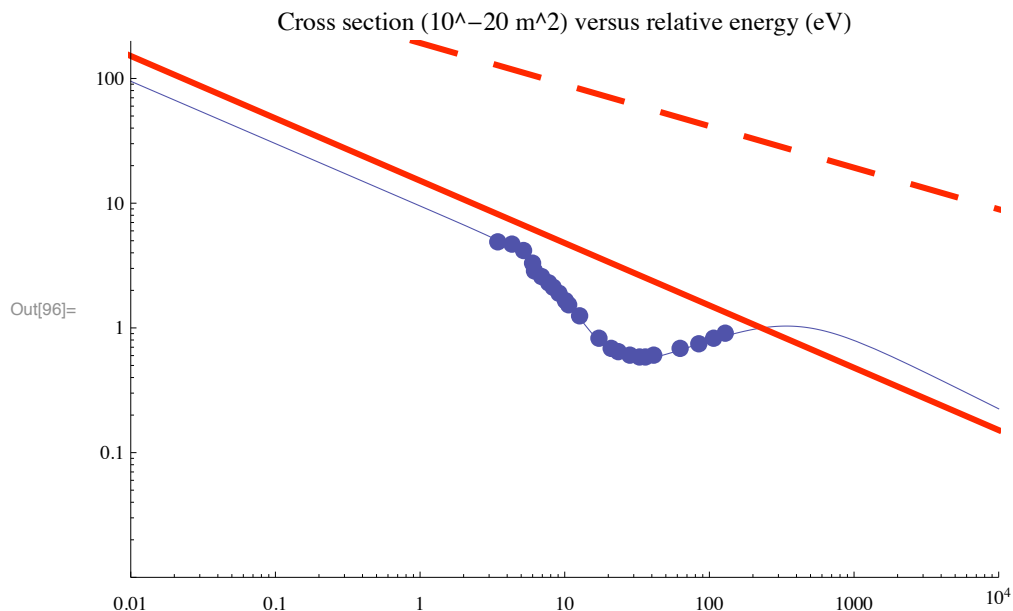
```

In[94]:= fitPT = 9.5 / enrel ^ 0.5 / (1 + (enrel / 7) ^ 4) ^ 0.35 *
          (1 + (enrel / 21.5) ^ 4) ^ 0.58 / (1 + (enrel / 400) ^ 2) ^ 0.5 + 1. * 10 ^ - 30;

In[95]:= fitPTPlot =
          LogLogPlot[fitPT, {enrel, 0.01, 10 000}, PlotRange -> {{0.01, 1000}, {0.01, 200}}];

In[96]:= Show[dataPTPlot2, fitPTPlot, langevinQPlot,
          PlotLabel -> "Cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]

```



The portion of this cross section at energies above ~ 200 eV is adjusted to give the production of fast H2 as observed by McClure (1963). See plot below. This fitting seems inconsistent with my choosing Williams and Dunbar (1966), rather than McClure, for fast H+ and fast H2+. McClure is our only source of fast H2 data.

fast H3+ + H2 -> slow, bound H3+* + fast H2 = vibrational excitation of slow H3+ by proton transfer (3)

This cross section is that obtained by a Peko and Champion (1997) (P&C) based on a crossed beam experiment that collects only slow ions and analyzes them by mass into H3+. The results are presented as a fraction of the total slow component of the initial H3+ + H2 reaction. P&C and others say that the H3+ produced by this process is vibrationally (and rotationally?) excited, i.e., in this energy range H3+ + H2 -> H3+* + H2 is an inelastic collision. P&C say that in the "spectator" model the H3+* is left with an internal energy of 5/9 of the collision energy and that this energy can lead to a competition between dissociation into H+ + H2 or H2+ + H and vibrational relaxation. Since the fractional energy lost in a momentum transfer collision is $2*m*M/(m+M)^2=12/25$, we will usually lump the proton transfer and elastic collisions together.

This is the higher energy component of Simko et al.(1997). If this really is a proton transfer collision, it results in vibrational excitation and in 180 deg scattering in CM mass and presumably has a threshold at the vibrational bending mode, i.e., at 0.31 eV. I have not found any theory relevant to H3+ + H2 collisions and so have no guidance as to the vibrational-rotational excitation (or anything else). For the somewhat related system of H2+ + H2, Bates and Reid, Proc. Roy. Soc. A 310, 1 (1969) seem to find a slow onset to vibrational excitation. On the other hand, Krstic and Schultz, J. Phys. B 32, 2515 (1999) find a rather sharp onset for vibrational excitation in collisions of H+ and H with H2.

As far as mobility of H3+ in H2 at low and moderate E/N is concerned, this ion-molecule combination behaves like that for elastic scattering in a potential similar to that of an alkali ion in H2 or in a rare gas with a weak repulsive core. However at E/N ~ 400 Td there is an anomalous behavior in which the mobility of H3+ and H+ approach each other. Phelps (1990) proposed this is caused by H3+* breakup. Peko et al (1997) noted that at low energies the cross section for proton transfer was approximately half the Langevin value. We expect that the contribution of this process to the effective momentum transfer cross section is twice the proton transfer value (as in the case of charge transfer by an electron) because of the observed production of a slow H3+ ion, i.e., effectively 180 deg scattering in CM.

In summary, we treat this process as a single step vibrational and rotational excitation in which the product H3+* has more internal energy than the incident H3+. The product H3+* is directed at 180 deg in CM and the product H2 is directed a 0 deg in CM. Their relative translational energy at the end of the first step is 4/9 times the initial relative translational energy. As discussed by P&C, this proton transfer model predicts that 5/9 of the initial relative translational energy ends up as internal energy of the product H3+*, rather than the fixed energy usually associated with inelastic collisions. This simplified model neglects the discrete nature of the vibrational and rotational levels of H3+*. I do not know of any quantum mechanical theory of this collision process.

- **Relative cross section from Peko and Champion (1997), Fig. 3a reaction (3)**

- **Digitize data from Peko and Champion (1995).**

This relative cross section curve Qt gives

```
In[97]:= qtdata ={{274.572, 1207.76}, {319.974, 1178.57},
  {355.647, 1141.27}, {379.97, 1094.25},
  {407.536, 1042.36}, {430.237, 1021.28},
  {443.209, 982.364}, {461.046, 958.042},
  {480.504, 941.826}, {490.233, 932.097},
  {521.042, 920.747}, {579.417, 902.91},
  {618.333, 888.316}, {639.413, 886.695},
  {673.465, 885.073}, {702.652, 883.452},
  {720.489, 885.073}, {744.811, 883.452},
  {825.887, 880.209}, {881.019, 883.452},
  {923.178, 881.83}, {957.23, 883.452}};

In[98]:= xscaledata ={{177.28, 880.209}, {947.501, 883.452}};

In[99]:= xscalegraph = Log[10,{2.0,120.}];

In[100]:= yscaledata ={{175.659, 881.83}, {178.902, 1219.11}};

In[101]:= yscalegraph = {0.0,1.0};

In[102]:= analyzeDigitizedData

In[103]:= data4Plot1 = ListLogLinearPlot[dataout, PlotRange -> {{2.0,150.},{0.0,1.0}},
  PlotLabel -> {"Cross section (10^-20 m^2) versus relative energy (eV)"}, ImageSize -> 432,
  PlotStyle -> PointSize[0.02]];
```

```
In[104]:= dataout // TableForm
```

```
Out[104]/TableForm=
```

```
3.3546 0.966348
4.27029 0.879803
5.16193 0.769213
5.87442 0.629803
6.8015 0.475955
7.67384 0.413455
8.22167 0.298073
9.03939 0.225961
10.0244 0.177882
10.5565 0.149036
12.435 0.115385
16.9595 0.0625
20.8572 0.0192303
23.3304 0.0144242
27.9599 0.00961516
32.6525 0.00480906
35.9001 0.00961516
40.8551 0.00480906
62.8666 -0.0048061
84.2751 0.00480906
105.446 1.33227 × 10-15
126.369 0.00480906
```

```
In[105]:= normData =
```

```
Abs[Table[{dataout[[j, 1]], (fitPT /. enrel -> dataout[[j, 1]]) * dataout[[j, 2]]},
{j, 1, Length[dataout]}] ];
```

```
In[106]:= data4Plot = ListLogLogPlot[normData, PlotRange -> {{0.01, 10000}, {0.01, 200.}},
PlotLabel -> {"Cross section (10-20 m2) versus relative energy (eV)"}, ImageSize -> 432,
PlotStyle -> PointSize[0.02]];
```

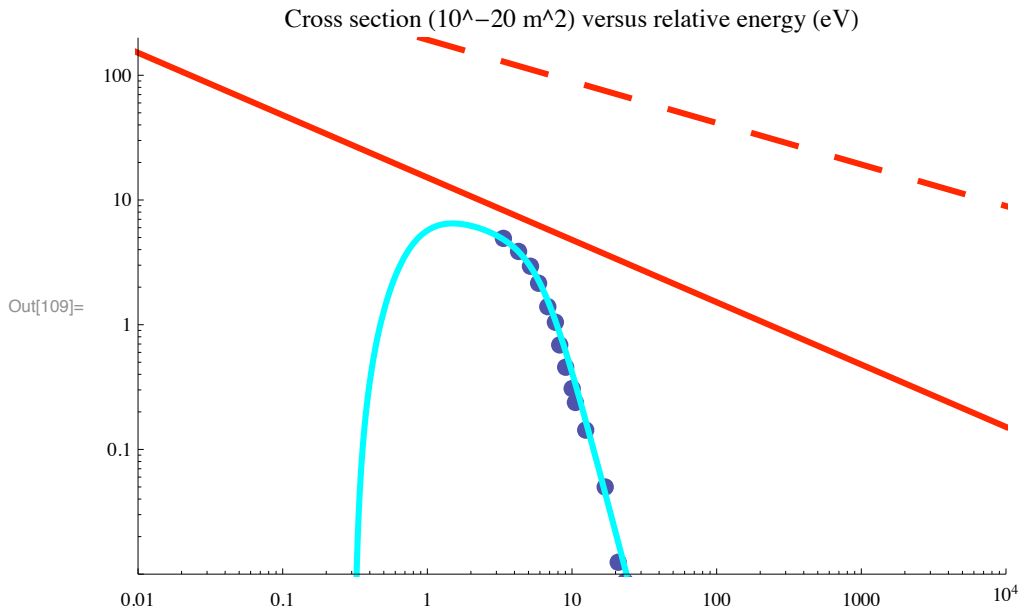
```
In[107]:= protonTransferFit = 10 * UnitStep[enrel - 0.31] *
enrel-0.5 / (1 + (0.6 / (enrel - 0.31))2) /
(1 + (enrel / 6.2)3.95)
```

```
Out[107]= 
$$\frac{10 \text{UnitStep}[-0.31 + \text{enrel}]}{\left(1 + \frac{0.36}{(-0.31 + \text{enrel})^2}\right) \text{enrel}^{0.5} (1 + 0.0007414 \text{enrel}^{3.95})}$$

```

```
In[108]:= protonTransferPlot = LogLogPlot[protonTransferFit, {enrel, 0.01, 10000},
PlotStyle -> {Hue[0.5], Thickness[0.007]}, PlotRange -> {{0.01, 10000.}, {0.01, 200}}];
```

```
In[109]:= Show[data4Plot, protonTransferPlot, langevinQPlot,
PlotLabel -> "Cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]
```



fast H3+ + H2 -> slow H+ + slow H2 + fast H2 = slow H3+* by proton transfer then dissociation. (4a)

This relative cross section is that obtained by Peko et al (1997) based on a crossed beam experiment that collects only slow ions and analyzes them by mass into H+ and H2+. The results are presented as a fraction of the total slow component of the initial H3+ + H2 reaction. I have not found measurements of the production of slow H+ other than P&C. The principle difference between this process and the previous one is that the internal energy of the H3+ after the collision is high enough so the H3+ is unstable and disintegrates.

We think of this as a two step process. The first step is the proton transfer process and is an inelastic collision in which the product H3+* has more internal energy than the incident H3+. The proton transfer process is one in which the product H+* is directed at 180 deg in CM and the product H2 is directed at 0 deg in CM. Their relative translational energy at the end of the first step is 4/9 times the initial relative translational energy. As discussed by P&C, this proton transfer model predicts that 5/9 of the initial relative translational energy ends up as internal energy of the product H3+*. In the second step, the excited H3+* dissociates with a relative energy approximately equal to the excess of the excitation energy over the binding energy of 4.4 eV and with the usual conservation of momentum, etc. This simplified model neglects the discrete nature of the vibrational and rotational levels of H3+*. I do not know of any quantum mechanical theory of this collision process.

- Relative cross section from Peko et al (1998), Fig.3 reaction (4a)

- Digitize data of Peko and Champion.

```
Import["Peko97Fig3.bmp"];
```

```
Show[%];
```

The cross section curve gives

```

In[110]:= qtdata ={{272.95, 889.938}, {316.731, 912.639},
{354.026, 948.313}, {379.97, 993.715},
{405.914, 1048.85}, {428.616, 1060.2},
{443.209, 1102.36}, {461.046, 1112.09},
{477.261, 1118.57}, {490.233, 1120.19},
{521.042, 1066.68}, {577.795, 1032.63},
{618.333, 1014.79}, {641.034, 1003.44},
{671.843, 996.958}, {702.652, 995.337},
{722.11, 992.093}, {744.811, 987.229},
{825.887, 979.121}, {881.019, 979.121},
{923.178, 975.878}, {957.23, 966.149}};

In[111]:= xscaledata ={{177.28, 881.83}, {947.501, 883.452}};

In[112]:= xscalegraph = Log[10,{2.,120.}];

In[113]:= yscaledata ={{177.28, 880.209}, {178.902, 1219.11}};

In[114]:= yscalegraph = {0.0,1.0};

In[115]:= analyzeDigitizedData

In[116]:= data5Plot = ListLogLinearPlot[dataout, PlotRange -> {{2.,150.},{0.0,1.0}}, PlotStyle -> PointSize[0.02], Ime
PlotLabel -> {"Cross section (10^-20 m^2) versus relative energy (eV)"}];

In[117]:= dataout // TableForm

Out[117]//TableForm=
3.3258 0.0287075
4.1973 0.0956917
5.11765 0.200955
5.87442 0.334924
6.74311 0.497611
7.608 0.531102
8.22167 0.655504
9.03939 0.684215
9.85311 0.703335
10.5565 0.708115
12.435 0.550223
16.8139 0.449751
20.8572 0.39711
23.5323 0.363619
27.7198 0.344493
32.6525 0.33971
36.2108 0.330138
40.8551 0.315785
62.8666 0.291861
84.2751 0.291861
105.446 0.282292
126.369 0.253584

In[118]:= normData5 = Table[{dataout[[j, 1]], (fitPT /. enrel -> dataout[[j, 1]]) * dataout[[j, 2]]},
{j, 1, Length[dataout]}];

In[119]:= data5Plot = ListLogLogPlot[normData5, PlotRange -> {{0.01,10000},{0.01,200.}},
PlotLabel -> {"Cross section (10^-20 m^2) versus relative energy (eV)"}, ImageSize -> 432,
PlotStyle->PointSize[0.02]];

```

Note that the following Huber et al data have been reduced from their Fig. 1 data to give the slow H2+ formation only.

```
In[120]:= huberHpData = {{90., 0.15}, {450., 0.2}};
```

```
In[121]:= huberHpPlot = ListLogLogPlot[huberHpData, PlotRange -> {{0.01, 10 000}, {0.01, 200.}},
  ImageSize -> 432, PlotStyle -> {Hue[0.3], PointSize[0.02]}];
```

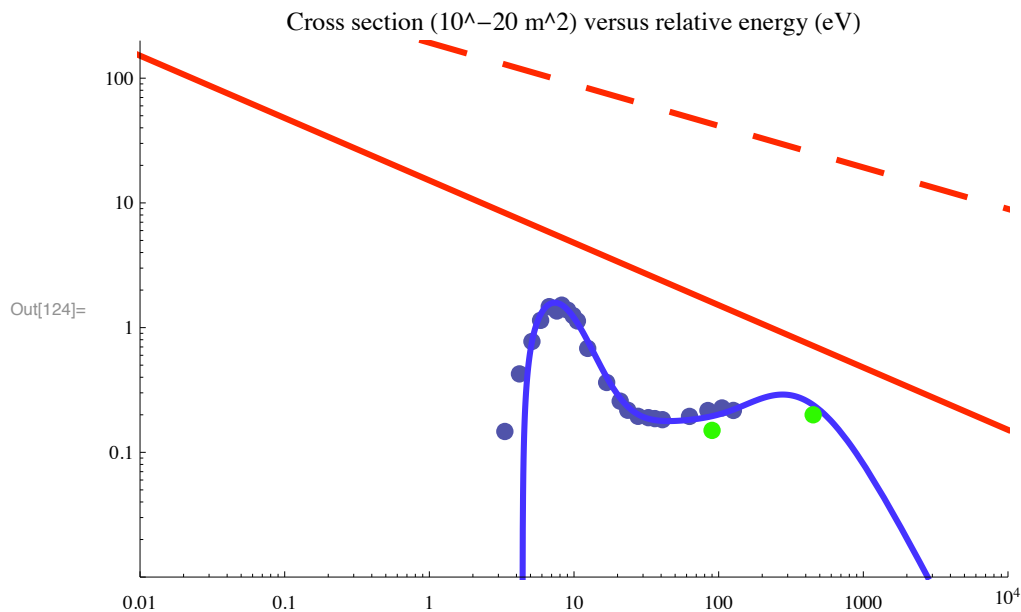
```
In[122]:= slowHpFit = 1.3 * UnitStep[enrel - 4.4] *
  enrel ^ 0.6 / (1 + (2 / (enrel - 4.4) ^ 1.1)) /
  (1 + (enrel / 8.) ^ 4.05) ^ 1.0 * (1 + (enrel / 21.) ^ 4) ^ 0.9 *
  (1 + (enrel / 120) ^ 3.5) ^ 0.4 / (1 + (enrel / 350) ^ 1.9) ^ 2
```

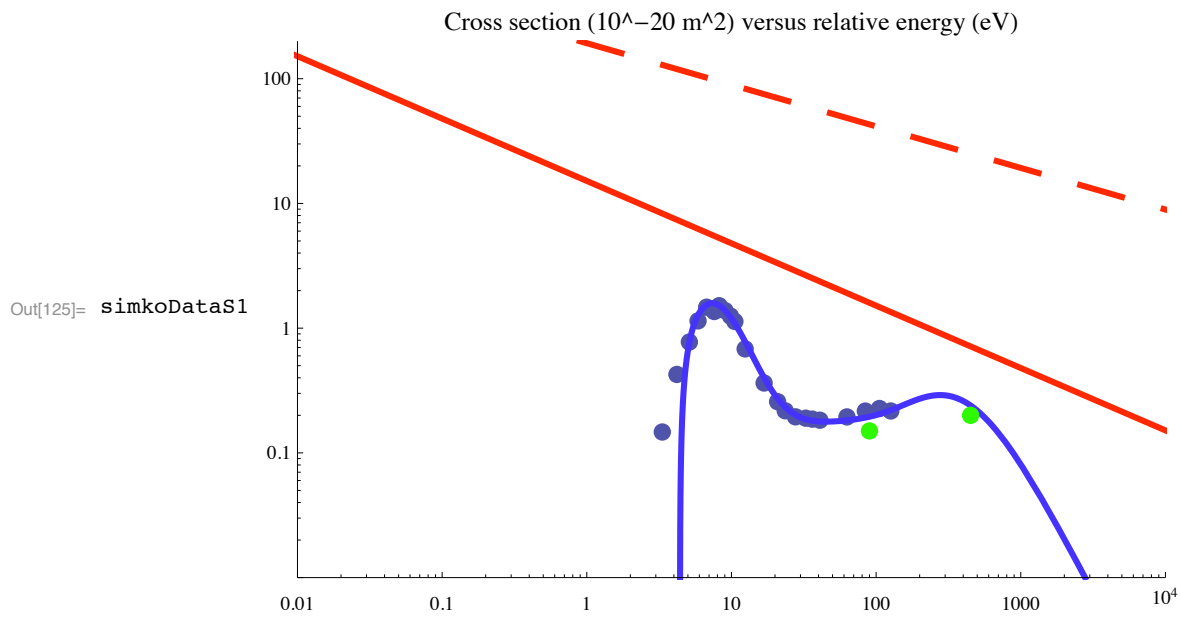
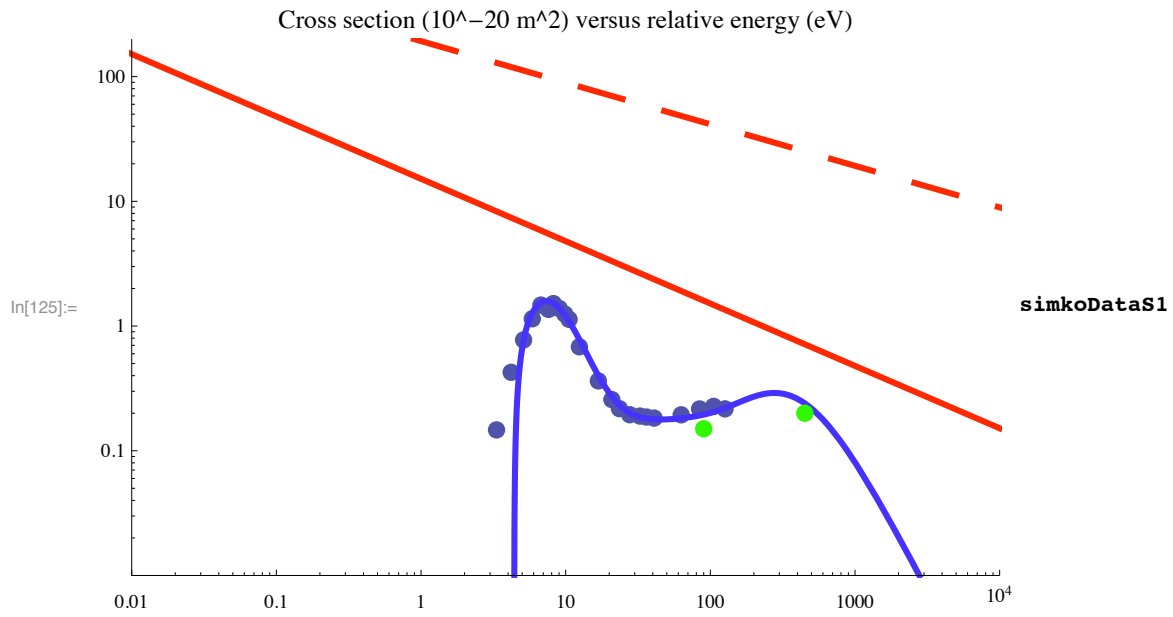
```
Out[122]= 
$$\frac{1.3 \text{enrel}^{0.6} (1 + 5.28282 \times 10^{-8} \text{enrel}^{3.5})^{0.4} (1 + 5.14189 \times 10^{-6} \text{enrel}^4)^{0.9} \text{UnitStep}[-4.4 + \text{enrel}]}{\left(1 + \frac{2}{(-4.4 + \text{enrel})^{1.1}}\right) (1 + 0.0000146646 \text{enrel}^{1.9})^2 (1 + 0.000220032 \text{enrel}^{4.05})^{1.0}}$$

```

```
In[123]:= slowHpFitPlot = LogLogPlot[slowHpFit, {enrel, 0.01, 10 000.},
  PlotStyle -> {Hue[0.7], Thickness[0.007]}, PlotRange -> {{0.01, 10 000.}, {0.01, 200}}];
```

```
In[124]:= Show[data5Plot, slowHpFitPlot, langevinQPlot, huberHpPlot,
  PlotLabel -> "Cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]
```





■ From Simko et al (1997)

```
ln[126]:= simkoDataS1=Import["simkoqchgtranhp.dat", "Table"];
```

```
In[127]:= simkoDataS1 // TableForm
```

```
Out[127]/TableForm=
```

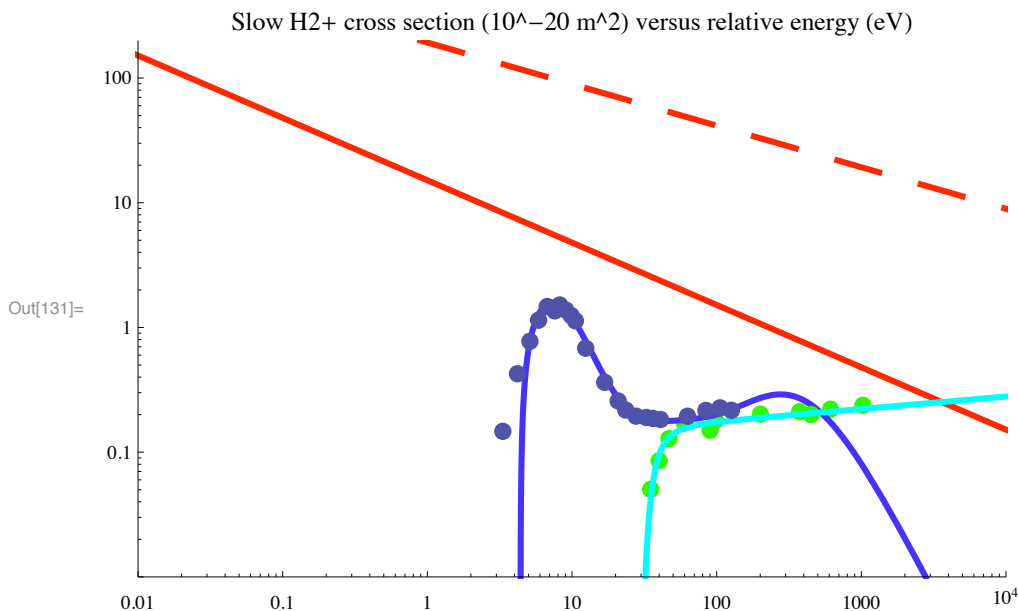
```
34.9699 5.03505 × 10-22
40.0278 8.53051 × 10-22
46.8428 1.28192 × 10-21
59.9329 1.70843 × 10-21
98.0153 1.79052 × 10-21
200.478 2.01557 × 10-21
374.928 2.11183 × 10-21
613.165 2.21331 × 10-21
1025.5 2.37583 × 10-21
```

```
In[128]:= simkoS1DataPlot = ListLogLogPlot[Table[{{%[[j,1]],%[[j,2]]*fac},{j,Length[%]}], PlotRange->{{0.01,10000}},
PlotLabel -> "Cross section (10-20 m2) versus relative energy (eV)", ImageSize -> 432, PlotStyle->{Hu
```

```
In[129]:= simkoS1Fit= 0.14*UnitStep[enrel-30]/(1+(70/(enrel-30)2)*(1+(enrel/10)2)0.05 + 1.*10-30;
```

```
In[130]:= simkoS1FitPlot = LogLogPlot[simkoS1Fit, {enrel, 0.01, 10000},
PlotStyle -> {Hue[0.5], Thickness[0.007]}, PlotRange -> {{0.01, 10000}, {0.01, 200}}];
```

```
In[131]:= Show[simkoS1DataPlot, slowHpFitPlot, langevinQPlot,
huberHpPlot, simkoS1FitPlot, data5Plot, PlotLabel ->
"Slow H2+ cross section (10-20 m2) versus relative energy (eV)", ImageSize -> 432]
```



fast H3+ + H2 → slow H2+ + slow H + fast H2 = slow H3+*by proton transfer then dissociation. (4b)

This relative cross section is that obtained by Peko et al (1997) based on a crossed beam experiment that collects only slow ions and analyzes them by mass into H2+ and H+. The results of P&C are presented in their Fig. 3a as a fraction of the total slow component of the initial H3+ + H2 reaction labeled INC. Huber et al measure the slow H2+ formation cross section at energies from 120 to 500 eV in CM.

In the first step of this two step model, the collision appears to be one in which the H3+ projectile and H2 target are not significantly deflected during proton transfer to H2. In CM the unstable H3+ is at 180 deg and the H2 is at 0. Then the H and H2+ fragments fly apart more or less isotropically with a few eV relative energy. There is much uncertainty in this model, e.g., the amount of internal energy of the molecular fragments.

Peko and Champion had no way to distinguish the products slow H2+ + slow H + fast H2 from the products slow H2+ + fast H + fast H2, i.e., no way to distinguish proton abstraction followed by dissociation of the H3+ (the present process) from electron charge transfer followed by dissociation of the H3 (the next process). It seems to me that Vogel and Meierjohann (1978) should have seen any fast H2 at their $\theta_1 = \theta_2 = 0$ for 10 keV H3+ + H2.

- **Cross section from Peko et al (1997), Fig. 3 reaction (4b), (5), and (6)**

- **Digitize data points and reconstruct plot.**

The relative cross section curve gives

```
In[132]:= qtdata ={{272.95, 880.209}, {316.731, 886.695},
  {354.026, 886.695}, {379.97, 888.316},
  {404.293, 888.316}, {426.994, 896.424},
  {443.209, 891.559}, {459.424, 907.775},
  {477.261, 917.504}, {490.233, 925.611},
  {521.042, 988.85}, {579.417, 1042.36},
  {618.333, 1074.79}, {639.413, 1091.01},
  {673.465, 1099.11}, {702.652, 1100.74},
  {722.11, 1103.98}, {744.811, 1110.46},
  {827.509, 1118.57}, {881.019, 1120.19},
  {923.178, 1121.81}, {958.852, 1133.17}};

In[133]:= xscaledata ={{175.659, 881.83}, {947.501, 883.452}};

In[134]:= xscalegraph = Log[10,{2.0,120.}];

In[135]:= yscaledata ={{177.28, 880.209}, {178.902, 1219.11}};

In[136]:= yscalegraph = {0.0,1.0};

In[137]:= analyzeDigitizedData

In[138]:= data3Plot1 =ListLogLinearPlot[dataout, PlotRange -> {{2.,150.},{0.0,1.0}}, ImageSize -> 432,
  PlotLabel -> {"Cross section (10^-20 m^2) versus relative energy (eV)"},
  PlotStyle -> PointSize[0.02]];
```



```
In[139]:= dataout // TableForm
```

```
Out[139]/TableForm=
```

```
3.35094 1.33227 × 10-15
4.22696 0.0191383
5.15167 0.0191383
5.91176 0.0239214
6.72592 0.0239214
7.58664 0.0478458
8.26809 0.0334906
9.01075 0.0813394
9.90498 0.110047
10.6106 0.133968
12.4944 0.320569
17.0294 0.478461
20.934 0.574153
23.4108 0.622014
28.0455 0.645914
32.7419 0.650724
36.302 0.660284
40.9476 0.679405
63.496 0.703335
84.3377 0.708115
105.474 0.712896
127.448 0.746416
```

```
In[140]:= normData6 =
```

```
Abs[Table[{dataout[[j, 1]], (fitPT /. enrel -> dataout[[j, 1]]) * dataout[[j, 2]]},
{j, 1, Length[dataout]}]]];
```

```
In[141]:= data6Plot = ListLogLogPlot[normData6, PlotRange -> {{0.01, 10000}, {0.01, 200.}},
PlotLabel -> {"Cross section (10-20 m2) versus relative energy (eV)"}, ImageSize -> 432,
PlotStyle -> PointSize[0.02]]];
```

```
In[142]:= slowH2pFit =
```

```
0.3 * UnitStep[enrel - 6.2] / (1 + (5 / (enrel - 6.2) ^ 2)) *
(1 + (enrel / 10) ^ 2) ^ 0.12 / (1 + (enrel / 2000) ^ 1)
```

```
Out[142]= 
$$\frac{0.3 \left(1 + \frac{\text{enrel}^2}{100}\right)^{0.12} \text{UnitStep}[-6.2 + \text{enrel}]}{\left(1 + \frac{5}{(-6.2 + \text{enrel})^2}\right) \left(1 + \frac{\text{enrel}}{2000}\right)}$$

```

```
In[143]:= slowH2pPlot = LogLogPlot[slowH2pFit, {enrel, 2.5, 10 000},
PlotStyle -> {Hue[0.8], Thickness[0.007]}, PlotRange -> {{0.01, 10 000}, {0.01, 200}}];
```

Note that the following Huber et al data have been reduced from their Fig. 1 data to give the slow H2+ formation only.

```
In[144]:= huberH2pData = {{90., 0.3}, {450., 0.4}};
```

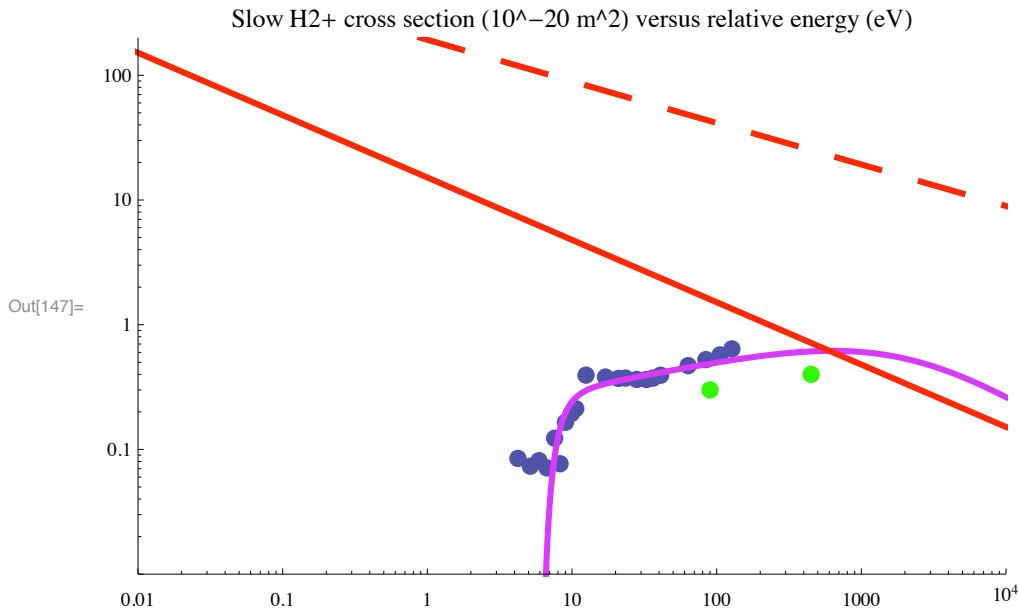
```
In[145]:= huberH2Data // TableForm
```

```
Out[145]/TableForm=
```

```
huberH2Data
```

```
In[146]:= huberH2pPlot = ListLogLogPlot[huberH2pData, PlotRange -> {{0.01, 10 000}, {0.01, 200.}},
ImageSize -> 432, PlotStyle -> {Hue[0.3], PointSize[0.02]}];
```

```
In[147]:= Show[data6Plot, huberH2pPlot, slowH2pPlot, langevinQPlot, PlotLabel ->
  "Slow H2+ cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]
```



Heim and Stori, J. Appl. Phys. say that the total H2+ cross section is small on the $\sim 1\text{E-}20$ m² scale at energies from 40 to 150 eV.

From Simko et al (1997)

```
In[148]:= Import["simkoqchgtranh2p.dat", "CSV"] // TableForm
```

```
Out[148]/TableForm=
  1.00002E+01    5.04820E-22
  1.09441E+01    7.77133E-22
  1.30998E+01    1.31651E-21
  1.67656E+01    2.07518E-21
  2.14516E+01    2.83273E-21
  3.06881E+01    3.51239E-21
  5.13291E+01    3.95553E-21
  9.60151E+01    4.67230E-21
  1.79619E+02    5.79007E-21
  3.28564E+02    6.83961E-21
  5.62105E+02    8.68318E-21
  1.02848E+03    1.18442E-20
```

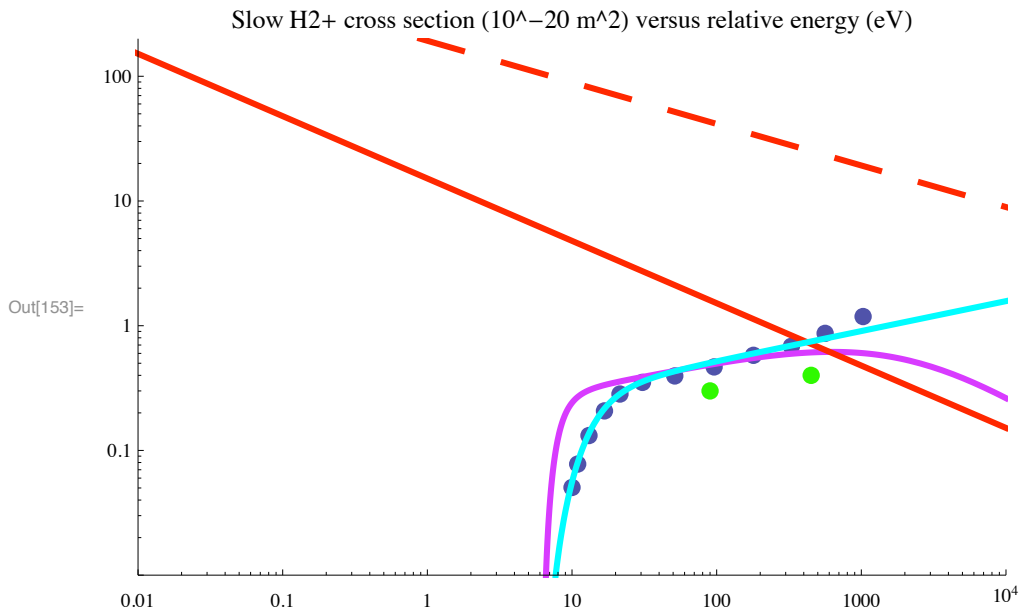
```
In[149]:= simkoDataS2=Import["simkoqchgtranh2p.dat", "Table"];
```

```
In[150]:= simkoS2DataPlot = ListLogLogPlot[Table[{{%[[j,1]],%[[j,2]]*fac},{j,Length[%]}], PlotRange -> {{0.01,10000}
  PlotLabel -> {"Cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432,
  PlotStyle->PointSize[0.02]];
```

```
In[151]:= simkoS2Fit= 0.3*UnitStep[enrel-6.2]/(1+(70/(enrel-6.2)^2))*(1+(enrel/10)^2)^0.12 + 1.*10^-3C
```

```
In[152]:= simkoS2FitPlot = LogLogPlot[simkoS2Fit, {enrel, 0.01, 10 000},
  PlotStyle -> {Hue[0.5], Thickness[0.007]}, PlotRange -> {{0.01, 10 000}, {0.01, 200}}];
```

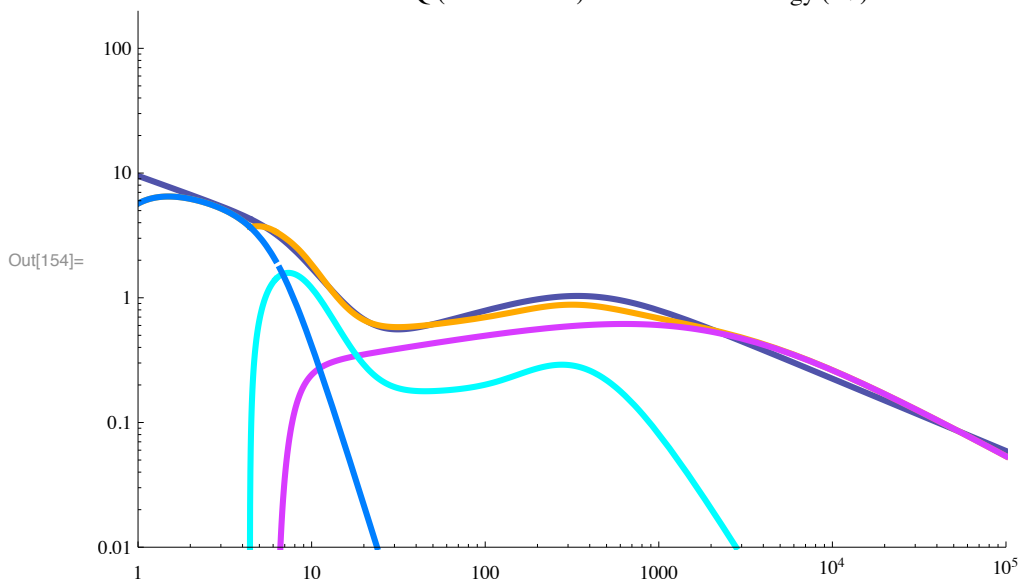
```
In[153]:= Show[simkoS2DataPlot, huberH2pPlot, slowH2pPlot, langevinQPlot, simkoS2FitPlot, PlotLabel -> "Slow H2+ cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]
```



■ Check of sum of proton transfer fits versus total proton transfer

```
In[154]:= checkPTPlot = LogLogPlot[{fitPT, slowH2pFit + slowHpFit + protonTransferFit,
  slowH2pFit, slowHpFit, protonTransferFit}, {enrel, 1., 100 000},
  ImageSize -> 432, PlotStyle -> {{Thickness[0.007]}, {Hue[0.1], Thickness[0.007]}},
  {Hue[0.8], Thickness[0.007]}, {Hue[0.5], Thickness[0.007]}},
  {Hue[0.6], Thickness[0.007]}}, PlotRange -> {{1., 100 000}, {0.01, 200}},
  PlotLabel -> "Comparison of sum of proton transfer fits with fit to
  \ntotal transfer Q (10^-20 m^2) versus relative energy (eV)"]
```

Comparison of sum of proton transfer fits with fit to
total transfer Q (10^{-20} m²) versus relative energy (eV)



Heim and Stori, *J. Appl. Phys.* 72, 3330 (1992) agree with this result and say that the total H₂⁺ cross section is small on the $\sim 10^{-20}$ m² scale at energies from 40 to 150 eV.

fast H₃⁺ + H₂ → slow H₂⁺ + fast H + fast H₂ = slow H₂⁺ by charge transfer + dissociation of fast H₃ (5)

Peko and Champion had no way to distinguish the products slow H₂⁺ + slow H + fast H₂ from the products slow H₂⁺ + fast H + fast H₂, i.e., no way to distinguish proton abstraction followed by dissociation of the slow H₃⁺ (the previous process) from electron charge transfer followed by dissociation of the fast H₃ (the present process). They propose that the charge transfer is important only at energies above 50 eV because it is a nonresonant process. Vogel and Meierjohann (1978) attribute all of their signal at 10 keV to charge transfer. Probably one could transform the fragment velocity distributions of Volger and Meierjohann (1978) for 10 keV collisions from rectangular LAB coordinates to spherical CM coordinates, but I do not have plans to try. Note that we prefer to assume that only the observed H₂⁺ by Huber et al (1980) belongs here, not their total apparent charge transfer signal. Huber et al raise the possibility of H₃⁺ dissociation to form H₂⁺ that immediately undergoes resonant charge transfer.

I do not know what to assume for this cross section and have taken a guess that leads to rough agreement below. Presumably one could use the theory of Rapp and Francis *J. Chem. Phys.* 37, 2631 (1962) as a best guess. I do not know whether the correction of Pullins et al, *Z. Phys. Chem.* 214, 1279 (2000) applies. Because this is a nonresonant charge transfer collision, Peko and Champion predict that it will only be important at energies above 50 eV. At low energies, it should be significantly smaller than that for the P&C fast H production process.

In the first step of this two step model, the collision is one in which the H3+ projectile and H2 target are not significantly deflected during electron transfer from the H2 to the H3+. In CM the unstable H3 is at 0 deg and the H2+ is at 180. Then the H and H2 fragments fly apart more or less isotropically with a few eV relative energy. There is much uncertainty in this model, e.g., the amount of internal energy of the molecular fragments.

```
In[155]:= fastHctFit = 0.025 * UnitStep[enrel - 6.2] *
           enrel ^ 0.53 / (1 + (50 / (enrel - 6.2) ^ 1.1)) /
           (1 + (enrel / 15 000) ^ 2) ^ 0.9
```

```
Out[155]= 
$$\frac{0.025 \text{enrel}^{0.53} \text{UnitStep}[-6.2 + \text{enrel}]}{\left(1 + \frac{50}{(-6.2 + \text{enrel})^{1.1}}\right) \left(1 + \frac{\text{enrel}^2}{225000000}\right)^{0.9}}$$

```

According to Rapp and Francis, J. Chem. Phys. 37, 2631 (1962), the nonresonant charge transfer cross section varies as enrel^2 at low energies and as $(a + b \ln(v))^2$, i.e., as the resonant charge transfer cross section, for high energies. The following function is an approximation to this model. However, it is much too sharply peaked in energy to give a good fit to experiment. Probably one could get a reasonable fit to experiment if there were other similar functions with a spread in the energies at which they peaked. We will not use the following formula.

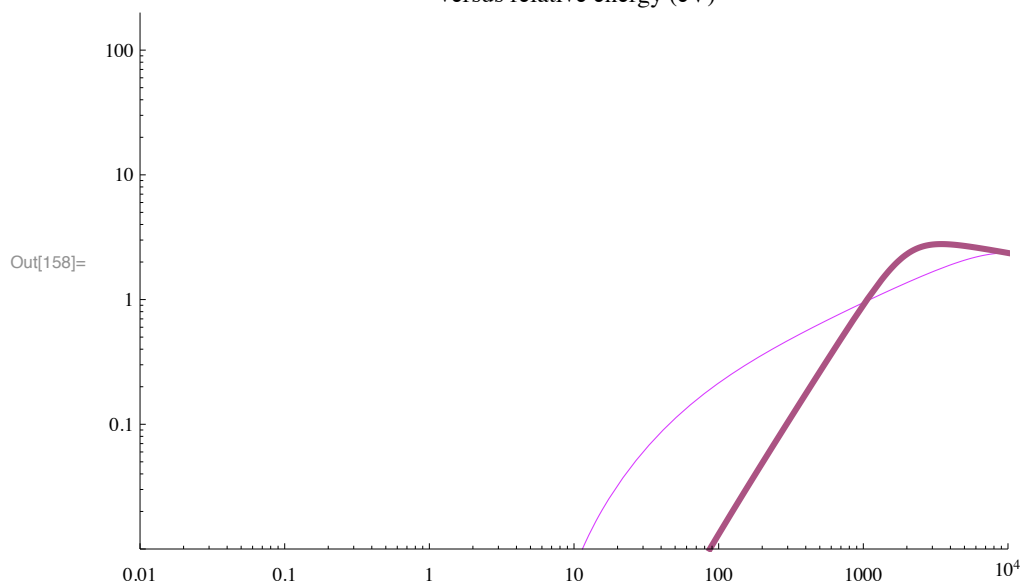
```
In[156]:= fastHctFit2 = 15. * UnitStep[enrel - 6.2] / enrel ^ 0.2 / (1 + (2000. / (enrel - 6.2)) ^ 4) ^ 0.5 /
           (1 + (enrel / 150 000) ^ 2) ^ 1.1 + 1. * 10 ^ -30;
```

```
In[157]:= fastHctFit2 /. enrel -> 100
```

```
Out[157]= 0.0131352
```

```
In[158]:= fastHctFitPlot = LogLogPlot[{fastHctFit, fastHctFit2}, {enrel, 2.5, 100 000},
   PlotStyle -> {Hue[0.8], Thickness[0.007], Dashing[{0.05, 0.05]}},
   PlotLabel -> "Cross section for fast H by charge transfer
   (10^-20 m^2)\n versus relative energy (eV)", ImageSize -> 432,
   PlotRange -> {{0.01, 10 000}, {0.01, 200}}]
```

Cross section for fast H by charge transfer (10^{-20} m^2)
versus relative energy (eV)



fast H3+ + H2 -> fast H+ + 2 fast H + slow H2 - CID of H3+ - similar to (1)

The reason for invoking this process is to fit try to both the sum of the H3+ destruction cross sections of Williams et al (1984) and the fast H atom production as measured by Williams and Dunbar (1966), i.e., we want a process producing more fast H atoms per collision than those discussed above. The assumption of a significant cross section appears to be inconsistent with the observation by Volger and Meierjohann (1978) that the production of fast H+ + 2 fast H atoms "makes only a negligible contribution" to the fast particle production compared to fast H + fast H2 production at 10 keV. I do not know how to resolve this problem.

Here the first step is the excitation of the H3+ and the second is the dissociation into fast H+ and 2 fast H atoms. This collision is assumed to be one in which the H3+ projectile and H2 target are not significantly deflected during excitation of the H3+ to a dissociating state. The loss of energy by the H3+ in the first step is expected to be roughly 10 eV. Then the H+ and 2 H fragments probably fly apart more or less isotropically in the H3+ CM with a few eV energy. There is much uncertainty in the applicability of this model.

■ Data from McClure (1963) for fast H production as read visually in 1985

```
In[159]:= mcClureDatafH = {{2000., 4.2}, {2800., 5.2}, {4000., 6.0}, {6000., 7.2},
      {8000., 8.3}, {12000., 9.5}, {20000., 9.1}, {28000., 8.4}, {40000., 6.8}};
```

```
In[160]:= mcClureDatafH // TableForm
```

```
Out[160]//TableForm=
  2000.  4.2
  2800.  5.2
  4000.  6.
  6000.  7.2
  8000.  8.3
 12000.  9.5
 20000.  9.1
 28000.  8.4
 40000.  6.8
```

```
In[161]:= mcClureHPlot = ListLogLogPlot[mcClureDatafH, PlotRange -> {{0.02,100000},{0.01,200.0}},
      PlotStyle->{Hue[0.1], PointSize[0.02]}, ImageSize -> 432];
```

```
In[162]:= fast2HFit = 0.017 * UnitStep[enrel - 8.8]
      enrel ^ 0.53 / (1 + (50 / (enrel - 8.8) ^ 1.1)) /
      (1 + (enrel / 24000) ^ 2) ^ 0.9
```

```
Out[162]= 
$$\frac{0.017 \text{enrel}^{0.53} \text{UnitStep}[-8.8 + \text{enrel}]}{\left(1 + \frac{50}{(-8.8 + \text{enrel})^{1.1}}\right) \left(1 + \frac{\text{enrel}^2}{576000000}\right)^{0.9}}$$

```

In the following plots this function is doubled to account for the two fast H atoms produced.

```
In[163]:= fast2HFitPlot = LogLogPlot[2 * fast2HFit, {enrel, 2.5, 100000},
      PlotStyle -> {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05]}],
      PlotRange -> {{0.01, 100000}, {0.01, 200}}];
```

```
In[164]:= totalHFfitPlot = LogLogPlot[(2 * fast2HFit + fastH2pFit + fastHctFit), {enrel, 2.5, 100 000},
    PlotStyle -> {Hue[0.5], Thickness[0.007]}, PlotRange -> {{0.01, 100 000}, {0.01, 200}}];
```

■ Fast H production from ORNL Rept. 8086

```
In[165]:= Import["Redbookvoll1pg52.txt", "CSV"] // TableForm
```

```
Out[165]//TableForm=
  Energy      Velocity      Cross      Section
  (eV/amu)    {cm/s}      (cm^2)
  1.5E+03    5.42E+07    3.20E-16
  2.0E+03    6.21E+07    4.26E-16
  4.0E+03    8.79E+07    6.94E-16
  7.0E+03    1.16E+08    8.90E-16
  1.0E+04    1.39E+08    9.69E-16
  1.3E+04    1.58E+08    9.96E-16
  2.0E+04    1.96E+08    9.02E-16
  4.0E+04    2.78E+08    5.77E-16
  7.0E+04    3.68E+08    3.56E-16
  1.0E+05    4.39E+08    2.62E-16
  2.0E+05    6.21E+08    1.45E-16
  4.0E+05    8.78E+08    7.79E-17
  6.0E+05    1.08E+09    5.48E-17
```

```
In[166]:= Drop[Import["Redbookvoll1pg52.txt", "Table"], 2];
```

```
In[167]:= ornlq3fAPlot = ListLogLogPlot[Table[{#[[j, 1]], #[[j, 3]] * 10^16}, {j, Length[%]}],
    PlotRange -> {{0.02, 100 000}, {0.01, 200.0}}, PlotStyle -> plotColorsPoints[{{7}}];
```

■ Fast H and H+ production from Simko et al (1997)

```
In[168]:= Import["simkoqdissochp.dat", "CSV"] // TableForm
```

```
Out[168]//TableForm=
  5.84763E+00    4.93411E-22
  6.55054E+00    1.28718E-21
  8.20362E+00    2.90730E-21
  1.02716E+01    5.82468E-21
  1.43813E+01    1.13905E-20
  2.10440E+01    1.63079E-20
  3.36520E+01    1.62920E-20
  6.72684E+01    1.31107E-20
  1.05156E+02    1.08123E-20
  2.29843E+02    8.29204E-21
  4.39449E+02    7.52355E-21
  7.34834E+02    7.33742E-21
  1.05082E+03    7.33198E-21
```

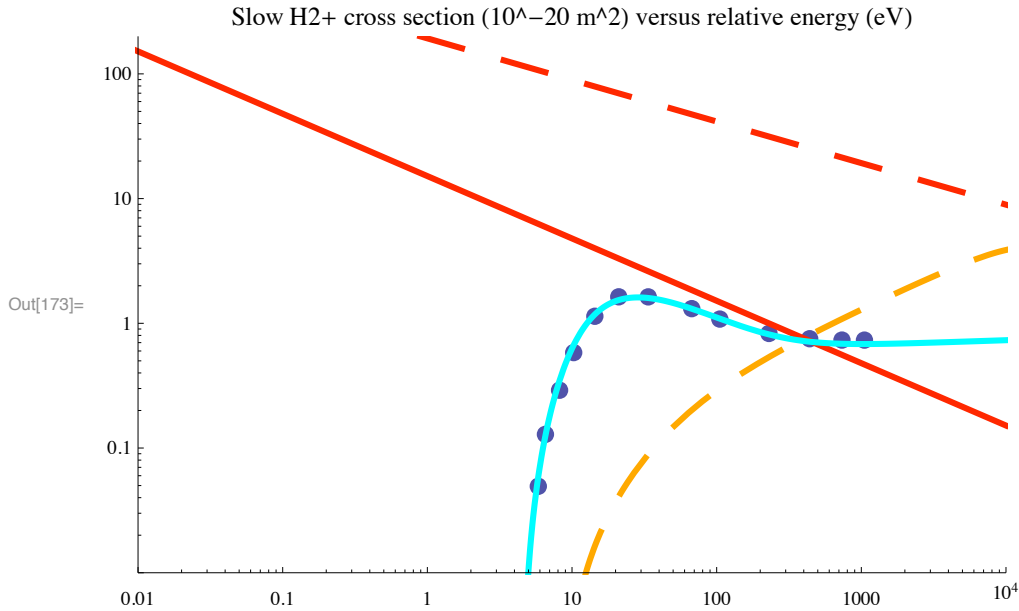
```
In[169]:= simkoDataF1=Import["simkoqdissochp.dat", "Table"];
```

```
In[170]:= simkoF1DataPlot = ListLogLogPlot[Table[{#[[j, 1]], #[[j, 2]]*fac}, {j, Length[%]}], PlotRange -> {{0.01, 10000}
    PlotLabel -> {"Cross section (10^-20 m^2) versus relative energy (eV)"}, ImageSize -> 432,
    PlotStyle->PointSize[0.02]];
```

```
In[171]:= simkoF1Fit= 2.2*UnitStep[enrel-4.4]/(1+(75/(enrel-4.4)^2))/(1+(enrel/28)^2)^0.27(1+(enrel/280
```

```
In[172]:= simkoF1FitPlot = LogLogPlot[simkoF1Fit, {enrel, 0.01, 10000},
    PlotStyle -> {Hue[0.5], Thickness[0.007]}, PlotRange -> {{0.01, 10000}, {0.01, 200}}];
```

```
In[173]:= Show[simkoF1DataPlot, fast2HFitPlot, langevinQPlot, simkoF1FitPlot, PlotLabel ->
    "Slow H2+ cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]
```



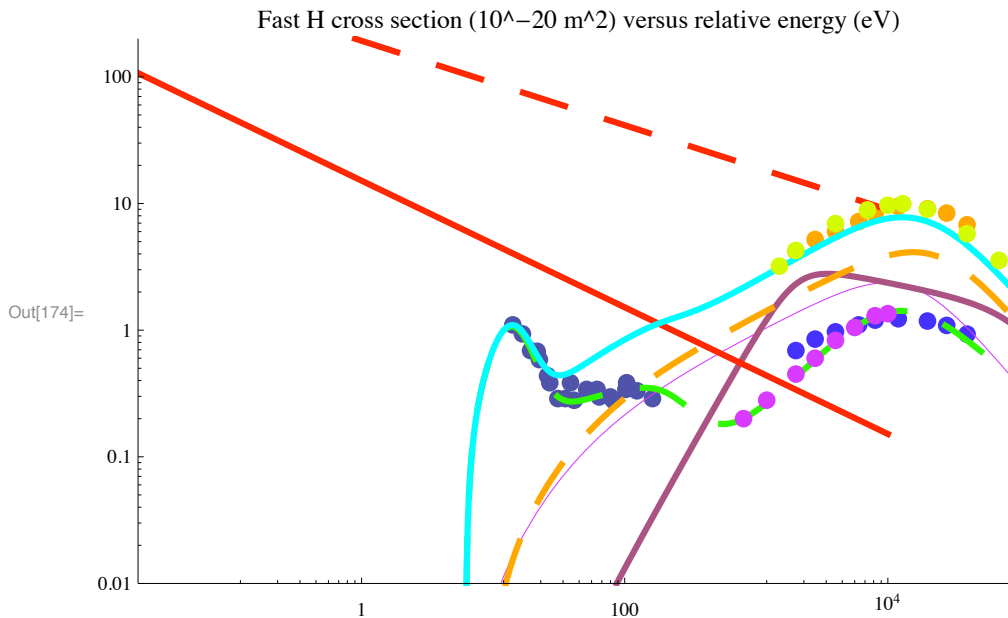
fast H3+ + H2 -> total fast H production [measured by McClure & by Williams](#)

Here we compare the fast H results with the present high energy models. This is a check and not a new cross section for the set.


```

In[174]:= Show[mcClurefHPlot, pekofH2pPlot, mcClurefH2pPlot,
fastHctFitPlot, fastH2pFitPlot, williamsfH2pPlot, langevinQPlot,
fast2HFitPlot, totalfHFitPlot, ornlq3fAPlot, PlotLabel ->
"Fast H cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]

```



The fit here is not perfect, but it did not seem worthwhile to try harder to adjust the various component cross sections. The energy dependences of several components are almost pure guesses. Also, there is considerable disagreement as to some of the measured cross sections.

fast H3+ + H2 -> total fast H2 production **measured by McClure & by Williams**

Here we compare our model cross sections for fast H2 production with experiment. This is a test of the recommended cross sections and is not a cross section to be added to the set.

From our previous fits

```

In[175]:= totalfH2Fit = fastHpFit + fitPT + fastHctFit;

```

```

In[176]:= totalfH2FitPlot = LogLogPlot[totalfH2Fit, {enrel, 1., 100 000},
PlotStyle -> {Hue[0.8], Thickness[0.007]}, PlotRange -> {{1., 100 000}, {0.01, 200}}];

```

■ Data from McClure (1963) for fast H2 production as read visually in 1985

```

In[177]:= mcClureDatafH2 = {{2000., 2.35}, {2800., 2.75}, {4000., 3.15}, {6000., 3.6},
{8000., 4.0}, {12 000., 4.3}, {20 000., 3.6}, {28 000., 3.05}, {40 000., 2.1}};

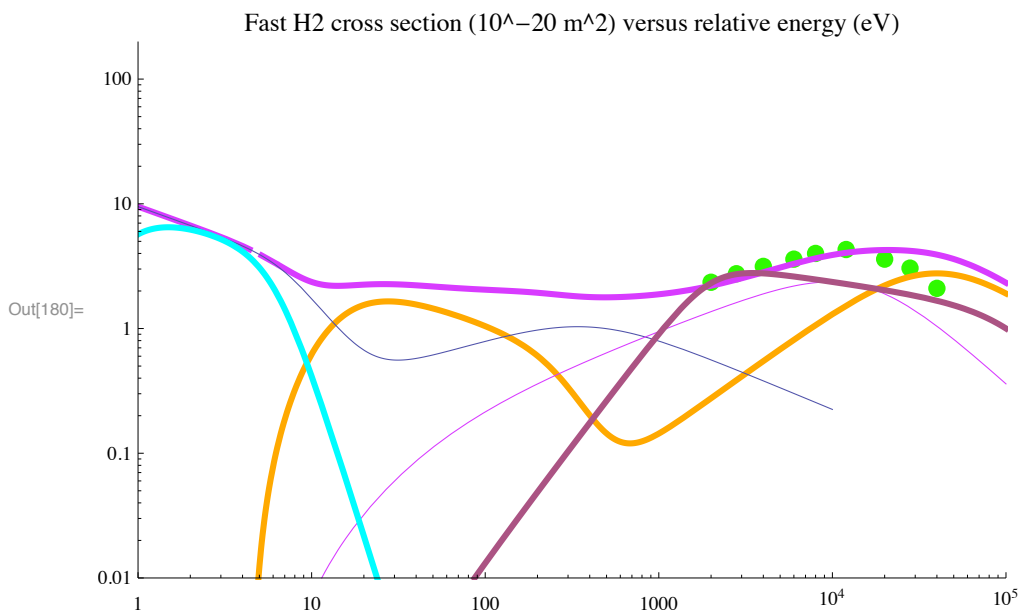
```

```
In[178]:= mcClureDatafH2 // TableForm
```

```
Out[178]/TableForm=
  2000.  2.35
  2800.  2.75
  4000.  3.15
  6000.  3.6
  8000.  4.
 12 000. 4.3
 20 000. 3.6
 28 000. 3.05
 40 000. 2.1
```

```
In[179]:= mcClurefH2Plot = ListLogLogPlot[mcClureDatafH2, PlotRange -> {{1.,100000},{0.01,200.0}},
  PlotStyle->{Hue[0.3], PointSize[0.02]}, ImageSize -> 432];
```

```
In[180]:= Show[mcClurefH2Plot, totalfH2FitPlot, fastHpPlot,
  fitPTPlot, fastHctFitPlot, protonTransferPlot, PlotLabel ->
  "Fast H2 cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]
```



The fit here is not perfect, but it did not seem worth while to try harder to adjust the various component cross sections. The energy dependences of several components are almost pure guesses. Also, there is considerable disagreement as to some of the measured cross sections.

fast H3+ + H2 → slow H2+ + fast H3+ + e ionization

We assume that this is a long range stripping collision where there is no significant deflection of the fast H3+ as it loses an energy equal to the ionization potential of H2, i.e., 15.6 eV, plus the energy of the free electron, e.g., 30 eV, at high collision energies.

From Gordeev et al (1958) as tabulated in the "old" Oak Ridge Red Book. The threshold is the ionization potential of H2, i.e., 15.6 eV.

```
In[181]:= gordeevQe = {{1000 * 2 / 5, 0.13}, {3000 * 2 / 5, 0.36}, {6000 * 2 / 5, 0.72},
  {10 000 * 2 / 5, 1.1}, {30 000 * 2 / 5, 2.6}, {60 000 * 2 / 5, 3.6}, {100 000 * 2 / 5, 4.3}};
```

```
In[182]:= gordeevQe // TableForm
```

```
Out[182]/TableForm=
```

```
400    0.13
1200   0.36
2400   0.72
4000   1.1
12 000 2.6
24 000 3.6
40 000 4.3
```

```
In[183]:= gordeevQePlot = ListLogLogPlot[gordeevQe, PlotRange -> {{1., 100000}, {0.01, 200.0}},
  PlotStyle -> {Hue[0.3], PointSize[0.02]}, ImageSize -> 432];
```

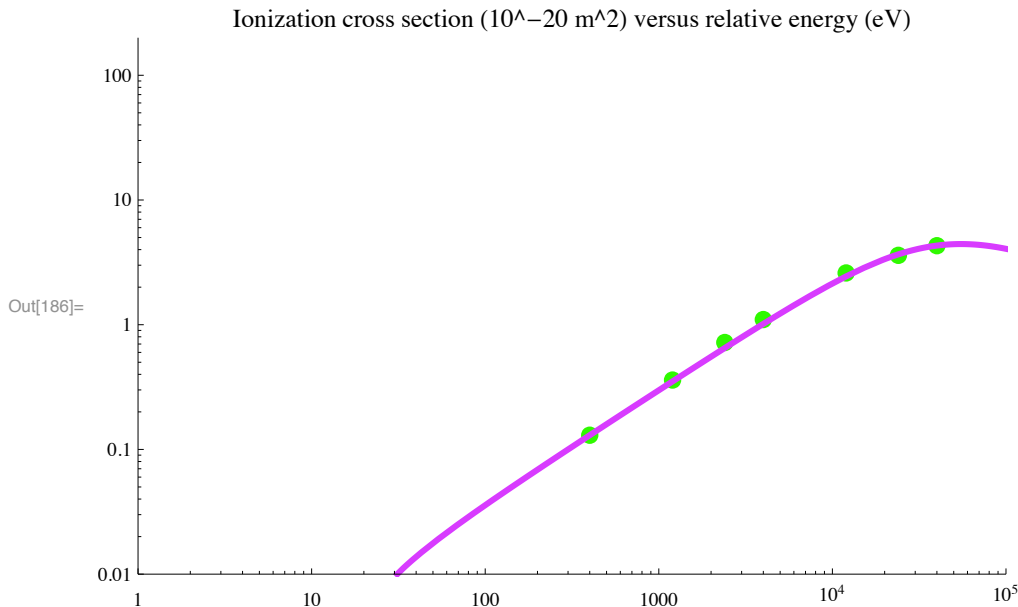
```
In[184]:= ionizationFit = 0.0006 * UnitStep[enrel - 15.6]
  enrel ^ 0.9 / (1 + (5 / (enrel - 15.6) ^ 1)) /
  (1 + (enrel / 42 000) ^ 1.5)
```

```
Out[184]= 
$$\frac{0.0006 \text{ enrel}^{0.9} \text{ UnitStep}[-15.6 + \text{enrel}]}{\left(1 + \frac{5}{-15.6 + \text{enrel}}\right) \left(1 + 1.16179 \times 10^{-7} \text{ enrel}^{1.5}\right)}$$

```

```
In[185]:= ionizationFitPlot = LogLogPlot[ionizationFit, {enrel, 1., 100 000},
  PlotStyle -> {Hue[0.8], Thickness[0.007]}, PlotRange -> {{1., 100 000}, {0.01, 200}}];
```

```
In[186]:= Show[gordeevQePlot, ionizationFitPlot, PlotLabel ->
  "Ionization cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]
```



Heim and Stori, J. Appl. Phys. 72, 3330 (1992) agree with this result and say that the total H₂⁺ cross section is small on the ~1E-20 m² scale at energies from 40 to 150 eV.

```
fromtex=(10^20*2.6*10^-24 UnitStep[w3 - 39.]*w3^0.9/(1 + 12.5/(w3 - 15.6))/(1+ (w3/105000.)^1
ionizationFitPlotTex = LogLogPlot[fromtex, {enrel, 1., 100 000},
  PlotStyle -> {Hue[0.5], Thickness[0.007], Dashing[ {.1, .1}]},
  PlotRange -> {{1., 100 000}, {0.01, 200}}];
Show[ionizationFitPlot, ionizationFitPlotTex]
```

fast H₃⁺ + e → 3 H or H₂ + H dissociative recombination

There is much current discussion about the dissociative recombination of electrons with H₃⁺. A recent review by M. Larsson, Phil. Trans. Royal Soc. Lond. A 358, 2433 (2000) cite merged-beam, storage-ring results as giving $\alpha(300\text{ K}) = 1.15\text{E-}7\text{ cm}^3/\text{s}$ while flowing afterglow experiments currently give $1\text{E-}8$ to $2\text{E-}8\text{ cm}^3/\text{s}$. It has been proposed (apparently not published) that the recombination coefficient is very sensitive to rotational excitation of the H₃⁺ and that the merged beam apparatus has “rotationally excited” (not vibrationally excited) H₃⁺ with a large recombination coefficient. Even more recently papers by Glosik et al, Chem. Phys. Lett. 331, 209 (2000) and J. Phys. B (submitted) (2001) claim that electron recombination to vibrationally relaxed H₃⁺ is a three-body process in which H₂ removes energy from a metastable H₃ to produce a dissociating state. The merged beam experiments give the neutral products as 3 H (75%) and H₂ + H (25%). The beam experiments yielding a large recombination coefficients show a lot of structure with a roughly $1/\text{enrel}$ behavior or a $T^{-(0.5)}$ variation.

fast H3+ + H2 → Balmer alpha dissociative excitation

From Table 5 of Williams et al (1982). The threshold is the excitation potential of H2, i.e., 12.1 eV plus the threshold for H formation of 6.2 eV, i.e., 18.3 eV. The cross section given here is the sum of the "projectile excitation- sigma P" in which the emission is Doppler shifted by an amount determined by an H atom with the unperturbed projectile velocity plus the "target excitation - sigmaT" in which there is no measurable Doppler shift as if the emitting H atom is randomly directed with a low velocity. From Williams et al, these components are roughly equal. I would assume the same angular distribution of products as for the second reaction in our list, i.e., no deflection of the projectile and target.

```
!! Halpha2.txt
```

```
In[187]:= Import["Halpha2.txt", "CSV"] // TableForm
```

```
Out[187]/TableForm=
```

```
ExcitatiOn Of Balmer alpha in H3+ + H2 cOllisiOns
```

```
Williams
```

```
Geddes
```

Energy (keV)	sigmaT (x10E-18 CM2)	sigmaP(3s) (x10E-18 CM2)	sigmaP(3d) + 0.12sigmaP(3p) (x10E-18 CM2)	sigmaP (x10E-18 CM2)
3	3.87	0.15	2.27	0.09
4	3.85	0.12	2.27	0.18
5	3.85	0.15	2.62	0.09
6	3.92	0.15	2.88	0.10
7	4.05	0.16	3.15	0.07
8	3.80	0.13	3.15	0.03
9	3.85	0.07	3.28	0.03
10	4.00	0.12	3.37	0.03
12	4.03	0.06	3.68	0.04
14	4.34	0.05	4.09	0.04
15	4.72	0.17	4.16	0.04
16	4.92	0.16	4.41	0.08
18	5.15	0.20	4.51	0.05
20	5.38	0.20	4.86	0.05
22.5	5.45	0.14	5.23	0.05
25	5.88	0.21	5.44	0.05
30	6.54	0.07	6.14	0.08
35	7.15	0.14	6.33	0.09
40	7.78	0.16	6.64	0.07
45	8.20	0.11	6.61	0.07
50	8.50	0.14	6.58	0.07
55	8.68	0.09	6.72	0.07
60	9.11	0.10	6.70	0.07
65	9.56	0.14	6.75	0.07
70	9.66	0.10	7.10	0.07
75	9.93	0.13	7.14	0.07
80	9.90	0.10	7.32	0.07
90	10.04	0.11	7.37	0.10
100	10.05	0.10	7.19	0.14

```
In[188]:= halphaTable = Drop[Import["Halpha2.txt", "table"], 4];
```

```
Dimensions [%]
```

```
In[189]:= williamsQHalpha = Table[{halphaTable[[j, 1]] * 1000 * 2 / 5,  
(halphaTable[[j, 2]] + halphaTable[[j, 8]]) * 0.01}, {j, 1, 29}];
```

```
In[190]:= williamsQAlphaPlot = ListLogLogPlot[williamsQAlpha, PlotRange -> {{1.,100000},{0.0001,2.0}},
PlotStyle->{Hue[0.3], PointSize[0.02]}, ImageSize -> 432];
```

```
In[191]:= halphaFit = 0.0027 * UnitStep[enrel - 18.3] *
enrel ^ 0.47 / (1 + (5 / (enrel - 18.3) ^ 1)) /
(1 + (enrel / 70 000) ^ 2.)
```

```
Out[191]= 
$$\frac{0.0027 \text{enrel}^{0.47} \text{UnitStep}[-18.3 + \text{enrel}]}{\left(1 + \frac{5}{-18.3 + \text{enrel}}\right) \left(1 + 2.04082 \times 10^{-10} \text{enrel}^{2.}\right)}$$

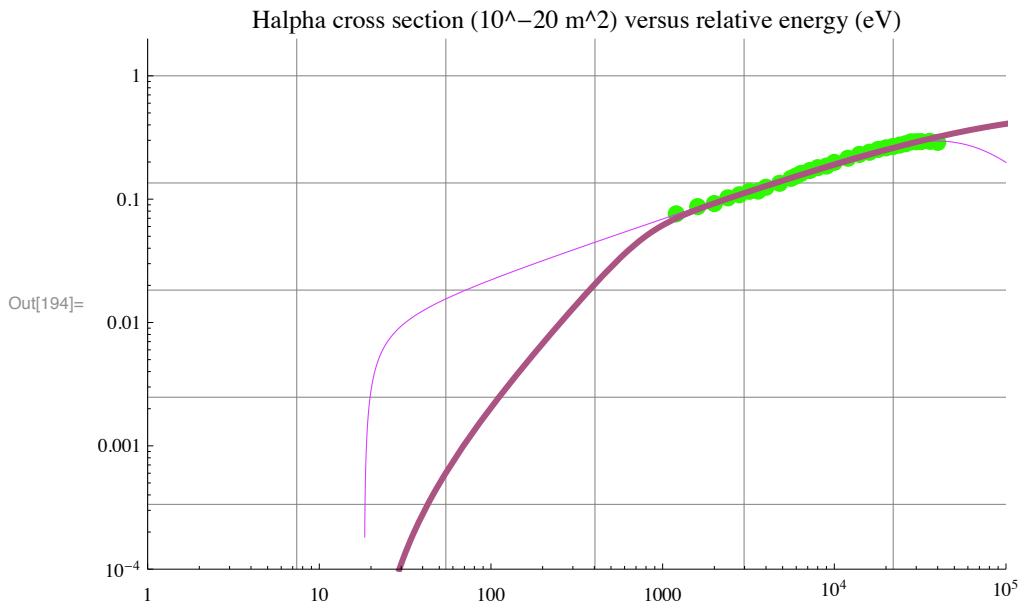
```

A fit with a much smaller cross section near threshold is

```
In[192]:= halphaFit2:=10^20*0.7*10^-26*UnitStep[w3-45.8] * (w3-45.8)^1.5/(1+(w3/2000.)^4)^.26/(1+(w3/2500
```

```
In[193]:= halphaFitPlot = LogLogPlot[{halphaFit, halphaFit2}, {enrel, 1., 100 000},
PlotStyle -> {Hue[0.8], Thickness[0.007]}, PlotRange -> {{1., 100 000}, {0.0001, 2}}];
```

```
In[194]:= Show[williamsQAlphaPlot, halphaFitPlot, GridLines -> Automatic, PlotLabel ->
"Alpha cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]
```



Note that the contributions of the target excitation σ_{T} , i.e., the component not Doppler shifted, and the projectile excitation σ_{P} , Doppler shifted, are comparable at the lowest energy of Williams et al.

fast H3+ + H2 → Lyman alpha dissociation and excitation

From Fig. 8 of Dunn, Geballe, and Pretzer, Phys. Rev. 128? 2200 (1962). The threshold is the excitation potential of H(n=3), i.e., 10.2 eV plus the threshold for H formation of 6.2 eV, i.e., 16.4 eV. The data points are from my visual digitization in 1985. These authors did not measure a Doppler shift. I would assume the same angular distribution of products as for the second reaction in our list, i.e., no deflection of the projectile and target. Note that these photons (along with the Lyman band from H2) can contribute to the electron production at the cathode.

```
In[195]:= dunnLymanData =
{{240., 0.196}, {400., 0.246}, {800., 0.272}, {1200., 0.28}, {1600., 0.304}, {2000., 0.33}};
```

```
In[196]:= dunnLymanData // TableForm
```

```
Out[196]/TableForm=
  240.  0.196
  400.  0.246
  800.  0.272
 1200.  0.28
 1600.  0.304
 2000.  0.33
```

```
In[197]:= dunnQHLYmanPlot = ListLogLogPlot[dunnLymanData, PlotRange -> {{1.,100000},{0.01,200.0}},
  PlotStyle->{Hue[0.3], PointSize[0.02]}, ImageSize -> 432];
```

Revised 08/12/07 by raising threshold to be more in line with revised excitation cross sections for H+ and H2+.

```
In[198]:= lymanFit = 0.0012 * UnitStep[enrel - 30] *
  enrel ^ 1. / (1 + (50 / (enrel - 30) ^ 1)) /
  (1 + (enrel / 250) ^ 4.) ^ 0.26 *
  (1 + (enrel / 1800) ^ 4) ^ 0.25 / (1 + (enrel / 20 000) ^ 2)
```

```
Out[198]=
  0.0012 enrel1 ·  $\left(1 + \frac{\text{enrel}^4}{10\,497\,600\,000\,000}\right)^{0.25}$  UnitStep[-30 + enrel]
   $\left(1 + \frac{50}{-30 + \text{enrel}}\right) \left(1 + \frac{\text{enrel}^2}{400\,000\,000}\right) \left(1 + 2.56 \times 10^{-10} \text{enrel}^4\right)^{0.26}$ 
```

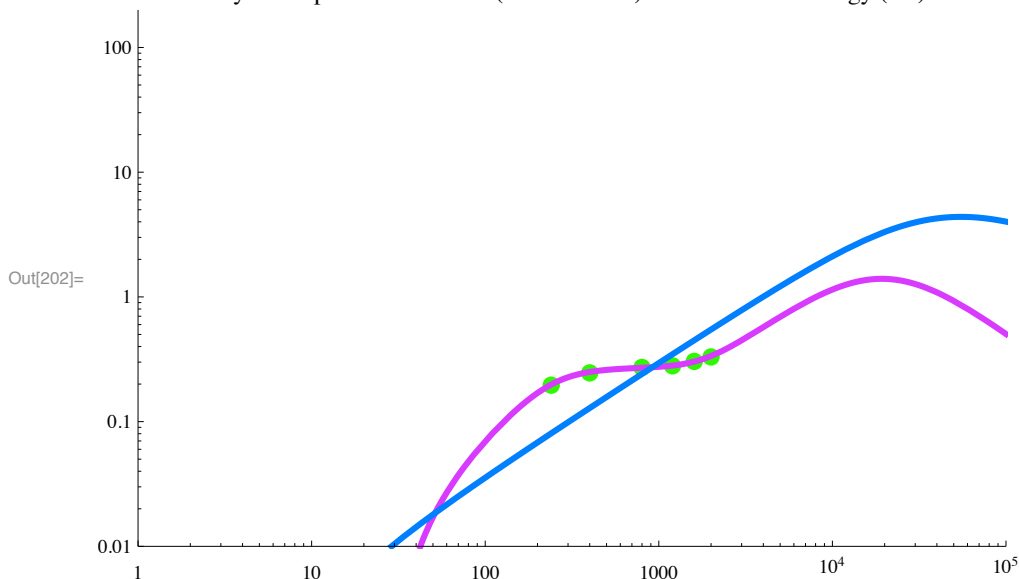
```
In[199]:= lymanFitPlot = LogLogPlot[lymanFit, {enrel, 1., 100 000},
  PlotStyle -> {Hue[0.8], Thickness[0.007]}, PlotRange -> {{1., 100 000}, {0.01, 200}}];
```

```
In[200]:= fit2006=(2.6*10^(-24)*UnitStep[epsilon - 39]*epsilon^(0.9)/(1 + 12.5/(epsilon - 15.6))/(1 +
```

```
In[201]:= fit2006Plot=LogLogPlot[fac*fit2006,{enrel,1.,100000}, PlotStyle -> {Hue[0.6], Thickness[0.00
```

```
In[202]:= Show[dunnQHLYmanPlot, lymanFitPlot, fit2006Plot, PlotLabel ->
  "Lyman alpha cross section (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]
```

Lyman alpha cross section (10⁻²⁰ m²) versus relative energy (eV)



Here there is a lot of guessing as to the low and high energy behavior.

Momentum transfer cross section for H3+ + H2 from mobility data

Note that this momentum transfer cross section is not part of our recommended set. At low E/N elastic collisions and vibrational excitation via proton transfer are assumed to determine the H3+ mobility in H2. The fit to mobility data could probably be improved, but I do not have an ion transport code for taking all of the necessary factors into account.

■ Potential models for mobility

From the ratio of the peak mobility to the low E/n limit one seems to need either a 16-4 potential or a $\gamma = 0.1$ with a 12-6-4 potential. See Fig. 5-3-1 of McDaniel and Mason (1973) and the corresponding figure of Mason and McDaniel (1988). The peak mobility of $16 \text{ cm}^2/\text{V}\cdot\text{s}$ at NTP occurs at $E/n = 150 \text{ Td}$, a drift velocity of $64e4 \text{ cm/s}$, and $T_{\text{eff}} = 4000 \text{ K}$. The later is roughly consistent with a dissociation energy of $\text{H5}^+ \rightarrow \text{H3}^+ + \text{H2}$ of 0.35 eV from Johnsen and Biondi (1976). Elford and Miloy get 0.25 eV and cite an equilibrium distance of 3 \AA . A problem in fitting mobility theory to the H3+ in H2 data, as pointed out in the literature, is the low mobility at low E/N compared to Langevin.

```
In[203]:= mramu = 3 * 2 / (3 + 2);
          amu = 1.661 * 10^-27;
          mr = mramu * amu;
          qe = 1.602 * 10^-19;
          ng = 2.69 * 10^25;          (*m^-3*)

          !! h3ph2mobility.txt
```



```
In[208]:= Import["h3ph2mobility.txt", "CSV"] // TableForm
```

```
Out[208]/TableForm=
```

H3+ - H2		Experimental Data		Derived		Quantities	
T = 300 K							
E/N	K0	vd	Teff	K0	Omega(11)	dLnK0/DLnTeff	
5.00	11.3	1.52	300	11.3	86.3	0.02	
6.00	11.3	1.82	400	11.4	74.1	0.09	
8.00	11.3	2.43	500	11.7	64.6	0.14	
10.0	11.3	3.04	600	12.0	57.5	0.18	
12.0	11.3	3.64	800	12.8	46.7	0.22	
15.0	11.3	4.55	1000	13.5	39.6	0.25	
20.0	11.3	6.07	1200	14.1	34.6	0.23	
25.0	11.3	7.59	1500	14.7	29.7	0.18	
30.0	11.3	9.11	2000	15.3	24.7	0.12	
40.0	11.4	12.3	2500	15.7	21.5	0.08	
50.0	11.7	15.7	3000	15.8	19.5	0.05	
60.0	12.1	19.5	4000	16.0	16.7	0.00	
80.0	13.4	28.8	5000	15.8	15.1	-0.09	
100	14.7	39.5	6000	15.4	14.2	-0.22	
120	15.5	50.0	8000	14.4	13.1	-0.22	
150	16.0	64.5	10000	13.8	12.2	-0.09	
200	15.5	83.3	12000	13.7	11.3	-0.04	
250	14.3	96.1	15000	13.7	10.1	0.02	
300	13.8	111	20000	13.9	8.60	0.11	
400	13.9	149					

Reference: 14 and 2

Accuracy: The total error in the experimental data is believed not to exceed $\pm 2\%$ for $E/N \leq 100$ Td and $\pm 6\%$ for $E/N > 100$ Td.

```
In[209]:= mobilityExpt1 =
Table[Take[Drop[Drop[Import["h3ph2mobility.txt", "Table"], 4], -5][[j]], 2], {j, 1, 20}];
```

We need to normalize the mobility to unit density and MKS units.

```
In[210]:= mobilityExpt2 =
Table[{mobilityExpt1[[j, 1]], mobilityExpt1[[j, 2]] * 2.69 * 10^19 * 10^2}, {j, 1, 20}];
```

```
In[211]:= mobilityExptPlot = ListLogLinearPlot[mobilityExpt2,
PlotRange -> {{1., 1000.}, {0., 5. * 10^22}}, PlotStyle -> PointSize[0.02]];
```

We need the energy at the highest E/n for which we believe the data, $E/n = 300$ Td.

```
In[212]:= kTeffHigh =
0.0258 + 1/3 * (2 * amu) * (mobilityExpt2[[19, 1]] * 10^-21 * mobilityExpt2[[19, 2]])^2 / qe
```

```
Out[212]= 0.665053
```

```
In[213]:= kTeffLow =
0.0258 + 1/3 * (2 * amu) * (mobilityExpt2[[1, 1]] * 10^-21 * mobilityExpt2[[1, 2]])^2 / qe
```

```
Out[213]= 0.0258 + 5.00173 * 10^-8 E/N^2 K0^2
```

Theoretical mobility to be fit to experiment**!! OmegaN - 4. txt**

We choose $N = 14$, although 12 might be better.

```
In[214]:= Import["OmegaN-4.txt", "table"] // TableForm
```

Out[214]/TableForm=

TABLE !!!! Omega (1,1) * T*	IV. THIS	Collision PAGE	Integrals HAS	for BEEN	(n, PROFREAD	4) AGAINST	Potential PUBLISHEE
	n=6	n=10	n=14	n=16	n=300		
0.01	24.741	18.227	16.538	15.769	13.776		
0.02	17.267	12.78	11.573	11.024	9.6074		
0.03	13.951	10.37	9.3812	8.9307	7.7747		
0.04	11.973	8.9336	8.0771	7.6861	6.6884		
0.05	10.632	7.9548	7.1885	6.8386	5.9506		
0.06	9.6469	7.2303	6.534	6.214	5.4082		
0.07	8.8816	6.6715	6.0249	5.7297	4.9883		
0.08	8.2604	6.2183	5.6149	5.339	4.6509		
0.09	7.7394	5.8447	5.2787	5.0161	4.3722		
0.1	7.2913	5.5257	4.9897	4.745	4.1373		
0.15	5.6789	4.421	4.0087	3.815	3.3439		
0.2	4.6263	3.7185	3.4021	3.249	2.878		
0.25	3.8791	3.2114	2.9699	2.8501	2.5606		
0.3	3.3196	2.827	2.6422	2.5493	2.3299		
0.35	2.8962	2.5262	2.3836	2.3124	2.1517		
0.4	2.5659	2.2848	2.1759	2.1225	2.0108		
0.45	2.3012	2.0842	2.0075	1.956	1.8957		
0.5	2.088	1.9252	1.8649	1.837	1.8009		
0.6	1.7671	1.5745	1.6449	1.6309	1.6529		
0.7	1.5369	1.4916	1.4826	1.483	1.544		
0.8	1.3681	1.3544	1.3606	1.3684	1.4609		
0.9	1.2387	1.2483	1.2638	1.2791	1.3961		
1.	1.1374	1.163	1.1886	1.2069	1.3444		
1.2	0.98964	1.0386	1.0735	1.1005	1.2675		
1.4	0.8885	0.9507	0.99396	1.0252	1.2137		
1.6	0.81438	0.8855	0.93462	0.96927	1.1747		
1.8	0.75829	0.83726	0.88897	0.92626	1.145		
2.	0.71435	0.79838	0.85326	0.89217	1.1216		
2.5	0.63692	0.72906	0.7894	0.83211	1.0812		
3.	0.58595	0.68339	0.74696	0.79208	1.0557		
3.5	0.54943	0.65052	0.71653	0.76339	1.0381		
4.	0.52171	0.62536	0.69337	0.74169	1.0252		
4.5	0.49956	0.60532	0.6749	0.72445	1.0155		
5.	0.48166	0.58883	0.65975	0.71031	1.0078		
6.	0.44337	0.56287	0.63583	0.6881	0.99663		
8.	0.41457	0.52743	0.60345	0.65813	0.98295		
10	0.3881	0.50301	0.58122	0.63776	0.97486		
20	0.31987	0.43811	0.52225	0.58402	0.95823		
40	0.26237	0.38335	0.47218	0.5385	0.94823		
60	0.23364	0.3546	0.44555	0.51417	0.94384		
80	0.21495	0.33547	0.42765	0.49773	0.94111		
100	0.20135	0.32131	0.41428	0.48539	0.93916		
200	0.16378	0.28087	0.37545	0.44922	0.93379		
400	0.13258	0.24529	0.34028	0.41591	0.92905		
600	0.11694	0.22649	0.32122	0.39759	0.92642		
800	0.1069	0.21399	0.30833	0.38508	0.92458		
1000	0.09967	0.20475	0.29868	0.37565	0.92316		

```
In[215]:= omegaN4 = Transpose[Drop[Import["OmegaN-4.txt", "table"], 5]];
```

```
In[216]:= omega1 = Transpose[{omegaN4[[1]], omegaN4[[4]]}];
```

Now we try N = 12

```
In[217]:= omega12 = Transpose[Drop[Import["omega12.txt", "table"], 4]];
```

```
In[218]:= omega1 = Transpose[{omega12[[1]], omega12[[2]]}];
```

The well depth for the H3+-H2 potential has been determined by Johnsen and Biondi (1976) from H5+ stability measurements as 0.35 eV, so we will use that as a first guess for our mobility model. These Omega(1,1) are normalized to $\text{Pi} \cdot \text{rmin}^2$ versus the temperature in units of the well depth. The rmin and well depth epsilon are adjustable parameters that are to be found by trial and error. The final epsilon and rmin are the first entries in the following lists.

```
In[219]:= epsilon = {0.3, 0.3, 0.3, 0.3, 0.25}[[1]]; (*eV*)
```

```
In[220]:= kTgas = 0.0258; (*eV*)
```

```
In[221]:= rmin = {2.22, 2.25, 2.3, 2.35, 2.35}[[1]] * 10^-10; (*m*)
```

```
In[222]:= mgas = 2 * amu;
```

Next we calculate a table of Teff and mobility normalized to unit gas density.

```
In[223]:= mobilityTheor1 = Table[{omega1[[j, 1]] * epsilon,
  3 * qe / (8 * Pi * rmin^2) (Pi / (2 * mr * epsilon * omega1[[j, 1]] * qe))^0.5 / omega1[[j, 2]]},
  {j, 1, Length[omega1]}];
```

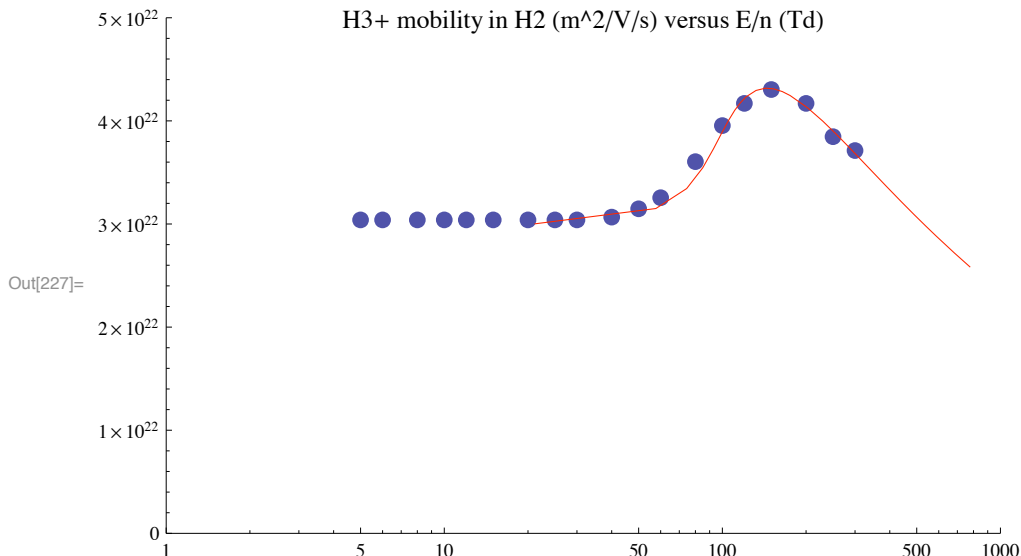
We now convert the kTeff/e into E/N values using the Wannier expression to find the drift velocity and the mobility to find E/N.

```
In[224]:= vd[kTeff_] := If[kTeff - kTgas > 0, Sqrt[2 * qe / mgas * (kTeff - kTgas)], 1]
```

```
In[225]:= mobilityTheor2 = Table[{10^21 * vd[mobilityTheor1[[j, 1]]] / mobilityTheor1[[j, 2]],
  mobilityTheor1[[j, 2]]}, {j, 1, Length[omega1]}];
```

```
In[226]:= mobilityTheorPlot = ListLogLinearPlot[mobilityTheor2, Joined -> True,
  PlotRange -> {{1., 1000.}, {0., 5. * 10^22}}, PlotStyle -> {Hue[1], PointSize[0.02]}];
```

```
In[227]:= Show[mobilityExptPlot, mobilityTheorPlot,
  PlotLabel -> "H3+ mobility in H2 (m^2/V/s) versus E/n (Td)", ImageSize -> 432]
```



These plots show that we do not fit the apparent turn up in experimental mobility at $E/n > \sim 300$ Td. I propose that the behavior is caused by H3+ breakup into H+ and H2 and the the breakup is facilitated by the build up of internal energy of the drifting H3+.

■ Cross section corresponding to theoretical mobility

!! QViehlandN - 4. txt

Here we are using $N = 14$

```
In[228]:= Import["QViehlandN-4.txt", "CSV"] // TableForm
```

```
Out[228]//TableForm=
```

Table 11-4 Cross Sections $V(l)*$ for (n						4) Potentials
Vieland et al (1979)						
$E*$	n = 6	n = 10	n = 14	n = 18	n = 300	
$Q(1)*$						
0.01	37.59	27.62	25.11	23.97	20.99	
0.02	26.38	19.41	17.61	16.79	14.67	
0.03	21.40	15.78	14.30	13.63	11.89	
0.04	18.43	13.62	12.33	11.74	10.23	
0.06	14.90	11.05	9.997	9.516	8.280	
0.08	12.79	9.526	8.609	8.192	7.122	
0.1	11.35	8.484	7.664	7.290	6.335	
0.2	7.786	5.987	5.324	5.060	4.402	
0.3	6.298	4.752	4.290	4.077	3.557	
0.4	5.551	4.070	3.676	3.493	3.059	
0.6	3.845	3.346	3.017	2.803	2.475	
0.8	2.736	2.575	2.476	2.406	2.132	
1	2.104	2.051	2.022	2.003	1.903	
2	1.063	1.123	1.161	1.187	1.338	
3	0.8040	0.8852	0.9365	0.9717	1.166	
4	0.6903	0.7807	0.8378	0.8776	1.102	
6	0.5825	0.6817	0.7450	0.7894	1.048	
8	0.5273	0.6309	0.6978	0.7451	1.020	
10	0.4917	0.5982	0.6677	0.7169	1.005	
20	0.4038	0.5179	0.5944	0.6493	0.9746	
40	0.3344	0.4536	0.5364	0.5967	0.9593	
60	0.2991	0.4201	0.5060	0.5693	0.9533	
80	0.2760	0.3977	0.4856	0.5509	0.9497	
100	0.2592	0.3811	0.4704	0.5370	0.9472	
200	0.2122	0.3335	0.4262	0.4966	0.9406	
400	0.1727	0.2916	0.3863	0.4596	0.9351	
600	0.1527	0.2694	0.3647	0.4394	0.9323	
800	0.1398	0.2547	0.3502	0.4256	0.9304	
1000	0.1305	0.2438	0.3392	0.4152	0.929	

```
In[229]:= qmN4 = Transpose[Drop[Import["QViehlandN-4.txt", "table"], 4]];
```

```
In[230]:= qm1 = Transpose[{qmN4[[1]], qmN4[[4]]}];
```

Here we are trying $N = 12$

```
In[231]:= Import["Q12_4.txt", "CSV"] // TableForm
```

```
Out[231]/TableForm=
```

```
%Table 11-2 Cross Sections Q(1)* for (12 6 4) Potentials
Vieland et al (1979) for gamma = 0 .i.e. for 12-4 potential
```

E*	Q(1)*
0.01	26.07
0.02	18.30
0.03	14.87
0.04	12.83
0.06	10.41
0.08	8.965
0.1	7.981
0.2	5.545
0.3	4.470
0.4	3.834
0.6	3.166
0.8	2.518
1	2.043
2	1.149
3	0.9148
4	0.8125
6	0.7165
8	0.6676
10	0.6362
20	0.5596
40	0.4985
60	0.4666
80	0.4451
100	0.4292
200	0.3831
400	0.3420
600	0.3200
800	0.3052
1000	0.2942

```
In[232]:= qm12 = Transpose[Drop[Import["Q12_4.txt", "table"], 5]];
```

```
In[233]:= qm1 = Transpose[{qm12[[1]], qm12[[2]]}];
```

Note that the following table is limited to energies from near the minimum of 0.026 to the maximum of $kT_{\text{eff}} = 0.9$ eV, corresponding to the range of the experimental E/N.

```
In[234]:= qm2 = Table[{qm1[[j, 1]] * epsilon, 10^20 * qm1[[j, 2]] * Pi * rmin^2}, {j, 5, 16}];
```

```
In[235]:= qmFitPlot = ListLogLogPlot[qm2, PlotRange -> {{0.01, 100 000}, {0.01, 200.}},
ImageSize -> 432, PlotStyle -> {Hue[0.6], PointSize[0.02]}];
```

Elastic cross section (including rotational excitation)

Following Simko et al (1997) we need generate an elastic cross section that fits the cross section derived from mobility data at low energies and drops rapidly at the onset of vibrational excitation. The details of the transfer from this “elastic” scattering to the vibrational excitation roughly follow the cross sections chosen by Simko et al (1997) to fit H3+ mobility and diffusion data in H2.

```
In[236]:= qElasticFit = 22 / enrel ^ 0.5 / (1 + (enrel / 0.4) ^ 4);
```

```
In[237]:= qElasticFitPlot = LogLogPlot[qElasticFit, {enrel, 0.01, 100 000},  
PlotStyle -> {Hue[0.3], Thickness[0.007]}, PlotRange -> {{0.01, 100 000}, {0.01, 200}}];
```

Note that at the lowest energies shown, this cross section is significantly larger (~50%) than Langevin. Perhaps proton transfer and rotational excitation are large enough to effectively increase the momentum transfer scattering, although I don't understand how.

■ Compare with Janev, Reiter, and Samm

```
In[238]:= sigmaCIDHp1 = 18.5 (**10^-20*) * Exp[-54.5/enrel^1.65] / enrel^0.63 / (1 + 4.66 * 10^-6 * enrel^1.93) * (1 - (
```

```
Out[238]= 
$$\frac{18.5 e^{-\frac{54.5}{\text{enrel}^{1.65}}} \left(1 - \frac{29.8073}{\text{enrel}^{2.32}}\right)^{4.06}}{\text{enrel}^{0.63} (1 + 4.66 \times 10^{-6} \text{enrel}^{1.93})}$$

```

```
In[239]:= sigmaCIDHp2 = 3.84 (**10^-20*) * Exp[-44.2/enrel^0.48] / (1 + 7.49 * 10^-11 * enrel^1.85 + 7.55 * 10^-28 * enr
```

```
Out[239]= 
$$\frac{3.84 e^{-\frac{44.2}{\text{enrel}^{0.48}}}}{1 + 7.49 \times 10^{-11} \text{enrel}^{1.85} + 7.55 \times 10^{-28} \text{enrel}^{4.6}}$$

```

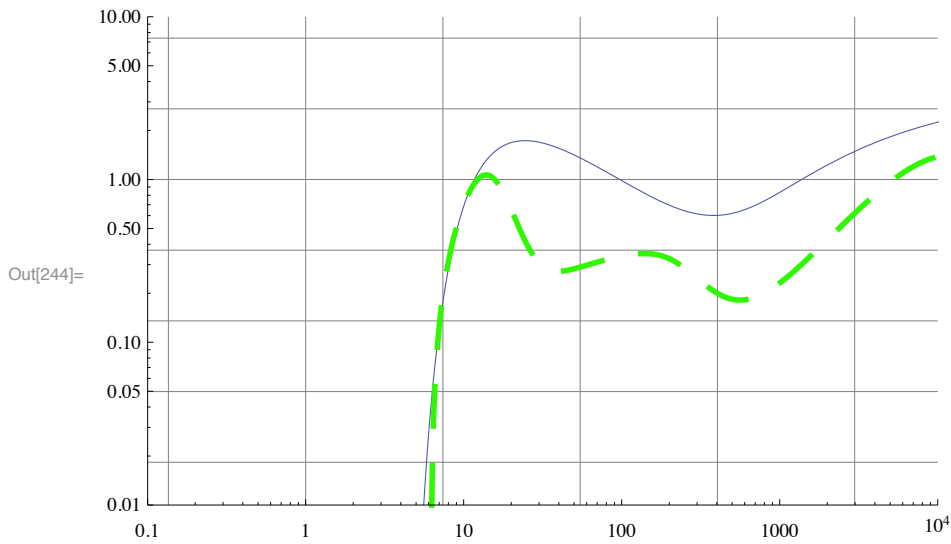
```
In[240]:= Plot[Abs[sigmaCIDHp1], {enrel, 0.1, 1000}, PlotRange -> {{0.1, 1000}, {0, 2}}, TextStyle -> FontSize -> 12
```

```
In[241]:= Plot[sigmaCIDHp2, {enrel, 0.1, 1000}, PlotRange -> {{0.1, 1000}, {0, 1}}, TextStyle -> FontSize -> 12];
```

```
In[242]:= sigmaCIDHp = sigmaCIDHp1 + sigmaCIDHp2;
```

```
In[243]:= janevCIDHpPlot = LogLogPlot[Abs[sigmaCIDHp], {enrel, 0.1, 100000}, PlotRange -> {{0.1, 10000}, {10^-2,
```

```
In[244]:= Show[janevCIDHpPlot, fastH2pFitPlot, GridLines->Automatic, ImageSize->400]
```



Summary

- Compare the sum of our H3+ destruction with Williams et al (1984) H3+ destruction

```
In[245]:= williamsH3pDestData = {{2500. * 2 / 5, 2.96}, {5000. * 2 / 5, 3.47}, {7500. * 2 / 5, 4.13},
    {10 000. * 2 / 5, 4.72}, {15 000. * 2 / 5, 5.3}, {20 000. * 2 / 5, 6.02}, {30 000. * 2 / 5, 7.2},
    {40 000. * 2 / 5, 7.6}, {60 000. * 2 / 5, 7.0}, {80 000. * 2 / 5, 6.4}, {100 000. * 2 / 5, 5.7}};
```

```
In[246]:= williamsH3pDestPlot =
    ListLogLogPlot [williamsH3pDestData, PlotRange -> {{0.02, 100 000}, {0.01, 200.}},
    ImageSize -> 432, PlotStyle -> PointSize[0.02]];
```

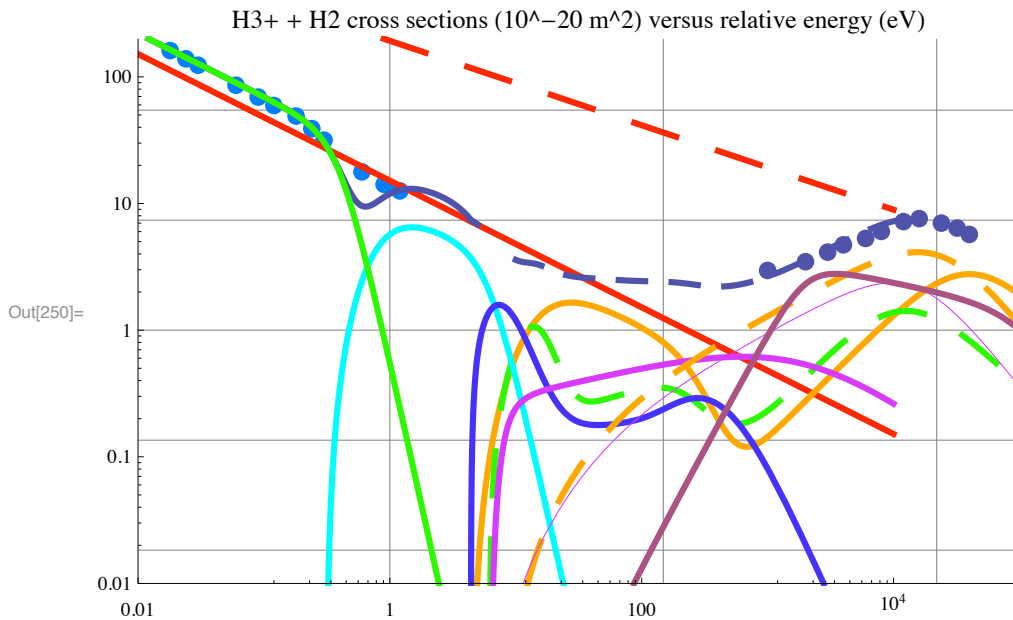
```
In[247]:= sumFits = fastHpFit + fastH2pFit + 2 * protonTransferFit +
    slowHpFit + slowH2pFit + fast2HFit + fastHctFit + qElasticFit;
```

```
In[248]:= sumFitsPlot1 = LogLogPlot [Evaluate [sumFits], {enrel, 0.01, 5.},
    PlotStyle -> Thickness[0.007], PlotRange -> {{0.01, 10 000}, {0.01, 200}}];
```

```
In[249]:= sumFitsPlot2 = LogLogPlot [Evaluate [sumFits], {enrel, 10., 10 000.}, PlotStyle ->
    {Thickness[0.007], Dashing[{0.03, 0.03]}], PlotRange -> {{0.01, 10 000}, {0.01, 200}}];
```



```
In[250]:= Show[qmFitPlot, williamsH3pDestPlot, langevinQPlot, fastHpPlot, fastH2pFitPlot,
protonTransferPlot, slowHpFitPlot, slowH2pPlot, fast2HFitPlot, sumFitsPlot1,
sumFitsPlot2, fastHctFitPlot, qElasticFitPlot, GridLines -> Automatic, PlotLabel ->
"H3+ + H2 cross sections (10^-20 m^2) versus relative energy (eV)", ImageSize -> 432]
```



Apparently the following did not work

```
ShowLegend[qmFitPlot,
{{Hue[1.0], "Langevin"}, {Hue[0.3], "Elastic"}}, LegendPosition -> {1.2, 0.5},
LegendSize -> {1., .3}, LegendLabel -> "H3+ - H2 Cross Sections",
PlotStyle -> Thickness[0.07], LegendOrientation -> Vertical, LegendShadow -> None}];
```

Note that the black curve is equal to the effective momentum transfer cross section at energies below about 5 eV. At higher energies, the dashed black curve is the sum of the cross sections leading to attenuation of an H3+ beam.

There are many uncertainties in these results. For example the dip in the sum of the elastic and vibrational excitation cross sections just below 1 eV seems much too narrow in energy, although the "area" seems roughly OK and the structure is comparable to that shown by Simko et al (1997).

A crucial question in the modeling of the behavior of H3+ in H2 under the influence of an electric field or in an afterglow situation is whether a significant fraction of the collisions lead to vibrational cooling of the H3+ that is excited by proton transfer collisions. Proton transfer measurements give cross sections between 1/4 (Vestal et al at low energies) and 1/2 (Peko and Champion at 4 eV) of Langevin. The proton transfer reaction is envisioned as a long range collision with nearly straight line trajectories. We are left asking whether there is a short range part of the Langevin scattering that could cause vibrational relaxation, e.g., scattering from the repulsive part of the potential barrier. A problem with vibrational relaxation in H3+ + H2 collisions is that the vibrational spacings seem very different so that resonant energy transfer (VV) seems unlikely and one must invoke vibrational-translational transfer (VT) or rotational excitation (VR).

This listing of reactions for H3+ has not considered H3+ + H. The possible proton transfer reaction H3+ + H -> H2+ + H2 appears to be exothermic by about 1.7 eV. I have no idea as to its energy dependence. The energy to be dissipated in the product H2+ could lead to dissociation at relatively low collision energies. Other possible reactions are vibrational relaxation of the H3+ and collisional dissociation of the H3+. Hopefully, the models will not have to consider H3+ + H collisions.

■ Continuous energy loss approximation (added 7/4/06)

I have not found my notes on the continuous energy loss approximation for H3+ + H2 and so rederive it. I include the known energy loss cross sections times their energy losses, but do not include elastic scattering or reactions.

```
In[251]:= I3[enrel_] = 16.4*lymanFit + 18.3*halphFit + 15.6*ionizationFit;
```

```
In[252]:= energyLossFitHi = 0.04*UnitStep[enrel - 15.6] * (enrel - 15.6)^0.9 / (1 + (enrel/300)^4)^0.14 * (1 + (enrel/1
```

```
Out[252]:= 
$$\frac{0.04 (-15.6 + \text{enrel})^{0.9} \left(1 + \frac{\text{enrel}^4}{3321506250000}\right)^{0.12} \text{UnitStep}[-15.6 + \text{enrel}]}{\left(1 + \frac{\text{enrel}^4}{8100000000}\right)^{0.14}}$$

```

As a rough approximation to rotational and vibrational excitation energy loss, we use the low energy behavior of H+ + H2. We double the I3[enrel] to allow for other excited states.

```
In[253]:= energyLossFit=2*1.*10^-20*energyLossFitHi+1.2*10^-20*enLab^0.45/(1+(enLab/10))/enLab->5*en
```

$$\text{Out[253]=} \frac{1.8124 \times 10^{-20} \text{enrel}^{0.45}}{1 + \frac{\text{enrel}}{4}} + \frac{8. \times 10^{-22} (-15.6 + \text{enrel})^{0.9} \left(1 + \frac{\text{enrel}^4}{3321506250000}\right)^{0.12} \text{UnitStep}[-15.6 + \text{enrel}]}{\left(1 + \frac{\text{enrel}^4}{8100000000}\right)^{0.14}}$$

For comparison, we consider llin[enlab]

```
In[254]:= llin[enLab_] = 1.2*10^-20*enLab^0.45*(1+(enLab/350)^4)^0.02+ 1.*10^-30;
```

```
In[255]:= energyLossPlot = LogLogPlot [
  {13[enrel], fac * energyLossFit, fac * llin[enLab] / enLab -> 5 * enrel / 2, energyLossFitHi},
  {enrel, 0.01, 10000.}, PlotStyle -> plotColorsLines,
  PlotRange -> {{0.01, 10000}, {0.01, 200}}, ImageSize -> 500];
```

■ Negative ion formation

It should be kept in mind that nearly all of the H- cross section measurements were designed to collect H- only from the near forward direction so that the experiment does not measure H-production in large angle scattering characteristic of target ionization. Only van Zyl et al measure all energy H-.

From Fig. 8 of Alvarez et al, Phys. Rev. A 14, 602 (1976).

```
In[256]:= Import["alvarez76fig8.dat", "Table"];
```

```
In[257]:= % // TableForm
```

```
Out[257]/TableForm=
```

```
1.98283 × 108 2.53666 × 10-22
2.77197 × 108 1.5798 × 10-22
3.38618 × 108 8.35245 × 10-23
3.89932 × 108 4.36281 × 10-23
4.35812 × 108 3.01254 × 10-23
4.76283 × 108 2.33636 × 10-23
```

```
In[258]:= alvarezData =
  Table[{mh2 * (#[[j, 1]] / 100) ^ 2 / (2 * qe) / {qe -> 1.602 * 10^-19, mh2 -> 2 * 1.673 * 10^-27},
    #[[j, 2]]}, {j, Length[#]} &[%];
```

In Fig. 8 of Alvarez et al, Phys. Rev. A 14, 602 (1976) these authors analyzed data in Williams and Dunbar, Phys. Rev 149, 62 (1966) to obtain

```
In[259]:= williamsDunbarData = Import["williamsdunbaralvarez76fig8.dat", "Table"];
```

In[260]:= % // TableForm

Out[260]/TableForm=

3.43836×10^7	1.20663×10^{-23}
4.10073×10^7	2.66352×10^{-23}
4.83677×10^7	3.95799×10^{-23}
5.58302×10^7	3.0649×10^{-23}
6.11918×10^7	3.86924×10^{-23}
7.13114×10^7	3.91637×10^{-23}
7.72986×10^7	6.77007×10^{-23}
8.60577×10^7	7.34777×10^{-23}
9.21506×10^7	6.46655×10^{-23}
9.88927×10^7	6.69847×10^{-23}
1.06946×10^8	8.86054×10^{-23}
1.13012×10^8	9.28543×10^{-23}
1.25159×10^8	9.18319×10^{-23}
1.37345×10^8	7.11259×10^{-23}
1.5957×10^8	9.3056×10^{-23}
1.77088×10^8	1.09615×10^{-22}

In[261]:= **williamsDunbarData =**

```
Table[{mh2 * (#[[j, 1]] / 100) ^ 2 / (2 * qe) /. {qe -> 1.602 * 10^-19, mh2 -> 2 * 1.673 * 10^-27},
      #[[j, 2]]}, {j, Length[#]}] &[%];
```

Note that a factor of ~ 2 in magnitude would bring these two data set into moderately good agreement in the energy region of near overlap.

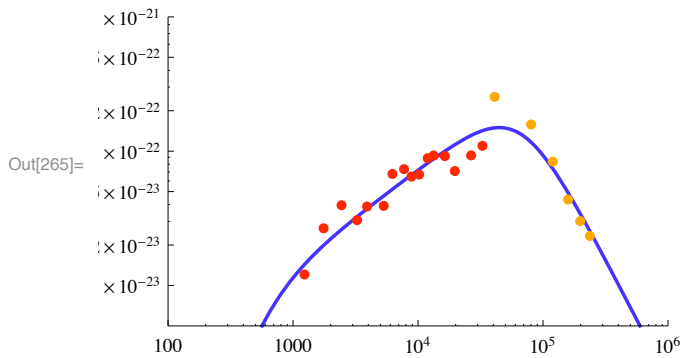
In[262]:= **exptDataPlot = ListLogLogPlot[{williamsDunbarData, alvarezData},
 PlotRange -> {{100, 1. * 10^6}, {5 * 10^-24, 10^-21}}, PlotStyle -> plotColorsPoints];**

In[263]:= **fitExpt = 4.5 * 10^-23 *
 (en / 5000) ^ 0.7 / (1 + (en / 65000) ^ (2.5)) / (1 + (500 / (en - 50)) ^ 2) UnitStep[en - 50];**

In[264]:= **fitExptPlot = LogLogPlot[fitExpt, {en, 100, 10^6},
 PlotStyle -> plotColorsLines[[5]], PlotRange -> {{100, 10^6}, {5 * 10^-24, 1 * 10^-21}}];**

```
In[265]:= Show[fitExptPlot, exptDataPlot,  
  PlotLabel -> "Cross section for H2+ + H2 -> H- (m^2) vs laboratory energy (eV)"]
```

Out[265]= Cross section for H2+ + H2 -> H- (m²) vs laboratory energy (eV)



```
In[266]:= Export["H2H3pQdata100910_7.pdf", EvaluationNotebook[]]
```

```
runtime = SessionTime[] - startclock
```

```
Quit[]
```

4 H- collisions with H2

H- + H2 collisions

Setup notebook environment

```
In[3]:= a = 1;
```

```
In[4]:= ClearAll["Global`*"];
```

```
In[5]:= Remove["Global`*"];
```

```
In[6]:= startclock = SessionTime[];
```

```
In[7]:= Off[General::spell];
```

```
In[8]:= Off[General::spell1];
```

```
In[9]:= today = StringForm["`~/`~/`~ `~:``:``", Date][[2]],  
Date][[3]], Date][[1]], Date][[4]], Date][[5]], N[Date][[6]], 2]
```

```
Out[9]= 12/2/2010 19:17:2.21063`2.
```

```
In[10]:= SetDirectory["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\h2lowcurrent"]
```

```
Out[10]= c:\\users\\avp\\documents\\Mathbook\\hydrogen\\h2lowcurrent
```

```
In[11]:= plotColorsLines = {  
  (*1-red*) {Hue[0.0], Thickness[0.007], Dashing[{}]},  
  (*2-orange*) {Hue[0.1], Thickness[0.007], Dashing[{}]},  
  (*3-green*) {Hue[0.3], Thickness[0.007], Dashing[{}]},  
  (*4-cyan*) {Hue[0.5], Thickness[0.007], Dashing[{}]},  
  (*5-dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{}]},  
  (*6-purple*) {Hue[0.8], Thickness[0.007], Dashing[{}]},  
  (*7-black*) {Thickness[0.007], Dashing[{}]},  
  (*8-dash red*) {Hue[0.0], Thickness[0.007], Dashing[{0.05, 0.05}]},  
  (*9-dash orange*) {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05}]},  
  (*10-dash green*) {Hue[0.3], Thickness[0.007], Dashing[{0.05, 0.05}]},  
  (*11-dash cyan*) {Hue[0.5], Thickness[0.007], Dashing[{0.05, 0.05}]},  
  (*12-dash dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{0.05, 0.05}]},  
  (*13-dash purple*) {Hue[0.8], Thickness[0.007], Dashing[{0.05, 0.05}]},  
  (*14-dash black*) {(*CMYKColor[0,0,0,1],*)Thickness[0.007], Dashing[{0.02, 0.02}]}};
```

```
In[12]:= plotColorsPoints = {  
  (*1-red*) {Hue[0.0], PointSize[0.02]},  
  (*2-orange*) {Hue[0.1], PointSize[0.02]},  
  (*3-green*) {Hue[0.3], PointSize[0.02]},  
  (*4-cyan*) {Hue[0.5], PointSize[0.02]},  
  (*5-dk blue*) {Hue[0.7], PointSize[0.02]},  
  (*6-purple*) {Hue[0.8], PointSize[0.02]},  
  (*7-yellow*) {Hue[0.2], PointSize[0.02]},  
  (*8-black*) {PointSize[0.02]}  
};
```

```
In[13]:= SetDirectory["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\H2HnCollisions"]
```

```
Out[13]:= c:\users\avp\documents\Mathbook\hydrogen\H2HnCollisions
```

The following should be the same as in Phelps, J. Phys. Chem. Ref. Data 19, 653 (1990).

```
In[15]:= data88=Drop[Drop[Import["HnH2Q88.xls", "XLS"][[1]], 6], -12];
```

```
In[16]:= fac = 1. * 10^20;
```

■ Momentum transfer cross section

```
In[17]:= momentumtrans88=Table[{#[[j,1]],#[[j,3]]/fac},{j,Length[#]}&[data88];
```

```
In[18]:= momentumtrans88Plot=ListLogLogPlot[momentumtrans88,PlotRange->{{0.0099,10000},{0.099/fac,100}},PlotStyle->plotColorsPoints[[1]]];
```

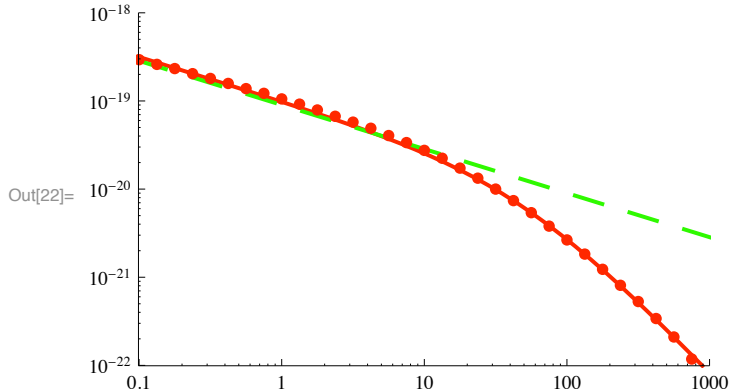
```
In[19]:= momentumTransFit[wn_] = 10 / fac / Sqrt[wn] / (1 + wn / 50)^1.2
```

$$\text{Out[19]} = \frac{1. \times 10^{-19}}{\left(1 + \frac{wn}{50}\right)^{1.2} \sqrt{wn}}$$

```
In[20]:= momentumTransFitTable = Table[{1. * 10^(j/8), momentumTransFit[10^(j/8)]}, {j, -8, 40}];
```

```
In[21]:= momentumTransFitPlot = LogLogPlot[{momentumTransFit[wn], 9.01 * 10^-20 / Sqrt[wn]}, {wn, 0.099, 10000}, PlotRange -> {{0.099, 1000}, {0.0099 / fac, 100 / fac}}, PlotStyle -> plotColorsLines[[{1, 10}]]];
```

```
In[22]:= Show[momentumTransFitPlot, momentumtrans88Plot]
```



■ Detachment cross section

This cross section is based on Phelps, J. Phys. Chem. Ref. Data 19, 653 (1990). The data sources included Hug and Champion and ??? and Gilbody.

```
In[23]:= detachment88=Table[{data88[[j,1]],data88[[j,2]]/fac},{j,Length[data88]}];
```

```
In[24]:= detachment88Plot=ListLogLogPlot[detachment88,PlotRange->{{1,10^6},{0.0099/fac,100/fac}},PlotStyle->plotColorsPoints[[2]]];
```

```
In[25]:= Import["gealy&vanzyl87table2.txt", "CSV"] // TableForm
```

```
Out[25]/TableForm=
```

2.000	9.99 ±10%	2.08 ±11%	20.7 ±15%
1.414	9.83 ±14%	2.56 ±10%	25.2 ±17%
1.000	9.54 ±16%	3.27 ±11%	31.2 ±19%
0.707	8.89 ±15%	4.55 ±11%	40.5 ±19%
0.500	8.02 ±15%	5.64 ±11%	45.2 ±18%
0.354	6.94 ± 15%	7.31 ±10%	50.7 ±18%
0.250	6.20 ±16%	9.26 ±10%	57.4 ± 19%
0.177	5.16 ±18%	12.2 ±11%	62.9 ±21%
0.125	4.46 ±17%	15.9 ±18%	70.9 ±25%
0.088	3.70 ±19%	20.3 ±14%	75.0 ±24%
0.063	2.48 ±24%	27.4 ±17%	68.1 ±29%

H- detachment in collisions with H₂ (col 2) and H (col 4) in !E-16 cm²

```
In[26]:= Drop[Import["gealy&vanzyl87table2.txt", "Table"], -1];
```

```
In[27]:= detachgealyvanzyl = Table[{{%[[j, 1]] * 1000, %[j, 2]] * 10^-20}, {j, Length[%]}];
```

```
In[28]:= detachgealyvanzylPlot = ListLogLogPlot[%,
  PlotRange -> {{1, 10^6}, {10^-22, 10^-18}}, PlotStyle -> plotColorsPoints[[3]]];
```

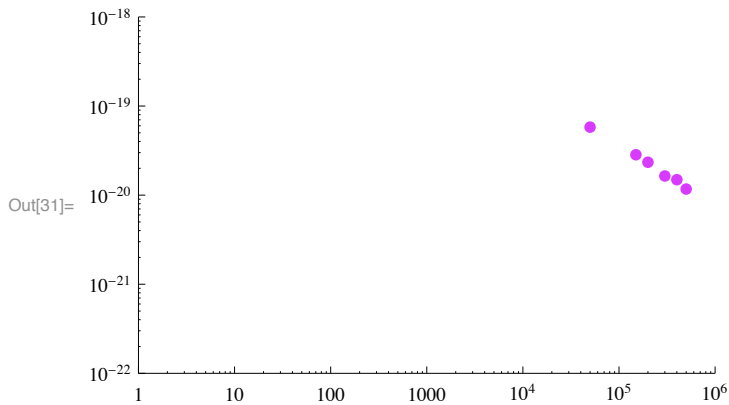
```
In[29]:= heinemeierTable1 = {{50, 5.8}, {150, 2.84}, {200, 2.34}, {300, 1.64}, {400, 1.49}, {500, 1.17}}
```

```
Out[29]= {{50, 5.8}, {150, 2.84}, {200, 2.34}, {300, 1.64}, {400, 1.49}, {500, 1.17}}
```

```
In[30]:= heinemeierTable = Table[{{%[[j, 1]] * 1000, %[j, 2]] * 10^-16 / 10000}, {j, Length[%]}]
```

```
Out[30]= {{50000, 5.8 * 10^-20}, {150000, 2.84 * 10^-20}, {200000, 2.34 * 10^-20},
  {300000, 1.64 * 10^-20}, {400000, 1.49 * 10^-20}, {500000, 1.17 * 10^-20}}
```

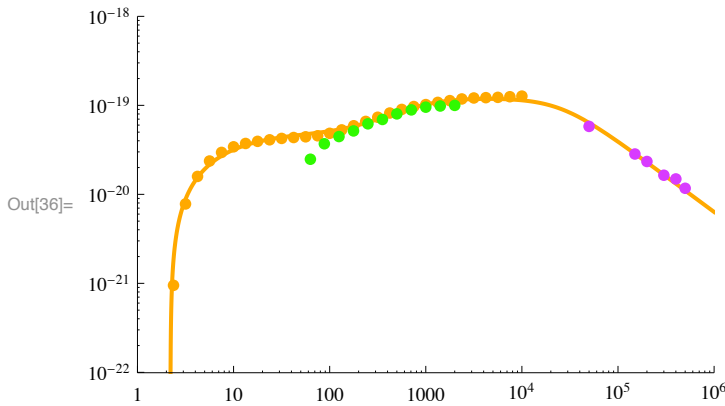
```
In[31]:= heinemeierPlot = ListLogLogPlot[%,
  PlotRange -> {{1, 10^6}, {10^-22, 10^-18}}, PlotStyle -> plotColorsPoints[[6]]]
```



```
In[32]:= detachment88Plot=ListLogLogPlot[detachment88,PlotRange->{{1,10^6},{0.0099/fac,100/fac}},
  PlotStyle->plotColorsPoints[[2]]];
```



```
In[33]:= detachmentFit [wn_] = UnitStep [wn - 2.2] * 5. * 10^-20 / (1 + 4.5 / (wn - 2.2)) *
      (1 + (wn / 170)^2)^0.25 / (1 + (wn / 1000)^2)^0.25 / (1 + (wn / 25 000)^2)^0.4
      5. * 10^-20 (1 + wn^2 / 28 900)^0.25 UnitStep [-2.2 + wn]
Out[33]:= (1 + 4.5 / (-2.2+wn)) (1 + wn^2 / 625 000 000)^0.4 (1 + wn^2 / 1 000 000)^0.25
In[34]:= detachmentFitTable = Table[{10^(j / 8), detachmentFit [10^(j / 8)]}, {j, -8, 56}];
In[35]:= detachmentFitPlot = LogLogPlot[{detachmentFit [wn]}, {wn, 1, 10^6},
      PlotRange -> {{1, 10^6}, {0.0099 / fac, 100 / fac}}, PlotStyle -> plotColorsLines [[2]]];
In[36]:= Show[detachmentFitPlot, detachment88Plot, heinemeierPlot, detachgealyvanzylPlot]
```



This plot is in approximate agreement with Williams, Phys. Rev. 154,9 (1967) and with Hug, Doverspike, and Champion (1983) at low energies

■ **Halp**ha excitation cross section

From Geddes, Hill, and Gilbody, J. Phys. D 14, 4837 (1981), we get

```
In[37]:= Import ["Geddes&Hill&Gilbody81JPD.txt", "CSV"] // TableForm
```

Out[37]/TableForm=

Energy (keV)	2s (H) (10-17CM)	2s (H2) (10-17CM2)	2La (H2)	3s (H2) (10-17CM2)	3Ha (H2) (10-18CM2)	(10-18)
3.0	2.23	2.35	6.73			
5.0	2.34	2.52	6.05	2.52	4.10	
7.5	2.50	2.73	5.31			
10.0	2.58	2.93	4.91	2.48	3.33	
12.5	2.67	3.14	4.82			
15.0	2.72	3.24	4.55	2.23	3.29	
17.5	2.81	3.27	4.64			
20.0	2.88	3.40	4.52	2.14	3.61	
22.5	2.99	3.45	4.61			
25.0	2.99	3.47	4.58	2.03	3.58	
27.5	3.04	3.49				
30.0	3.04	3.50				

```

In[38]:= data = Delete[
  Drop[Drop[Import["Geddes&Hill&Gilbody81JPD.txt", "Table"], 4], -3], {{2}, {4}, {6}, {8}}]
Out[38]= {{5., 2.34, 2.52, 6.05, 2.52, 4.1},
  {10., 2.58, 2.93, 4.91, 2.48, 3.33}, {15., 2.72, 3.24, 4.55, 2.23, 3.29},
  {20., 2.88, 3.4, 4.52, 2.14, 3.61}, {25., 2.99, 3.47, 4.58, 2.03, 3.58}}

In[39]:= geddesHalpahaData = Table[#[[j, 1]] * 1000, #[[j, 6]] * 10^-22], {j, Length[#]} &[data]
Out[39]= {{5000., 4.1 * 10^-22}, {10000., 3.33 * 10^-22},
  {15000., 3.29 * 10^-22}, {20000., 3.61 * 10^-22}, {25000., 3.58 * 10^-22}}

In[40]:= geddesHalpahaPlot = ListLogLogPlot[geddesHalpahaData, PlotRange ->
  {{10, 100000}, {0.99 * 10^-22, 1.01 * 10^-20}}, PlotStyle -> plotColorsPoints[[4]];

```

For comparison we look at the H + H2 and H+ + H2 excitation cross sections.

```

In[41]:= qAha[wA_] :=
  (UnitStep[wA - 26.] * (1.77 * 10^-27. * (wA - 26.)^3 / (wA / 230. + 1)^4 + (5.5 * 10^-26. * wA)) +
  1. * 10^-30)
In[42]:= q1ha[w1_] :=
  6. * 10^-28 * UnitStep[w1 - 50] (w1 - 50)^2 / (1 + (w1 / 700)^4)^0.5 * (1 + (w1 / 3000)^4)^0.25
  5 + 1. * 10^-30
Out[43]= 5.

```

We propose the following for Halpaha excitation by H-

```

In[44]:= qnhal[wn_] := 9. * 10^-28 * UnitStep[wn - 50]
  (wn - 50)^2 / (1 + (wn / 700)^4)^0.5 / (1 + (wn / 3000)^4)^0.04 * (1 + (wn / 30000)^3)^0.4

```

or

```

In[45]:= qnha[wn_] := 2.1 * 10^-21 *
  UnitStep[wn - 50] / (1 + 100 / (wn - 50)^1) / (1 + (wn / 200))^0.5 * (1 + (wn / 16000)^3)^0.48

```

```

In[46]:= halpahaFitTable = Table[{10^(j / 8), qnha[10^(j / 8)]}, {j, -8, 40}];

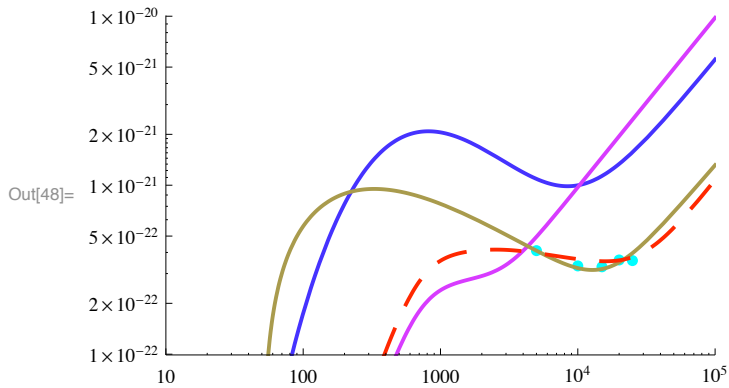
```

```

In[47]:= atomIonPlot = LogLogPlot[{qAha[w], q1ha[w], qnha[w], qnhal[w]},
  {w, 0.099, 100000}, PlotRange -> {{0.099, 100000}, {0.0099 / fac, 100 / fac}},
  PlotStyle -> plotColorsLines[[{5, 6, 7, 8}]]];

```

```
In[48]:= Show[geddesHalpPlot, atomIonPlot]
```



dark yellow - H⁻ + H₂ -> H α , blue - H + H₂ -> H α , purple - H + + H₂ -> H α

The low energy behavior for the adopted (red) H⁻ + H₂ -> H α cross section is purely a **prejudiced** guess based on the H⁺ behavior.

```
In[49]:= summaryTable =
  Table[{momentumTransFitTable[[j, 1]], momentumTransFitTable[[j, 2]], detachmentFitTable[[j, 2]], halpFitTable[[j, 2]]}, {j, Length[momentumTransFitTable]}];
```

```
In[50]:= Export["NegIonXSect.txt", summaryTable, "Table"]
```

```
Out[50]= NegIonXSect.txt
```

I should check high energy parts of H⁺ and H excitation!!!!

■ Charge transfer

Charge transfer to form H₂⁻ is unlikely and will be neglected. Note that many processes besides H⁻ + H₂ -> H₂⁻ + H are listed in the literature as charge transfer.

■ Energy loss function

We know nothing about inelastic collisions of H⁻ with H₂ and will neglect them

■ Fast H atom production

We assume that this is the same as collisional detachment, although it might not be the same.

```
In[51]:= qnfa[wn_] := qnse[wn]
```

■ Surface destruction of the H⁻ and reflection as H atoms

We probably have no information on this process. We assume complete destruction of the H⁻ and, if it were important, use the data for H⁺ reflection as H.

```
In[52]:= Quit[]
```

Cross sections for H + H2 collisions

Setup notebook environment

```
a = 1;

ClearAll["Global`*"];

Remove["Global`*"];

startclock = SessionTime[];

Off[General::spell];

Off[General::spell1];

today = StringForm["`"/`"/` ` `:``:``", Date][[2]],
  Date][[3]], Date][[1]], Date][[4]], Date][[5]], Date][[6]]]

12/2/2010 16:21:14.7833445`8.922347648469067
```

```

SetDirectory["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\h2hcollisions"]
c:\\users\\avp\\documents\\Mathbook\\hydrogen\\h2hcollisions

plotColorsLines = {
  (*1-red*) {Hue[0.0], Thickness[0.007], Dashing[{}]},
  (*2-orange*) {Hue[0.1], Thickness[0.007], Dashing[{}]},
  (*3-green*) {Hue[0.3], Thickness[0.007], Dashing[{}]},
  (*4-cyan*) {Hue[0.5], Thickness[0.007], Dashing[{}]},
  (*5-dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{}]},
  (*6-purple*) {Hue[0.8], Thickness[0.007], Dashing[{}]},
  (*7-black*) {Thickness[0.007], Dashing[{}]},
  (*8-dash red*) {Hue[0.0], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*9-dash orange*) {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*10-dash green*) {Hue[0.3], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*11-dash cyan*) {Hue[0.5], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*12-dash dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*13-dash purple*) {Hue[0.8], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*14-dash black*) {Thickness[0.007], Dashing[{0.02, 0.02}]}];

plotColorsPoints = {
  (*1-red*) {Hue[0.0], PointSize[0.02]},
  (*2-orange*) {Hue[0.1], PointSize[0.02]},
  (*3-green*) {Hue[0.3], PointSize[0.02]},
  (*4-cyan*) {Hue[0.5], PointSize[0.02]},
  (*5-dk blue*) {Hue[0.7], PointSize[0.02]},
  (*6-purple*) {Hue[0.8], PointSize[0.02]},
  (*7-yellow*) {Hue[0.2], PointSize[0.02]},
  (*8-black*) {PointSize[0.02]}
};

fac=10^20;

```

Total Q for elastic and inelastic scattering of H by H2 from Krstic and Schultz (1999), Fig. 1a

This data does not appear to be available in tabulated form so we digitize the graphs in Fig. 1 of J. Phys. B, 32 , 2415 (1999).

■ Integrated total scattering

```

Drop[Import["krsticfig1totalHn.dat", "Table"], -1];

krsticHTotal=Transpose[Table[{#[[All,1]],#[[All,2]]*(0.529)^2}]];

krsticHTotalPlot=ListLogLogPlot[krsticHTotal,PlotRange->{{0.1,100.},{1.,1000.}},
  PlotLabel->{"Total elastic Q (10^-20 m^2) versus Erel (eV)",
  ImageSize -> 400, PlotStyle->PointSize[0.02],PlotStyle->plotColorsPoints[[2]], DisplayFur

Drop[Import["krsticfig1aelasticHn.dat", "Table"], -1];

krsticHElastic=Transpose[Table[{#[[All,1]],#[[All,2]]*(0.529)^2}]];

krsticHElasticPlot=ListLogLogPlot[krsticHElastic, PlotRange->{{0.1,100.},{1.,1000.}},
  PlotLabel->{"Total elastic Q (10^-20 m^2) versus Erel (eV)", PlotStyle->plotColorsPoints
  ImageSize -> 400, PlotStyle->PointSize[0.02], DisplayFunction->Identity];

Show[krsticHTotalPlot, krsticHElasticPlot, DisplayFunction->$DisplayFunction];

```

Momentum transfer scattering

```

Drop[Import["krsticfig1bqmelasticHn.dat", "Table"], -1];

krsticHqMElastic=Transpose[Table[{{#[All,1]},#[All,2]}*(0.529)^2}]];

krsticHqMElasticPlot=ListLogLogPlot[krsticHqMElastic,PlotRange->{{0.1,100.},{0.01,100.}},
  PlotLabel->{"Elastic Qm (10^-20 m^2) versus Erel (eV)"},
  ImageSize -> 400, PlotStyle->PointSize[0.02],PlotStyle->plotColorsPoints[[2]], DisplayFur

Drop[Import["krsticfig1bqmtotalHn.dat", "Table"], -1];

krsticHqMTotal=Transpose[Table[{{#[All,1]},#[All,2]}*(0.529)^2}]];

krsticHqMTotalPlot=ListLogLogPlot[krsticHqMTotal, PlotRange->{{0.1,100.},{0.01,100.}},
  PlotLabel->{"Total Qm (10^-20 m^2) versus Erel (eV)"}, PlotStyle->plotColorsPoints[[2]],
  ImageSize -> 400, PlotStyle->PointSize[0.02], DisplayFunction->Identity];

Show[krsticHqMElasticPlot, krsticHqMTotalPlot, DisplayFunction->$DisplayFunction];

```

Note that QmTotal include the contribution of vibrational excitation, but not rotational excitation.

■ Ratio of momentum transfer to total cross sections

First consider the ratio of the elastic momentum transfer to total elastic cross sections to quantitatively determine the effect of the angular distributions with momentum transfer weighting.

```

ratioQmoQtelastic=Table[{0.1*10^(j/8),Interpolation[krsticHqMElastic,
InterpolationOrder->1][0.095*10^(j/8)]/
Interpolation[krsticHElastic,InterpolationOrder->1][0.095*10^(j/8)]}, {j,1,3*8}]

{{0.133352, 0.349882}, {0.177828, 0.324664}, {0.237137, 0.297571}, {0.316228, 0.264732},
{0.421697, 0.222048}, {0.562341, 0.18483}, {0.749894, 0.151636}, {1., 0.119665},
{1.33352, 0.0864849}, {1.77828, 0.0582735}, {2.37137, 0.0415158}, {3.16228, 0.0297344},
{4.21697, 0.0221525}, {5.62341, 0.0170938}, {7.49894, 0.0128514}, {10., 0.00941599},
{13.3352, 0.00726906}, {17.7828, 0.00546653}, {23.7137, 0.00425241}, {31.6228, 0.00347893},
{42.1697, 0.00251936}, {56.2341, 0.0017735}, {74.9894, 0.00122584}, {100., 0.000978355}}

ratioQmoQtelasticPlot=ListLogLogPlot[ratioQmoQtelastic, PlotRange->{{0.1,100},{0.0001,1}},
PlotStyle->plotColorsPoints[[1]], DisplayFunction->Identity];

```

```
ratioQmoQtElasticPlot=ListLogLogPlot[ratioQmoQtVib, PlotRange->{{0.1,100},{0.001,10}},
PlotStyle->plotColorsPoints[5],DisplayFunction->Identity];
```

ListLogLogPlot::lprn: ratioQmoQtVib is not a list of numbers or pairs of numbers. >>

```
fitQmoQtElasticPlot=LogLogPlot[0.4/(1+(enLab/0.33)^2)^0.53, {enLab,0.1,100}, PlotRange->{{0.
PlotStyle->plotColorsLines[1]};
```

■ Vibrational Excitation

■ Vibrational excitation from Phelps (1990)

```
Drop[Import["H2HPhelps1990.txt", "Table"], 2];
```

```
phelpsH2HVib01=Transpose[Table[{{%[[All,1]],%[[All,4]]}]]];
```

```
phelpsH2HVib01Plot=ListLogLogPlot[phelpsH2HVib01,PlotRange->{{0.1,10000.},{0.01,10.}},
PlotLabel->{"Vibrational excit (10-20 m2) versus Erel (eV)", ImageSize -> 400, PlotSty
```

■ Vibrational excitation from K&S (1999)

Vibrational excitation from Fig. 5. [Convert to LAB energies.](#)

```
Import["krsticfig5vib01.dat", "Table"]
```

```
{{0.966557, 0.00992283}, {1.24498, 1.08785}, {1.57606, 4.62051},
{2.04752, 2.81674}, {2.84501, 2.8228}, {4.4276, 2.96172}, {6.01366, 3.10471},
{8.07487, 3.48239}, {11.474, 4.18124}, {17.6532, 4.69405}, {26.5539, 4.92396},
{39.4963, 4.82656}, {62.8888, 4.52425}, {99.0178, 3.96288}}
```

```
krsticHVib01=Transpose[Table[{{%[[All,1]]*3/2,%[[All,2]]*(0.529)^2}]]];
```

```
krsticHVib01Plot=ListLogLogPlot[krsticHVib01,PlotRange->{{0.1,10000.},{0.01,10.}},
  PlotLabel->{"Vibrational excit (10^-20 m^2) versus Erel (eV)", ImageSize -> 400, PlotSty
Show[krsticHVib01Plot, phelpsH2HVib01Plot, DisplayFunction->$DisplayFunction];
```

This shows that our 1990 estimate is as much as a factor of ~ 4 larger than the theory of K&S (1999).

Next, consider the ratio of the vibrational momentum transfer to total vibrational cross sections to quantitatively determine the effect of the angular distributions with momentum transfer weighting.

```
krsticQmVib=Drop[Table[{0.1*10^(j/8)*3/2,(Interpolation[krsticHqMTotal,InterpolationOrder->1]
Interpolation[krsticHqMElastic,InterpolationOrder->1][0.1*10^(j/8)])}, {j,7,3*8-1}],2];
krsticQmVibPlot=ListLogLogPlot[%, PlotRange->{{0.1,10000},{0.01,10}},PlotStyle->plotColorsPoi
```

A useful result from K&S is the total vibrational excitation given by their difference in the total cross sections

```
differenceQt=Table[{0.1*10^(j/8)*3/2,(Interpolation[krsticHTotal,InterpolationOrder->1][0.1*1
Interpolation[krsticHElastic,InterpolationOrder->1][0.1*10^(j/8)])}, {j,7,3*8-1}];
krsticHTotalDiffPlot=ListLogLogPlot[%, PlotRange->{{0.1,10000},{0.01,10}},PlotStyle->plotCol
fitVibrationTotal=(UnitStep[enLab-3/2*0.52]*8/(1+(8/(enLab-3/2*0.52))^1)/(1+(enLab/5)^2)^0.2
(*/(1+(enLab/150)^2.2)^0.3*));
fitVibrationPlot=LogLogPlot[fitVibrationTotal, {enLab,0.01,10000}, PlotRange->{{0.01,100},{0
PlotStyle->plotColorsLines[[7]], PlotPoints->10000];
Show[krsticQmVibPlot, krsticHTotalDiffPlot, krsticHVib01Plot, phelpsH2HVib01Plot, fitVibrati
```

black - total vib. excit of K&S; green - vib Qm from K&S; orange - vib 0-1 from K&S; blue - Phelps (1990); black line - fit to total vib. excit.

The K&S (1999) theory for the sum of the vibrational excitation cross sections and the estimates of Phelps (1990) for 0-1 are not too different for energies below ~ 10 eV.

We note that the data is versus enRel

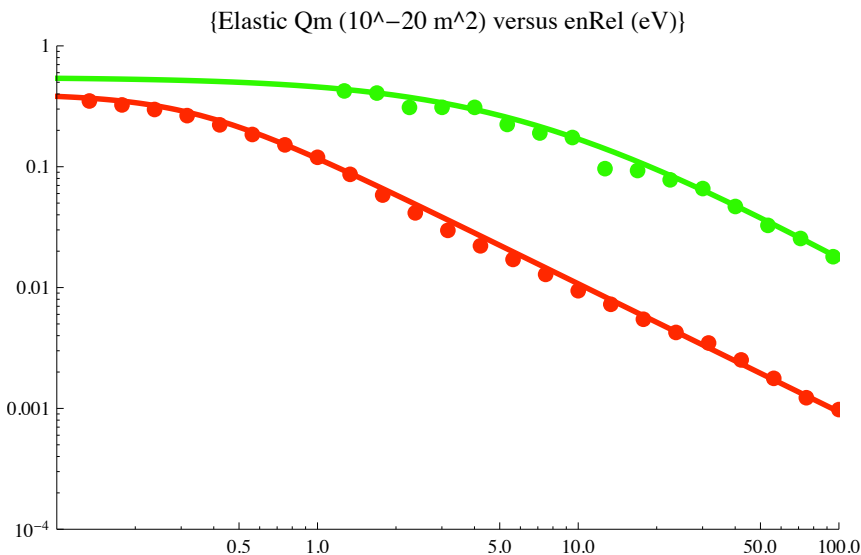
```
ratioQmoQtDiff=Table[{0.095*10^(j/8),(Interpolation[krsticHqMTotal,InterpolationOrder->1][0.0
Interpolation[krsticHqMElastic,InterpolationOrder->1][0.095*10^(j/8)])/
(Interpolation[krsticHTotal,InterpolationOrder->1][0.095*10^(j/8)]-
Interpolation[krsticHElastic,InterpolationOrder->1][0.095*10^(j/8)])}, {j,9,3*8}];
```

Here we had to delete the first few points because they were negative.

```
ratioQmoQtDiffPlot=ListLogLogPlot[ratioQmoQtDiff, PlotRange->{{0.1,100},{0.001,10}}, PlotSty
fitQmoQtDiff[enRel_]=(0.55/(1+(enRel/6.)^1)^1.2)
0.55
-----
(1 + 0.166667 enRel) ^1.2
fitQmoQtDiffPlot=LogLogPlot[fitQmoQtDiff[enRel], {enRel,0.1,100}, PlotRange->{{0.1,100},{0.0
PlotStyle->plotColorsLines[[3]]];
```



```
Show[ratioQmoQtelasticPlot, fitQmoQtElasticPlot, ratioQmoQtDiffPlot, fitQmoQtDiffPlot,
PlotLabel->{"Elastic Qm (10^-20 m^2) versus enRel (eV)", ImageSize -> 400]
```



red - Qm/Qt ratio from elastic scattering; green - Qm/Qt ratio from sum of vibrational excitation; not shown - blue - Qm/Qt ratio from lowest vibrational excitation only.

The values of this ratio in green are done using digitized K&S data, although the values are the small differences of rather large quantities. The larger ratios for the vibrational data are consistent with the lower relative differential cross sections at small angles for vibrational excitation. The shift to higher energies for the break in the fitted elastic curve relative to the fitted vibrational excitation curve is not understood. Presumably the drop in the fitted curves at the higher energies is because of the decrease in the rainbow angle as the collision energy increases. These decreases are important because they reduce the contributions of the inelastic processes to the effective momentum transfer cross section. Note that the decrease with increasing energy is much slower for H + H₂ than for H + H₂⁺.

■ Rotational excitation

From Phelps (1990) in 10⁻²⁰ m² versus LAB energy.

```
phelpsH2H1990 = Drop[Import["H2HPhelps1990.txt", "Table"], 2];
phelpsH2HRot02=Transpose[Table[{{%[[All,1]],%[[All,2]]}}]];
phelpsH2HRot02Plot=ListLogLogPlot[phelpsH2HRot02,PlotRange->{{0.01,10000.},{0.001,100.}},
PlotLabel->{"Rotational excit (10^-20 m^2) versus ELab (eV)", ImageSize -> 400, PlotStyl
phelpsH2HRot13=Transpose[Table[{phelpsH2H1990[[All,1]],phelpsH2H1990[[All,3]]}]];
phelpsH2HRot13Plot=ListLogLogPlot[phelpsH2HRot13,PlotRange->{{0.01,10000.},{0.001,100.}},
PlotLabel->{"Rotational excit (10^-20 m^2) versus ELab (eV)", ImageSize -> 400, PlotStyl
```

■ Rotational excitation from Fowler and Wroe, J. Phys. B 29, L851 (1996)

There have been several theoretical papers on rotational excitation in H + H₂ collisions since my 1990 review. Forrey et al, Ap. J. 489, 1000 (1997) favor the results of Flower and Wroe, J. Phys. B 29, L101 (1996) over Sun and Dalgarno, Ap. J. 427, 1053 (1994). From Fowler and Wroe (1996) as plotted by Forrey et al, Ap. J. 489, 1000 (1997) in 10⁻²⁰ m² versus COM energy in deg K.

```
fowlerH2HRot02 = Import["fowlerfig2arot02.dat", "Table"];
```

Convert to eV and LAB energy

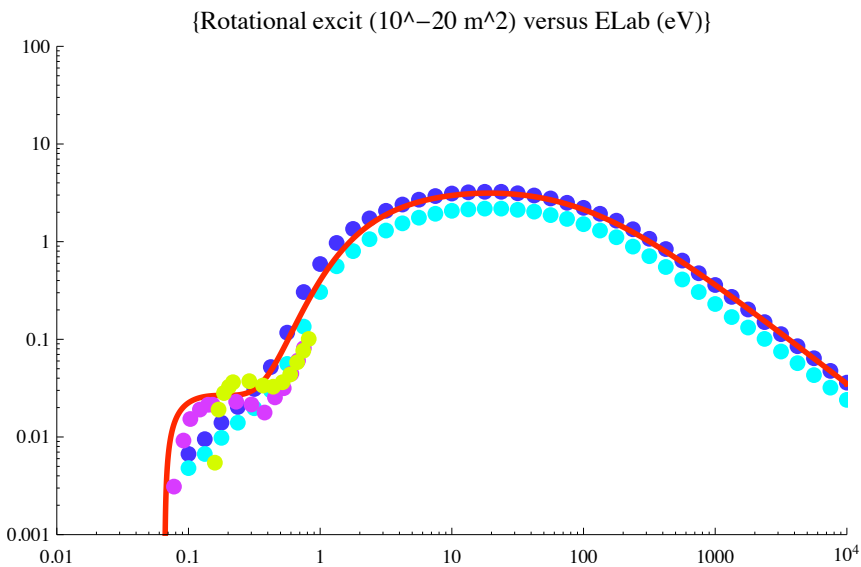
```
fowlerH2HRot02=Transpose[Table[{#[[All,1]]/11600*3/2,#[[All,2]]}]];
fowlerH2HRot02Plot=ListLogLogPlot[fowlerH2HRot02,PlotRange->{{0.01,10000.},{0.001,100.}},
  PlotLabel->{"Rotational excit (10^-20 m^2) versus ELab (eV)"}, ImageSize -> 400, PlotStyl
fowlerH2HRot13 = Import["fowlerfig2brot13.dat", "Table"];
fowlerH2HRot13=Transpose[Table[{#[[All,1]]/11600*3/2,#[[All,2]]}]];
fowlerH2HRot13Plot=ListLogLogPlot[fowlerH2HRot13,PlotRange->{{0.01,10000.},{0.001,100.}},
  PlotLabel->{"Rotational excit (10^-20 m^2) versus ELab (eV)"}, ImageSize -> 400, PlotStyl
```

Fit to theory

```
fitH2HRot02=(UnitStep[enLab-0.066]*0.04/(1+(0.02/(enLab-0.066))^1)*(1+(enLab/0.36)^4.7)/(1+(
  1+(enLab/80))^1.25);
```

Here I attempted to follow Fowler near threshold, although thi region is no important in our model. The 0-2 cross section fit will be multiplied by 5/3 to approximated the group of rotational transitions.

```
fitH2HRot02Plot=LogLogPlot[fitH2HRot02, {enLab,0.01,10000}, PlotRange->{{0.01,10000.},{0.001,
  PlotLabel->{"Rotational excit (10^-20 m^2) versus ELab (eV)"}, ImageSize -> 400, PlotStyl
Show[phelpsH2HRot02Plot, phelpsH2HRot13Plot, fitH2HRot02Plot, fowlerH2HRot02Plot, fowlerH2HR
```



The next question is, what Q_m/Q_t ratio should I assume for rotational excitation? I will use the results for vibrational excitation, because Chu and Dalgarno, Ap. J. 199, 637 (1975) show a differential cross section for rotational excitation that increases with angle, leading to a larger ratio than for their elastic scattering.

■ Lyman alpha excitation in H + H₂

From Phelps (1990)

```
h2h2pCTData = Drop[Import["h2hPhelps1990.txt", "Table"], 2];
```

```

Transpose[%];

h2hLymanAlphaData=Transpose[Join[{{%[[1]]},{%[[8]]}}]];

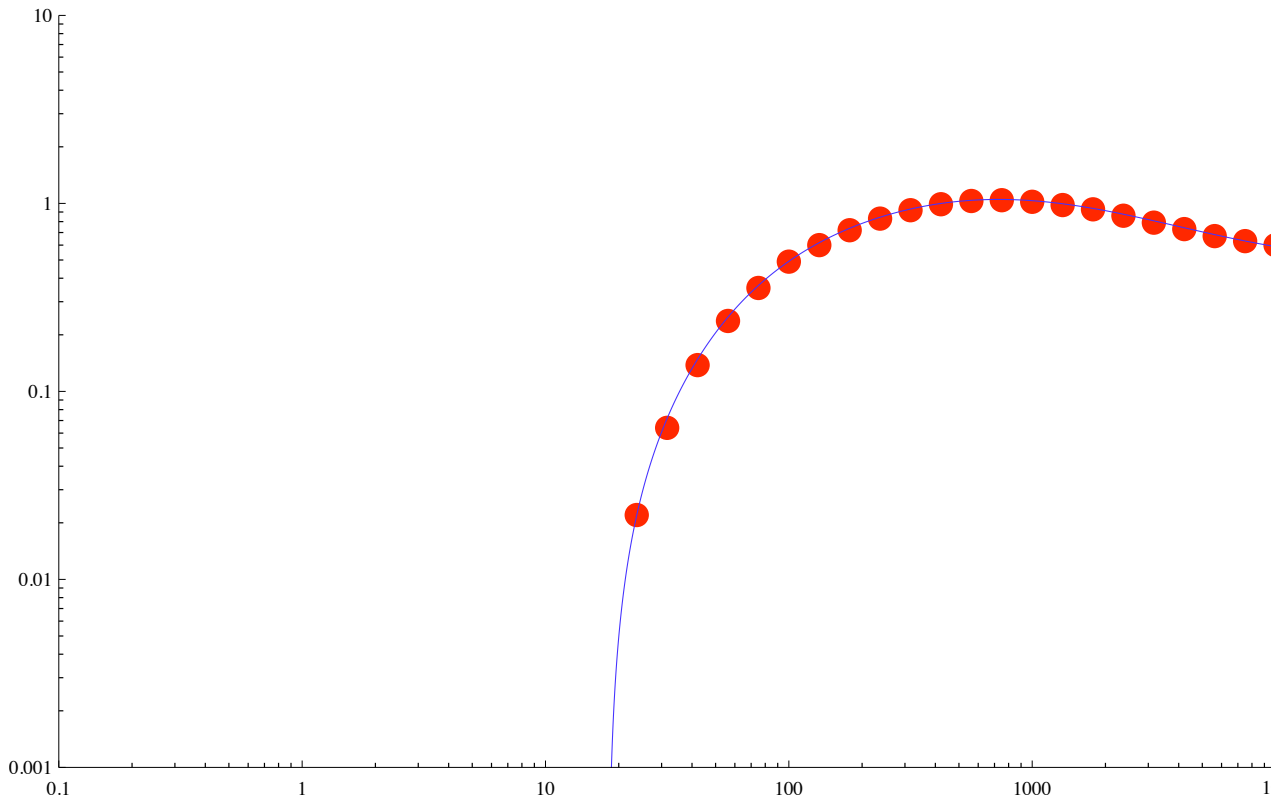
h2hLymanAlphaDataPlot =ListLogLogPlot[h2hLymanAlphaData, PlotStyle->plotColorsPoints[[1]],
PlotRange->{{0.1,10000},{.001,10}}];

h2hLymanAlphaFit:=2.0*10^-23*UnitStep[wM-18.0]*(wM-18.0)^1.45/(1+(wM/50.)^2)^.45/(1+(wM/700)^
(1+wM/15000) //wM ->enlab

h2hLymanAlphaFitPlot=LogLogPlot[10^20*h2hLymanAlphaFit,{enlab,0.1,10000},PlotStyle->plotColor
PlotRange->{{0.1,10000},{.001,10}},PlotPoints->10000,DisplayFunction->Identity];

Show[h2hLymanAlphaDataPlot, h2hLymanAlphaFitPlot,ImageSize->600]

```



■ Halpha excitation

- fast H + H₂ -> fast H(n=3) + H₂ by small-angle (long range) collisional excitation - Balmer alpha excitation.

From file H2MULTIBEAMSpatial041706.nb we get the following. Presumably it came from van Zyl et al.

```

qAxB[wA_] :=
  (UnitStep[wA - 26.] * (1.77 * 10^-27. * (wA - 26.)^3 / (wA / 230. + 1)^4 + (5.5 * 10^-26. * wA)) +
  1. * 10^(-30))

qAxBPlot =
  LogLogPlot[qAxB[w1], {w1, 10, 100 000}, PlotRange -> {{10, 100 000}, {10^-23, 10^-20}}];

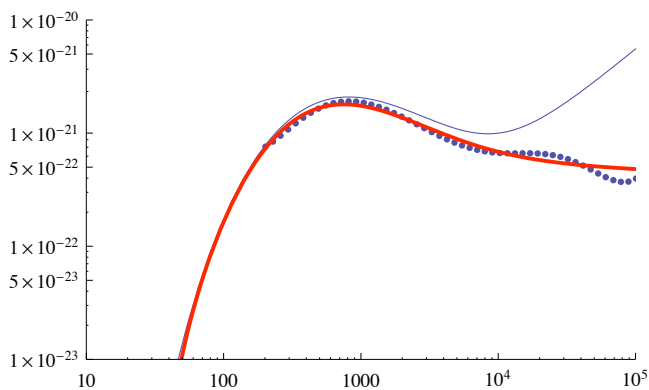
qAxBNew[wA_] :=
  UnitStep[wA - 26.] * 1.77 * 10^-27. * (wA - 26.)^3 / (wA / 240. + 1)^4.25 * (1 + (wA / 5000)^1.2)

```

```
qAxBNewPlot = LogLogPlot[qAxBNew[w1], {w1, 10, 100 000},
  PlotRange -> {{10, 100 000}, {10^-23, 10^-20}}, PlotStyle -> plotColorsLines[[1]]];
```

This would produce a fast H atom excited to the $n=3$ state and emitting Balmer alpha. We assume that this results in small angle scattering, i.e., it does not contribute significantly compared to the elastic scattering energy loss. This assumption is critical and is based on data by Gilbody et al.

```
Drop[Import["ornl6086H2H-Halpha.txt", "Table"], 1];
Drop[Import["ornl6086H2H-HalphaS.txt", "Table"], 1];
Table[{{#[[j, 1]], (#[[j, 2]] + #2[[j, 2]]) / 10 000}, {j, Length[#]}] &[% , %];
ornlH2HHalphaPlot = ListLogLogPlot[%, PlotRange -> {{10, 100 000}, {10^-23, 10^-20}}];
Show[ornlH2HHalphaPlot, qAxBPlot, qAxBNewPlot]
```



The ORNL differ considerably from my interpretation of van Zyl at high energies!!!

■ H2 near uv excitation

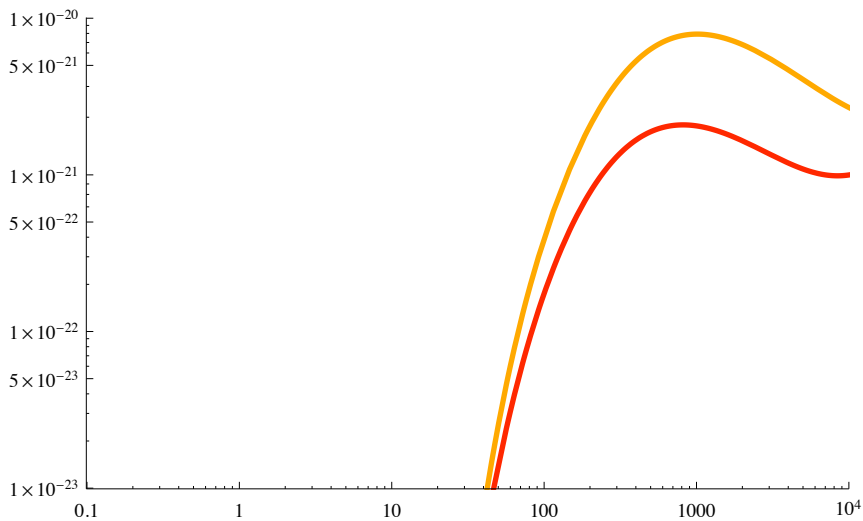
On the basis of the comparisons of the spatial scans for the uv continuum and our model results we propose the following

```
qAuv[wA_] := UnitStep[wA - 26.] (3*10^-27 (wA - 26.)^3 / (wA/300. + 1)^4 + (5.5*10^-26*wA)) + 1.*10
```

This is intended to increase the cross section for H + H2 by about a factor of 2 at low energies and a factor of ~ 4 at high energies.

```
fitsPlot = LogLogPlot[{qAxB[wA], qAuv[wA]}, {wA, 0.1, 10000}, PlotRange -> {{0.099, 10000}, {.99*10^-23,
  ImageSize -> 400, PlotStyle -> plotColorsLines};
```

```
Show[(*uvExcitCalcPlot,*)fitsPlot]
```



■ Momentum transfer scattering of H by H2

■ From Phelps (1990)

```
h2hPhelpsData = Drop[Import["h2hPhelps1990.txt", "Table"], 2];
```

```
Transpose[%];
```

```
h2hMomentumTransferData=Transpose[Join[{{%[[1]]}},{{%[[12]]}}];
```

```
h2hMomentumTransferPhelpsPlot =ListLogLogPlot[h2hMomentumTransferData, PlotStyle->plotColors  
PlotRange->{{0.1,10000},{.001,100}}];
```

```
h2hMomentumTransferFit[enLab_]=7.*10^-20/enLab^0.35/(1+enLab/18)/(1+enLab/1000)^0.5 + 1.*10^
```

$$1. \times 10^{-30} + \frac{7. \times 10^{-20}}{\left(1 + \frac{\text{enLab}}{1000}\right)^{0.5} \left(1 + \frac{\text{enLab}}{18}\right) \text{enLab}^{0.35}}$$

```
h2hMomentumTransferFitPlot =LogLogPlot[fac*h2hMomentumTransferFit[enLab], {enLab, 0.1, 10000
```

■ Total momentum transfer from Krstic (1999)

```
h2hKrsticTotQmData = Drop[Import["krsticfig1bqmtotalhn.dat", "Table"], -1];
```

Convert to 10⁻²⁰ m² and LAB energy

```
h2hKrsticTotQm=Transpose[Table[{h2hKrsticTotQmData[[All,1]]*3/2,h2hKrsticTotQmData[[All,2]]*}
```

```
h2hKrsticTotQmPlot =ListLogLogPlot[h2hKrsticTotQm, PlotStyle->plotColorsPoints[[4]], PlotRan
```

```
h2hKrsticTotalFit[enLab_]=13.*10^-20/enLab^0.35/(1+(enLab/1))^0.6/(1+(enLab/200))^0.8 + 1.*1
```

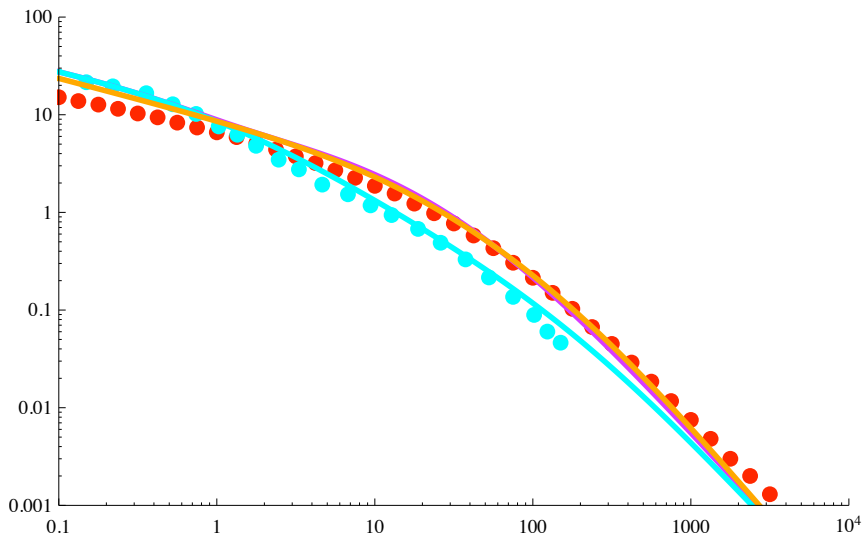
$$1. \times 10^{-30} + \frac{1.3 \times 10^{-19}}{\left(1 + \frac{\text{enLab}}{200}\right)^{0.8} \text{enLab}^{0.35} (1 + \text{enLab})^{0.6}}$$

```
h2hKrsticTotalFitPlot =LogLogPlot[fac*h2hKrsticTotalFit[enLab], {enLab, 0.1, 10000}, PlotSty
PlotRange->{{0.1,10000},{.001,100}}, PlotPoints->10000, DisplayFunction->Identity];
```

I need to add the contribution of rotational excitation to the momentum transfer cross section

```
qmSum=fac*h2hKrsticTotalFit[enLab]+(5/3*fitH2HRot02*fitQmoQtDiff[enRel])/enRel->2/3*enLab;
h2hqmRotPlot =LogLogPlot[qmSum, {enLab,0.066,10000}, PlotStyle->plotColorsLines[[6]], PlotRa
h2hKrsticQmSumFit[enLab_]=9.*10^-20/enLab^0.42/(1+(enLab/15))^0.7/(1+(enLab/200))^0.8 + 1.*1
h2hKrsticQmSumFitPlot =LogLogPlot[fac*h2hKrsticQmSumFit[enLab], {enLab, 0.1, 10000}, PlotSty
```

```
Show[h2hMomentumTransferPhelpsPlot, (*h2hMomentumTransferFitPlot,*) h2hKrsticTotQmPlot, h2hq
h2hKrsticTotalFitPlot, h2hKrsticQmSumFitPlot, ImageSize->400, DisplayFunction->$DisplayFunct
```



red points - Qm Phelps (1990); cyan points - total Qm K&S; cyan curve - our fit to total Qm of K&S; purple curve - sum of total Qm of K&S and Qm from rot. excit.; orange curve - simplified fit to sum curve.

■ Energy loss function

■ Including elastic recoil

```
lossFcn=Drop[Import["Phelps90Table9.txt","Table"],3];
totalLossFcn=Table[{lossFcn[[j,1]],lossFcn[[j,7]]},{j,Length[lossFcn]};
totalLossFcnPlot=ListLogLogPlot[totalLossFcn,PlotRange->{{.1,10000},{0.5,200}},PlotStyle->p
```

The following is a fit to the total energy loss function of Phelps (1990).

```
fitTotalLossFcn=3.4*enLab^0.7/(1+(enLab/4)^1.5)^(.3)*(1+(enLab/1900)^2)^.6/(1+(enLab/3000)^3)
fitTotalLossFcnPlot=LogLogPlot[fitTotalLossFcn,{enLab,.1,10000},PlotRange->{{.1,10000},{.5,200}}
Show[fitTotalLossFcnPlot,totalLossFcnPlot,ImageSize->400,DisplayFunction->$DisplayFunction];
```

■ Inelastic only, i.e., not including elastic recoil

For the multibeam model, we want the inelastic contribution to the energy loss function

```
lossFcn=Drop[Import["Phelps90Table9.txt","Table"],3];
inelasticLossFcn=Table[{lossFcn[[j,1]],lossFcn[[j,6]]},{j,Length[lossFcn]};
inelasticLossFcnPlot=ListLogLogPlot[inelasticLossFcn,PlotRange->{{.1,10000},{0.5,200}},Plot
```

```

fitInelasticLossFcn=0.52*(enLab)^0.625 (*10^-20 eV m^2*)
0.52 enLab^0.625

fitInelasticLossFcnPlot=LogLogPlot[fitInelasticLossFcn,{enLab,.1,10000},PlotRange->{{.1,10000}

Show[fitInelasticLossFcnPlot,inelasticLossFcnPlot,ImageSize->400,DisplayFunction->$DisplayFu

```

This estimate includes the contributions of rotational and vibrational excitation. Does the vibrational estimate need to be changed because of the lower peak vibrational excitation cross section? I conclude that the change in vibrational excitation cross section at energies (~1 eV) where it is important to the energy loss function are small. At higher energies (~ 100 eV) the change in vibrational excitation is a factor ~ 2, but the contribution to the energy loss function is small. Therefore, I have made no changes in my model.

■ Ionization from VanZyl et al (1981) (as tabulated in Phelps (1990)) and from Brehm et al (1995)

```

phelpsTable8=Drop[Import["h2hPhelps1990.txt","Table"],2];

Transpose[%];

h2hElectronProductionData=Transpose[Join[{{%[[1]]},{%[[11]]/fac}}]];

h2hH2pElectronVanZylData=Import["vanzyl181fig8h2p.dat","Table"];

h2hH2pElectronVanZylDataPlot =ListLogLogPlot[h2hH2pElectronVanZylData, PlotStyle->plotColors
PlotRange->{{10,100000},{.0001/fac,10/fac}}, DisplayFunction->Identity];

```

qAe2

```

h2hH2pElectronVanZylFit[enLab_]=1.5*10^-26*(enLab-27)^1.55*UnitStep[enLab-27]/
(1+(enLab/10000)^1)^1.4;

```

From H2CrossSections.nb we find. The fit is not quite as good as the preceding cell.

```

h2hElectronProductionFit[wA_] =
UnitStep[wA - 22.] * (9. * 10^-27 * (wA - 22) ^ 2 / ((wA / 5000) + 1) ^ 5 + (5. * 10^-29. * wA ^ 2) );

h2hH2pElectronVanZylFitPlot =LogLogPlot[h2hH2pElectronVanZylFit[enLab], {enLab, 0.1, 100000}
PlotStyle->plotColorsLines[[1]], PlotRange->{{10,100000},{.0001/fac,10/fac}}, DisplayFuncio

```

Production of fast H+ + electron + slow H2, i.e., conversion of H to H+ with small energy loss.

```

h2hHpElectronVanZylData=Import["vanzyl181fig8hp.dat","Table"];

h2hHpElectronVanZylDataPlot =ListLogLogPlot[h2hHpElectronVanZylData, PlotStyle->plotColorsPo
PlotRange->{{10,100000},{.0001/fac,10/fac}}, DisplayFunction->Identity];

```

qAe1

```

h2hHpElectronVanZylFit[enLab_]=8.*10^-26*(enLab-32)^1.55*UnitStep[enLab-32]/
(1+(enLab/3000)^3)*(1+(enLab/6500)^3)^0.67

```

$$8. \times 10^{-26} (-32 + \text{enLab})^{1.55} \left(1 + \frac{\text{enLab}^3}{274\,625\,000\,000}\right)^{0.67} \text{UnitStep}[-32 + \text{enLab}]$$

$$1 + \frac{\text{enLab}^3}{27\,000\,000\,000}$$

```

h2hHpElectronVanZylFitPlot =LogLogPlot[h2hHpElectronVanZylFit[enLab], {enLab, 0.1, 100000},
PlotStyle->plotColorsLines[[3]], PlotRange->{{10,100000},{.0001/fac,10/fac}}, DisplayFuncio

```

Van zyl H- + H2+ production


```

h2hHnH2pVanZylData=Import["vanzyl81fig8hn.dat","Table"];
h2hHnH2pVanZylDataPlot =ListLogLogPlot[h2hHnH2pVanZylData, PlotStyle->plotColorsPoints[[4]],
PlotRange->{{10,100000},{.0001/fac,10/fac}}, DisplayFunction->Identity];

```

The following fit has been modified at low energies to take into account the data of Brem et al (1995)

qAN2

```

h2hHnH2pVanZylFit=3.*10^-22/(1+250/(enLab-27)^1.55)*UnitStep[enLab-27]/
(1+(enLab/350)^3)^0.55+ 3.*10^-28*(enLab-450)^1.98*UnitStep[enLab-450]/
(1+(enLab/5000)^2)^1.4

```

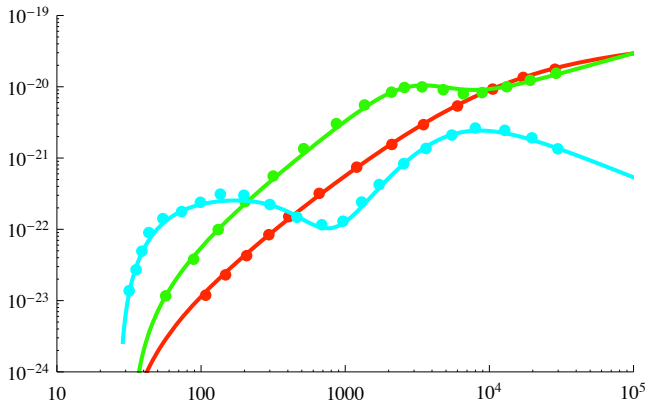
$$\frac{3. \times 10^{-28} (-450 + \text{enLab})^{1.98} \text{UnitStep}[-450 + \text{enLab}]}{\left(1 + \frac{\text{enLab}^2}{25000000}\right)^{1.4}} + \frac{3. \times 10^{-22} \text{UnitStep}[-27 + \text{enLab}]}{\left(1 + \frac{250}{(-27 + \text{enLab})^{1.55}}\right) \left(1 + \frac{\text{enLab}^3}{42875000}\right)^{0.55}}$$

```

h2hHnH2pVanZylFitPlot =LogLogPlot[h2hHnH2pVanZylFit, {enLab, 0.1, 100000},
PlotStyle->plotColorsLines[[4]](*, PlotRange->{{0.1,100000},{.0001/fac,10/fac}}*);

```

```
Show[h2hH2pElectronVanZylFitPlot , h2hH2pElectronVanZylDataPlot ,
h2hHpElectronVanZylDataPlot , h2hHpElectronVanZylFitPlot ,
h2hHnH2pVanZylDataPlot , h2hHnH2pVanZylFitPlot ]
```



■ Data from Brehm et al (1995)

Brehm et al, 28, 1517 (1995) show additional excit channels, i.e., $H3+ + e$ and $H+ + H-$.

■ $H + H2 \rightarrow H3+ + e$.

```
brehmh3pTableRel=Import["brehmfig4ah3p.dat","Table"];
```

These are relative energies and cm^2 , so we need to convert to LAB energies and m^2 .

```
brehmh3pTable = Table[{3/2 * #[[j, 1]], #[[j, 2]] / 100}, {j, 8}] &[brehmh3pTableRel];
```

```
h3pProductionPlot =ListLogLogPlot[brehmh3pTable, PlotStyle->plotColorsPoints[[6]],
PlotRange->{{10,1000},{.0001/fac,10/fac}}];
```

qAe3

```
h3pProductionFit[enLab_]=1.7*10^-21*Exp[-((enLab-19.1)/2)^2]+1.*10^-30;
```

```
h3pFitPlot =LogLogPlot[h3pProductionFit[enLab], {enLab, 1, 100}, PlotStyle->plotColorsLines[
PlotRange->{{10,1000},{.0001/fac,10/fac}}];
```

```
Show[h3pProductionPlot , h3pFitPlot]
```

```
intH3pFit = Integrate[h3pProductionFit[enLab], {enLab, 10, 30}]
```

6.02634×10^{-21}

```
brehmh2pTableRel=Import["brehmfig4ah2p.dat","Table"];
```

These are relative energies and cm^2 , so we need to convert to LAB energies and m^2 .

```
brehmh2pTable = Table[{3/2 * #[[j, 1]], #[[j, 2]] / 10 000}, {j, 8}] &[brehmh2pTableRel];
```

```
h2pBrehmProductionPlot =ListLogLogPlot[brehmh2pTable, PlotStyle->plotColorsPoints[[1]],
PlotRange->{{10,1000},{.0001/fac,10/fac}},PlotMarkers->{"■"}];
```

```
brehmhpTableRel=Import["brehmfig4ahp.dat", "Table"];
```

These are relative energies and cm², so we need to convert to LAB energies and m².

```
brehmhpTable = Table[{3 / 2 * #[[j, 1]], #[[j, 2]] / 10 000}, {j, 8}] &[brehmhpTableRel];
hpBrehmProductionPlot =ListLogLogPlot[brehmhpTable, PlotStyle->plotColorsPoints[[3]],
PlotRange->{{10,1000},{.0001/fac,10/fac}},PlotMarkers->{"■"}];
brehmHnH2pTableRel=Import["brehmfig3ah2p.dat", "Table"];
```

These are relative energies and cm², so we need to convert to LAB energies and m².

```
brehmHnH2pTable = Table[{3 / 2 * #[[j, 1]], #[[j, 2]] / 10 000}, {j, 8}] &[brehmHnH2pTableRel];
hnH2pBrehmProductionPlot =ListLogLogPlot[brehmHnH2pTable, PlotStyle->plotColorsPoints[[4]],
PlotRange->{{10,1000},{.0001/fac,10/fac}},PlotMarkers->{"■"}];
brehmHnHpTableRel=Import["brehmfig3ahp.dat", "Table"];
```

These are relative energies and cm², so we need to convert to LAB energies and m².

```
brehmHnHpTable = Table[{3 / 2 * #[[j, 1]], #[[j, 2]] / 10 000}, {j, 8}] &[brehmHnHpTableRel];
hnHpBrehmProductionPlot =ListLogLogPlot[brehmHnHpTable, PlotStyle->plotColorsPoints[[5]],
PlotRange->{{10,1000},{.0001/fac,10/fac}},PlotMarkers->{"■"}];
```

qAN1

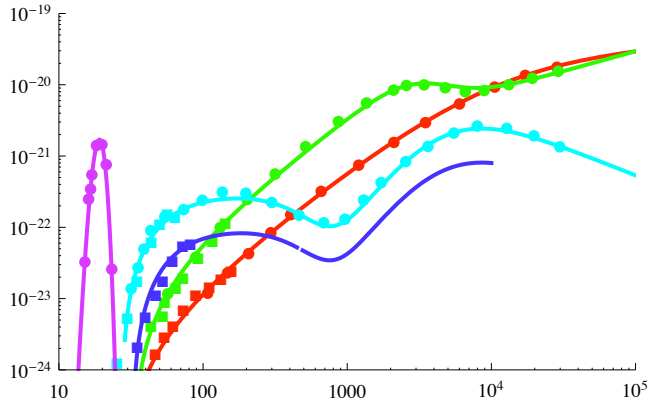
```
h2hHnHpVanZylFit=1.*10^-22/(1+300/(enLab-32)^1.55)*UnitStep[enLab-32]/
(1+(enLab/350)^3)^0.55+ 1.*10^-28*(enLab-450)^1.98*UnitStep[enLab-450]/
(1+(enLab/5000)^2)^1.4
```

$$\frac{1. \times 10^{-28} (-450 + \text{enLab})^{1.98} \text{UnitStep}[-450 + \text{enLab}]}{\left(1 + \frac{\text{enLab}^2}{25000000}\right)^{1.4}} + \frac{1. \times 10^{-22} \text{UnitStep}[-32 + \text{enLab}]}{\left(1 + \frac{300}{(-32 + \text{enLab})^{1.55}}\right) \left(1 + \frac{\text{enLab}^3}{42875000}\right)^{0.55}}$$

The high energy portion of this cross section parallels the H- + H2+ curve and is only a guess based on the Brehm at al proposal of similarity.

```
h2hHnHpVanZylFitPlot =LogLogPlot[h2hHnHpVanZylFit, {enLab, 1, 10000}, PlotStyle->plotColorsL
PlotRange->{{10,1000},{.0001/fac,10/fac}}];
```

```
Show[h2hH2pElectronVanZylFitPlot , h2hH2pElectronVanZylDataPlot ,
h2hHpElectronVanZylDataPlot , h2hHpElectronVanZylFitPlot ,
h2hHnH2pVanZylDataPlot , h2hHnH2pVanZylFitPlot , h2pBrehmProductionPlot ,
hpBrehmProductionPlot , hnH2pBrehmProductionPlot , h2hHnHpVanZylFitPlot ,
hnHpBrehmProductionPlot , h3pProductionPlot , h3pFitPlot]
```



```
Quit[]
```

Notes from MBHCAsymmDoppler081709_7.nb. on 08/20.09, the trial contribution to new j3[p,q] was

```
(*loss of fast H to production of new, H3+,
j3[p,q] from jA[p,3+q] by H +H2 -> e +H3+ associative ionization*)
If[dele <= 1, -Total[Table[gioniz * jA[p, k] * n * delx * qAe3[dele * (k - 1)],
{k, Floor[17 / dele], Floor[21 / dele]}]], 0] +
If[dele > 1, -gioniz * intQAe3 * jA[p, Floor[19 / dele] + 1] * n * delx / dele, 0] +
```

Analytical fits to H2 - H2 cross sections from JPCRD 1990

Setup notebook environment

```
In[1]:= a = 1;

In[2]:= ClearAll["Global`*"];

In[3]:= Remove["Global`*"];

In[4]:= startclock = SessionTime[];

In[5]:= Off[General::spell];

In[6]:= Off[General::spell1];

In[7]:= today = StringForm["`"/`"/` ``:``:``", Date][[2]],
           Date][[3]], Date][[1]], Date][[4]], Date][[5]], Date][[6]]
Out[7]= 12/10/2010 20:33:37.6185201`9.327976594792087

In[8]:= SetDirectory["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\h2h2Collisions"]
Out[8]= c:\\users\\avp\\documents\\Mathbook\\hydrogen\\h2h2Collisions

In[9]:= plotColorsLines = {
  (*1-red*) {Hue[0.0], Thickness[0.007], Dashing[{}]},
  (*2-orange*) {Hue[0.1], Thickness[0.007], Dashing[{}]},
  (*3-green*) {Hue[0.3], Thickness[0.007], Dashing[{}]},
  (*4-cyan*) {Hue[0.5], Thickness[0.007], Dashing[{}]},
  (*5-dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{}]},
  (*6-purple*) {Hue[0.8], Thickness[0.007], Dashing[{}]},
  (*7-black*) {Thickness[0.007], Dashing[{}]},
  (*8-dash red*) {Hue[0.0], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*9-dash orange*) {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*10-dash green*) {Hue[0.3], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*11-dash cyan*) {Hue[0.5], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*12-dash dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*13-dash purple*) {Hue[0.8], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*14-dash black*) {Thickness[0.007], Dashing[{0.02, 0.02}]}];

In[10]:= plotColorsPoints = {
  (*1-red*) {Hue[0.0], PointSize[0.02]},
  (*2-orange*) {Hue[0.1], PointSize[0.02]},
  (*3-green*) {Hue[0.3], PointSize[0.02]},
  (*4-cyan*) {Hue[0.5], PointSize[0.02]},
  (*5-dk blue*) {Hue[0.7], PointSize[0.02]},
  (*6-purple*) {Hue[0.8], PointSize[0.02]},
  (*7-black*) {PointSize[0.02]},
  (*8-dash red*) {Hue[0.0], PointSize[0.02]},
  (*9-dash orange*) {Hue[0.1], PointSize[0.02]},
  (*10-dash green*) {Hue[0.3], PointSize[0.02]},
  (*11-dash cyan*) {Hue[0.5], PointSize[0.02]},
  (*12-dash dk blue*) {Hue[0.7], PointSize[0.02]},
  (*13-dash purple*) {Hue[0.8], PointSize[0.02]},
  (*14-dash black*) {PointSize[0.02]}];
```

H2 + H2 -> Halpha

From J. Phys. Chem. Ref. Data (1990)

```

In[11]:= Import["H2H2Phelps1990.txt", "CSV"] // TableForm
Out[11]/TableForm=
  "1990 data for H2 + H2 from Phelps, JPCRD"

0.1      1.00E-09    1.00E-09    0.063    1.00E-09    1.00E-09    1.00E-09    1.00E-09    1.0
0.1334   1.00E-09    1.00E-09    0.12     1.00E-09    1.00E-09    1.00E-09    1.00E-09    1
0.1778   1.00E-09    1.00E-09    0.196    1.00E-09    1.00E-09    1.00E-09    1.00E-09
0.237    1.00E-09    1.00E-09    0.3      0.009       1.00E-09    1.00E-09    1.00E-09    1.00E-
0.316    1.00E-09    1.00E-09    0.45     0.0197      1.00E-09    1.00E-09    1.00E-09    1.00
0.422    1.00E-09    1.00E-09    0.655    0.039       1.00E-09    1.00E-09    1.00E-09    1.00
0.562    1.00E-09    1.00E-09    0.92     0.069       1.00E-09    1.00E-09    1.00E-09    1.00E
0.75     1.00E-09    1.00E-09    1.27     0.12        0.0051      1.00E-09    1.00E-09    1.00E-09
1        1.00E-09    1.00E-09    1.7      0.214       0.0124      1.00E-09    1.00E-09    1.00E-09
1.334    1.00E-09    1.00E-09    2.17     0.365       0.0285      1.00E-09    1.00E-09    1.00E-0
1.778    1.00E-09    1.00E-09    2.68     0.64        0.065       1.00E-09    1.00E-09    1.00E-09
2.371    1.00E-09    1.00E-09    3.2      1.08        0.13        0.004       1.00E-09    1.00E-09    1.
3.162    1.00E-09    1.00E-09    3.63     1.74        0.24        0.019       1.00E-09    1.00E-09    1
4.217    1.00E-09    1.00E-09    3.75     2.63        0.39        0.082       1.00E-09    1.00E-09    1
5.623    1.00E-09    1.00E-09    3.6      3.65        0.53        0.245       1.00E-09    1.00E-09    1.
7.5      1.00E-09    1.00E-09    3.25     4.47        0.64        0.55        1.00E-09    1.00E-09    1.00
10       1.00E-09    1.00E-09    2.75     4.9         0.71        1.07        1.00E-09    1.00E-09    1.00E-
13.34    1.00E-09    1.00E-09    2.22     4.75        0.71        1.52        1.00E-09    1.00E-09    1.
17.78    0.0006     0         1.68     4.15        0.65        1.82        0         0.0009     0         2.68
23.7     0.0033     0         1.23     3.38        0.57        2.04        0         0.003      0         2.1
31.6     0.0144     0         0.89     2.66        0.455       2.15        0         0.0058     0         1.59
42.1     0.036      0.0009    0.625    2.02        0.335       2.21        0         0.0095     0.0009    1.19
56.2     0.075      0.0065    0.435    1.48        0.225       2.2         0         0.0125     0.0065    0.87
75       0.134      0.0255    0.295    1.08        0.148       2.15        0         0.0155     0.0255    0.63
100      0.215      0.0515    0.197    0.765       0.095       2.04        0         0.0185     0.0515    0.445
133.4    0.31       0.082     0.128    0.54        0.059       1.9         0         0.0214     0.082     0.315
177.8    0.425      0.113     0.082    0.363       0.037       1.74        0.00075    0.0247    0.11375
237      0.57       0.143     0.051    0.24        0.0225      1.57        0.0013     0.0278    0.1443    0.
316      0.705      0.175     0.0315   0.157       0.0137      1.4         0.0021     0.0308    0.1771
422      0.83       0.21      0.0193   0.102       0.0085      1.25        0.0034     0.0343    0.2134    0
562      0.97       0.247     0.0115   0.053       0           1.11        0.0055     0.0373    0.2525    0.034
750      1.11       0.284     0.009    0.037       0           0.96        0.009      0.0405    0.293     0.0202
1000     1.23       0.323     0         0.0217      0           0.825       0.0153     0.0443    0.3383    0.0114
1334     1.36       0.363     0         0.0128      0           0.715       0.0243     0.048     0.3873    0.0065
1778     1.48       0.405     0         0.0075      0           0.605       0.0385     0.0517    0.4435    0.0034
2371     1.6        0.445     0         0           0           0.515       0.06       0.056     0.505     0.0019
3162     1.71       0.487     0         0           0           0.435       0.091      0.0597    0.578     0.00103
4217     1.85       0.533     0         0           0           0.36        0.135      0.0635    0.668     0.00056
5623     2.03       0.59      0         0           0           0.3         0.193      0.0675    0.783     0.0003
7499     2.24       0.665     0         0           0           0.252       0.268      0.0733    0.933     0.00016
10000    2.5        0.77      0         0           0           0.212       0.37       0.0775    1.14      0.000085

In[12]:= h2h2Data=Drop[Import["H2H2Phelps1990.txt", "Table"], 3];
In[13]:= h2h2HalpahaData=Table[{h2h2Data[[j, 1]], h2h2Data[[j, 9]]}, {j, Length[h2h2Data]}];

```

```
In[14]:= h2h2HalpahaDataPlot =ListLogLogPlot[h2h2HalpahaData, PlotStyle->plotColorsPoints[[4]],
PlotRange->{{0.1,10000},{.0001,1}}];
```

Only the higher energy points represent an extrapolation of the experiments of Williams, Geddes, and Gilbody, J. Phys. B 16, L765 (1983).

```
In[15]:= h2h2HalpahaExpt=Take[h2h2HalpahaData,-3];
```

```
In[16]:= h2h2HalpahaExptPlot =ListLogLogPlot[h2h2HalpahaExpt, PlotStyle->plotColorsPoints[[5]],
PlotRange->{{0.1,10000},{.0001,1}}];
```

Now consider various fits to the points from 1990 and from high energy experiments. We first fit the 1990 listing.

```
In[17]:= qMxB1[wM_] =
UnitStep[wM - 18.] * 1. * 10^-22 * wM^0.23 / ((15 / (wM - 18.) ^0.8) + 1) ^1.25 + 1. * 10^(-30);
```

Fitting the high energy data from experiment, but raising the threshold gives

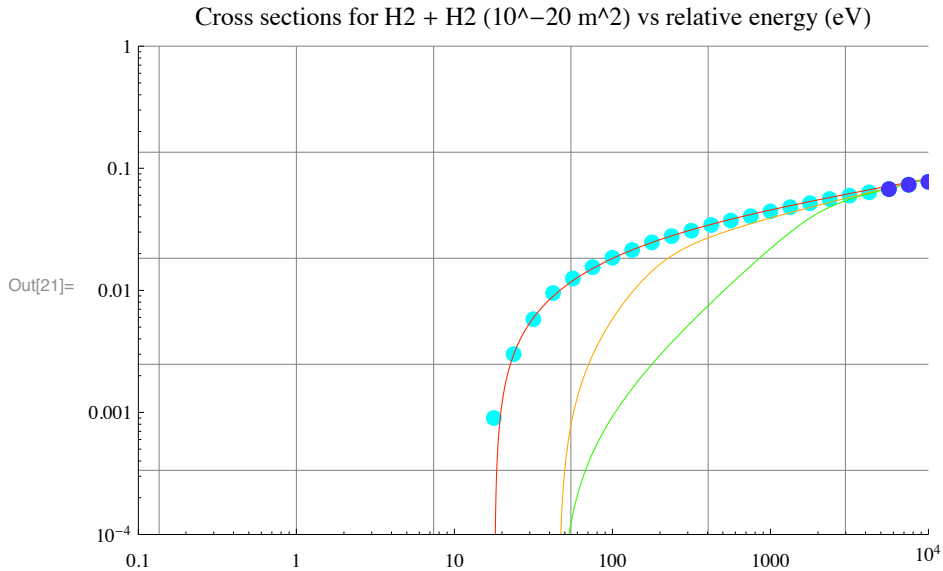
```
In[18]:= qMxB2[wM_] :=0.7*10^-24*UnitStep[wM-45.8]*(wM-45.8)^1.11/(1+(wM/200.)^4)^.2/(1+(wM/250000)^1)^
```

Fitting the high energy data from experiment, raising the threshold, and lowering the cross section at lower energy gives

```
In[19]:= qMxB3[wM_] :=1.1*10^-25*UnitStep[wM-45.8]*(wM-45.8)^1.11/(1+(wM/2000.)^4)^.2/(1+(wM/250000)^1)
```

```
In[20]:= h2h2pCTFitPlot=LogLogPlot[{10^20*qMxB1[wM],10^20*qMxB2[wM],10^20*qMxB3[wM]},{wM,0.1,10000},
PlotStyle->plotColorsPoints, PlotRange->{{0.1,10000},{.0001,Automatic}}];
```

```
In[21]:= Show[h2h2HalphaDataPlot, h2h2pCTFitPlot, h2h2HalphaExptPlot, ImageSize->400,
PlotLabel-> "Cross sections for H2 + H2 (10^-20 m^2) vs relative energy (eV)",
GridLines->Automatic]
```



■ Elastic scattering

```
In[22]:= h2h2ElasticData=Table[{h2h2Data[[j,1]],h2h2Data[[j,11]]},{j,Length[h2h2Data]}];
```

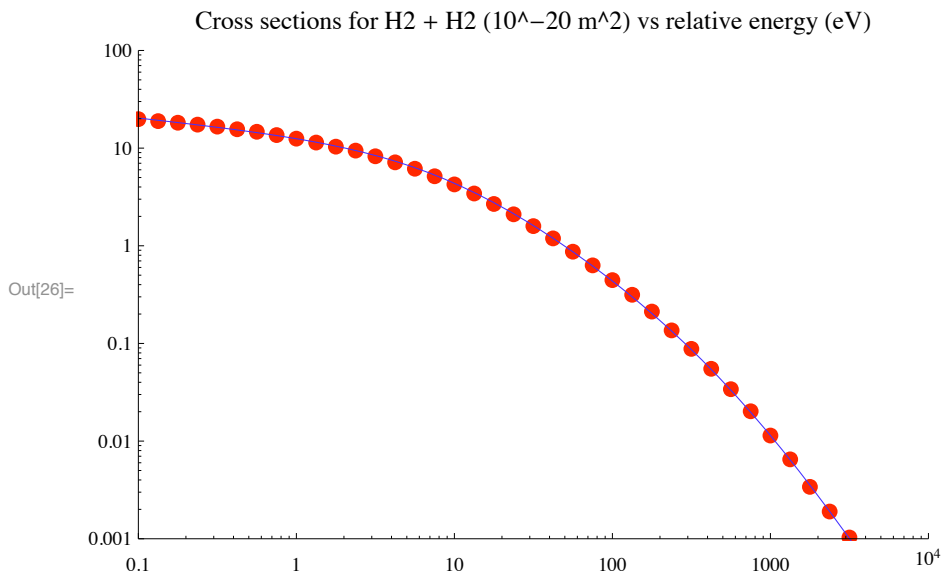
```
In[23]:= h2h2ElasticDataPlot =ListLogLogPlot[h2h2ElasticData, PlotStyle->plotColorsPoints[[1]],
PlotRange->{{0.1,10000},{.001,100}}];
```

```
In[24]:= qmH2H2Phelps[wM_] :=(4.5*10^-19/(wM/.001+1)^.17/(wM/9+1)^1./(wM/650+1)^1.3)
```

```
In[25]:= h2h2ElasticFitPlot=LogLogPlot[10^20*qmH2H2Phelps[wM],{wM,0.1,10000}, PlotStyle->plotColorsPo
PlotRange->{{0.1,10000},{.0001,100}}];
```



```
In[26]:= Show[h2h2ElasticDataPlot, h2h2ElasticFitPlot, ImageSize->400,
PlotLabel-> "Cross sections for H2 + H2 (10^-20 m^2) vs relative energy (eV)"]
```



■ Energy loss function for H2 + H2

For the multibeam model, we want the inelastic contribution to the energy loss function

```
Import["H2H2Q88.txt", "CSV"] // TableForm
```

```
In[27]:= lossFcn=Drop[Drop[Import["H2H2Q88.txt", "Table"], 6], -3];
```

```
In[28]:= inelasticLossFcn=Table[{lossFcn[[j, 1]], lossFcn[[j, 17]]}, {j, Length[lossFcn]}];
```

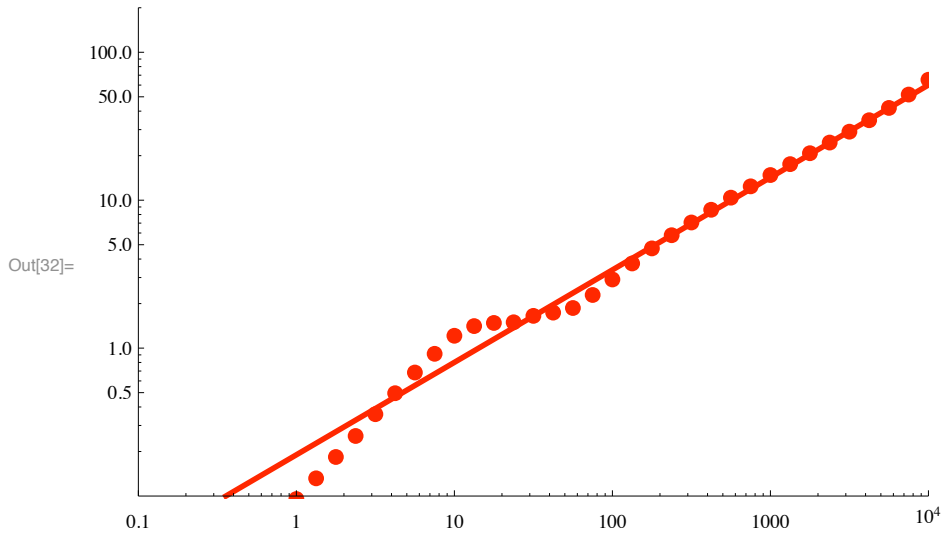
```
In[29]:= inelasticLossFcnPlot=ListLogLogPlot[inelasticLossFcn, PlotRange->{{.1, 10000}, {0.5, 200}}, Plot
```

```
In[30]:= fitInelasticLossFcn=0.19*(enLab)^0.625 (*10^-20 eV m^2*)
```

```
Out[30]= 0.19 enLab0.625
```

```
In[31]:= fitInelasticLossFcnPlot=LogLogPlot[fitInelasticLossFcn, {enLab, .1, 10000}, PlotRange->{{.1, 10000
```

```
In[32]:= Show[fitInelasticLossFcnPlot,inelasticLossFcnPlot,ImageSize->400]
```



■ H2 + H2 dissociation.

Note that the cross section of $2.5E-16 \text{ cm}^2$ at 10 keV given in Fig. 4 of McClure, Phys. Rev. 134, A1226 (1964) is that for production of fast H atoms. The cross section for H2 dissociation is $1.17E-16 \text{ cm}^2$. This says that the cross section for H2 destruction from Phelps (1990) is therefore too high by 2.14. However, Williams, Geddes, and Gilbody, J. Phys. B 17, 811 (1984) give values agreeing with the larger value of McClure. Therefore, we should not divide by 2.14.

```
In[33]:= h2h2DissocData=Table[{h2h2Data[[j,1]],h2h2Data[[j,2]]},{j,Length[h2h2Data]}];
```

```
% // TableForm
```

```
In[34]:= h2h2DissocDataPlot =ListLogLogPlot[h2h2DissocData, PlotStyle->plotColorsPoints[[4]], PlotRan
```

```
In[35]:= qMfA[wM_] =
```

```
UnitStep[wM - 18.] * 3. * 10^-21 * wM^0.23 / ((200 / (wM - 18.)^1) + 1)^1.25 + 1. * 10^(-30);
```

```
In[36]:= qMfA2[wM_] =
```

```
UnitStep[wM - 46.] * 3. * 10^-21 * wM^0.23 / ((500 / (wM - 46.)^1) + 1)^1.25 + 1. * 10^(-30);
```

```
In[37]:= h2h2DissocFitPlot=LogLogPlot[{1.*10^20*qMfA[wM],1.*10^20*qMfA2[wM]},{wM,0.1,10000},
PlotStyle->plotColorsPoints, PlotRange->{{0.1,10000},{.0001,Automatic}}];
```

■ Williams and Gilbody (1984)

```
In[38]:= Import["Williams&Gilbody84JPB.txt", "CSV"] // TableForm
```

Out[38]//TableForm=

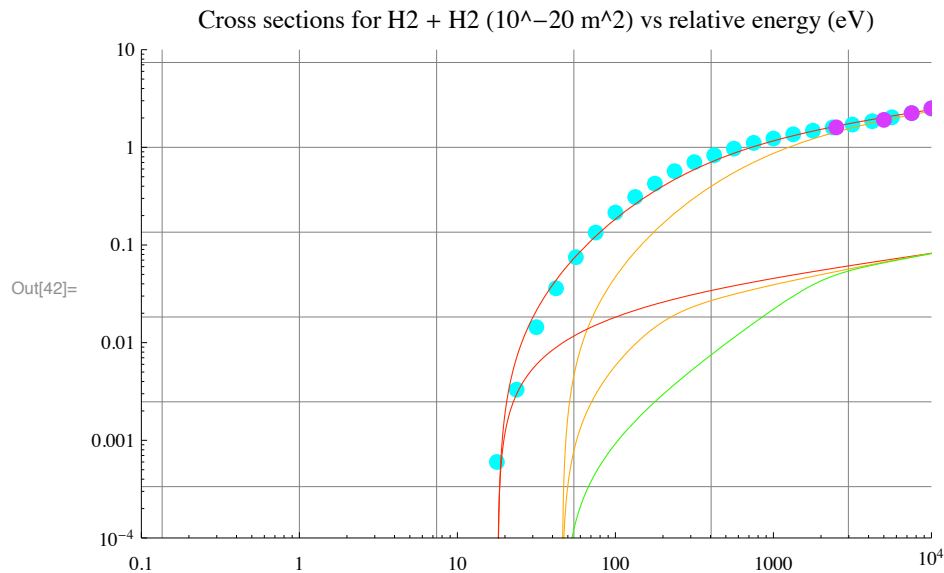
Energy (keV)	QD (H2) x10 ⁻¹⁶ cm ²	QD (H2+)	QD (H3+)	QHH	QH
2.5	1.60	8.04	2.96	0.0001	0.0001
5	1.91	8.37	3.47	1.24	2.68
7.5	2.24	8.68	4.13	1.34	2.94
10	2.51	8.16	4.72	1.37	3.11
15	2.68	7.93	5.30	1.30	2.94
20	3.07	7.93	6.02	1.44	3.33
30	3.47	8.69	7.22	1.44	3.47
40	3.57	7.58	7.58	1.27	3.22
50	3.50	6.74	7.16	1.06	2.85
60	3.42	5.93	7.00	0.79	2.15
70	3.31	5.18	6.51	0.76	2.18
80	3.14	4.56	6.30	0.84	2.17
90	3.06	4.13	5.85	0.66	1.72
100	2.98	3.75	5.52	0.73	1.68

```
In[39]:= h2h2Williams=Drop[Import["Williams&Gilbody84JPB.txt","Table"],2]; (*10^-20 m^2*)
```

```
In[40]:= williamsh2h2DissocData = Table[{{[j, 1]} * 1000, {[j, 2]}}, {j, Length[%]}];
```

```
In[41]:= williamsh2h2DissocDataPlot =ListLogLogPlot[williamsh2h2DissocData, PlotStyle->plotColorsPoin
PlotRange->{{0.1,10000},{.0001,10}}];
```

```
In[42]:= Show[h2h2DissocDataPlot, h2h2DissocFitPlot, h2h2pCTFitPlot, williamsh2h2DissocDataPlot,
ImageSize->400, PlotLabel-> "Cross sections for H2 + H2 (10^-20 m^2) vs relative energy (eV)
GridLines->Automatic]
```



■ H2 + H2 -> Ionization

Electron production from J. Phys. Chem. Ref. Data (1990)

```
In[43]:= h2h2IonizData=Table[{h2h2Data[[j,1]],h2h2Data[[j,10]]},{j,Length[h2h2Data]}];
```

```
In[44]:= h2h2IonizDataPlot =ListLogLogPlot[h2h2IonizData, PlotStyle->plotColorsPoints[[1]],
PlotRange->{{0.1,10000},{.0001,1}}];
```

Now consider various fits to the points from 1990 and from high energy experiments. We first fit the 1990 listing.

```
In[45]:= qMie[wM_] = UnitStep[wM - 35] * 1.5 * 10^-21 / (1 + (100 / (wM - 35))^2.) * (1 + (wM / 250))^0.5;
```

```
In[46]:= h2h2IonizFitPlot=LogLogPlot[10^20*qMie[wM], {wM, 0.1, 10000},
  PlotStyle->plotColorsLines[[1]], PlotRange->{{0.1, 10000}, {.0001, Automatic}}];
```

H2+ production from J. Phys. Chem. Ref. Data (1990)

```
In[47]:= h2h2h2pData=Table[{h2h2Data[[j, 1]], h2h2Data[[j, 3]]}, {j, Length[h2h2Data]}];
```

```
In[48]:= % // TableForm
```

Out[48]//TableForm=

0.1	$1. \times 10^{-9}$
0.1334	$1. \times 10^{-9}$
0.1778	$1. \times 10^{-9}$
0.237	$1. \times 10^{-9}$
0.316	$1. \times 10^{-9}$
0.422	$1. \times 10^{-9}$
0.562	$1. \times 10^{-9}$
0.75	$1. \times 10^{-9}$
1	$1. \times 10^{-9}$
1.334	$1. \times 10^{-9}$
1.778	$1. \times 10^{-9}$
2.371	$1. \times 10^{-9}$
3.162	$1. \times 10^{-9}$
4.217	$1. \times 10^{-9}$
5.623	$1. \times 10^{-9}$
7.5	$1. \times 10^{-9}$
10	$1. \times 10^{-9}$
13.34	$1. \times 10^{-9}$
17.78	0
23.7	0
31.6	0
42.1	0.0009
56.2	0.0065
75	0.0255
100	0.0515
133.4	0.082
177.8	0.113
237	0.143
316	0.175
422	0.21
562	0.247
750	0.284
1000	0.323
1334	0.363
1778	0.405
2371	0.445
3162	0.487
4217	0.533
5623	0.59
7499	0.665
10 000	0.77

```
In[49]:= h2h2h2pDataPlot =ListLogLogPlot[h2h2h2pData, PlotStyle->plotColorsPoints[[4]],
      PlotRange->{{0.1,10000},{.0001,1}}];
```

Now consider various fits to the points from 1990 and from high energy experiments. We first fit the 1990 listing.

```
In[50]:= qMi2[wM_] = UnitStep[wM - 35] * 1.5 * 10^-21 / (1 + (100 / (wM - 35))^2.) * (1 + (wM / 250))^0.5;
```

```
In[51]:= h2h2h2pFitPlot=LogLogPlot[10^20*qMi2[wM], {wM,0.1,10000},
      PlotStyle->plotColorsLines[[4]], PlotRange->{{0.1,10000},{.0001,Automatic}}];
```

H+ production from J. Phys. Chem. Ref. Data (1990)

```
In[52]:= h2h2hpData=Table[{h2h2Data[[j,1]],h2h2Data[[j,8]]},{j,Length[h2h2Data]}];
```

```
In[53]:= % // TableForm
```

```
Out[53]/TableForm=
```

0.1	$1. \times 10^{-9}$
0.1334	$1. \times 10^{-9}$
0.1778	$1. \times 10^{-9}$
0.237	$1. \times 10^{-9}$
0.316	$1. \times 10^{-9}$
0.422	$1. \times 10^{-9}$
0.562	$1. \times 10^{-9}$
0.75	$1. \times 10^{-9}$
1	$1. \times 10^{-9}$
1.334	$1. \times 10^{-9}$
1.778	$1. \times 10^{-9}$
2.371	$1. \times 10^{-9}$
3.162	$1. \times 10^{-9}$
4.217	$1. \times 10^{-9}$
5.623	$1. \times 10^{-9}$
7.5	$1. \times 10^{-9}$
10	$1. \times 10^{-9}$
13.34	$1. \times 10^{-9}$
17.78	0
23.7	0
31.6	0
42.1	0
56.2	0
75	0
100	0
133.4	0
177.8	0.00075
237	0.0013
316	0.0021
422	0.0034
562	0.0055
750	0.009
1000	0.0153
1334	0.0243
1778	0.0385
2371	0.06
3162	0.091
4217	0.135
5623	0.193
7499	0.268
10 000	0.37

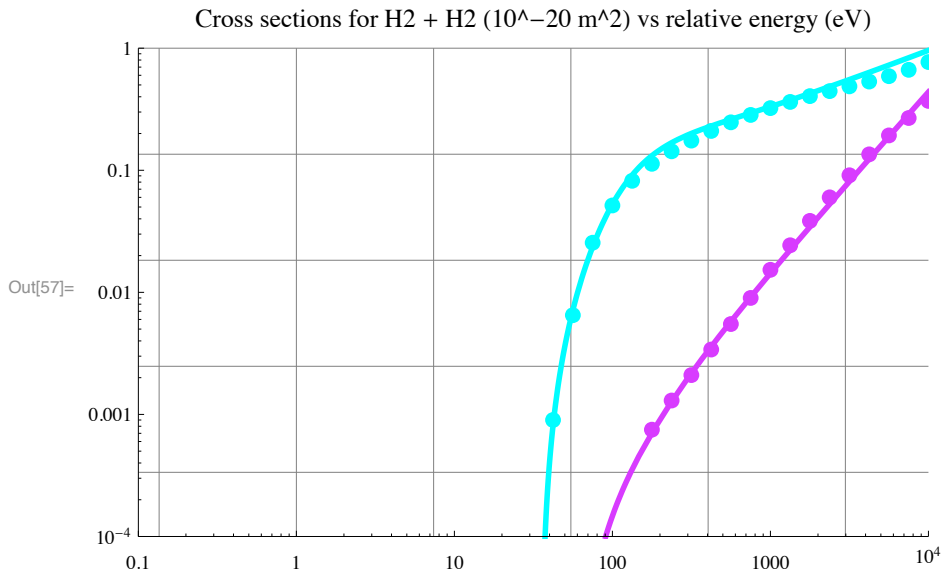
```
In[54]:= h2h2hpDataPlot =ListLogLogPlot[h2h2hpData, PlotStyle->plotColorsPoints[[6]],
PlotRange->{{0.1,10000},{.0001,1}}];
```

Now consider various fits to the points from 1990 and from high energy experiments. We first fit the 1990 listing.

```
In[55]:= qMil[wM_] = UnitStep[wM - 60] * 7. * 10^-27 * (wM - 60)^1.45;
```

```
In[56]:= h2h2hpFitPlot=LogLogPlot[10^20*qMil[wM], {wM,0.1,10000},
PlotStyle->plotColorsLines[[6]], PlotRange->{{0.1,10000},{.0001,Automatic}}];
```

```
In[57]:= Show[(*h2h2IonizDataPlot, h2h2IonizFitPlot,*)h2h2h2pDataPlot, h2h2h2pFitPlot, h2h2hpDataPlo
ImageSize->400, PlotLabel-> "Cross sections for H2 + H2 (10^-20 m^2) vs relative energy (eV)
GridLines->Automatic]
```



■ Ion pair formation H2 + H2 -> H- + ? (H+ + H2)?

S. Hayakawa, M. Kogo, A. Matsumoto, and T. Sugiura, In. J. Mass Spectrom. and Ion Processes 84, 113 (1988).

```
In[58]:= Import["hayakawa88fig4.dat", "CSV"] // TableForm
```

Out[58]/TableForm=

3.97334E+02	2.22844E-24
5.94162E+02	5.66643E-24
1.00900E+03	1.14496E-23
2.00041E+03	1.79869E-23
3.04193E+03	3.55438E-23
5.05080E+03	1.22899E-22

Hayakawa	Int. J. Mass Spect.&Ion Proc 84	113 (1988)
----------	---------------------------------	------------

```
In[59]:= Drop[Import["hayakawa88fig4.dat", "Table"], -1];
```

```
In[60]:= hayakawaPlot = ListLogLogPlot[%, PlotRange -> {{100, 10 000}, {10^-24, 2. * 10^-22}}];
```

```
In[61]:= qM1N[enLab_] =
```

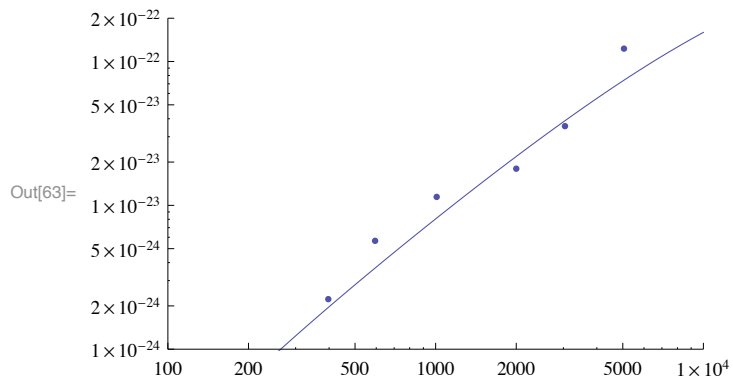
$$9. \cdot 10^{-24} \cdot ((\text{enLab} - 30) / 1000)^{1.5} / (1 + \text{enLab} / 30000)^2 \cdot \text{UnitStep}[\text{enLab} - 30]$$

Out[61]=

$$\frac{2.84605 \times 10^{-28} (-30 + \text{enLab})^{1.5} \text{UnitStep}[-30 + \text{enLab}]}{\left(1 + \frac{\text{enLab}}{30000}\right)^2}$$

```
In[62]:= plotqM1N = LogLogPlot[%, {enLab, 100, 10 000}];
```

```
In[63]:= Show[hayakawaPlot, plotqM1N]
```



Hayakawa et al claim from their magnetic and energy analysis that the H_- and H_+ had half the energy of the incident H_2 . They obtain absolute cross sections with a factor of 2 uncertainty. Their experiment would miss any large angle scattering.

```
In[64]:= Quit[]
```


Electron yields for ions of H2

Here we want to obtain analytic approximations to the experimental electron yields per particle for H⁺, H₂⁺, H₃⁺, and H atoms incident on metals such as Cu and Au. These data files were assembled from 1992 to 2001 and the date of this file is 2001. See Correspondence/??91-??92/SECONDARY.DOC for old notes.

Setup notebook environment

```
In[1]:= a = 1;
```

```
In[2]:= ClearAll["Global`*"];
```

```
In[3]:= Remove["Global`*"];
```

```
In[4]:= startclock = SessionTime[];
```

```
In[5]:= Off[General::spell];
```

```
In[6]:= Off[General::spell1];
```

```
In[7]:= now := StringForm["`~/`~/`~ `~:~:~`", Date][[2]],
      Date][[3]], Date][[1]], Date][[4]], Date][[5]], Date][[6]]]
```

```
In[8]:= plotColorsLines = {
  (*1*) {Red, Thickness[0.007], Dashing[{}]},
  (*2*) {Hue[0.1], (*Orange,*)Thickness[0.007], Dashing[{}]},
  (*3*) {Green, Thickness[0.007], Dashing[{}]},
  (*4*) {Cyan, Thickness[0.007], Dashing[{}]},
  (*5*) {Blue, Thickness[0.007], Dashing[{}]},
  (*6*) {Magenta, Thickness[0.007], Dashing[{}]},
  (*7*) {Yellow, Thickness[0.007], Dashing[{}]},
  (*8*) {Pink, Thickness[0.007], Dashing[{}]},
  (*9*) {Black, Thickness[0.004], Dashing[{}]},
  (*10-dash*) {Red, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*11-dash*) {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*12-dash*) {Green, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*13-dash*) {Cyan, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*14-dash*) {Blue, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*15-dash*) {Purple, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*16-dash*) {Yellow, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*17-dash*) {Pink, Thickness[0.007], Dashing[{0.02, 0.02}]},
  (*18-dash*) {Black, Thickness[0.007], Dashing[{0.02, 0.02]}}
};
```

```
In[9]:= plotColorsPoints = {
  (*1*) {Red, PointSize[0.02]},
  (*2*) {Hue[0.1], PointSize[0.02]},
  (*3*) {Green, PointSize[0.02]},
  (*4*) {Cyan, PointSize[0.02]},
  (*5*) {Blue, PointSize[0.02]},
  (*6*) {Magenta, PointSize[0.02]},
  (*7*) {Yellow, PointSize[0.02]},
  (*8*) {Pink, PointSize[0.02]},
  (*9*) {Black, PointSize[0.02]},
  (*10*) {Red, PointSize[0.014]},
  (*11*) {Hue[0.1], PointSize[0.014]},
  (*12*) {Green, PointSize[0.014]},
  (*13*) {Cyan, PointSize[0.014]},
  (*14*) {Blue, PointSize[0.014]},
  (*15*) {Purple, PointSize[0.014]},
  (*16*) {Yellow, PointSize[0.014]},
  (*17*) {Pink, PointSize[0.014]},
  (*18*) {Black, PointSize[0.014]}
};
```

Shape gives surface, color gives ion

```
In[10]:= SetDirectory["c:\users\avp\documents\mathbook\hydrogen\surfaceeffects\gammaions\"]
```

```
Out[10]= c:\users\avp\documents\mathbook\hydrogen\surfaceeffects\gammaions
```

From Vol. 3, p. 12 for H+ and H2+ on Mo

```
In[11]:= Import["ORNL6088v3pc12.txt", "CSV"] // TableForm
```

```
Out[11]/TableForm=
```

3.0E-02	1E-9	3.3E-02	2.9E-01	1E-9
5.0E-02	6.3E-02	3.4E-02	2.8E-01	4.0E-02
7.0E-02	7.2E-02	3.5E-02	2.7E-01	4.2E-02
1.0E-01	8.3E-02	3.8E-02	2.6E-01	4.3E-02
2.0E-01	1.1E-01	5.2E-02	2.5E-01	5.4E-02
4.0E-01	1.6E-01	9.8E-02	2.5E-01	8.0E-02
7.0E-01	2.1E-01	1.7E-01	2.6E-01	1.3E-01
1.0E+00	2.5E-01	2.4E-01	2.8E-01	1.8E-01
2.0E+00	3.9E-01	4.5E-01	4.0E-01	3.3E-01
4.0E+00	6.2E-01	7.6E-01	6.0E-01	5.7E-01
7.0E+00	8.4E-01	1.05E00	8.5E-01	8.7E-01
1.0E+01	9.8E-01	1.25E00	1.0E00	1.1E00
2.0E+01	1.2E+00	1.7E00	1.5E00	1.7E00
4.0E+01	1.4E+00	2.4E00	2.1E00	2.2E00
7.0E+01	1.5E00	3.0E00	1E-9	1E-9
1.0E+02	1.5E00	3.0E00	1E-9	1E-9
1.2E+02	1.4E00	2.8E00	1E-9	1E-9

keV H+ H2+ He+ O+

ORNL Report 6088 Vol 3 P12 (1985)

Secondary electron coefficient (electron/ion)

```
In[12]:= Drop[Import["ORNL6088v3pc12.txt", "Table"], -3];
```

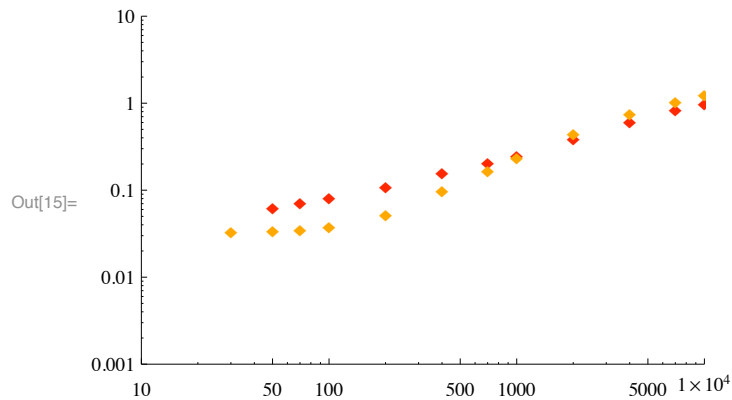
For H+ on Mo

```
In[13]:= hplusTable = Table[{{%[[j, 1]] * 1000, %[j, 2]}}, {j, Length[%]}];
```

For H2+ on Mo

```
In[14]:= h2plusTable = Table[{{%[[j, 1]] * 1000, %[j, 3]}}, {j, Length[%]}];
```

```
In[15]:= ornl6088Plot = ListLogLogPlot[{hplusTable, h2plusTable},
  PlotRange -> {{10, 10^4}, {0.001, 10}}, PlotStyle -> plotColorsPoints, PlotMarkers -> {"♦"}]
```



```
In[16]:= SetDirectory["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\h2lowcurrent"]
```

```
Out[16]= c:\\users\\avp\\documents\\Mathbook\\hydrogen\\h2lowcurrent
```

```
In[17]:= now
```

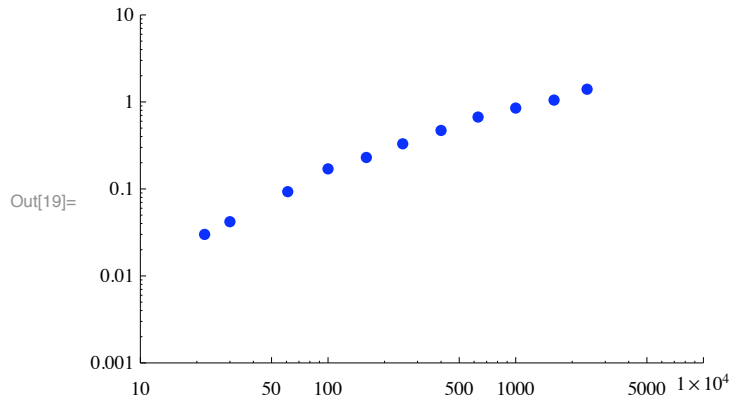
```
Out[17]:= 9/16/2011 22:42:18.112593`9.01055556845577
```

```
!! H2gamH0.dat
```

```
Mo, PlotMarkers -> {"◆"}, Cu - circle, Au - PlotMarkers->{"■"}
```

```
In[18]:= eYieldH0CuRay = Drop[Import["H2gamH0.dat", "Table"], 1];
```

```
In[19]:= eYieldH0CuRayPlot = ListLogLogPlot[eYieldH0CuRay,  
PlotRange -> {{10, 10000}, {0.001, 10}}, PlotStyle -> plotColorsPoints[[5]]]
```



```
In[20]:= Import["H2gamHp.dat", "CSV"] // TableForm
```

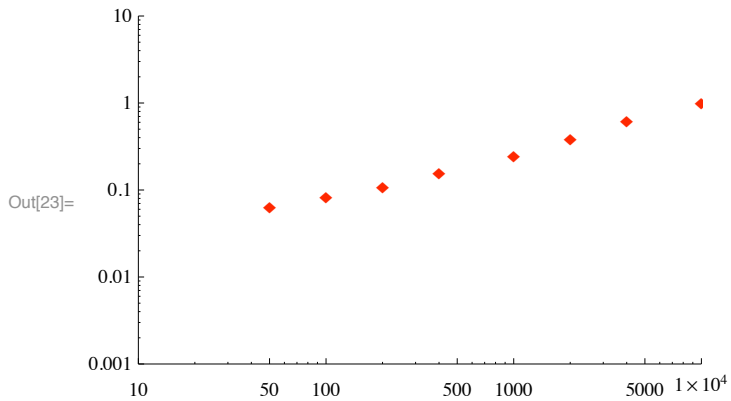
```
Out[20]//TableForm=
```

```
" gamma for H+ beams
  50      0.065 ORNL-5206 -Mo
  100     0.083
  200     0.11
  400     0.16
 1000     0.25
 2000     0.39
 4000     0.63
10000      1
 5500     0.7 Perdix et al      '69-Mo
10000     0.9
 1500     0.25 Ray and Barnett   '71
 5000     0.6
10000     1.2
  40      0.054 Mahadavan et al   '65
  200     0.13
 1600     0.33
  100     0.02 Winter - Au
  150     0.021
  500     0.06
  800     0.07
 1000     0.14
 2000     0.33
 3000     0.55
 4000     0.7
 6000      1
 8000     1.1
  17      0.0052 Ray              Barnett      Van Zyl
  25      0.02
  40      0.04 - Cu with H2
  65      0.077
 100      0.125
 160      0.2
 250      0.29
 400      0.4
 630      0.5
 1000     0.75
 1700     1.05
```

```
In[21]:= Take[Import["H2gamHp.dat", "Table"], {2, 9}];
```

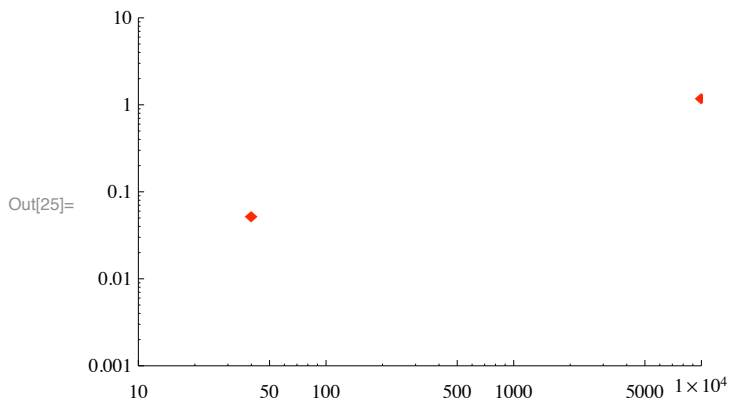
```
In[22]:= eYieldHpMoORNL =
  Table[#[[j, 1]], #[[j, 2]], {j, 8}] &[Take[Import["H2gamHp.dat", "Table"], {2, 9}]];
```

```
In[23]:= eYieldHpMoORNLPLOT =
ListLogLogPlot[eYieldHpMoORNLPLOT, PlotRange -> {{10, 10 000}, {0.001, 10}},
PlotStyle -> plotColorsPoints, PlotMarkers -> {"♦"}]
```



```
In[24]:= eYieldHpMoPerdix = Table[Take[Drop[Import["H2gamHp.dat", "Table"], 5][[j]], 2], {j, 9, 10}];
```

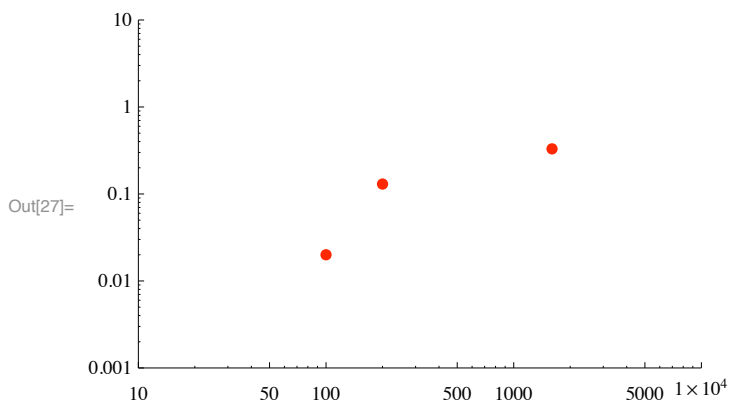
```
In[25]:= eYieldHpMoPerdixPlot =
ListLogLogPlot[eYieldHpMoPerdix, PlotRange -> {{10, 10 000}, {0.001, 10}},
PlotStyle -> plotColorsPoints, PlotMarkers -> {"♦"}]
```



```
In[26]:= eYieldHpCuRay71 = Table[Take[Drop[Import["H2gamHp.dat", "Table"], 5][[j]], 2], {j, 11, 13}];
```

```
Out[26]= {{200, 0.13}, {1600, 0.33}, {100, 0.02}}
```

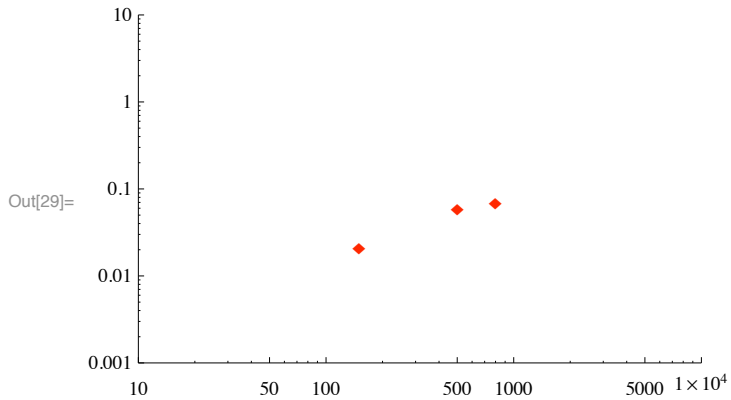
```
In[27]:= eYieldHpCuRay71Plot = ListLogLogPlot[eYieldHpCuRay71,
PlotRange -> {{10, 10 000}, {0.001, 10}}, PlotStyle -> plotColorsPoints]
```



```
In[28]:= eYieldHpMoMahadevan =
  Table[Take[Drop[Import["H2gamHp.dat", "Table"], 5][[j]], 2], {j, 14, 16}]
```

```
Out[28]:= {{150, 0.021}, {500, 0.06}, {800, 0.07}}
```

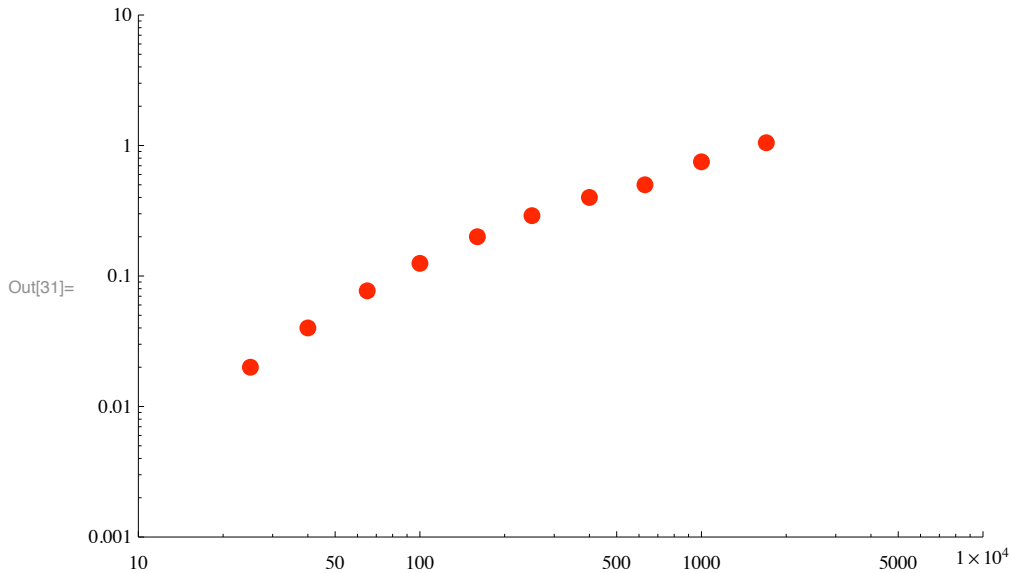
```
In[29]:= eYieldHpMoMahadevanPlot =
  ListLogLogPlot[eYieldHpMoMahadevan, PlotRange -> {{10, 10000}, {0.001, 10}},
  PlotStyle -> plotColorsPoints, PlotMarkers -> {"♦"}]
```



- From Ray et al (1979) for H+ on gas covered Cu of unknown cleanliness.

```
In[30]:= eYieldHpCuRay79 = Table[Take[Drop[Import["H2gamHp.dat", "Table"], 5][[j]], 2], {j, 24, 33}];
```

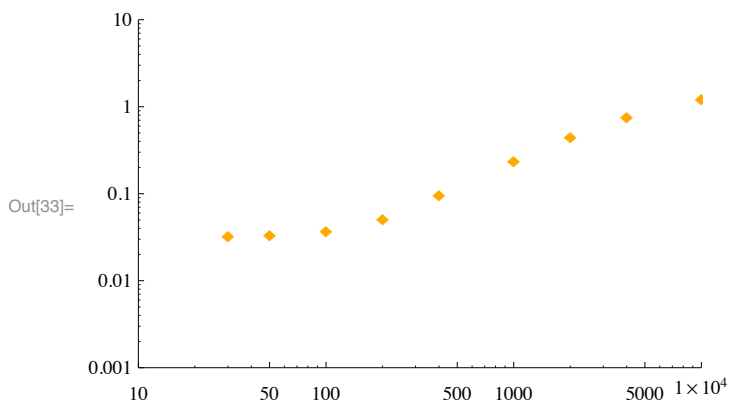
```
In[31]:= eYieldHpCuRay79Plot = ListLogLogPlot[eYieldHpCuRay79,
  PlotRange -> {{10, 10 000}, {0.001, 10}}, PlotStyle -> plotColorsPoints, ImageSize -> 432]
```



There have been proposals that the hydrogen atoms act independently when they strike the surface. This would mean that for a molecular ion H_m^+ there will be m atoms each with an energy of $1/m$ of the molecule. In order to convert the observed yields into yields for the atomic ion we would multiply the yields by m and divide the ion energies by m . If the yield is a linear function of energy, the function should be unchanged by this transformation. We do not make this scaling.

```
In[32]:= eYieldH2pMoORNL =
  Table[{1 / m, m} * Take[Drop[Import["H2gamH2p.dat", "Table"], 5][[j]], 2], {j, 1, 9}] /. m -> 1;
```

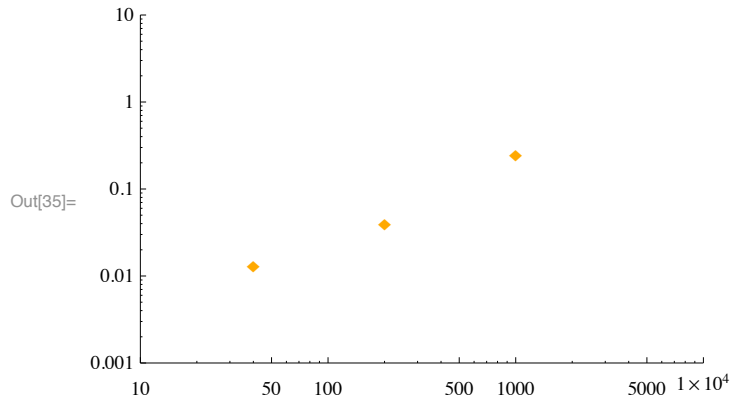
```
In[33]:= eYieldH2pMoORNLPLOT =
  ListLogLogPlot[eYieldH2pMoORNL, PlotRange -> {{10, 10 000}, {0.001, 10}},
  PlotStyle -> plotColorsPoints[[2]], PlotMarkers -> {"♦"}]
```



```
In[34]:= eYieldH2pMoMahadevan = Table[
  {1 / m, m} * Take[Drop[Import["H2gamH2p.dat", "Table"], 5][[j]], 2], {j, 10, 12}] /. m -> 1;
```

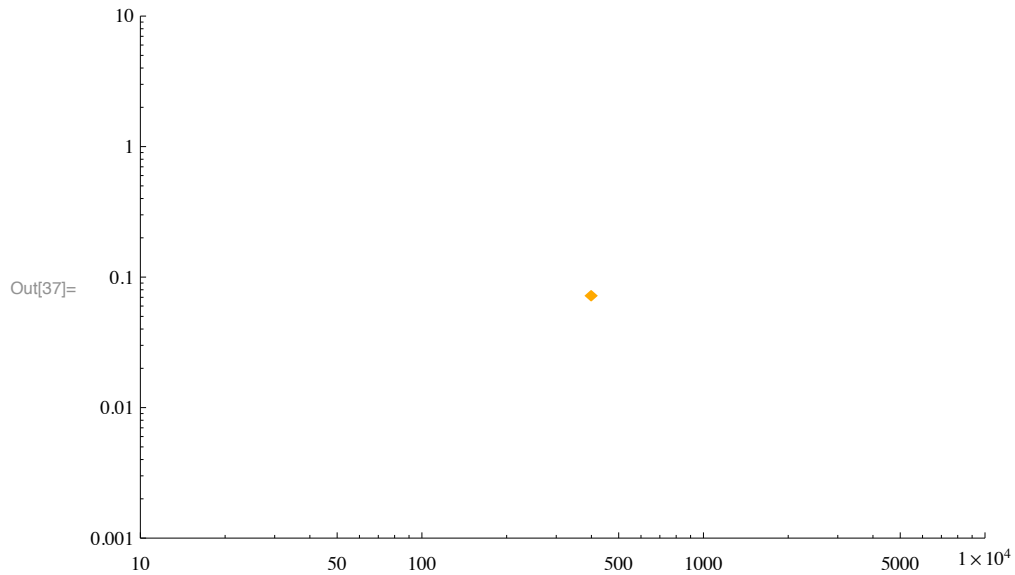


```
In[35]:= eYieldH2pMoMahadevanPlot = ListLogLogPlot[%, PlotRange -> {{10, 10 000}, {0.001, 10}},
  PlotStyle -> plotColorsPoints[[2]], PlotMarkers -> {"♦"}]
```



```
In[36]:= eYieldH2pMoVance =
  Table[{1 / m, 1 / m} * Take[Drop[Import["H2gamH2p.dat", "Table"], 5][[j]], 2], {j, 13, 13}] /.
  m -> 1;
```

```
In[37]:= eYieldH2pMoVancePlot = ListLogLogPlot[%, PlotRange -> {{10, 10 000}, {0.001, 10}},
  PlotStyle -> plotColorsPoints[[2]], ImageSize -> 432, PlotMarkers -> {"♦"}]
```



From ORNL

```
In[38]:= Import["H2gamH2p.dat", "CSV"] // TableForm
```

```
Out[38]//TableForm=
```

```
%Secondary emission coefficient for ion and
neutral atom beams from literature
  Energy      Gamma      Author
%      eV
"H2+
  30          0.033 ORNL-5206 -Mo
  50          0.034
  100         0.038
  200         0.052
  400         0.098
  1000        0.24
  2000        0.45
  4000        0.76
  10000       1.25
  40          0.013 Mahadavan et al      '65
  200         0.04
  1000        0.25
  400         0.073 Vance                '68
  100         0.012 Winter - Au
  200         0.015
  1000        0.07
  1600        0.12
  2000        0.22
  4000        0.8
  6000        1.2
  8000        1.5
  10000       1.7
```

```
In[39]:= SetDirectory[NotebookDirectory[]]
```

```
Out[39]= C:\Users\avp\Documents\Mathbook\HYDROGEN\SurfaceEffects\GammaIons
```

■ From Winter et al for Au

From Lakits, Aumayr, and Winter, Rev. Sci. Instr. 60, 3151 (1989). Their data are plotted against eV/amu as would be appropriate as proposed by the independent atom model. We have chosen to multiply by the amu to be consistent with our other data.

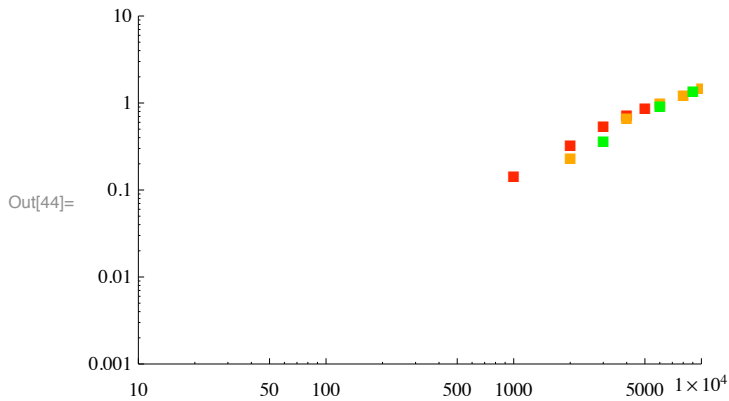
```
In[40]:= eYieldAuLakits = Import["Lakits&Winter89RSIfig5a.txt", "Table"];
```

```
In[41]:= eYieldHpAuLakits = Table[{{#[[j, 1]] * 1000 * 1, #[[j, 2]]}, {j, Length[#]}} &[eYieldAuLakits];
```

```
In[42]:= eYieldH2pAuLakits = Table[{{#[[j, 1]] * 1000 * 2, #[[j, 3]]}, {j, Length[#]}} &[eYieldAuLakits];
```

```
In[43]:= eYieldH3pAuLakits = Table[{{#[[j, 1]] * 1000 * 3, #[[j, 4]]}, {j, Length[#]}} &[eYieldAuLakits];
```

```
In[44]:= eYieldHpAuLakitsPlot =
  ListLogLogPlot[{eYieldHpAuLakits, eYieldH2pAuLakits, eYieldH3pAuLakits},
    PlotRange -> {{10, 10 000}, {0.001, 10}}, PlotStyle -> plotColorsPoints, PlotMarkers -> "■"]
```

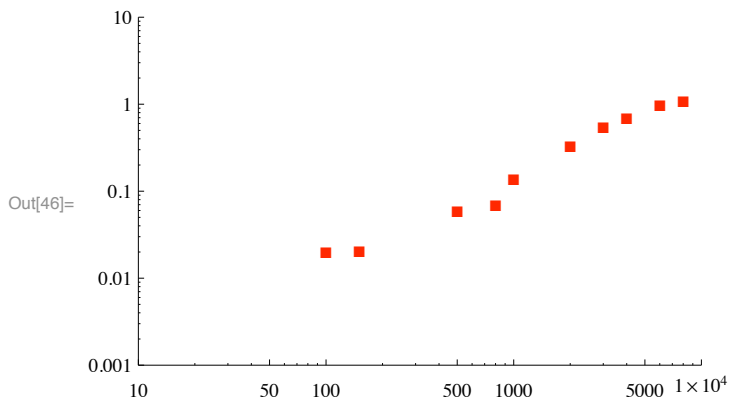


■ From Winter et al on Au of unknown cleanliness.

```
In[45]:= eYieldHpAuWinter = Table[Take[Drop[Import["H2gamHp.dat", "Table"], 5][[j]], 2], {j, 13, 22}]
```

```
Out[45]= {{100, 0.02}, {150, 0.021}, {500, 0.06}, {800, 0.07}, {1000, 0.14},
  {2000, 0.33}, {3000, 0.55}, {4000, 0.7}, {6000, 1}, {8000, 1.1}}
```

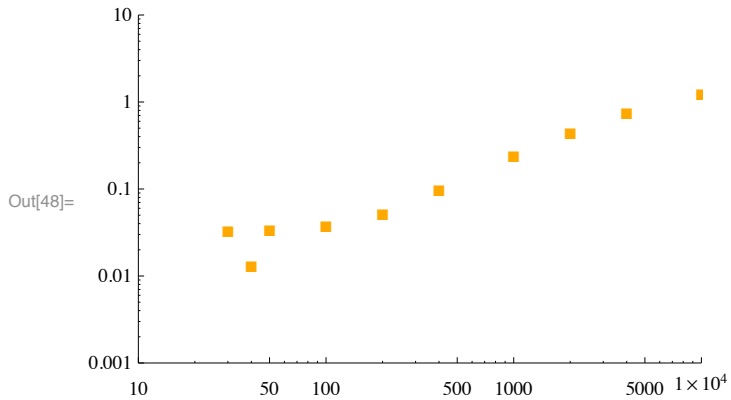
```
In[46]:= eYieldHpAuWinterPlot = ListLogLogPlot[%, PlotRange -> {{10, 10 000}, {0.001, 10}},
  PlotStyle -> plotColorsPoints[[1]], PlotMarkers -> "■"]
```



Here we have the option for Hm+ of scaling the energy by 1/m so as to plot the yield as if the H particles were acting independently and/or with equal yield for H and H+. For now we take m=1.

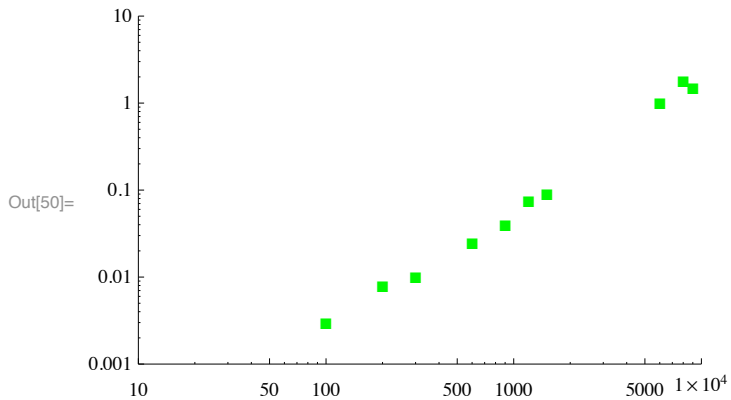
```
In[47]:= eYieldH2pAuWinter = Table[
  {1 / m, m} * Take[Drop[Import["H2gamH2p.dat", "Table"], 5][[j]], 2], {j, 1, 10}] /. m -> 1;
```

```
In[48]:= eYieldH2pAuWinterPlot = ListLogLogPlot[%, PlotRange -> {{10, 10 000}, {0.001, 10}},
  PlotStyle -> plotColorsPoints[[2]], PlotMarkers -> "■"]
```



```
In[49]:= eYieldH3pAuWinter = Table[
  {1 / m, m} * Take[Drop[Import["H2gamH3p.dat", "Table"], 5][[j]], 2], {j, 1, 10}] /. m -> 1.;
```

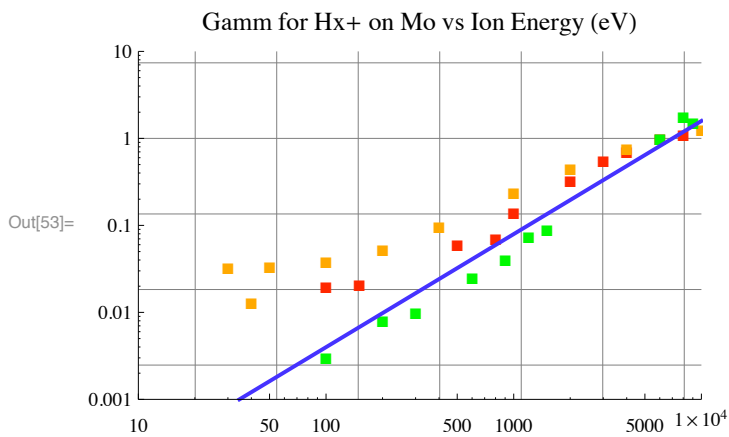
```
In[50]:= eYieldH3pAuWinterPlot =
  ListLogLogPlot[eYieldH3pAuWinter, PlotRange -> {{10, 10 000}, {0.001, 10}},
  PlotStyle -> plotColorsPoints[[3]], PlotMarkers -> {"■"}]
```



```
In[51]:= fitCleanAu = 1. * 10^-5 * eng^1.3;
```

```
In[52]:= fitCleanAuPlot = LogLogPlot[fitCleanAu, {eng, 1, 10 000},
  PlotRange -> {{10, 10 000}, {0.001, 10}}, PlotStyle -> {Hue[0.7], Thickness[0.007]}];
```

```
In[53]:= summaryAuPlot =
Show[eYieldHpAuWinterPlot, eYieldH2pAuWinterPlot, eYieldH3pAuWinterPlot, fitCleanAuPlot,
GridLines -> Automatic, PlotLabel -> "Gamm for Hx+ on Mo vs Ion Energy (eV)"]
```



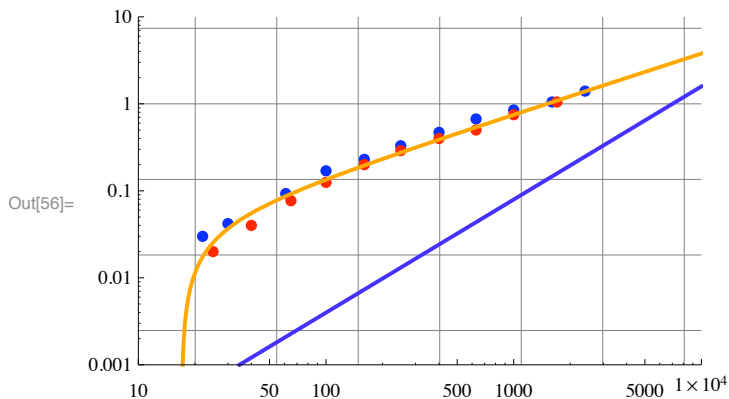
The previous plot shows that H⁺ and H₂⁺ data are consistent with a high γ at low energies, whereas the H₃⁺ data continues to drop at low energies.

■ Gas covered Cu

```
In[54]:= fitDirtyCu = 6. * 10^-3 * UnitStep[eng - 17] * eng^0.7 / (1 + 10. / (eng - 17)) + 1. * 10^-30;
```

```
In[55]:= fitDirtyCuPlot = LogLogPlot[fitDirtyCu, {eng, 1, 10 000},
PlotRange -> {{10, 10 000}, {0.001, 10}}, PlotStyle -> {Hue[0.1], Thickness[0.007]}];
```

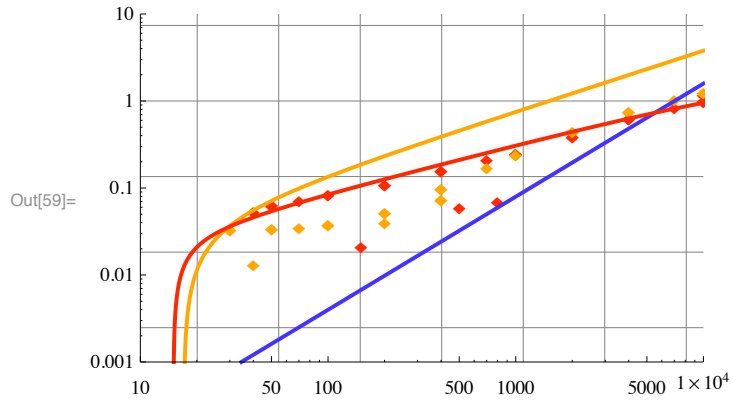
```
In[56]:= summaryCuPlot = Show[eYieldH0CuRayPlot, eYieldHpCuRay79Plot,
fitDirtyCuPlot, fitCleanAuPlot, GridLines -> Automatic]
```



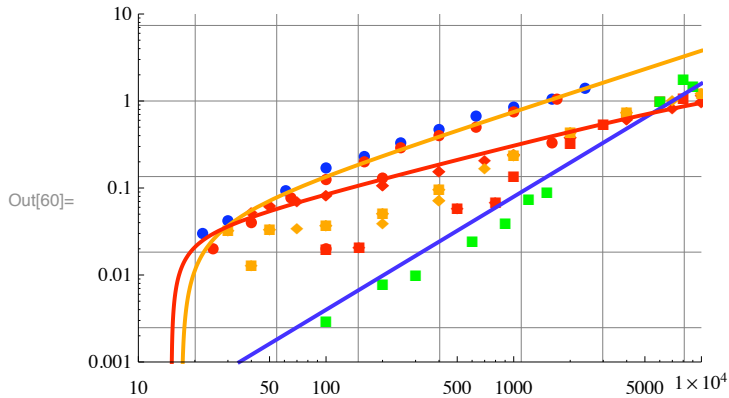
```
In[57]:= fitMo = 7. * 10^-3 * UnitStep[eng - 15] * eng^0.55 / (1 + 5. / (eng - 15))^0.8 / (1 + (eng / 60 000));
```

```
In[58]:= fitMoPlot = LogLogPlot[fitMo, {eng, 1, 10 000},
PlotRange -> {{10, 10 000}, {0.001, 10}}, PlotStyle -> plotColorsLines[[1]]];
```

```
In[59]:= summaryMoPlot = Show[ eYieldHpMoORNLPLOT , eYieldHpMoPerdixPlot , eYieldHpMoMahadevanPlot ,
    eYieldH2pMoORNLPLOT , eYieldH2pMoMahadevanPlot , eYieldH2pMoVancePlot ,
    orn16088Plot , fitDirtyCuPlot , fitCleanAuPlot , fitMoPlot , GridLines -> Automatic]
```



```
In[60]:= summaryPlot = Show[ eYieldHOCuRayPlot, eYieldHpMoORNLPLOT, eYieldHpMoPerdixPlot,
    eYieldHpCuRay71Plot, eYieldHpCuRay79Plot, eYieldHpMoMahadevanPlot,
    eYieldHpAuWinterPlot, eYieldH2pMoORNLPLOT, ornl6088Plot, eYieldH2pMoMahadevanPlot,
    eYieldH2pMoVancePlot, eYieldH2pAuWinterPlot, eYieldH3pAuWinterPlot,
    fitDirtyCuPlot, fitCleanAuPlot, fitMoPlot, GridLines -> Automatic]
```



blue - Mo; orange - gas covered Cu;

Mo, PlotMarkers \rightarrow {"◆"}, Cu - circle, Au - PlotMarkers \rightarrow {"■"}

■ Drift tube measurements of γ ion for hydrogen

```
In[61]:= SetDirectory [NotebookDirectory []]
```

```
Out[61]:= C:\Users\avp\Documents\Mathbook\HYDROGEN\SurfaceEffects\GammaIons
```

The latest measurements I have found are those of Yoshida et al, J. Phys. B 28, 2478 (1995) who repeat some of the measurements of Shimozuma et al, J. Phys. B 10, 1671 (1977).

The following are visual average of badly scatered data for Au

```
In[62]:= Import ["shimozuma77fig6a.dat", "Table"];
```

```
In[63]:= shimozumaAuGammaIon = Table[{{%[[j, 1]], %[[j, 2]]}, {j, Length[%]}}];
```

```
In[64]:= Import ["shimozuma77fig6b.dat", "Table"];
```

```
In[65]:= shimozumaAuGammaTotal = Table[{{%[[j, 1]], %[[j, 2]]}, {j, Length[%]}}];
```

From D. J. Rose, Proc. 3rd Int. Conf. Ionization Phenomena Gases, Venice 1957, p. 28 for Mo

```
In[66]:= Import ["rose57icpig3.dat", "Table"];
```

```
In[67]:= roseMoGammaTotal = Table[{{%[[j, 1]] / 0.356, %[[j, 2]]}, {j, Length[%]}}];
```

```
In[68]:= gammaMoTotal = ListLogLogPlot[{roseMoGammaTotal},
    PlotStyle  $\rightarrow$  plotColorsPoints[[3]], PlotRange  $\rightarrow$  {{50, 2000}, {10^-4, 0.1}},
    PlotLabel  $\rightarrow$  "Hydrogen  $\gamma$ Total vs E/N (Td)", PlotMarkers  $\rightarrow$  {"◆"}];
```

From Tagashira and Lucas, Brit. J. Appl. Phys. 2, 867 (1969)

```
In[69]:= Import ["Tagashira&Lucas69BritJAPFig3b.dat", "Table"];
```

```

In[70]:= tagashiraAlTotal = Table[{#[[j, 1]] / 0.356, #[[j, 2]]}, {j, Length[%]}];
In[71]:= Import["Tagashira&Lucas69BritJAPFig3c.dat", "Table"];
In[72]:= tagashiraAlIon = Table[{#[[j, 1]] / 0.356, #[[j, 2]]}, {j, Length[%]}];
In[73]:= gammaAlIon = ListLogLogPlot[{tagashiraAlIon(*,tagashiraAlTotal*)},
  PlotStyle -> plotColorsPoints[{{2, 4}}], PlotRange -> {{50, 2000}, {10^-4, 0.1}},
  PlotLabel -> "Hydrogen  $\gamma$ Ion vs E/N (Td)", PlotMarkers -> {"▲"}];
In[74]:= gammaAlTotal = ListLogLogPlot[{tagashiraAlTotal},
  PlotStyle -> plotColorsPoints[{{2, 4}}], PlotRange -> {{50, 2000}, {10^-4, 0.1}},
  PlotLabel -> "Hydrogen  $\gamma$ Ion and  $\gamma$ Total vs E/N (Td)", PlotMarkers -> {"▲"}];

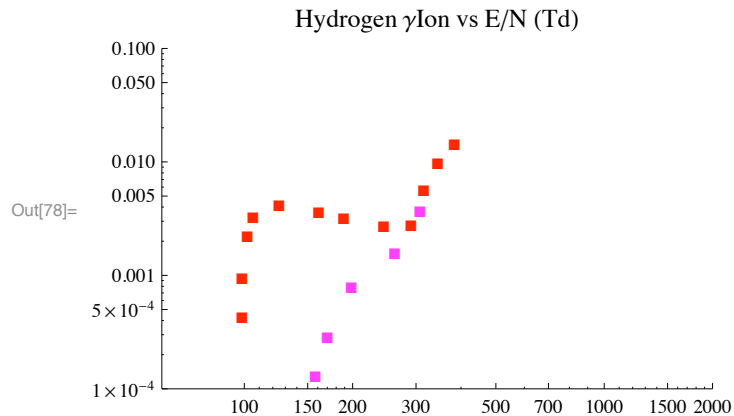
```

From Morgan and Williams, Proc. Phys. Soc. 85, 443 (1965) for Au electrodes

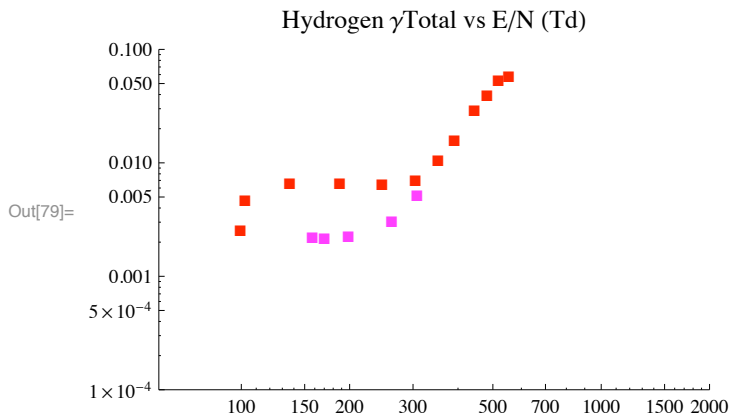
```

In[75]:= morganData = Import["Morgan&Williams65ProcPhysSocTable1.txt", "Table"];
In[76]:= morganAuGammaIon = Table[{#[[j, 1]] / 0.356, #[[j, 2]] * 10^-4}, {j, Length[#]}] &[morganData];
In[77]:= morganAuGammaTotal =
  Table[{#[[j, 1]] / 0.356, (#[[j, 2]] * 10^-4 + #[[j, 3]] * 10^-3)}, {j, Length[#]}] &[
    morganData];
In[78]:= gammaAuIon = ListLogLogPlot[{shimozumaAuGammaIon, morganAuGammaIon},
  PlotStyle -> plotColorsPoints[{{1, (*5,*6)}], PlotRange -> {{59, 2000}, {10^-4, 0.1}},
  PlotLabel -> "Hydrogen  $\gamma$ Ion vs E/N (Td)", PlotMarkers -> {"■"}]

```




```
In[79]:= gammaAuTotal = ListLogLogPlot[{shimozumaAuGammaTotal, morganAuGammaTotal},
  PlotStyle → plotColorsPoints[{{1, (*5,*6)}}], PlotRange → {{59, 2000}, {10^-4, 0.1}},
  PlotLabel → "Hydrogen  $\gamma$ Total vs E/N (Td)", PlotMarkers → {"■"}]
```

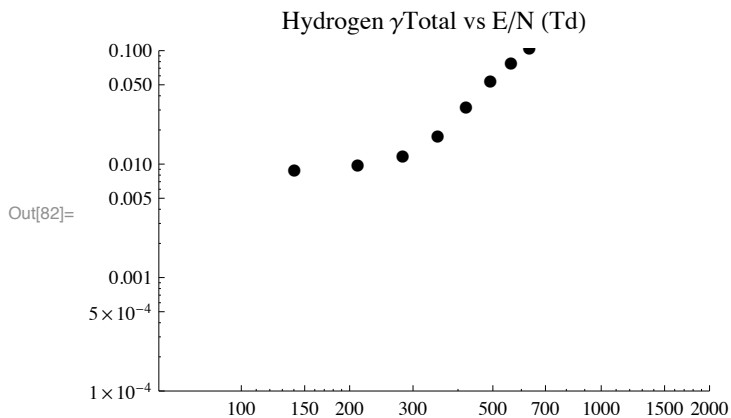


From Folkhard and Haydon, Australian J. Phys. 24, 527 (1970) for Cu electrodes

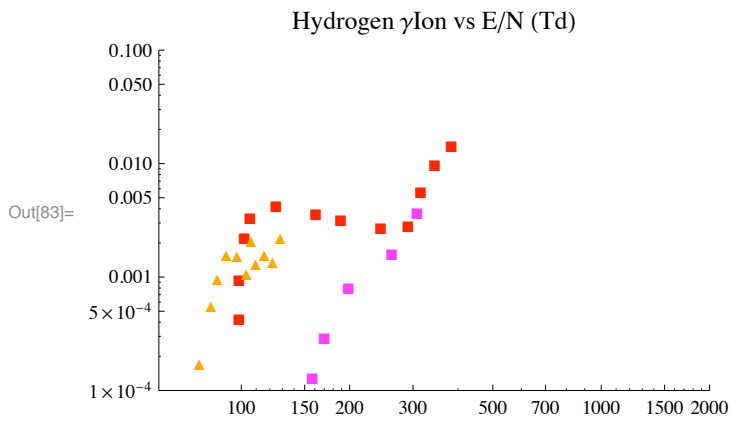
```
In[80]:= folkhardData = Import["Folkhard&Haydon71AustJPhys.txt", "Table"];
```

```
In[81]:= folkhardCuGammaTotal =
  Table[{{#[[j, 1]] / 0.356, #[[j, 3]]}, {j, Length[#] - 2}} &[folkhardData];
```

```
In[82]:= gammaCuTotal = ListLogLogPlot[folkhardCuGammaTotal,
  PlotStyle → plotColorsPoints[[9]], PlotRange → {{59, 2000}, {10^-4, 0.1}},
  PlotLabel → "Hydrogen  $\gamma$ Total vs E/N (Td)", PlotMarkers → {"●"}]
```

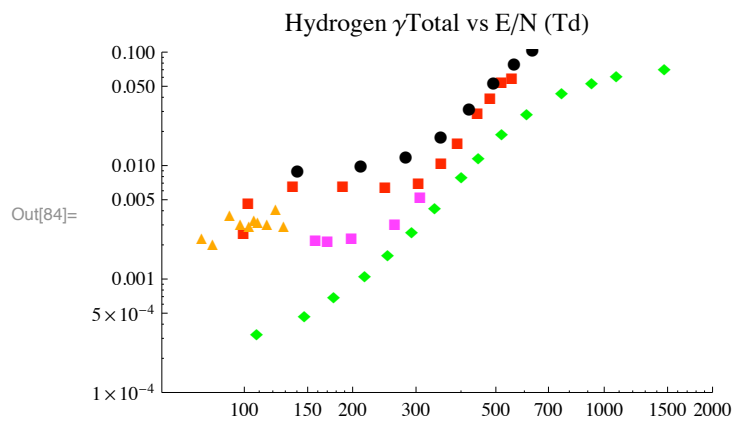


```
In[83]:= gammaIon = Show[gammaAuIon, gammaAlIon]
```



Mo, PlotMarkers \rightarrow {"◆"}; Au - PlotMarkers \rightarrow {"■"}; Al - PlotMarkers \rightarrow {"▲"}; Cu - PlotMarkers \rightarrow {"▼"}

```
In[84]:= gammaTotal = Show[gammaAuTotal, gammaMoTotal, gammaAlTotal, gammaCuTotal]
```



These swarm data show that yields for Mo and Au are drastically different at low E/N (~130 Td). The differences for swarm experiments are similar to the differences for Mo and Cu from beam experiments at 30 to 50 eV. Some swarm experiments show a sharp cutoff at low energies that may or may not be present with beams of H and H+.

Fletcher and Blevin, J. Phys. D 14, 27 (1981) find a large increase in $\gamma_{\text{lon}}/\gamma_{\text{Photon}}$ at 200-300 Td for stainless steel. This change occurs at the same E/N as the rise in this ratio found by Shimozuma et al, but is more drastic. It is also the E/N range (~ 300 Td) at which the kinetics model in Phelps (2009) shows a switch in cathode flux from H3+ at low E/N to H+ at higher E/N.

We should look for changes in ion flux properties at E/N ~ 100 Td, e.g., a switch from H5+ to H3+ with increasing E/N.

💡 Is there any theory for secondary electron production by H+ and H? Can theory explain the large values for H and H+ incident on Cu compared to Mo? INSPEC did not yield useful references.

The large γ_{lon} values found for Au and Cu surfaces at low E/N and the resultant low particle energies are presumably the result of collisions of H3+ with the cathode, i.e., our model yields low H+, fast H, and H2+ fractions at the low E/N. An Auger process involving H3+ and Cu or Au would be essentially independent of H3+ energy. Other possibilities are associative ionization or chemi-ionization process. However, the energetics look wrong and the literature does not consider such a process, e.g., the proton affinity of a Cu surface is not considered in H atom - Cu surface discussions and H- producton apparently is not observed. These considerations do not explain the apparent rapid drop in γ_{lon} near E/N = 100 Td, which may be an experimental artifact. From transient current waveforms in H2 at lower E/N, Morgan attributes the large γ_{Total} for Au at ~ 150 Td to photoelectrons and says γ_{lon} is small .

📄 Simko et al (1997) disagree with our conclusion that H3+ dominates the ion flux at the cathode at E/N < 300 Td and say the H+ flux is lager.

Using ion beams and an Au target, Winter et al did not see the high γ_{lon} with H3+ at 50 eV that he saw with H+ and H2+. Using swarm techniques and an Au target, Shimozuma et al saw high values at E/N = 150 Td, but Morgan and Williams did not.

We are left with considerable uncertainty regarding ion-induced electron emission by H3+ at E/N < 300 Td and energies below 500 eV. Fortunately, our model says that H3+ is only about 1/3 of the ion flux for the conditions of the Jelenkovic and Phelps cathode fall experiment.

In[85]:= Quit []

Reflection of fast H atoms at a surface

Beware: The later parts of this are old and may not have been reconstructed properly.

The problem is to formulate empirical expressions for the energy dependent boundary conditions for a multibeam model used to solve for the ion and atom energy distributions for low pressure discharges in H₂.

Setup notebook environment

```
In[1]:= a = 1;
```

```
In[2]:= ClearAll["Global`*"];
```

```
In[3]:= Remove["Global`*"];
```

```
In[4]:= startclock = SessionTime[];
```

```
In[5]:= Off[General::spell];
```

```
In[6]:= Off[General::spell1];
```

```
In[7]:= today = StringForm["~/~/~ :~:~", Date][[2]],  
Date][[3]], Date][[1]], Date][[4]], Date][[5]], Date][[6]]
```

```
Out[7]= 9/18/2011 19:58:6.5987788`8.572038543261836
```

```

In[8]:= SetDirectory [NotebookDirectory []]
Out[8]:= C:\Users\avp\Documents\Mathbook\HYDROGEN\SurfaceEffects\HAtomReflection

In[9]:= plotColorsLines = {
  (*1-red*) {Hue[0.0], Thickness[0.007], Dashing[{}]},
  (*2-orange*) {Hue[0.1], Thickness[0.007], Dashing[{}]},
  (*3-green*) {Hue[0.3], Thickness[0.007], Dashing[{}]},
  (*4-cyan*) {Hue[0.5], Thickness[0.007], Dashing[{}]},
  (*5-dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{}]},
  (*6-purple*) {Hue[0.8], Thickness[0.007], Dashing[{}]},
  (*7-black*) {Thickness[0.007], Dashing[{}]},
  (*8-dash red*) {Hue[0.0], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*9-dash orange*) {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*10-dash green*) {Hue[0.3], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*11-dash cyan*) {Hue[0.5], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*12-dash dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*13-dash purple*) {Hue[0.8], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*14-dash black*) {(*CMYKColor[0,0,0,1],*)Thickness[0.007], Dashing[{0.02, 0.02}]}];

In[10]:= plotColorsPoints = {
  (*1-red*) {Hue[0.0], PointSize[0.02]},
  (*2-orange*) {Hue[0.1], PointSize[0.02]},
  (*3-green*) {Hue[0.3], PointSize[0.02]},
  (*4-cyan*) {Hue[0.5], PointSize[0.02]},
  (*5-dk blue*) {Hue[0.7], PointSize[0.02]},
  (*6-purple*) {Hue[0.8], PointSize[0.02]},
  (*7-yellow*) {Hue[0.2], PointSize[0.02]},
  (*8-black*) {PointSize[0.02]}
};

```

Backscattered atom energy distribution.

We begin by fitting the TRIM calculations of Eckstein and Verbeek with an empirical formula and a number of trials. This formula is compared with the results published by several authors.

- Eckstein and Verbeek (1984) Fig 2.16 of FE for D+ → Ni. Empirically, we found that in order to give their FN values by integration over energy, these values must be increased by a factor of 40 equal to the number of channels (20) times an unaccounted for factor of 2. Again we assume that the reflection coefficients for D and H are the same.

```
In[11]:= eckstein30Data = Drop[Import["eckstein_verbeek84fig216_30ev.dat", "Table"], -1];
```

See tabulation below

```
In[12]:= eckstein30Data = Table[#{#[j, 1], #[j, 2] * 40}, {j, 19}] &[eckstein30Data];
```

```
In[13]:= eckstein30List = Transpose[eckstein30Data][[2]];

```

```
In[14]:= eckstein100Data = Drop[Import["eckstein_verbeek84fig216_100ev.dat", "Table"], -1];
```

```
In[15]:= eckstein100Data = Table[#{#[j, 1], #[j, 2] * 40}, {j, 19}];
```

```
In[16]:= eckstein100List = Transpose[eckstein100Data][[2]];

```

```
In[17]:= eckstein300Data = Drop[Import["eckstein_verbeek84fig216_300ev.dat", "Table"], -1];
```

```

In[18]:= eckstein300Data = Table[{{%[[j, 1]], %[[j, 2]] * 40}, {j, 19}}];
In[19]:= eckstein300List = Transpose[eckstein300Data][[2]];
In[20]:= eckstein1000Data = Drop[Import["eckstein_verbeek84fig216_1kev.dat", "Table"], -1];
In[21]:= eckstein1000Data = Table[{{%[[j, 1]], %[[j, 2]] * 40}, {j, 19}}];
In[22]:= eckstein1000List = Transpose[eckstein1000Data][[2]];
In[23]:= eckstein3000Data = Drop[Import["eckstein_verbeek84fig216_3kev.dat", "Table"], -1];
In[24]:= eckstein3000Data = Table[{{%[[j, 1]], %[[j, 2]] * 40}, {j, 19}}];
In[25]:= eckstein3000List = Transpose[eckstein3000Data][[2]];
In[26]:= eckstein10000Data = Drop[Import["eckstein_verbeek84fig216_10kev.dat", "Table"], -1];
In[27]:= eckstein10000Data = Table[{{%[[j, 1]], %[[j, 2]] * 40}, {j, 19}}];
In[28]:= eckstein10000List = Transpose[eckstein10000Data][[2]];
In[29]:= Length[%]
Out[29]= 19

In[30]:= eckstein84DataLogLogPlot = ListLogLogPlot[{eckstein30Data, eckstein100Data,
    eckstein300Data, eckstein1000Data, eckstein3000Data, eckstein10000Data},
    PlotStyle → plotColorsPoints, PlotRange → {{0.01, 1}, {0.01, 5}}];
In[31]:= eckstein84DataPlot = ListPlot[{eckstein30Data, eckstein100Data,
    eckstein300Data, eckstein1000Data, eckstein3000Data, eckstein10000Data},
    PlotStyle → plotColorsPoints, PlotRange → {{0, 1}, {0, 3}}];
In[32]:= eckstein84ExptData = Table[{Table[j * 0.05, {j, 20}][[j]], eckstein30List[[j]],
    eckstein100List[[j]], eckstein300List[[j]], eckstein1000List[[j]],
    eckstein3000List[[j]], eckstein10000List[[j]]}, {j, Length[eckstein30List]};
In[33]:= Export["Eckstein&Verbeek84.txt", eckstein84ExptData, "Table"]
Out[33]= Eckstein&Verbeek84.txt

```

```
In[34]:= TableForm[eckstein84ExptData, TableHeadings ->
  {None, {"rel en", "30 eV", "100 eV", "300 eV", "1000 eV", "3000 eV", "10000 eV"}}]
```

```
Out[34]/TableForm=
```

rel en	30 eV	100 eV	300 eV	1000 eV	3000 eV	10000 eV
0.05	0.0874252	0.11497	0.097006	0.0958084	0.0958084	0.101796
0.1	0.128144	0.186826	0.128144	0.190419	0.185629	0.162874
0.15	0.208383	0.222754	0.208383	0.221557	0.210778	0.162874
0.2	0.231138	0.245509	0.232335	0.245509	0.237126	0.176048
0.25	0.275449	0.262276	0.274252	0.271856	0.273054	0.16527
0.3	0.307784	0.308982	0.306587	0.308982	0.307784	0.178443
0.35	0.330539	0.34491	0.330539	0.329341	0.298204	0.148503
0.4	0.378443	0.371258	0.378443	0.371258	0.306587	0.141317
0.45	0.417964	0.433532	0.416768	0.432336	0.300599	0.117365
0.5	0.464672	0.463472	0.493412	0.45988	0.31976	0.0826348
0.55	0.525748	0.526948	0.523352	0.456288	0.329341	0.0958084
0.6	0.68024	0.608384	0.558084	0.506588	0.270659	0.0658684
0.65	0.8503	0.66946	0.613172	0.505388	0.240718	0.0562876
0.7	1.0503	0.78922	0.673056	0.443112	0.269461	0.0383234
0.75	1.4	0.873056	0.71018	0.464672	0.168862	0.0538924
0.8	2.12	0.973652	0.716168	0.445508	0.207186	0.0467068
0.85	2.22	0.97006	0.69102	0.390419	0.135329	0.0359282
0.9	1.34371	1.34371	0.617964	0.277844	0.0934132	0.0227545
0.95	0.148503	0.222754	0.147306	0.0514972	0.0191617	0.0191617

Try to fit the points with a universal formula

```
In[35]:= phelpsEn30Fit =
  40 * 0.013 * enrel ^ 0.4 * (1 + (enrel / 0.58) ^ 5.8) (1 + 0.1 / 0.92) / (1 + 0.1 / (0.92 - enrel));
```

To get a reasonable fit, it is necessary to greatly reduce the effect of the 3/2 power coefficient

```
In[36]:= phelpsEn30Fit = 40 * 0.013 * enrel ^ 0.4 *
  (1 + 21 (enrel) ^ 6) / (1 + 0.01 (enrel) ^ 1.5) (1 + 0.1 / 0.9) / (1 + 0.1 / (0.9 - enrel));
```

```
In[37]:= phelpsEn100Fit =
  40 * 0.013 * enrel ^ 0.4 * (1 + 6.8 (enrel) ^ 4) (1 + 0.1 / 0.92) / (1 + 0.1 / (0.92 - enrel));
```

The following is Ok

```
In[38]:= phelpsEn100Fit = 40 * 0.013 * enrel ^ 0.4 *
  (1 + 6.9 (enrel) ^ 4.5) / (1 + 0.01 (enrel) ^ 1.5) * (1 + 0.1 / 0.92) / (1 + 0.1 / (0.92 - enrel));
```

```
In[39]:= phelpsEn300Fit = 40 * 0.013 * enrel ^ 0.4 *
  (1 + 2.9 (enrel) ^ 3) / (1 + 0.01 (enrel) ^ 1.5) (1 + 0.1 / 0.92) / (1 + 0.1 / (0.92 - enrel));
```

```
In[40]:= phelpsEn1000Fit = 40 * 0.013 * enrel ^ 0.4 *
  (1 + 2.1 (enrel) ^ 2) / (1 + (enrel / 1.5) ^ 2) * (1 + 0.1 / 0.92) / (1 + 0.1 / (0.92 - enrel));
```

The following has the $en^{-3/2}$ high energy behavior from McCracken and Erent. The following fit is Ok.

```
In[41]:= phelpsEn1000Fit = 40 * 0.013 * enrel ^ 0.4 *
  (1 + 0.9 * (enrel) ^ 2) / (1 + 0.1 (enrel) ^ 1.5) * (1 + 0.1 / 0.92) / (1 + 0.1 / (0.92 - enrel));
```

```
In[42]:= phelpsEn3000Fit =
  40 * 0.013 * enrel ^ 0.4 / (1 + 0.69 (enrel) ^ 2) (1 + 0.1 / 0.92) / (1 + 0.1 / (0.92 - enrel));
```

The following has the $en^{-3/2}$ high energy behavior from McCracken and Erent. The fit is only somewhat worse than above. We need to effectively eliminate the growth,


```
In[43]:= phelpsEn3000Fit = 40 * 0.013 * enrel ^ 0.4 *
          (1 + 0.2 (enrel) ^ 2.) / (1 + 0.8 (enrel) ^ 1.5) (1 + 0.1 / 0.92) / (1 + 0.1 / (0.92 - enrel));
```

```
In[44]:= phelpsEn10000Fit =
          40 * 0.013 * enrel ^ 0.4 / (1 + 11.1 (enrel) ^ 2) (1 + 0.1 / 0.95) / (1 + 0.1 / (0.95 - enrel));
```

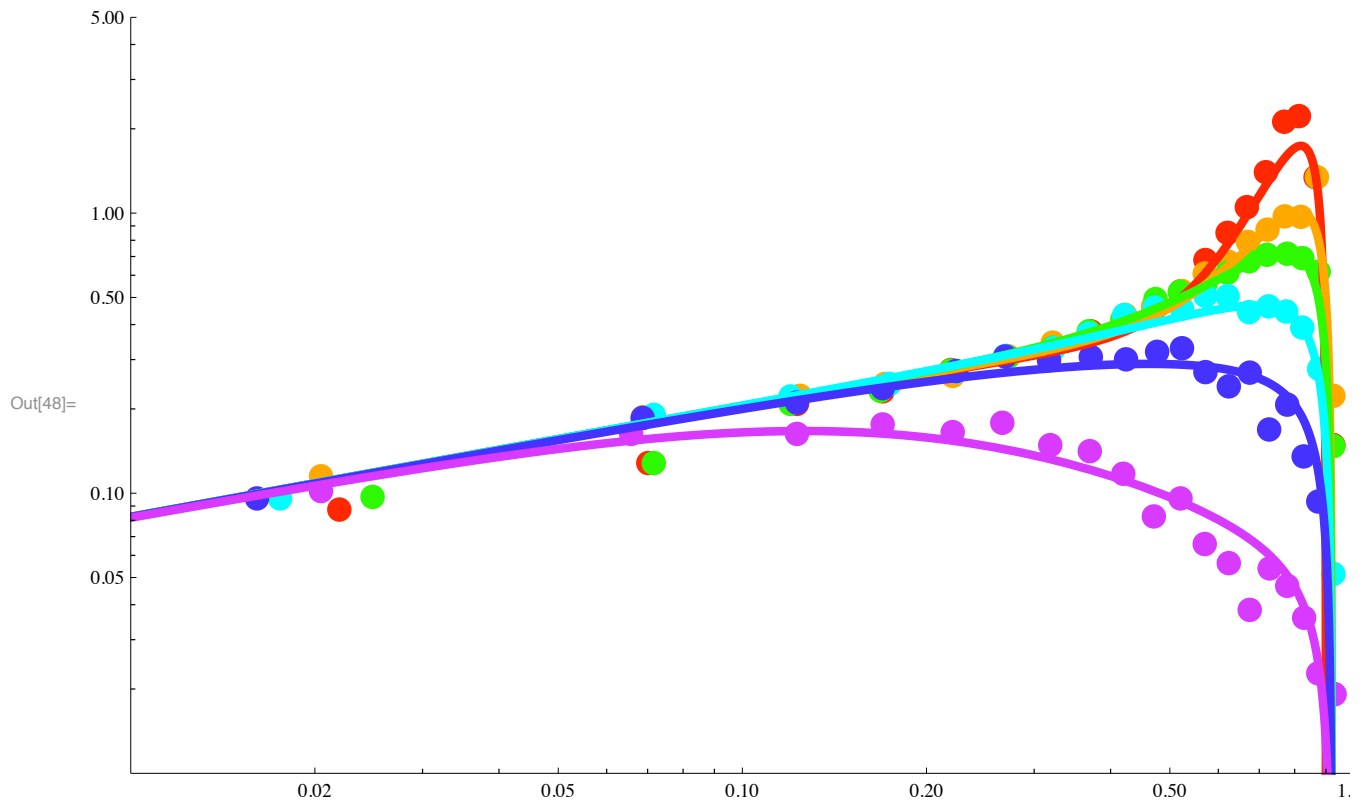
The following has the $en^{-3/2}$ high energy behavior from McCracken and Erent, but the fit is worse.

```
In[45]:= phelpsEn10000Fit = 40 * 0.013 * enrel ^ 0.4 *
          (1 + 2.8 (enrel) ^ 2.) / (1 + 8 * (enrel) ^ 1.5) (1 + 0.1 / 0.92) / (1 + 0.1 / (0.92 - enrel));
```

```
In[46]:= phelpsEn10000Fit = 40 * 0.013 * enrel ^ 0.4 *
          (1 + .1 (enrel) ^ 1.) / (1 + 8 * (enrel) ^ 1.5) (1 + 0.1 / 0.92) / (1 + 0.1 / (0.92 - enrel));
```

```
In[47]:= phelpsFitLogLogPlot = LogLogPlot[{phelpsEn30Fit, phelpsEn100Fit, phelpsEn300Fit,
          phelpsEn1000Fit, phelpsEn3000Fit, phelpsEn10000Fit (*,phelpsFit*)},
          {enrel, 0.01, 0.95}, PlotRange -> All, PlotStyle -> plotColorsLines];
```

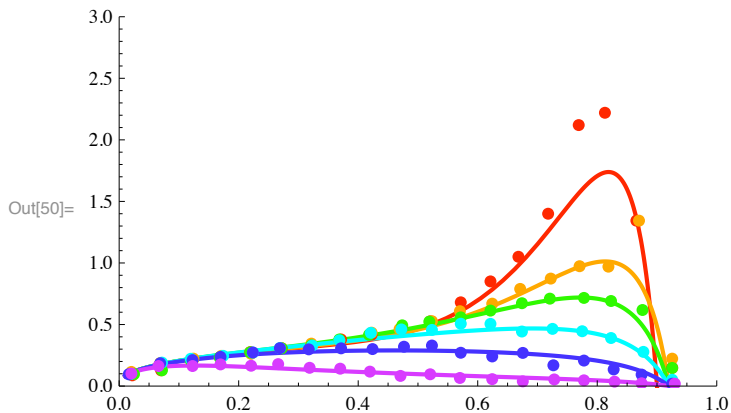
```
In[48]:= Show[eckstein84DataLogLogPlot, phelpsFitLogLogPlot, ImageSize -> 600]
```



Linear plot

```
In[49]:= phelpsFitPlot = Plot[{phelpsEn30Fit, phelpsEn100Fit,
          phelpsEn300Fit, phelpsEn1000Fit, phelpsEn3000Fit, phelpsEn10000Fit},
          {enrel, 0.01, 0.95}, PlotRange -> {{0, 1}, {0, 3}}, PlotStyle -> plotColorsLines];
```

```
In[50]:= Show[phelpsFitPlot, eckstein84DataPlot]
```



■ Trials

At the higher energies these are upper limits for the exponents listed next

```
In[51]:= table1 = {{30, 21.4}, {100, 7}, {300, 3}, {1000, 0.9}, {3000, 0.2}, {10 000, 0.1}}
```

```
Out[51]= {{30, 21.4}, {100, 7}, {300, 3}, {1000, 0.9}, {3000, 0.2}, {10 000, 0.1}}
```

The fits are not very sensitive to the following two tries

```
In[52]:= table1Fit := 30 / (en0 / 30) ^ 1
```

```
table1Fit := 27 / (en0 / 30) ^ 1
```

```
In[53]:= exponent = {{30, 6}, {100, 4.5}, {300, 3}, {1000, 2}, {3000, 2}, {10 000, 1}}
```

```
Out[53]= {{30, 6}, {100, 4.5}, {300, 3}, {1000, 2}, {3000, 2}, {10 000, 1}}
```

The fits are not very sensitive to the following two tries

```
exponentFit := 4.5 * (en0 / 100) ^ -0.3
```

```
In[54]:= exponentFit := 4.3 * (en0 / 100) ^ -0.28
```

```
exponentFit := 15 / en0 ^ 0.35
```

At the lower energies these are upper limits

```
In[55]:= table2 = {{30, 0.01}, {100, 0.01}, {300, 0.01}, {1000, 0.1}, {3000, 0.76}, {10 000, 8}}
```

```
Out[55]= {{30, 0.01}, {100, 0.01}, {300, 0.01}, {1000, 0.1}, {3000, 0.76}, {10 000, 8}}
```

The fits are not very sensitive to the following two tries

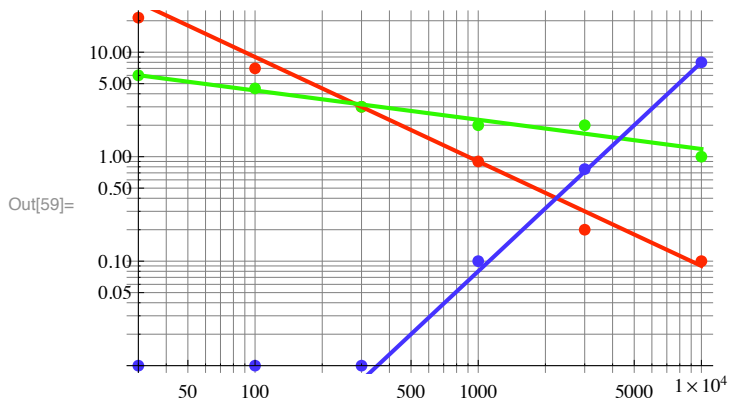
```
table2Fit := 6 * (en0 / 10 000) ^ 2
```

```
In[56]:= table2Fit := 8 * (en0 / 10 000) ^ 2
```

```
In[57]:= parameters = ListLogLogPlot[{table1, exponent, table2},
  PlotStyle → plotColorsPoints[{{1, 3, 5}}], GridLines → Automatic];
```

```
In[58]:= parameterFit = LogLogPlot[{table1Fit, exponentFit, table2Fit},
  {en0, 30, 10 000}, PlotStyle → plotColorsLines[{{1, 3, 5}}]]];
```

In[59]:= Show[parameters, parameterFit]



From early trials

```
phelpsFit :=
  40 * 0.013 * enrel ^ 0.4 * (1 + table1Fit * (enrel) ^ exponentFit) / (1 + table2Fit * (enrel) ^ 1.5)
  (1 + 0.1 / 0.92) / (1 + 0.1 / (0.92 - enrel))
```

The high energy limit of this formula does not work well for the high energy incident particles, so we try a different limiting form.

```
phelpsFit := 40 * 0.013 * enrel ^ 0.4 * (1 + table1Fit * (enrel) ^ exponentFit) /
  (1 + table2Fit * (enrel) ^ 1.5) (1 + 0.2 / 1) / (1 + 0.2 / (1 - enrel))
```

The following was installed in the cross section file

```
In[60]:= PhelpsFit := 0.52 * enrel ^ 0.4 *
  (1 + (900 / (en0 + 30)) * (enrel) ^ (17.9 / en0 ^ 0.3)) / (1 + (8 * 10 ^ -8 * en0 ^ 2) * (enrel) ^ 1.5)
  (1 - enrel / 0.95) / (1 - enrel / 1.05) UnitStep[.95 - enrel]
```

In[61]:= PhelpsFit

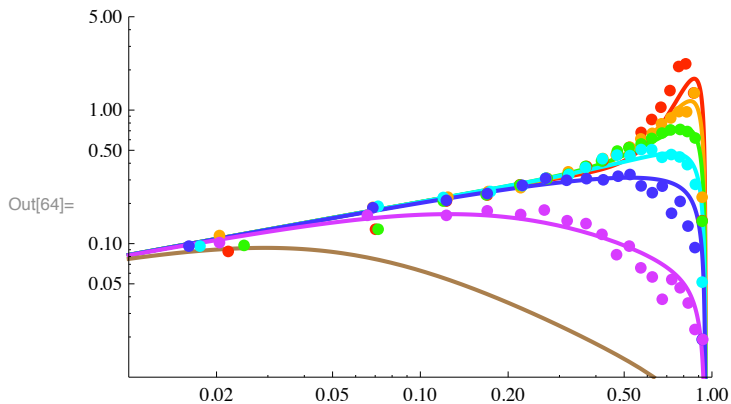
$$0.52 (1 - 1.05263 \text{ enrel}) \text{ enrel}^{0.4} \left(1 + \frac{900 \text{ enrel}^{\frac{17.9}{\text{en0}^{0.3}}}}{30 + \text{en0}} \right) \text{UnitStep}[0.95 - \text{enrel}]$$

Out[61]=
$$\frac{0.52 (1 - 1.05263 \text{ enrel}) \text{ enrel}^{0.4} \left(1 + \frac{900 \text{ enrel}^{\frac{17.9}{\text{en0}^{0.3}}}}{30 + \text{en0}} \right) \text{UnitStep}[0.95 - \text{enrel}]}{(1 - 0.952381 \text{ enrel}) \left(1 + \frac{\text{en0}^2 \text{ enrel}^{1.5}}{12500000} \right)}$$

```
In[62]:= Table[PhelpsFit /. en0 -> #[[j]], {j, Length[#]} &[ {30, 100, 300, 1000, 3000, 10000, 30000} ];
```

```
In[63]:= PhelpsFitPlot = LogLogPlot[%, {enrel, 0.01, 1},
  PlotRange -> {{0, 1}, {0.01, 5}}, PlotStyle -> plotColorsLines];
```

```
In[64]:= Show[phelpsFitPlot, eckstein84DataLogLogPlot]
```



```
In[65]:= phelpsFitTable = Table[{j * 0.01, phelpsFit /. {en0 -> 30, enrel -> j * 0.01},
  phelpsFit /. {en0 -> 100, enrel -> j * 0.01}, phelpsFit /. {en0 -> 300, enrel -> j * 0.01},
  phelpsFit /. {en0 -> 1000, enrel -> j * 0.01}, phelpsFit /. {en0 -> 3000, enrel -> j * 0.01},
  phelpsFit /. {en0 -> 10000, enrel -> j * 0.01}}, {j, 100}];
```

```
In[66]:= Export["FitToEckstein&Verbeek84.txt", phelpsFitTable, "Table"]
```

```
Out[66]:= FitToEckstein&Verbeek84.txt
```

Multiplying the following intergrated distributions by an arbitray factor of 40 forces a fit. Presumably a factor of 20 comes from the fact that the signal is distributed over 20 channels. Why the other factor of 2?

```
In[67]:= phelpsFitReflectionFraction =
  Table[{#[[j]], NIntegrate[(phelpsFit /. en0 -> #[[j]]], {enrel, 0, 0.95}], {j, Length[#]}] &[
    {1, 3, 10, 30, 100, 300, 1000, 3000, 10000, 30000}];
```

```
In[68]:= TableForm[phelpsFitReflectionFraction, TableHeadings -> {None, {"energy (eV)", "RN"}}]
```

```
Out[68]//TableForm=
energy (eV) RN
-----
1           0.358689
3           0.441025
10          0.548026
30          0.586082
100         0.511712
300         0.410745
1000        0.325987
3000        0.238939
10000       0.094115
30000       0.0226608
```

Alternatively, we can calculate the RN values using the tabulated phelpsFit values. This is the generic formula to be used in the calculation of fluxes and profiles.

```
In[69]:= phelpsFitReflectionFraction2 =
  Table[#[[j]], Total[Table[(phelpsFit /. {en0 -> #[[j]], enrel -> (k - 1) / (mc - 1)}],
    {k, 31}]] / mc /. mc -> 31], {j, Length[#]}] &[
  {1, 3, 10, 30, 100, 300, 1000, 3000, 10 000, 30 000}]] // TableForm
```

```
Out[69]//TableForm=
```

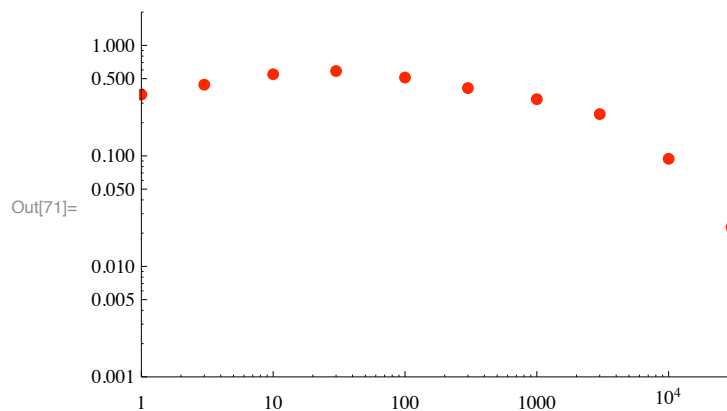
1	0.348979
3	0.429323
10	0.532956
30	0.568981
100	0.495733
300	0.397242
1000	0.314818
3000	0.230357
10 000	0.0900484
30 000	0.0208823
100 000	0.00267576

```
In[70]:= Export["PhelpsFitReflectionFraction.txt", phelpsFitReflectionFraction2, "Table"]
```

```
Out[70]= PhelpsFitReflectionFraction.txt
```

The high energy results are slightly too small according to Fig. 2.11 of Eckstein and Verbeek (1984)

```
In[71]:= phelpsFitReflectionFractionPlot = ListLogLogPlot[phelpsFitReflectionFraction,
  PlotRange -> {{1, 30 000}, {.001, 2}}, PlotStyle -> plotColorsPoints[[1]]]
```



From MBHCAsymmDoppler042610_7.nb and from jA[p,q] equations. Replace phelpsFitASS with phelpsFit. Set Reflection Factor = 1.

```
In[72]:= fit1A = phelpFit
```

$$0.52 (1 - 1.05263 \text{ enrel}) \text{ enrel}^{0.4} \left(1 + \frac{900 \text{ enrel}^{\frac{17.9}{\text{en0}^{0.3}}}}{30 + \text{en0}} \right) \text{UnitStep}[0.95 - \text{enrel}]$$

$$\frac{\text{Out[72]}=}{(1 - 0.952381 \text{ enrel}) \left(1 + \frac{\text{en0}^2 \text{ enrel}^{1.5}}{12500000} \right)}$$

In our kinetics model we use the reflection (r) of left-moving (i) atoms (A) resulting from ions striking a surface at position p (which is often at p=1)

```
In[73]:= rilAp[p_, q_] :=
  Sum[If[k > 1 && k >= q > 1 && p ≤ m - ma, fit1A[k, q] / mc * il[p, k], 0], {k, q, mc}]
```

Modify this to calculate RN and so check normalization, i.e., set il[p,k] = 1, note that the index p no longer matters.

```
rnq = fit1A[k, q] / mc /. {il[p, k] → 1, en0 → 30000, mc → 30}
```

```
Table[If[k > 1 && k >= q > 1, rnq, 0], {k, q, 30}]
```

■ Eckstein and Verbeek - RN values

I need to test against published RN values.

```
In[74]:= ecksteinVerbeek84RNData = Import["eckstein_verbeek84fig211.dat", "Table"];
```

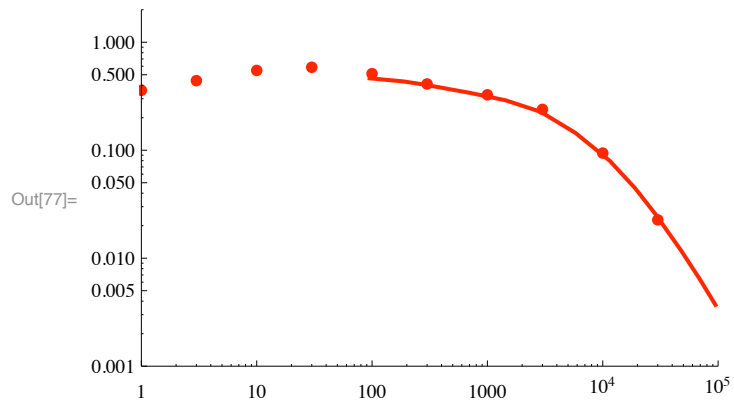
```
In[75]:= TableForm[%, TableHeadings → {None, {"energy (eV)", "RN"}}]
```

Out[75]/TableForm=

energy (eV)	RN
95.3469	0.463663
189.557	0.433148
284.331	0.405005
715.929	0.338745
1439.03	0.289825
2891.61	0.227114
5806.42	0.144455
11523.2	0.079659
19096.5	0.0444381
28598.1	0.0256285
47898.6	0.0117322
69333.6	0.00640541
94880.1	0.00369522

```
In[76]:= ecksteinVerbeek84RNPlot = ListLogLogPlot[%,
  PlotRange → {{1, 100000}, {0.001, 2}}, Joined → True, PlotStyle → plotColorsLines[[1]]];
```

```
In[77]:= Show[ecksteinVerbeek84RNPlot , helpsFitReflectionFractionPlot ]
```



- Aratari and Eckstein (1989)
- Attempt to scale our empirical FE and RN expressions

We divide the experimental magnitudes by a factor so as to fit the fractional reflection RN versus en_0 in their Fig. 5a. For this we assume an angular distribution of $\text{Cos}[\theta]$ per unit solid angle.

```

In[78]:= Import["aratari_eckstein_89_50.dat", "CSV"] // TableForm
Out[78]/TableForm=
  1.74520E-03    4.33840E-03
  1.69285E-01    5.63991E-02
  1.93717E-01    1.86551E-01
  2.21641E-01    3.86117E-01
  2.67016E-01    4.98915E-01
  3.24607E-01    6.16052E-01
  3.76963E-01    7.98265E-01
  4.45026E-01    9.37093E-01
  5.00873E-01    1.14100E+00
  5.37522E-01    1.27549E+00
  5.84642E-01    1.38829E+00
  6.28272E-01    1.56182E+00
  6.61431E-01    1.74837E+00
  6.89354E-01    1.94360E+00
  7.22513E-01    2.11280E+00
  7.67888E-01    2.26464E+00
  7.99302E-01    2.28200E+00
  8.30716E-01    2.26464E+00
  8.53403E-01    2.07809E+00
  8.86562E-01    1.90022E+00
  9.05759E-01    1.54881E+00
  9.26702E-01    1.24512E+00
  9.38918E-01    9.58785E-01
  9.47644E-01    7.50542E-01
  9.61606E-01    4.85900E-01
  9.82548E-01    1.95228E-01
  1.01047E+00    2.16920E-02
  1.06632E+00    -8.67679E-03
Aratari & Eckstein Fig 3(1989)

In[79]:= aratari50Data = Drop[Import["aratari_eckstein_89_50.dat", "Table"], -1];
In[80]:= aratari50Table = Table[{#[[j, 1]], #[[j, 2]] / 2}, {j, Length[%]}];
In[81]:= rn50 = NIntegrate[Interpolation[%, InterpolationOrder -> 1][x], {x, 0, 1}]
Out[81]= 0.513148

In[82]:= aratari400Data = Drop[Import["aratari_eckstein_89_400.dat", "Table"], -3];
In[83]:= aratari400Table = Table[{#[[j, 1]], #[[j, 2]] / 4}, {j, Length[%]}];
In[84]:= rn400 = NIntegrate[Interpolation[%, InterpolationOrder -> 1][x], {x, 0, 1}]
Out[84]= 0.362953

In[85]:= aratari800Data = Drop[Import["aratari_eckstein_89_800.dat", "Table"], -2];
In[86]:= aratari800Table = Table[{#[[j, 1]], #[[j, 2]] / 4.7}, {j, Length[#]}] &[aratari800Data];
In[87]:= rn800 = NIntegrate[Interpolation[%, InterpolationOrder -> 1][x], {x, 0, 1}]
Out[87]= 0.314943

In[88]:= aratari2000Data = Drop[Import["aratari_eckstein_89_2000.dat", "Table"], -3];
In[89]:= aratari2000Table = Table[{#[[j, 1]], #[[j, 2]] / 5.8}, {j, Length[%]}];

```



```
In[90]:= rn2000 = NIntegrate[Interpolation[%, InterpolationOrder -> 1][x], {x, 0, 1}]
```

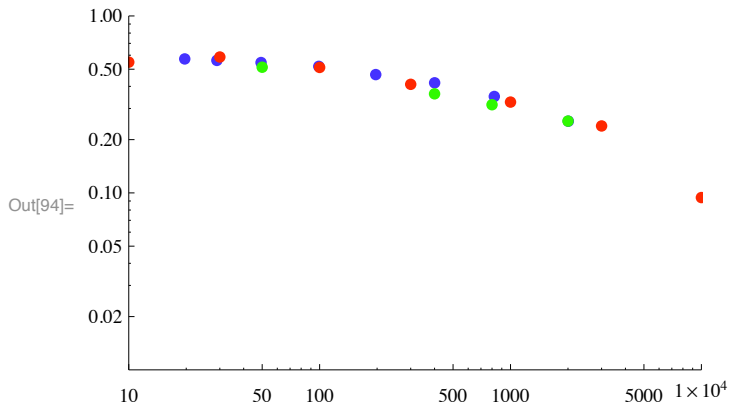
```
Out[90]= 0.25455
```

```
In[91]:= aratariCalcRNPlot = ListLogLogPlot[{{50, rn50}, {400, rn400}, {800, rn800}, {2000, rn2000}},
      PlotRange -> {{10, 10 000}, {0.01, 1}}, PlotStyle -> plotColorsPoints[[3]]];
```

```
In[92]:= Import["aratari89rnfig5.dat", "Table"];
```

```
In[93]:= aratari89RNPlot =
      ListLogLogPlot[%, PlotRange -> {{10, 10 000}, {0.01, 1}}, PlotStyle -> plotColorsPoints[[5]]];
```

```
In[94]:= Show[aratari89RNPlot, aratariCalcRNPlot, phelpsFitReflectionFractionPlot]
```

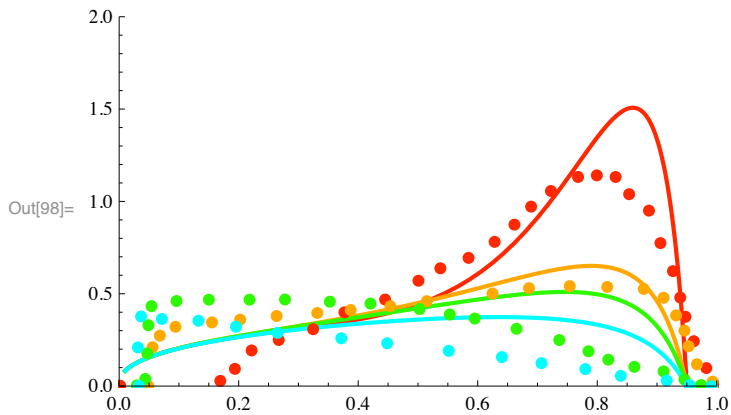


```
In[95]:= aratariTable2Plot =
      ListPlot[{aratari50Table, aratari400Table, aratari800Table, aratari2000Table},
      PlotStyle -> plotColorsPoints, PlotRange -> {{0, 1}, {0, 1}}];
```

```
In[96]:= Table[phelpsFit //. en0 -> #[[j]], {j, 4}] &[{50, 400, 800, 2000}];
```

```
In[97]:= phelpsFitPlot = Plot[%, {enrel, 0.01, 0.95},
      PlotRange -> {{0, 1}, {0, 2}}, PlotStyle -> plotColorsLines[{{1, 2, 3, 4}}];
```

```
In[98]:= Show[phelpsFitPlot, aratariTable2Plot]
```



These are very poor fits to the shapes. The average values do not count, because of our individual adjustment to calculated RN.

These are very poor fits, and I have no understanding as to why. The scaling laws in Eckstein and Verbeek (1984) and the text in Aratari and Eckstein (1989) say that there should be very little difference between H and D projectiles except on a metal of very low or very high mass.

■ Data of Oen and Robinson (1976) FE

```
In[99]:= Import["Oen&Robinson76-100eVFig5.dat", "CSV"] // TableForm
```

Out[99]/TableForm=

9.47358E-01	-6.20048E-01
2.99731E+00	-2.94227E-01
4.56911E+00	3.15849E+00
6.93253E+00	4.73823E+00
8.65957E+00	9.75687E+00
1.10165E+01	1.54054E+01
1.27515E+01	1.54163E+01
1.46467E+01	1.38632E+01
1.70087E+01	1.63819E+01
1.87392E+01	1.92096E+01
2.07896E+01	1.92225E+01
2.26814E+01	1.98603E+01
2.50503E+01	1.79972E+01
2.67882E+01	1.61301E+01
2.83581E+01	2.08348E+01
3.07130E+01	2.77353E+01
3.29122E+01	3.33829E+01
3.49756E+01	2.52581E+01
3.67131E+01	2.37040E+01
3.85989E+01	2.80976E+01
4.08105E+01	2.59206E+01
4.25331E+01	3.37561E+01
4.47348E+01	3.78387E+01
4.69490E+01	3.40967E+01
4.91372E+01	4.66300E+01
5.13404E+01	4.97737E+01
5.30904E+01	4.03949E+01
5.46522E+01	5.01074E+01
5.67091E+01	4.60514E+01
5.85924E+01	5.20100E+01
6.09727E+01	4.29482E+01
6.31690E+01	5.04737E+01
6.49015E+01	5.20495E+01
6.69360E+01	6.20779E+01
6.89895E+01	6.02128E+01
7.08747E+01	6.49194E+01
7.29217E+01	6.71231E+01
7.48085E+01	7.08908E+01
7.70057E+01	7.77903E+01
7.90422E+01	8.65668E+01
8.11126E+01	7.40602E+01
8.29804E+01	8.97213E+01
8.53543E+01	8.47284E+01
8.70798E+01	9.06860E+01
8.86556E+01	9.16348E+01
9.07921E+01	1.36719E+02
9.30257E+01	2.19988E+02
9.44686E+01	6.85113E+00
9.71614E+01	-3.30758E-01
9.88964E+01	-3.19897E-01

In[100]:= **Import**["Oen&Robinson76-100eVFig5.dat", "Table"];

In[101]:= **oen100Data** = **Table**[%[[j, 1]], %[[j, 2]] / 8000, {j, 50}];

```
In[102]:= rn100 = NIntegrate[Interpolation[%, InterpolationOrder -> 1][x], {x, 0, 100}]
```

```
Out[102]= 0.541176
```

```
In[103]:= oen100Data2 = Table[{#[[j, 1]] / 100, #[[j, 2]] * 100}, {j, 50}] &[oen100Data];
```

```
In[104]:= Import["Oen&Robinson76-5000eVFig5.dat", "CSV"] // TableForm
```

```
Out[104]//TableForm=
```

3.85679E+01	1.22493E-01
1.49114E+02	1.48883E-01
2.35714E+02	2.01624E-01
3.78119E+02	2.01668E-01
4.56682E+02	2.69909E-01
5.51605E+02	2.71489E-01
6.62615E+02	2.40516E-01
7.50116E+02	1.81628E-01
8.59999E+02	2.90189E-01
9.62333E+02	3.53787E-01
1.05762E+03	3.10406E-01
1.13667E+03	3.18182E-01
1.25534E+03	3.18219E-01
1.35864E+03	2.62437E-01
1.46929E+03	2.76425E-01
1.56486E+03	1.97384E-01
1.66750E+03	2.23773E-01
1.76998E+03	2.68766E-01
1.85788E+03	1.60266E-01
1.96094E+03	1.33941E-01
2.04724E+03	2.23891E-01
2.16674E+03	1.21602E-01
2.29216E+03	2.65827E-01
2.37167E+03	2.16239E-01
2.45914E+03	1.62003E-01
2.54650E+03	1.20170E-01
2.64118E+03	1.51207E-01
2.75971E+03	1.69848E-01
2.85489E+03	1.38870E-01
2.95743E+03	1.77661E-01
3.05996E+03	2.16453E-01
3.15506E+03	1.96327E-01
3.26612E+03	1.59152E-01
3.34548E+03	1.28169E-01
3.44804E+03	1.63860E-01
3.55136E+03	1.06528E-01
3.63867E+03	7.08957E-02
3.74124E+03	1.05036E-01
3.84455E+03	4.77037E-02
3.96315E+03	5.70428E-02
4.04250E+03	2.76101E-02
4.12954E+03	2.60867E-02
4.24756E+03	1.06743E-01
4.34266E+03	8.66179E-02
4.45365E+03	5.71949E-02
4.54093E+03	2.62142E-02
4.63586E+03	2.62437E-02
4.73881E+03	1.38725E-02
4.85761E+03	-1.59454E-03
4.94463E+03	-1.56756E-03

```
In[105]:= Import["Oen&Robinson76-5000eVFig5.dat", "Table"];
```

```
In[106]:= oen5000Data = Table[{#[[j, 1]], #[[j, 2]] / 5000}, {j, 50}];
```

```
In[107]:= rn5000 = NIntegrate [Interpolation [%, InterpolationOrder -> 1] [x], {x, 0, 5000}]
```

```
Out[107]= 0.162477
```

```
In[108]:= oen5000Data2 = Table[{#[[j, 1]] / 5000, #[[j, 2]] * 5000}, {j, 50}] &[oen5000Data];
```

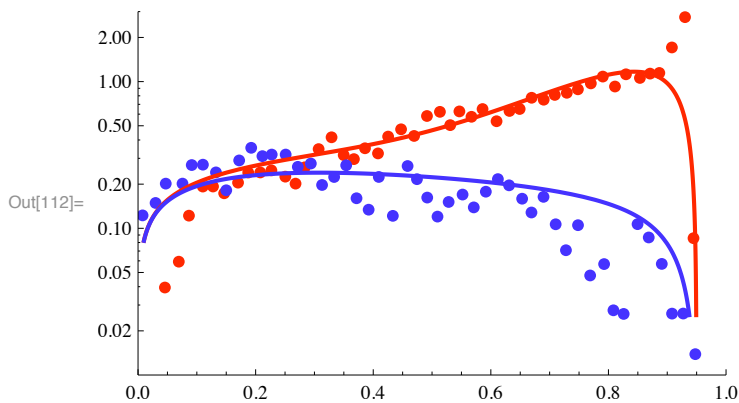
The agreement of the RN values with those shown in Fig. 5 indicates that I have finally gotten the scaling of the experiment correct.

```
In[109]:= oenDataPlot = ListLogPlot [{oen100Data2, oen5000Data2},
    PlotStyle -> plotColorsPoints [{{1, 5}}], PlotRange -> {{0, 1}, {0.01, 3}}];
```

```
In[110]:= Table[phelpsFit // . en0 -> #[[j]], {j, 2}] &[{{100, 5000}}];
```

```
In[111]:= phelpsFitPlot = LogPlot [%, {enrel, 0.01, 1}, PlotStyle -> plotColorsLines [{{1, 5}}]]];
```

```
In[112]:= Show[oenDataPlot, phelpsFitPlot]
```



The agreement is fair except near the maximum velocity.

■ Calculation of Verbeek, Eckstein, and Bhattacharya (1980)

These experiments and calculations are for scattering of H by Au, whereas our formula is for scattering of H by Ni. The theory says that energy should be scaled by $0.358/0.093 = 3.85$. $\text{scaled energy} = \text{enAu} * 0.093 = \text{enNi} * 0.358$ or $\text{enNi} = 0.26 * \text{enAu}$.

These data were obtained using H₂⁺ of twice the energy cited. It is assumed that the atom and ion act independently and produce equal effects.

These experimental data are said to be normalized such that the areas are proportional to RN.

■ 5000 eV data

```
In[113]:= expt5000 = Import ["verbeek80fig7ev5000.dat", "Table"];
```

```
In[114]:= rn5000expt = NIntegrate [Interpolation [expt5000, InterpolationOrder → 1] [x], {x, 0, 1}] * 8000
Out[114]= 0.222107
```

This value is close to the cited 0.217, The multiplier is 8000 eV, although it reminds me of the use of 8000 particles in the MC calculation.

```
In[115]:= verbeek5000Data = Table[{#[[j, 1]] * 5000, #[[j, 2]] * 8000 / 5000}, {j, Length[#]}] &[expt5000];
In[116]:= rn5000 = NIntegrate [Interpolation [%, InterpolationOrder → 1] [x], {x, 0, 5000}]
Out[116]= 0.222107
```

```
In[117]:= verbeek5000Data2 =
  Table[{#[[j, 1]] / 5000, #[[j, 2]] * 5000}, {j, Length[#]}] &[verbeek5000Data];
```

■ 8000 eV data

```
In[118]:= expt8000 = Import ["verbeek80fig7ev8000.dat", "Table"];
In[119]:= rn8000expt = NIntegrate [Interpolation [expt8000, InterpolationOrder → 1] [x], {x, 0, 1}] * 8000
Out[119]= 0.175424
In[120]:= verbeek8000Data = Table[{#[[j, 1]] * 8000, #[[j, 2]]}, {j, Length[#]}] &[expt8000];
In[121]:= rn8000 = NIntegrate [Interpolation [%, InterpolationOrder → 1] [x], {x, 0, 8000}]
Out[121]= 0.175424
```

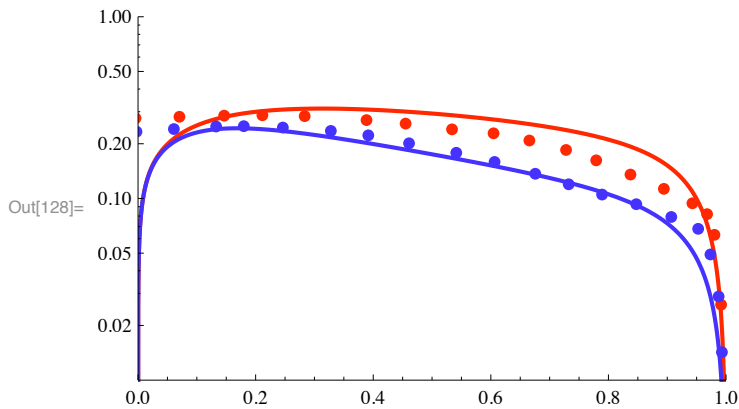
This value is close to the cited 0.174, The multiplier of 8000 reminds one of the use of 8000 particles in the MC calculation

```
In[122]:= verbeek8000Data2 =
  Table[{#[[j, 1]] / 8000, #[[j, 2]] * 8000}, {j, Length[#]}] &[verbeek8000Data];
```

The agreement of the RN values with those shown in Fig. 7 indicates that I have finally gotten the scaling of the experiment correct.

```
In[123]:= verbeekDataPlot =
  ListLogPlot [{verbeek5000Data2, verbeek8000Data2}, PlotStyle → plotColorsPoints [{1, 5}]];
In[124]:= phelpsFit2 := 1.3 * 40 * 0.013 * enrel ^ 0.4 * (1 + table1Fit * (enrel) ^ exponentFit) /
  (1 + table2Fit * (enrel) ^ 1.5) (1 + 0.1 / 1) / (1 + 0.1 / (1 - enrel))
In[125]:= Table [phelpsFit2 /. en0 → #[[j]], {j, 2}] &[{{5000 * 0.26, 8000 * 0.26}}];
In[126]:= Table [phelpsFit2 /. en0 → #[[j]], {j, 2}] &[{{5000, 8000}}];
In[127]:= phelpsFit2Plot = LogPlot [%, {enrel, 0.0, 1},
  PlotStyle → plotColorsLines [{1, 5}], PlotRange → {{0, 1}, {0.01, 1}}];
```

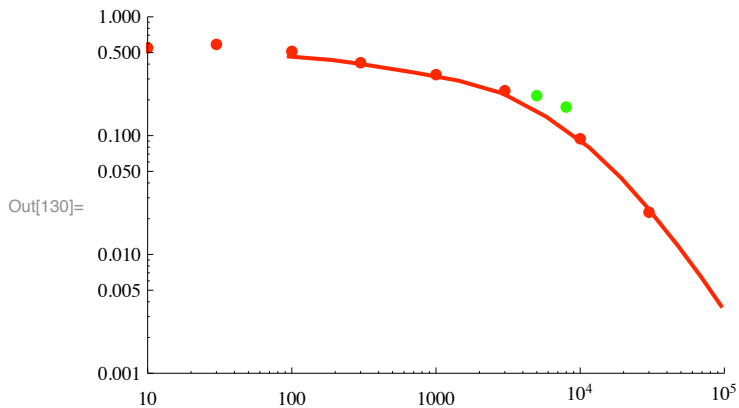
```
In[128]:= Show[phelpsFit2Plot, verbeekDataPlot]
```



Using energy scaling, the agreement with my formula is extremely bad. With no scaling the fit is only fair.

```
In[129]:= verbeekEckstein80RNPlot = ListLogLogPlot[{{5000, 0.217}, {8000, .174}},
  PlotRange -> {{10, 100 000}, {0.001, 1}}, PlotStyle -> plotColorsPoints[[3]]];
```

```
In[130]:= Show[verbeekEckstein80RNPlot, ecksteinVerbeek84RNPlot, phelpsFitReflectionFractionPlot]
```



The increase in the PhelpsFit by 1.3 is required because the RN values are larger than the values of Eckstein&Verbeek (1984).

- McCracken and Freeman, *J. Phys. B* 2, 661 (1969)

These authors use a simplified energy loss then scattering followed by energy loss model. They conclude that for high energy protons, the distribution in final energy goes as $E^{-(3/2)}$.


```
In[131]:= scale = 0.000001
```

```
Out[131]= 1. × 10-6
```

```
In[132]:= mcrackenTi20keV = Table[{#[[j, 1]] / 20, #[[j, 2]] * scale}, {j, Length[#]}] &[
  Import["mcrackenfreeman69fig4bti20kev.dat", "Table"]];
```

```
In[133]:= mcrackenTi40keV = Table[{#[[j, 1]] / 40, #[[j, 2]] * scale}, {j, Length[#]}] &[
  Import["mcrackenfreeman69fig4bti40kev.dat", "Table"]];
```

```
In[134]:= mcrackenTi60keV = Table[{#[[j, 1]] / 60, #[[j, 2]] * scale}, {j, Length[#]}] &[
  Import["mcrackenfreeman69fig4bti60kev.dat", "Table"]];
```

```
In[135]:= mcrackenNb20keV = Table[{#[[j, 1]] / 20, #[[j, 2]] * scale}, {j, Length[#]}] &[
  Import["mcrackenfreeman69fig4bnb20kev.dat", "Table"]];
```

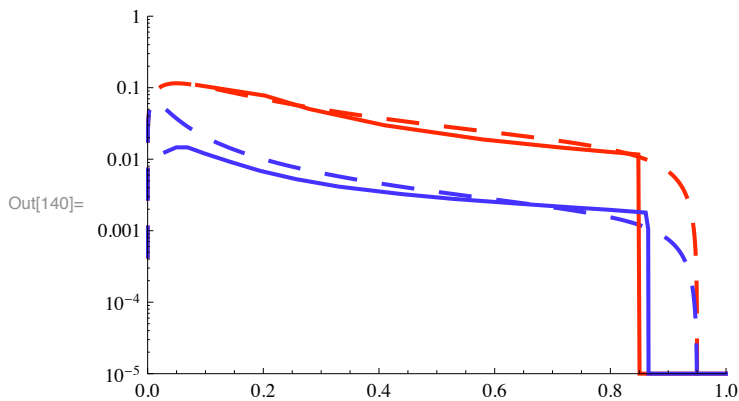
```
In[136]:= mcrackenNb40keV = Table[{#[[j, 1]] / 40, #[[j, 2]] * scale}, {j, Length[#]}] &[
  Import["mcrackenfreeman69fig4bnb40kev.dat", "Table"]];
```

```
In[137]:= mcrackenNb60keV = Table[{#[[j, 1]] / 60, #[[j, 2]] * scale}, {j, Length[#]}] &[
  Import["mcrackenfreeman69fig4bnb60kev.dat", "Table"]];
```

```
In[138]:= mcrackenPlot = ListLogPlot[{mcrackenTi20keV, (*mcrackenTi40keV,*)mcrackenTi60keV
  (*,mcrackenNb20keV,*) (*mcrackenNb40keV,*) (*mcrackenNb60keV*)},
  PlotRange → {{0, 1}, {10-5, 1}}, Joined → True, PlotStyle -> plotColorsLines[{{1, 5}}];
```

```
In[139]:= phelpsFit20keVPlot = LogPlot[{phelpsFit /. en0 → 20 000, phelpsFit /. en0 → 60 000},
  {enrel, 0, 1}, PlotStyle → plotColorsLines[{{8, 12}}], PlotRange → {{0, 1}, {10-5, 1}}];
```

```
In[140]:= Show[phelpsFit20keVPlot, mcrackenPlot]
```



Functional form of backscattered atom energy distribution.

From the experimental data of Eckstein and Verbeek (1984), I propose the following generic form.

```
In[141]:= rAtom[enRel_] := a * Exp[b * enRel]
```

From Fig. 2.16, I propose the b is positive at low incident energies and negative at high incident ion energies and a is of the order of 0.5. Possibly $a * \text{enRel} * \text{Exp}[b * \text{enRel}]$ would be better.

■ Mean energy of backscattered atoms

The advantage of this form relative to a one parameter formula is that one can vary the mean energy of the backscattered atoms. The upper limit in the following should probably be 0.95 not 1.0

```
In[142]:= meanBackEn:= Integrate[enRel*rAtom[enRel],{enRel,0,1}]/ Integrate[rAtom[enRel],{enRel,0,1}]
```

Typical values of b are -2 for 10 keV H ions and 2.5 for 30 eV H ions when considered as a fraction of the incident ion energy, both on nickel. The points given next are rough eyeball fits to the data of Fig. 2.16 of Eckstein and Verbeek.

```
In[143]:= bNiData={{30,2.5},{300,.9},{1000,.6},{10000,-2}};
```

```
In[144]:= bNiDataPlot=ListPlot[bNiData,PlotStyle->plotColorsPoints[[1]],DisplayFunction->Identity];
```

```
In[145]:= bNiDataLogPlot=ListLogLinearPlot[bNiData,PlotStyle->plotColorsPoints[[1]],DisplayFunction->]
```

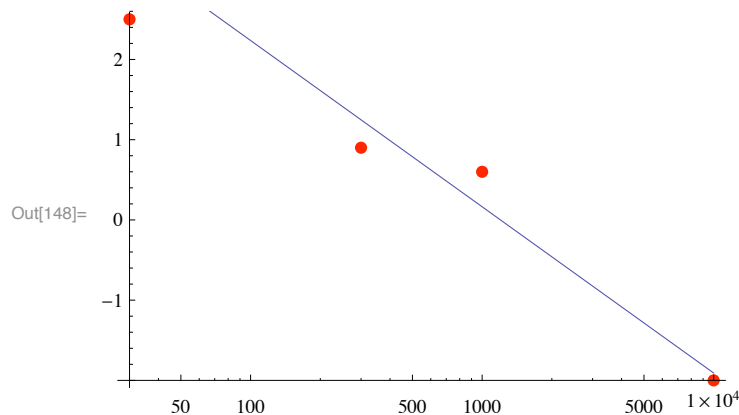
We now fit the mean energy data with

```
In[146]:= bNiFit=-.9*Log[(enLabNi/1200)]
```

```
Out[146]= -0.9 Log[ $\frac{\text{enLabNi}}{1200}$ ]
```

```
In[147]:= bNiFitPlot=LogLinearPlot[bNiFit,{enLabNi,10,10000},PlotRange->All,DisplayFunction->Identity]
```

```
In[148]:= Show[bNiDataLogPlot,bNiFitPlot]
```



Now let us look at some representative fits to the data of Fig. 2.16 of Eckstein and Verbeek.

```
In[149]:= Clear[enLab,en,a,b]
```

```
In[150]:= rAtom[enRel]
```

```
Out[150]= a eb enRel
```

Here the factor "a" includes the per relative energy interval cited in the ordinate of Fig. 2.16 for D+ on Ni. In general it is a function of enLab. I presume that the relative energy interval is 0.05, since there are 20 bins. From Fig. 2.16, I would expect that $RN = \int rAtom[enRel] d enRel \rightarrow \sum rAtom * 0.05 \sim 1.2E-2$ at $E0 = 300$ eV. For enLab=300 eV and Ni, from Fig. 2 of Eckstein and Biersack (1985), $RN = 0.45$. But $RN = \int rAtom[enRel] d enRel = \int rAtom[en/enLab] d en/enLab = \int rAtom[en/enLab]/enLab d en$, with an appropriate change in limits of integration.

```
In[151]:= bNiFit/.enLabNi->1000
```

```
Out[151]= 0.164089
```

```
In[152]:= rAtom[enRel]/.b->bNiFit
```

```
Out[152]= 12000.9 enRel a enLabNi-0.9 enRel
```

```
In[153]:= rAtom[enRel]/.{a->0.5*10^-2,b->bNiFit}
```

```
Out[153]= 0.005 × 12000.9 enRel enLabNi-0.9 enRel
```

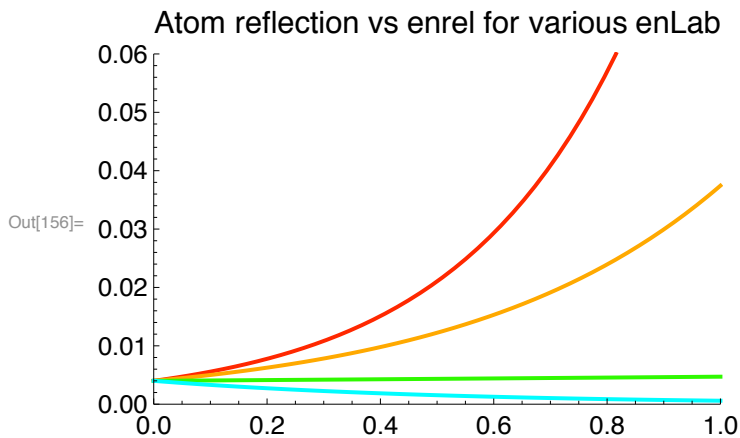
```
In[154]:= (rAtom[enRel]/.{a->0.5*10^-2,b->bNiFit})/.enLabNi->100
```

```
Out[154]= 0.005 × 120.9 enRel 250. enRel
```

```
In[155]:= (rAtom[enRel]/.{a->0.5*10^-2,b->bNiFit})/.enLabNi->100/.enRel->1
```

```
Out[155]= 0.0467986
```

```
In[156]:= modelNiReflectionPlot=Plot[{(rAtom[enRel]/.{a->0.4*10^-2,b->bNiFit})/.enLabNi->30,
rAtom[enRel]/.{a->0.4*10^-2,b->bNiFit}/.enLabNi->100, rAtom[enRel]/.{a->0.4*10^-2,b->bNiFit}
rAtom[enRel]/.{a->0.4*10^-2,b->bNiFit}/.enLabNi->10000},{enRel,0,1}, PlotRange->{{0,1},{0,6*
PlotStyle->{plotColorsLines[[1]],plotColorsLines[[2]],plotColorsLines[[3]],plotColorsLines[[4
PlotLabel-> "Atom reflection vs enrel for various enLab",TextStyle->{FontFamily->"Helvetica",}
```



One cannot brag about the similarity of these fits to Fig. 2.16, although the trend is there.

From the labels for Ni in Fig. 2.16 of Eckstein and Verbeek, the average energy of the backscattered atoms as a function of the incident energy is

```
In[157]:= enAvg={{30,.63},{100,.646},{300,577},{1000,.512},{3000,.438},{10000,.336}}
```

```
Out[157]= {{30, 0.63}, {100, 0.646}, {300, 577}, {1000, 0.512}, {3000, 0.438}, {10000, 0.336}}
```

```
In[158]:= exptNiMeanEnPlot=ListLogLinearPlot[enAvg,PlotRange->{{10,10000},{0,1}}, PlotStyle->plotColor
```

Assume

```
In[159]:= bNiFit = -0.9 * Log[ $\frac{\text{enLabNi}}{1200}$ ];
```

As of 12/13/10 19:55 the basis for this assumption is lost

Using our expression for the mean energy of the backscattered atoms and the scaled rAtom expression, the mean energies for backscattered H from H + incident on Au is

```
In[160]:= meanBackEnAu:= Integrate[enRel*rAtomAu,{enRel,0,1}]/ Integrate[rAtomAu,{enRel,0,1}]
```

```
In[161]:= meanBackEn/.b->bNiFit
```

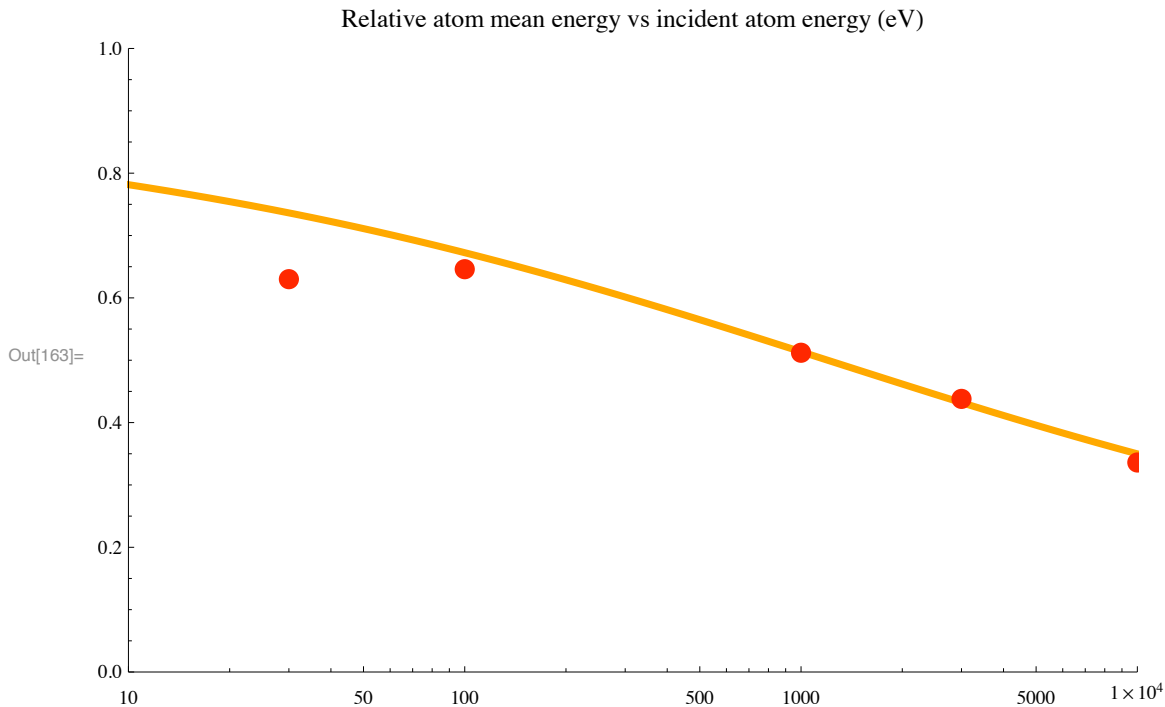
```
Out[161]= 
$$- \frac{1.11111 \left( 1 + \frac{590.559 \left( -1 - 0.9 \text{Log} \left[ \frac{\text{enLabNi}}{1200} \right] \right)}{\text{enLabNi}^{0.9}} \right)}{\left( -1 + \frac{590.559}{\text{enLabNi}^{0.9}} \right) \text{Log} \left[ \frac{\text{enLabNi}}{1200} \right]}$$

```

Something lost here

```
In[162]:= modelNiMeanEnPlot=LogLinearPlot[meanBackEn/.b->bNiFit,{enLabNi,10,10000}, PlotStyle->plotCol
PlotRange->{{10,10000},{0,1}}];
```

```
In[163]:= Show[modelNiMeanEnPlot,exptNiMeanEnPlot, ImageSize->500,
PlotLabel-> "Relative atom mean energy vs incident atom energy (eV)"]
```



This fit is good for incident energies equal to or greater than 100 eV.

■ Scaling to Au

We need to scale these results for nickel to those for gold. This is customarily done with $\text{enScale} = \text{enL} * \text{enLab}$, where from Table 2.1 $\text{enLNi} = 0.3575$ for nickel and $\text{enLAu} = 0.09305$ for gold. See Eckstein and Verbeek (1984).

```
In[164]:= Clear[enLabAu, enLabNi]
```

```
In[165]:= enLabAu=enLabNi*enLNi/enLAu
```

```
Out[165]= 
$$\frac{\text{enLabNi enLNi}}{\text{enLAu}}$$

```

```
In[166]:= denAuodenNi=D[enLabAu, enLabNi]
```

```
Out[166]= 
$$\frac{\text{enLNi}}{\text{enLAu}}$$

```

```
In[167]:= Clear[enLabAu, enLabNi, b]
```

```
In[168]:= enLNi = 0.3575;
```

```
In[169]:= enLAu = 0.09305;
```

```
In[170]:= bNiFit
```

```
Out[170]= -0.9 Log  $\left[ \frac{\text{enLabNi}}{1200} \right]$ 
```

I suspect that the scaling of the lowest energy data is not reliable. We will use this scaling anyhow. The distribution in energy of Au atoms is then

```
In[171]:= rAtomAu=a*Exp[bNiFit*enRel]*denAuodenNi /.enLabNi->enLabAu*enLAu/enLNI //Simplify
```

```
Out[171]= 3.84202 a e7.59247 enRel enLabAu-0.9 enRel
```

```
In[172]:= rAtomAu/.{enLabAu->30,enRel->0.5,a->5.*10^-2}
```

```
Out[172]= 1.85144
```

Note that while the denAuodenNi drops out of the mean energy it has a large effect on the reflected flux.

From our fits to RE and RN for H reflected from Au in files MultiBeamDoppler.nb and Multibeam>nb, we have

```
In[173]:= fitModelRE=0.5/(1+(enlab/7500)^(0.5))^2.8;
```

```
In[174]:= fitModelRN=0.6/(1+(enlab/30000)^(0.5))^3.0;
```

Using our expression for the mean energy of the backscattered atoms and the scaled rAtom expression, the mean energies for backscattered H from H + incident on Au is

```
In[175]:= meanBackEnAu:= Integrate[enRel*rAtomAu,{enRel,0,1}]/ Integrate[rAtomAu,{enRel,0,1}]
```

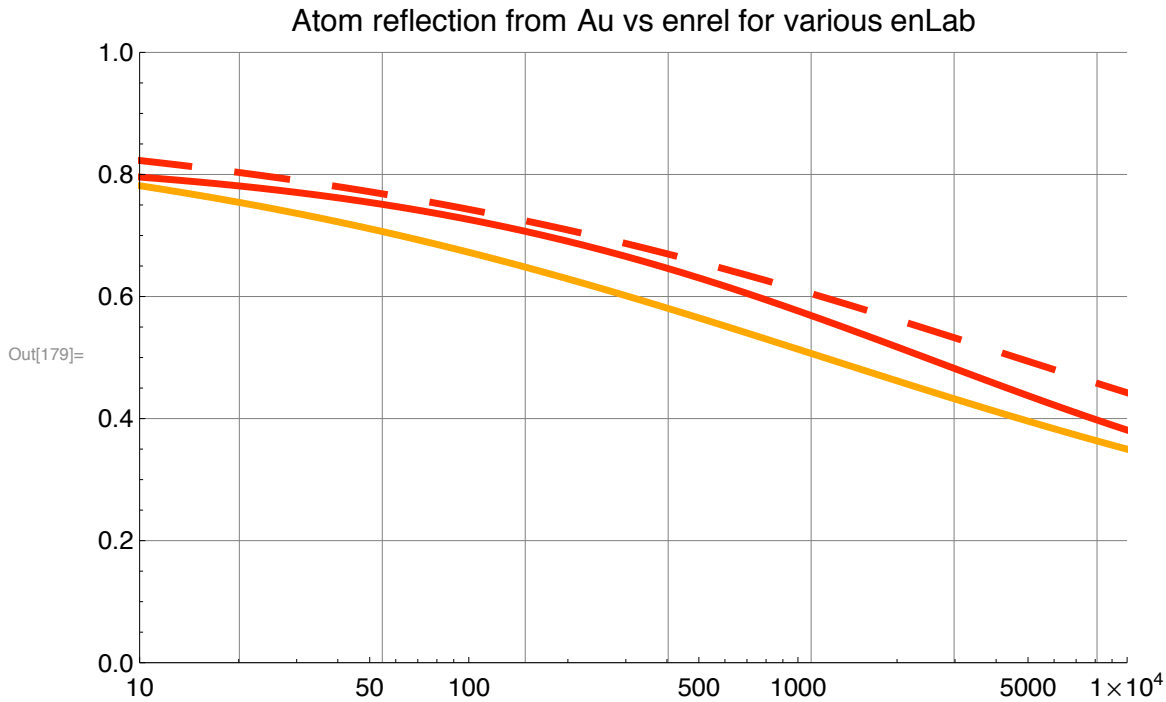
```
In[176]:= meanBackEnAu
```

```
Out[176]= -  $\frac{1. (13074.2 + 1. \text{enLabAu}^{0.9} - 1784.88 \text{Log}[\text{enLabAu}])}{\left(1. - \frac{1983.2}{\text{enLabAu}^{0.9}}\right) \text{enLabAu}^{0.9} (7.59247 - 0.9 \text{Log}[\text{enLabAu}])}$ 
```

```
In[177]:= modelAuMeanEnPlot=LogLinearPlot[Evaluate[meanBackEnAu], {enLabAu,10,10000},PlotRange->{{10,1},PlotStyle->plotColorsLines[[8]]];
```

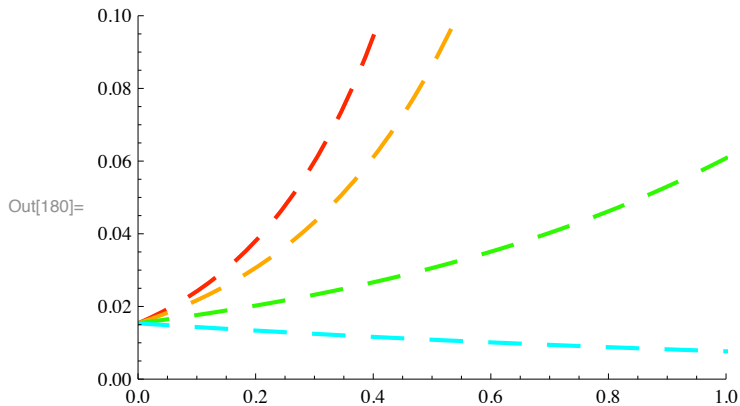
```
In[178]:= exptAuMeanEnPlot=LogLinearPlot[fitModelRE/fitModelRN,{enlab,10,10^4},PlotRange->{{10,10^4},{0},PlotStyle->plotColorsLines[[1]]];
```

```
In[179]:= Show[modelAuMeanEnPlot,exptAuMeanEnPlot,modelNiMeanEnPlot, ImageSize->500,
GridLines->Automatic, PlotLabel-> "Atom reflection from Au vs enrel for various enLab",
BaseStyle->{FontFamily->"Helvetica",FontSize->12}]
```

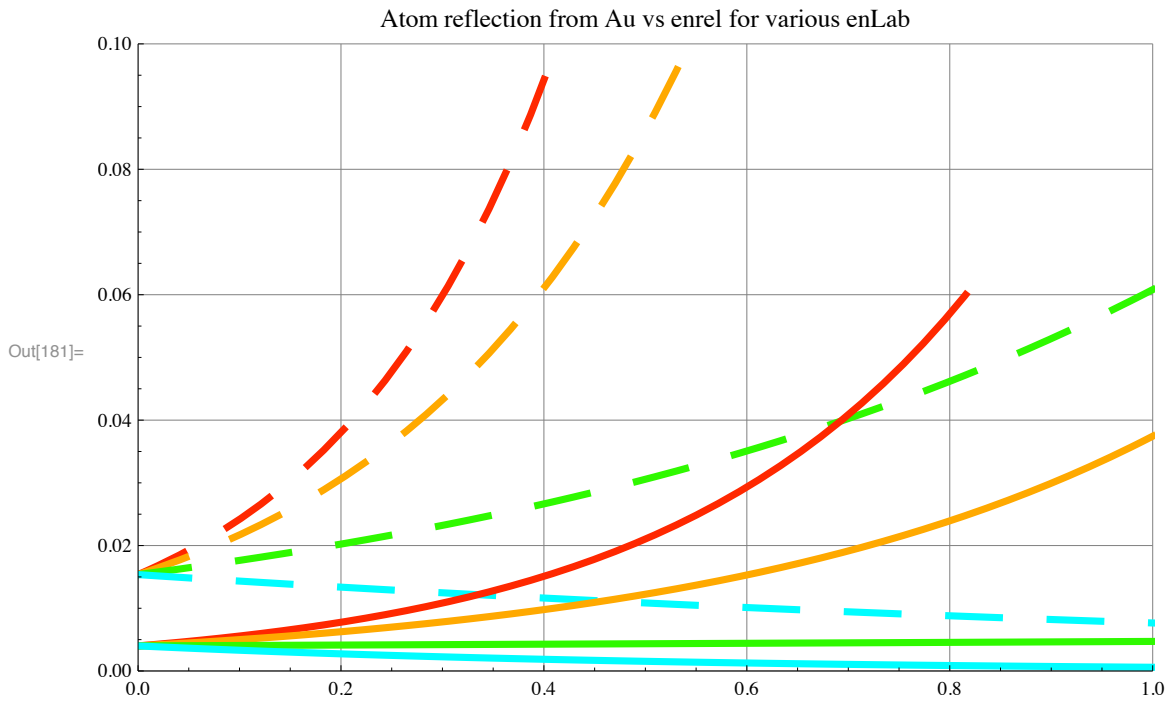


The Au model (red dash) is only rough fit to the Au experiment (red solid).

```
In[180]:= modelAuReflectionPlot=Plot[{rAtomAu/.{enLabAu->30,a->0.4*10^-2}, rAtomAu/.{enLabAu->100,a->0.4*10^-2},
rAtomAu/.{enLabAu->1000,a->0.4*10^-2}, rAtomAu/.{enLabAu->10000,a->0.4*10^-2}}, {enRel,0,1.},
PlotRange->{{0,1.},{0,0.1}}, PlotStyle->{plotColorsLines[[8]],plotColorsLines[[9]],plotColor:
plotColorsLines[[11]]}]
```



```
In[181]:= Show[modelAuReflectionPlot, modelNiReflectionPlot, ImageSize->500, GridLines->Automatic, PlotLabel-> "Atom reflection from Au vs enrel for various enLab"]
```



■ Number reflected RN

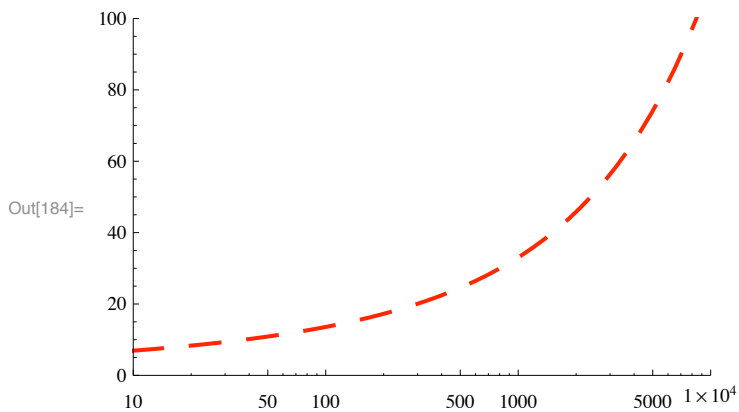
```
In[182]:= modelRNAu= Integrate[rAtomAu/.enRel->en/enLabAu,{en,0,enLabAu}]/.a->0.4*10^-2 //Simplify
```

$$\text{Out[182]= } \frac{30.478 \text{ enLabAu}^{0.1} - 0.0153681 \text{ enLabAu}^{1.1}}{7.59247 - 0.9 \text{ Log}[\text{enLabAu}]}$$

```
In[183]:= % /. enLabAu -> 10
```

Out[183]= 6.92298

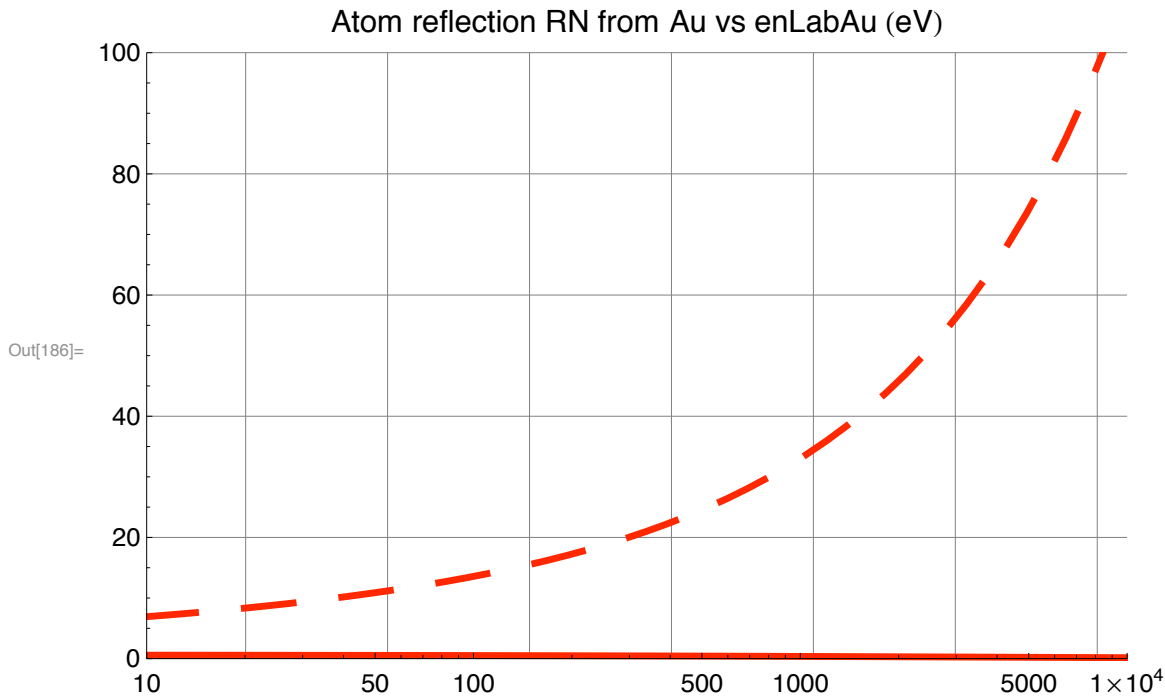
```
In[184]:= modelAuRNPlot=LogLinearPlot[modelRNAu, {enLabAu,10,10000},PlotRange->{{10,10000},{0,100}}, PlotStyle->plotColorsLines[[8]]]
```



```
In[185]:= exptAuRNPlot=LogLinearPlot[fitModelRN,{enlab,10,10^4},PlotRange->{{10,10^4},{0,1}}, PlotStyle->plotColorsLines[[1]]];
```



```
In[186]:= Show[modelAuRNPlot,exptAuRNPlot, ImageSize->500, GridLines->Automatic,
PlotLabel-> "Atom reflection RN from Au vs enLabAu (eV)", TextStyle->{FontFamily->"Helvetica"
```

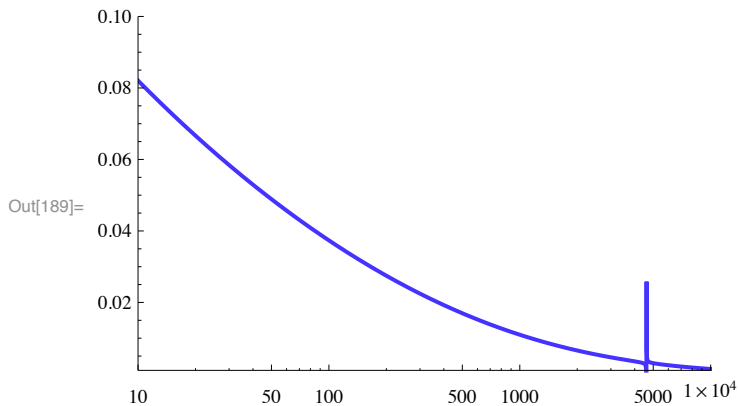


Something very wrong!!!

We therefore need to come up with an empirical $a[\text{enLab}]$ function. One approach would be to set it equal to the product of the reciprocal of the above expression and our empirical expression for RN.

```
In[187]:= a1=(7.59 - 0.9*Log[enLabAu])/(0.004*(7619*enLabAu^0.1 - 3.84*enLabAu))*0.6/(1+(enLabAu/30000
```

```
In[189]:= modela1Plot=LogLinearPlot[Evaluate[a1], {enLabAu,10,10000},PlotRange->{{10,10000},{0.001,0.1}
PlotStyle->plotColorsLines[[5]]]
```



```
In[190]:= rAtomAu1=(3.84*a1*E^(7.59*enRel))/enLabAu^(0.9*enRel)*0.004
```

```
Out[190]= 
$$\frac{2.304 e^{7.59 \text{ enRel}} \text{ enLabAu}^{-0.9 \text{ enRel}} (7.59 - 0.9 \text{ Log}[\text{enLabAu}])}{(1 + 0.0057735 \text{ enLabAu}^{0.5})^3 (7619 \text{ enLabAu}^{0.1} - 3.84 \text{ enLabAu})}$$

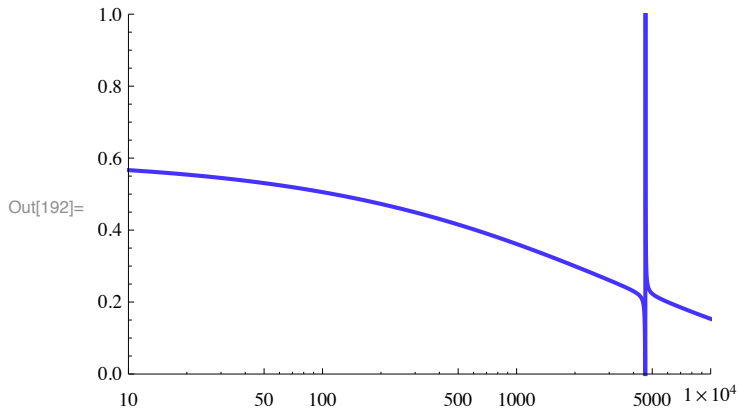
```

```
In[191]:= modelRNAu1= Integrate[rAtomAu1/.enRel->en/enLabAu,{en,0,enLabAu}]/Simplify
```

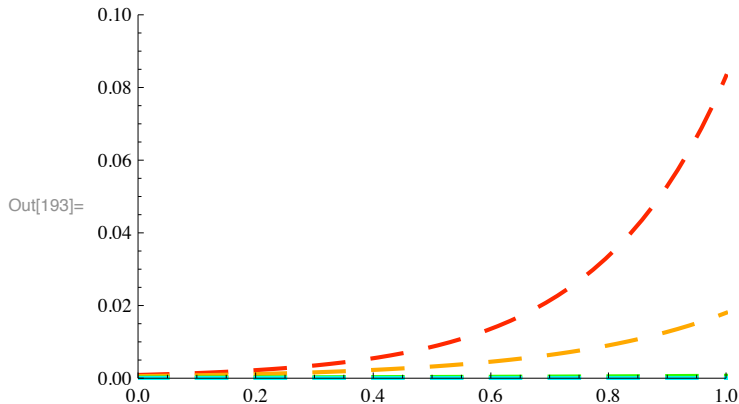
$$\text{Out[191]= } \frac{(-4102.23 \text{ enLabAu}^{0.1} + 2.0736 \text{ enLabAu}^{1.0}) (-8.43333 + 1. \text{ Log}[\text{enLabAu}])}{(1 + 0.0057735 \text{ enLabAu}^{0.5})^3 (7619. \text{ enLabAu}^{0.1} - 3.84 \text{ enLabAu}) (7.59 - 0.9 \text{ Log}[\text{enLabAu}])}$$

If the numerical accuracy were sufficient, the terms in the numerator would cancel two of the terms in the denominator leaving the empirical fit to RN and there would be no singularities in the following plot.

```
In[192]:= modelAu1RNPlot=LogLinearPlot[Evaluate[modelRNAu1], {enLabAu,10,10000},PlotRange->{{10,10000}}
PlotStyle->plotColorsLines[[5]]]
```



```
In[193]:= modelAuReflectionPlot=Plot[{rAtomAu1/.enLabAu->30, rAtomAu1/.enLabAu->100, rAtomAu1/.enLabAu
rAtomAu1/.enLabAu->10000}, {enRel,0,1.}, PlotRange->{{0,1.},{0,0.1}},
PlotStyle->{plotColorsLines[[8]],plotColorsLines[[9]],plotColorsLines[[10]],plotColorsLines
```



These values look much too small at small relative energies and at large incident energies.

■ Formulas for reflection of H resulting from incident H+ or H

In the following, k is the energy index for the initial ion. The reflected flux $RN[(k-1)*delE]$ is assumed spread evenly over the lower energy bins. The summation covers all energy bins above q in which there are initial ions. In the case of $H^+ + \text{surface} \rightarrow H$, we use

```
In[194]:= r1A[q_]:=Sum[fitRN[(k-1)*delE]/k*j1[m,k], {k,q,m}];
```

As a test assume

```
In[195]:= j1[m_,q_]=1;fitRN[en_]=1^en;m=13;delE=1;
```

```
In[196]:= Table[r1A[j],{j,1,m}]
```

```
Out[196]= {
  {
    1145993/360360, 785633/360360, 605453/360360, 485333/360360, 395243/360360,
    323171/360360, 263111/360360, 30233/51480, 11899/25740, 3013/8580, 431/1716, 25/156, 1/13
  }
}
```

```
In[197]:= N[Total[%]]
```

```
Out[197]= 13.
```

A second test is

```
In[198]:= j1[m_,q_]=If[q==5,1,0];
```

```
In[199]:= Table[r1A[j],{j,1,m}]
```

```
Out[199]= {
  {
    1/5, 1/5, 1/5, 1/5, 1/5, 0, 0, 0, 0, 0, 0, 0, 0
  }
}
```

In[200]:= **N[Total[%]]**

Out[200]= 1.

In[201]:= **r1A[q_]:=Sum[fitRN[(k-1)*delE]/k*j1[m,k]*(s1+s2*(If[k>1,2*(q-1)/(k-1),0]+If[q==1&&k==1,1,0])**

As a test assume

In[202]:= **j1[m_,q_]=1;fitRN[en_]=1^en;m=13;delE=1;s1=0;s2=0;s3=1;**

In[203]:= **Table[r1A[j],{j,1,m}]**

Out[203]= $\left\{ \frac{965813}{180180}, \frac{452993}{180180}, \frac{300533}{180180}, \frac{208133}{180180}, \frac{145763}{180180}, \right.$
 $\left. \frac{101411}{180180}, \frac{69071}{180180}, \frac{6473}{25740}, \frac{1999}{12870}, \frac{373}{4290}, \frac{35}{858}, \frac{1}{78}, 0 \right\}$

In[204]:= **N[Total[%]]**

Out[204]= 13.

In[205]:= **j1[m_,q_]=If[q==5,1,0];**

In[206]:= **Table[r1A[j],{j,1,m}]**

Out[206]= $\left\{ \frac{2}{5}, \frac{3}{10}, \frac{1}{5}, \frac{1}{10}, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 \right\}$

In[207]:= **N[Total[%]]**

Out[207]= 1.

■ Reflection of H resulting from incident H2+ or H2

The accepted model is that the incident molecule dissociates and that the fragments reflect as independent atoms or ions. Our problem is to find a simple way of expressing the conversion of incident H2+, j2[m,q], into reflected H jA[m,qprime].

In[208]:= **r2A[q_]:=Sum[If[OddQ[k],4*fitRN[(k-1)*delE]/(k-1)*j2[m,k],0]+If[EvenQ[k],4*fitRN[(k-1)*delE]**

As a test assume

In[209]:= **j2[m_,q_]=1;fitRN[en_]=1^en;m=13;delE=1;**

In[210]:= **Table[r2A[j],{j,1,m}]**

Out[210]= $\left\{ \frac{59}{5}, \frac{29}{5}, \frac{19}{5}, \frac{37}{15}, \frac{22}{15}, \frac{2}{3}, 0, 0, 0, 0, 0, 0, 0, 0 \right\}$

In[211]:= **N[Total[%]]**

Out[211]= 26.

A second test is

In[212]:= **j2[m_,q_]=If[q==5,1,0];**

```
In[213]:= Table[r2A[j], {j, 1, m}]
Out[213]= {1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}
```

```
In[214]:= N[Total[%]]
Out[214]= 2.
```

A third test is

```
In[215]:= j2[m_, q_] := If[q == 6, 1, 0];
In[216]:= Table[r2A[j], {j, 1, m}]
Out[216]= {2/3, 2/3, 2/3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}
```

```
In[217]:= N[Total[%]]
Out[217]= 2.
```

I do not understand this, but it seems to work!!!!

■ Reflection of H resulting from incident H3+

The accepted model is that the incident molecule dissociates and that the fragments reflect as independent atoms or ions. Our problem is to find a simple way of expressing the conversion of incident H3+, j2[m,q], into reflected H jA[m,qprime].

```
In[218]:= r3A[q_] := Sum[If[k >= 3 && IntegerQ[k/3], 9*fitRN[(k-1)*delE]/k*j3[m,k], 0] +
  If[k >= 3 && IntegerQ[(k+1)/3], 9*fitRN[(k-1)*delE]/(k-2)*j3[m,k], 0] +
  If[k >= 3 && IntegerQ[(k+2)/3], 9*fitRN[(k-1)*delE]/(k-1)*j3[m,k], 0], {k, 3*q, m}] + If[q == 1, 3*j3[r
```

As a test assume

```
In[219]:= j3[m_, q_] := 1; fitRN[en_] := 1^en; m = 13; delE = 1;
In[220]:= Table[r3A[j], {j, 1, m}]
Out[220]= {21, 12, 9/2, 3/2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}
In[221]:= N[Total[%]]
Out[221]= 39.
```

A second test is

```
In[222]:= j3[m_, q_] := If[q == 6, 1, 0];
In[223]:= Table[r3A[j], {j, 1, m}]
Out[223]= {3/2, 3/2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}
```

In[224]:= **N[Total[%]]**

Out[224]= 3.

A third test is

In[225]:= **j3[m_,q_]=If[q==7,1,0];**

In[226]:= **Table[r3A[j],{j,1,m}]**

Out[226]= $\left\{\frac{3}{2}, \frac{3}{2}, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0\right\}$

In[227]:= **N[Total[%]]**

Out[227]= 3.

A fourth test is

In[228]:= **j3[m_,q_]=If[q==8,1,0];**

In[229]:= **Table[r3A[j],{j,1,m}]**

Out[229]= $\left\{\frac{3}{2}, \frac{3}{2}, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0\right\}$

```
In[230]:= N[Total[%]]
```

```
Out[230]= 3.
```

I do not understand all of this, but it seems to work!!!!

reflection of H+ as fast H

■ 1992 Model

In Petrovic et al, Phys. Rev. Lett., 68, 325 (1992) for an AuPd cathode, we assumed the reflection of fast H+ as fast H with an energy of 2/3 of the incident H+ energy and 60% of the number, i.e., $RN = 0.6$. The mean energy of the reflected atoms is $2/3 = RE/RN$.

Assume reflection is independent of energy and neglect diffuse scattering

```
r1A[m_, q_] := 0.5 * j1[m, q] * reflectionFactor
```

Production of a reflected fast H atom from H+ (j1) incident on cathode. In order to partially take into account the spread in energies of the reflected atoms, we will take the mean energy of the reflected atoms as 2/3 of the available energy, i.e., 2/3 of the incident ion energy. In units of q this is 2/3*k in the summation. We also must take into account the atoms lost, i.e., assume 50% reflected.

```
r1A[m_, q_] = 0.5 * If[1 <= q <= m, Sum[If[Round[2/3*k] == q, (j1[m, k]), 0], {k, q+1, m}], 0] * reflectionFac
```

This assumption corresponds to $RN = 0.5$ and $RE = 0.33$. I do not find data for H on Au in Eckstein and Verbeek, J. Plasma Phys. and Nuclear Fusion: Special Issue 1984, p. 12. These values are in the general region shown for other surfaces.

■ NIFS Model - 2005

The following input values of RE and RN come from the NIFS data Web site under the category CURVES, in which one enters the incident atom mass, the target atom mass, and the angle of incidence (0 deg) and get a plot of their empirical fit to Monte Carlo calculations of the backscattering coefficients RN and RE. I then digitized the curves and fitted them as given below. They do not give data for incident molecules, so I will take them to be the same as for atoms of the same energy per atom.

```
In[231]:= Import [
    "c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceeffects\\HAtomReflection\\REHOnAu
    .dat", "CSV" ] // TableForm
```

```
Out[231]//TableForm=
  1.56537E+00    4.90951E-01
  8.71392E+00    4.56601E-01
  4.57266E+01    4.03533E-01
  2.07025E+02    3.13929E-01
  6.97332E+02    2.26126E-01
  2.28141E+03    1.39812E-01
  6.83237E+03    7.61031E-02
  2.23802E+04    3.13185E-02
  4.84257E+04    1.42561E-02
  9.58581E+04    7.00267E-03
```

```
In[232]:= rEmodel=Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceeffects\\HAtomReflecti
```

```
In[233]:= rEmodelPlot= ListLogLogPlot[rEmodel,PlotRange->{{1,10^5},{10^-3,1}},PlotStyle->plotColorsPoir
```

```
In[234]:= fitModelRE=0.5/(1+(enlab/7500)^(0.5))^2.8;
```

```
In[235]:= fitModelREPlot=LogLogPlot[fitModelRE,{enlab,1,10^5},PlotRange->{{1,10^5},{10^-3,1}}, PlotSty
```

This RE seems high compared to the 1/3 we assumed above.

```
In[236]:= Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceeffects\\HAtomReflection\\RNHC
```

```
Out[236]//TableForm=
  2.28179E+00    5.56887E-01
  3.91022E+01    5.53411E-01
  3.81634E+02    4.49483E-01
  1.62567E+03    3.22163E-01
  8.26437E+03    1.79092E-01
  2.77485E+04    8.55769E-02
  5.80428E+04    4.53073E-02
  1.00000E+05    2.52457E-02
```

```
In[237]:= rNmodel=Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceeffects\\HAtomReflecti
```

```
In[238]:= rNmodelPlot=ListLogLogPlot[rNmodel,PlotRange->{{1,10^5},{10^-3,1}},PlotStyle->plotColorsPoir
```

```
In[239]:= fitModelRN=0.6/(1+(enlab/30000)^(0.5))^3.0;
```

The following formula was replaced by formulas based on Eckstein and Biersack (1985) as of 05/03/07

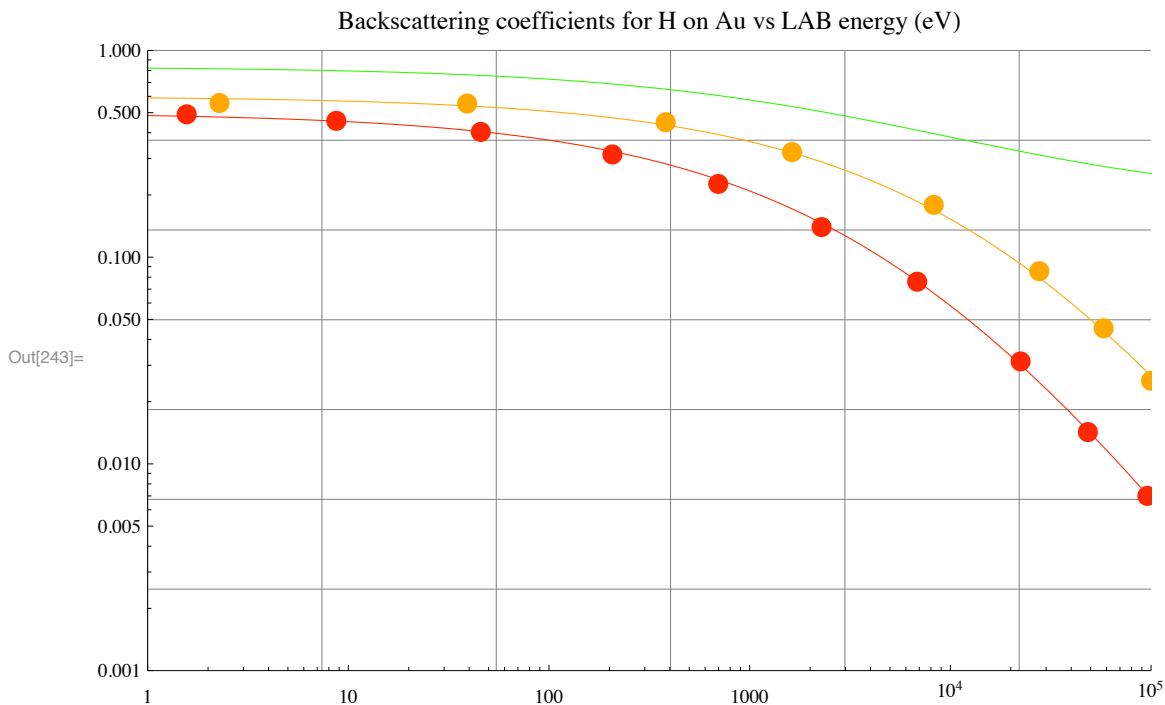
```
In[240]:= fitRN[enlab_]=0.6/(1+(enlab/30000)^(0.5))^3.0;
```

```
In[241]:= fitModelRNPlot=LogLogPlot[fitModelRN,{enlab,1,10^5},PlotRange->{{1,10^5},{10^-3,1}}, PlotSty
```

```
In[242]:= avgEnModelPlot=LogLogPlot[fitModelRE/fitModelRN,{enlab,1,10^5},PlotRange->{{1,10^5},{10^-3,1}
  PlotStyle->plotColorsPoints[[3]]];
```



```
In[243]:= Show[rEmodelPlot, rNmodelPlot, fitModelRNPlot, fitModelREPlot, avgEnModelPlot, ImageSize->500, Grid
PlotLabel-> "Backscattering coefficients for H on Au vs LAB energy (eV)"]
```



In the following fitModelRN replaces the $RN = 1/2$, fitModelRE replaces the $RE = 1/3$, and fitModelRE/fitModelRN replaces the $Re/RN = 2/3$.

```
r1A[m_, q_] = If[1 <= q <= m, (fitModelRN/.enlab->q*deLE) * Sum[If[Round[((fitModelRE/fitModelRN)/.en:
(j1[m, k]), 0], {k, q+1, m}], 0] * reflectionFactor;
```

Revision of 04/05/06. See notebook AtomReflection030906.nb. Here fitRE/fitRN = 1/2 because of uniform distribution, i.e., we do not have a choice for RE/RN. A further revision and simplification is

```
In[244]:= r1A[q_] := Sum[fitRN[(k-1)*deLE]/k*j1[m, k], {k, q, m}] * reflectionFactor;
```

To make this correspond to a uniform distribution in energy for the reflected H atoms, we divide by the number of bins k .

■ Eckstein and Biersack, Appl. Phys. A 38, 123 (1985).

The authors give rather larger RN values for H on various heavy metal surfaces than I had obtained from Eckstein and Verbeek (1984).

■ Reflection of H atoms by amorphous tungsten and gold

The following input values of RE and RN come from Eckstein and Beirsack (1985). They do not give data for incident molecules, so I will take them to be the same as for atoms of the same energy per atom.

For tungsten from Fig. 3 b

```
In[245]:= Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceeffects\\HAtomReflection\\REWE  
"CSV"]//TableForm
```

```
Out[245]/TableForm=
```

1.93444E-01	7.90168E-02
2.86275E-01	1.74880E-01
4.80777E-01	3.66515E-01
6.75976E-01	4.93151E-01
9.85834E-01	6.05289E-01
1.95422E+00	6.78806E-01
2.95806E+00	6.80497E-01
4.90083E+00	6.57872E-01
9.90522E+00	5.80731E-01
1.96580E+01	5.31816E-01
4.93404E+01	4.44794E-01
9.79422E+01	3.92596E-01
2.99924E+02	2.94349E-01
1.00506E+03	2.20807E-01

```
In[246]:= rEcalc=Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceeffects\\HAtomReflectic  
"Table"];
```

```
In[247]:= rEcalcWPlot= ListLogLogPlot[rEcalc,PlotRange->{{0.1,10^4},{10^-3,1}},PlotStyle->plotColorsPoi
```

We do not fit this because the fit is not used. From Fig. 3 a

```
In[248]:= Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceeffects\\HAtomReflection\\RNWE
"CSV"]//TableForm
```

```
Out[248]/TableForm=
```

2.01153E-01	1.56805E-01
3.03205E-01	3.09944E-01
5.09120E-01	5.80040E-01
7.02755E-01	7.24038E-01
1.00585E+00	8.24581E-01
2.02564E+00	8.57835E-01
3.06124E+00	8.59249E-01
4.97108E+00	8.45241E-01
9.83703E+00	7.87495E-01
1.98173E+01	7.47352E-01
5.04182E+01	7.09916E-01
9.97701E+01	6.61416E-01
2.93179E+02	5.52783E-01
9.77029E+02	4.45549E-01

```
In[249]:= rNcalc=Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceeffects\\HAtomReflectic
"Table"];
```

```
In[250]:= rNcalcWPlot=ListLogLogPlot[rNcalc,PlotRange->{{0.1,10^4},{10^-3,1}},PlotStyle->plotColorsPoi
```

The following formula is used in H2CrossSections.nb as of 05/03/07

```
In[251]:= fitRNW[enlab_]=0.95/(1+(0.4/enlab)^2)/(1+(enlab/7))^0.15/(1+(enlab/30000))^1.35;
```

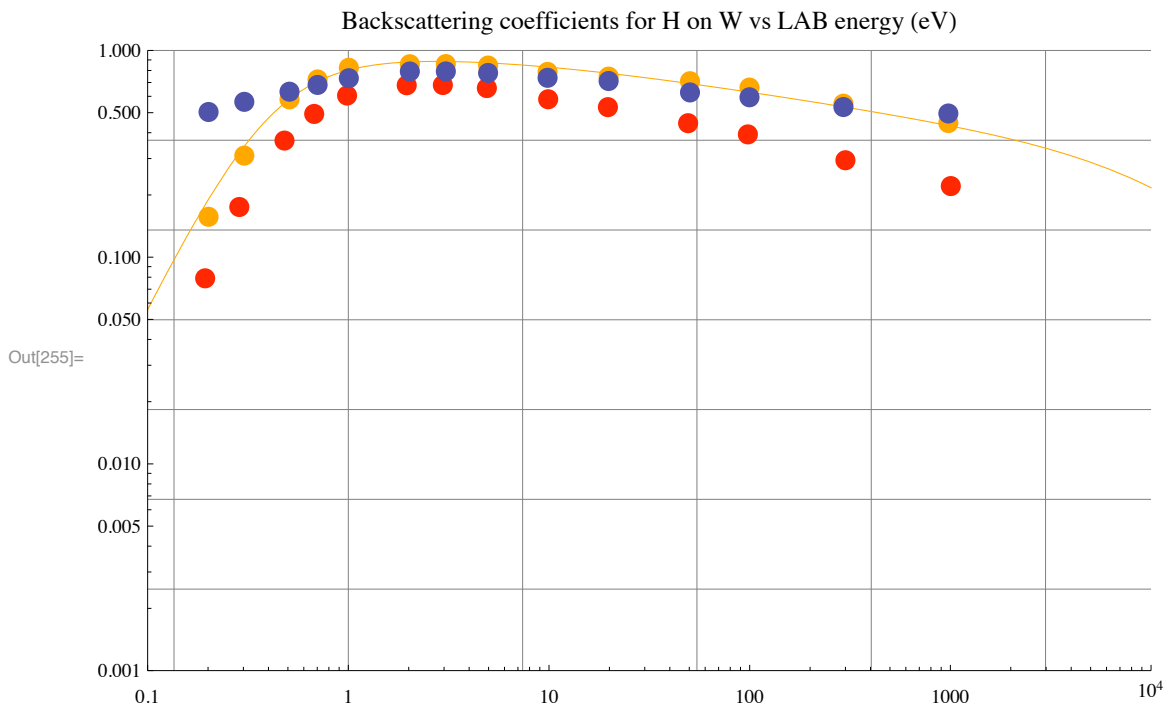
Here we have forced the fit to approach $(\text{enlab})^{-3/2}$ at energies above 30000 eV as predicted by theory and as shown by the universal plot. See Eckstein and Verbeek (1984).

```
In[252]:= fitCalcRNWPlot=LogLogPlot[fitRNW[enlab],{enlab,0.1,10^4},PlotRange->{{0.1,10^4},{10^-3,1}},
```

```
In[253]:= avgEnCalcWTable=Table[{rNcalc[[j,1]],rEcalc[[j,2]]/rNcalc[[j,2]],{j,Length[rEcalc]}};
```

```
In[254]:= avgEnCalcWPlot=ListLogLogPlot[avgEnCalcWTable,PlotRange->{{0.1,10^4},{10^-3,1}}, PlotStyle->
```

```
In[255]:= Show[rEcalcWPlot,rNcalcWPlot,fitCalcRNWPlot,avgEnCalcWPlot, ImageSize->500,GridLines->Automa
PlotLabel-> "Backscattering coefficients for H on W vs LAB energy (eV)"]
```



We use the energy scaling given by Eckstein and Verbeek (1984) to extrapolate the calculations of Eckstein and Biersack (1985) for tungsten to obtain $RN(enlab)$ for Au using the values of ϵ_{L} in their Table 2.1.

```
In[256]:= fitRNAu[enlab_]=0.95/(1+(0.4/(1.08*enlab))^2)/(1+((1.08*enlab/7))^0.15/(1+((1.08*enlab)/3)
```

■ Reflection of H atoms by amorphous carbon

The following input values of RE and RN come from Eckstein and Beirsack (1985). They do not give data for incident molecules, so I will take them to be the same as for atoms of the same energy per atom.

```
In[257]:= Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceEffects\\HAtomReflection\\RECI
"CSV"]//TableForm
```

```
Out[257]//TableForm=
  4.86904E-01    1.75438E-03
  6.77098E-01    1.60319E-02
  9.81221E-01    5.94225E-02
  1.45118E+00    1.46883E-01
  1.93195E+00    2.16629E-01
  2.91971E+00    2.86281E-01
  4.74887E+00    2.97893E-01
  9.77266E+00    2.62990E-01
  1.94114E+01    2.07840E-01
  4.96599E+01    1.44603E-01
  9.86495E+01    1.12193E-01
  2.97040E+02    6.86810E-02
  9.80512E+02    3.07573E-02
```

```
In[258]:= rEcalc=Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceEffects\\HAtomReflectic
"Table"];
```

```
In[259]:= rEcalcCPlot= ListLogLogPlot[rEcalc,PlotRange->{{0.1,10^4},{10^-3,1}},PlotStyle->plotColorsPoi
```

We do not fit this because the fit is not used.

```
In[260]:= Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceeffects\\HAtomReflection\\RNCF
"CSV"]//TableForm
```

Out[260]//TableForm=

3.90682E-01	1.59158E-03
5.07608E-01	1.13764E-02
7.09080E-01	6.89446E-02
9.93433E-01	1.93149E-01
1.52446E+00	3.88890E-01
1.95817E+00	5.03457E-01
3.01056E+00	6.17267E-01
5.06716E+00	6.18551E-01
1.00314E+01	5.16145E-01
1.98589E+01	4.30693E-01
4.96634E+01	3.34236E-01
9.83178E+01	2.78900E-01
2.99705E+02	1.90470E-01
9.82654E+02	9.87758E-02

```
In[261]:= rNcalc=Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceeffects\\HAtomReflectic
"Table"];
```

```
In[262]:= rNcalcCPlot=ListLogLogPlot[rNcalc,PlotRange->{{0.1,10^4},{10^-3,1}},PlotStyle->plotColorsPoi
```

The following formula is used in H2CrossSections.nb as of 05/03/07

```
In[263]:= fitRNC[enlab_]=0.8/(1+(1.4/enlab)^4)/(1+(enlab/5)^0.35/(1+(enlab/3000))^1.15;
```

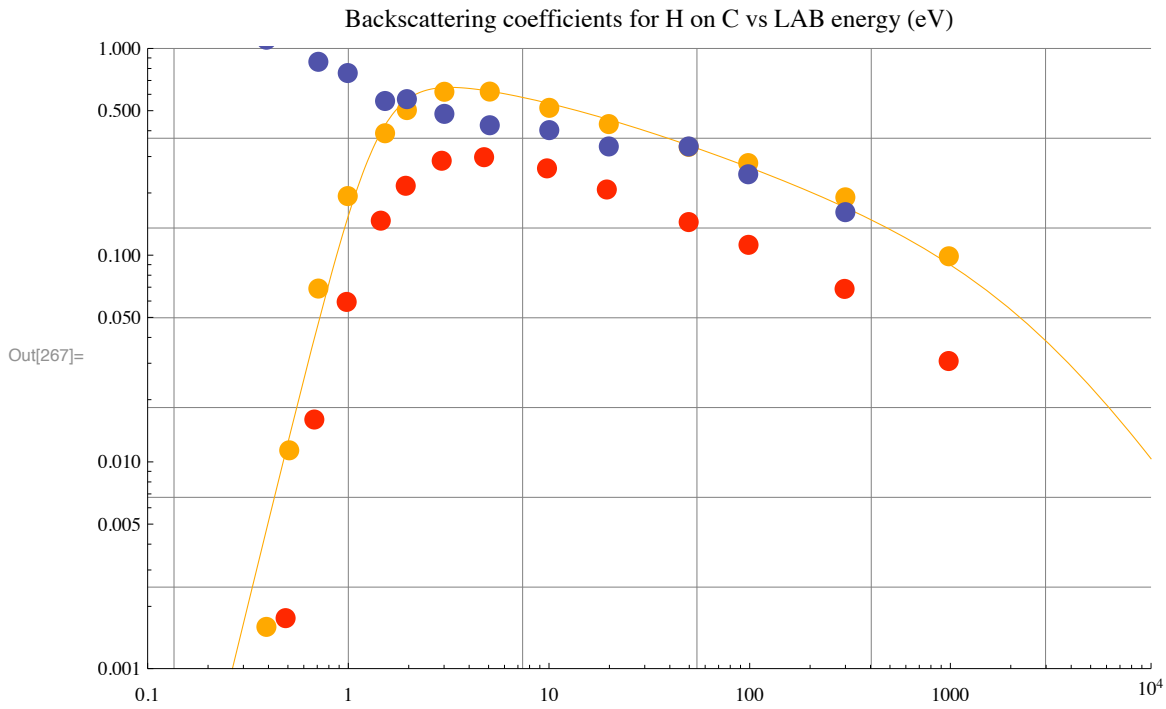
Here we have forced the fit to approach $(enlab)^{-3/2}$ at energies above 3000 eV as predicted by theory and as shown by the universal plot. See Eckstein and Verbeek (1984).

```
In[264]:= fitCalcRNCPlot=LogLogPlot[fitRNC[enlab],{enlab,0.1,10^4},PlotRange->{{0.1,10^4},{10^-3,1}},
```

```
In[265]:= avgEnCalcCTable=Table[{rNcalc[[j,1]],rEcalc[[j,2]]/rNcalc[[j,2]],{j,Length[rEcalc]}};
```

```
In[266]:= avgEnCalcCPlot=ListLogLogPlot[avgEnCalcCTable,PlotRange->{{0.1,10^4},{10^-3,1}}, PlotStyle->
```

```
In[267]:= Show[rEcalcCPlot,rNcalcCPlot,fitCalcRNCPlot,avgEnCalcCPlot, ImageSize->500,GridLines->Automa
PlotLabel-> "Backscattering coefficients for H on C vs LAB energy (eV)"]
```



■ Reflection of H atoms by nickel

The following input values of RE and RN come from Eckstein and Beirsack (1985). They do not give data for incident molecules, so I will take them to be the same as for atoms of the same energy per atom.

```
In[268]:= Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceeffects\\HAtomReflection\\RENi
"CSV"]//TableForm
```

```
Out[268]/TableForm=
```

1.95705E-01	1.51220E-02
2.95506E-01	5.92933E-02
3.88634E-01	1.19404E-01
4.93601E-01	1.86081E-01
6.82576E-01	3.10422E-01
9.75922E-01	4.43932E-01
1.95863E+00	6.12749E-01
2.99322E+00	6.22335E-01
5.06277E+00	5.80061E-01
9.97551E+00	5.40353E-01
1.99841E+01	4.54255E-01
3.05250E+01	4.02380E-01
5.07556E+01	3.62461E-01
1.03419E+02	3.04689E-01
3.11139E+02	2.26904E-01
1.01809E+03	1.35257E-01

```
In[269]:= rEcalc=Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceeffects\\HAtomReflectic
"Table"];
```

```
In[270]:= rEcalcNiPlot= ListLogLogPlot[rEcalc,PlotRange->{{0.1,10^4},{10^-3,1}},PlotStyle->plotColorsPc
```

We do not fit this because the fit is not used.

```
In[271]:= Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceeffects\\HAtomReflection\\RNNiE
"CSV"]//TableForm
```

```
Out[271]/TableForm=
```

1.93152E-01	4.48990E-02
2.93841E-01	1.37261E-01
3.94794E-01	2.45694E-01
4.89951E-01	3.56655E-01
6.73725E-01	5.48865E-01
9.81224E-01	7.17860E-01
1.46252E+00	8.26197E-01
1.96765E+00	8.46272E-01
2.93371E+00	8.57035E-01
4.95987E+00	8.19167E-01
9.83819E+00	7.83288E-01
1.97420E+01	6.98522E-01
3.01211E+01	6.44600E-01
4.86543E+01	6.01884E-01
9.87510E+01	5.43044E-01
2.95518E+02	4.46867E-01
9.80436E+02	3.08942E-01

```
In[272]:= rNcalc=Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\surfaceeffects\\HAtomReflection
"Table"];
```

```
In[273]:= rNcalcNiPlot=ListLogLogPlot[rNcalc,PlotRange->{{0.1,10^4},{10^-3,1}},PlotStyle->plotColorsPc
```

The following formula is used in H2CrossSections.nb as of 05/03/07

```
In[274]:= fitRNNi[enlab_]=0.95/(1+(0.6/enlab)^2.5)/(1+(enlab/10))^0.23/(1+(enlab/30000))^1.27;
```

Here we have forced the fit to approach $(enlab)^{-3/2}$ at energies above 3000 eV as predicted by theory and as shown by the universal plot. See Eckstein and Verbeek (1984).

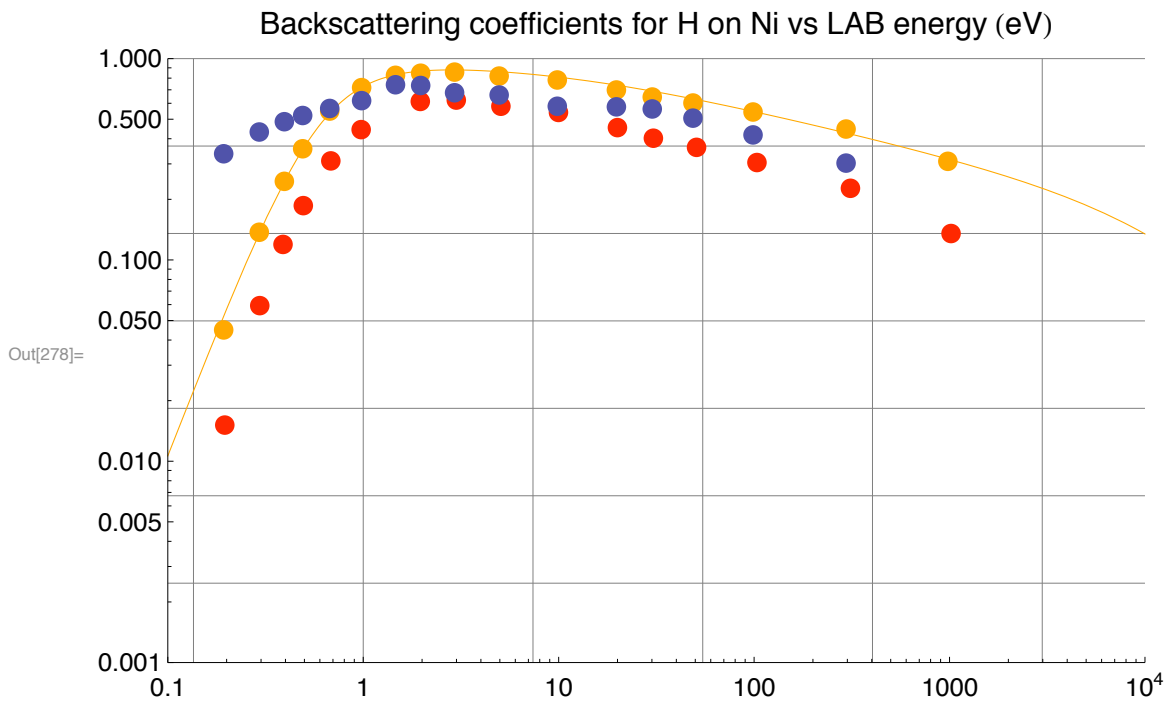
```
In[275]:= fitCalcRNNiPlot=LogLogPlot[fitRNNi[enlab],{enlab,0.1,10^4},PlotRange->{{0.1,10^4},{10^-3,1}},
```

```
In[276]:= avgEnCalcNiTable=Table[{rNcalc[[j,1]],rEcalc[[j,2]]/rNcalc[[j,2]]},{j,Length[rEcalc]}];
```

```
In[277]:= avgEnCalcNiPlot=ListLogLogPlot[avgEnCalcNiTable,PlotRange->{{0.1,10^4},{10^-3,1}}, PlotStyle
```



```
In[278]:= Show[rEcalcNiPlot,rNcalcNiPlot,fitCalcRNNiPlot,avgEnCalcNiPlot, ImageSize->500,GridLines->Au  
PlotLabel-> "Backscattering coefficients for H on Ni vs LAB energy (eV)", TextStyle->{FontFar
```



```
In[279]:= Quit[]
```

Electron yields for secondary and backscattered electrons

We want to assemble data for backscattered and secondary electrons resulting from incident electrons and then use this data to obtain analytic approximations for use in modeling.

Setup notebook environment

```
In[89]:= a = 1;
```

```
In[90]:= ClearAll["Global`*"];
```

```
In[91]:= Remove["Global`*"];
```

```
In[92]:= startclock = SessionTime[];
```

```
In[93]:= Off[General::spell];
```

```
In[94]:= Off[General::spell1];
```

```
In[95]:= now := StringForm["`~/`~/`~ `~:``:``", Date][[2]],
         Date][[3]], Date][[1]], Date][[4]], Date][[5]], Date][[6]]]
```

```
In[96]:= plotColorsLines = {
  (*1*) {Red, Thickness[0.007], Dashing[{}]},
  (*2*) {Hue[0.1], (*Orange,*)Thickness[0.007], Dashing[{}]},
  (*3*) {Green, Thickness[0.007], Dashing[{}]},
  (*4*) {Cyan, Thickness[0.007], Dashing[{}]},
  (*5*) {Blue, Thickness[0.007], Dashing[{}]},
  (*6*) {Purple, Thickness[0.007], Dashing[{}]},
  (*7*) {Yellow, Thickness[0.007], Dashing[{}]},
  (*8*) {Pink, Thickness[0.007], Dashing[{}]},
  (*9*) {Black, Thickness[0.004], Dashing[{}]},
  (*10-dash*) {Red, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*11-dash*) {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*12-dash*) {Green, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*13-dash*) {Cyan, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*14-dash*) {Blue, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*15-dash*) {Purple, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*16-dash*) {Yellow, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*17-dash*) {Pink, Thickness[0.007], Dashing[{0.02, 0.02}]},
  (*18-dash*) {Black, Thickness[0.007], Dashing[{0.02, 0.02]}}
};
```

```
In[97]:= plotColorsPoints = {
  (*1*) {Red, PointSize[0.02]},
  (*2*) {Hue[0.1], PointSize[0.02]},
  (*3*) {Green, PointSize[0.02]},
  (*4*) {Cyan, PointSize[0.02]},
  (*5*) {Blue, PointSize[0.02]},
  (*6*) {Purple, PointSize[0.02]},
  (*7*) {Yellow, PointSize[0.02]},
  (*8*) {Pink, PointSize[0.02]},
  (*9*) {Black, PointSize[0.02]},
  (*10*) {Red, PointSize[0.014]},
  (*11*) {Hue[0.1], PointSize[0.014]},
  (*12*) {Green, PointSize[0.014]},
  (*13*) {Cyan, PointSize[0.014]},
  (*14*) {Blue, PointSize[0.014]},
  (*15*) {Purple, PointSize[0.014]},
  (*16*) {Yellow, PointSize[0.014]},
  (*17*) {Pink, PointSize[0.014]},
  (*18*) {Black, PointSize[0.014]}
};
```

```
In[99]:= SetDirectory [NotebookDirectory []]
```

```
Out[99]= C:\Users\avp\Documents\Mathbook\HYDROGEN\SurfaceEffects\Secondary&BackscatteredElectrons
```

Secondary electrons not including backscattered electrons.

See reviews such as Thomas, E. W., Material Interaction for Fusion 1, 79, (1991) and Thomas, E W (1985) Particle Interactions with surfaces, ORNL Report No. 6088 Vol. 3. These data are also available at <http://www-cfadc.phy.ornl.gov/redbooks/redbooks.html>.

■ Dependence of total yield of secondaries on primary energy and angle of incidence.

Secondary yield versus primary energy (eV) for normal incidence on graphite. This does not include backscattered primary electrons. The dividing energy between secondary electrons δ and back scattered primary electrons η is usually taken to be 50 eV. See Thomas (1985). Most authors say that the angular distribution of product electrons has a cosine distribution.

For graphite: Woods, Hopkins, and McCracken, Surface Science 162, 928 (1985).

Data is very similar for an "as mounted" Poco (pyrolytic) graphite surface, such as used in our discharge experiments. The yields increase by roughly 50% for a 45 deg angle of incidence.

```
In[100]:= Import ["Woods&McCracken85Fig4.dat", "CSV"] // TableForm
```

```
Out[100]/TableForm=
```

4.40049E+01	2.38901E-01		
7.25102E+01	3.07292E-01		
1.00921E+02	3.54631E-01		
1.36010E+02	4.39857E-01		
1.64345E+02	4.70353E-01		
2.10087E+02	5.12411E-01		
2.79543E+02	5.21811E-01		
3.79330E+02	5.22759E-01		
4.87743E+02	5.12118E-01		
5.87412E+02	4.86750E-01		
6.91425E+02	4.62430E-01		
8.45287E+02	4.28584E-01		
1.01866E+03	3.91559E-01		
1.18990E+03	3.64011E-01		
1.39806E+03	3.44844E-01		
1.62577E+03	3.31973E-01		
1.85566E+03	3.23310E-01		
2.00748E+03	3.17887E-01		
Woods	Hopkins	& McCracken	
Surface Science 162	928	(1985)	

```
In[101]:= woodsData = Drop [Import ["Woods&McCracken85Fig4.dat", "Table"], -3];
```

```
In[102]:= woodsYieldPlot = ListLogLogPlot [woodsData, PlotRange -> {{1, 10000}, {0.01, 2}},
PlotStyle -> {Hue[1], PointSize[0.04]}, ImageSize -> 432, PlotMarkers -> {"♦"},
PlotLabel -> "Secondary electron yield  $\delta$  vs primary energy (eV) for normal incidence",
GridLines -> Automatic];
```

The following is my fit versus primary energy enp to this data from Woods et al:

```
In[103]:= fitSecondaryGraphite [enp_] = 0.6 * (enp / 100) ^ 0.8 / (1 + (enp / 300)) ^ 1.5
```

$$\text{Out[103]= } \frac{0.0150713 \text{ enp}^{0.8}}{\left(1 + \frac{\text{enp}}{300}\right)^{1.5}}$$

```
In[104]:= fitSecondaryPlot = LogLogPlot [fitSecondaryGraphite [en], {en, 1, 10^4},
      PlotRange -> {{1, 100 000}, {0.01, 2}}, PlotStyle -> plotColorsLines [[1]]];
```

Based on Sternglass (1954), Kollath (1956) gives a semiempirical fit of

```
In[105]:= empiricalfitδ = maxYield * 2.72 ^ 2 * (enp / enmax) * Exp[-2 * (enp / enmax) ^ 0.5]
```

$$\text{Out[105]= } \frac{7.3984 e^{-2 \left(\frac{\text{enp}}{\text{enmax}}\right)^{0.5}} \text{ enp maxYield}}{\text{enmax}}$$

The two constants are adjusted for an eye fit near the maximum and appear to differ from literature values.

```
In[106]:= empiricalfitδGraphite = empiricalfitδ /. {enmax -> 340, maxYield -> 0.53}
```

$$\text{Out[106]= } 0.0115328 e^{-0.108465 \text{ enp}^{0.5}} \text{ enp}$$

```
In[107]:= empiricalfitPlot = LogLogPlot [empiricalfitδGraphite, {enp, 1, 10^4},
      PlotRange -> {{1, 100 000}, {0.01, 2}}, PlotStyle -> plotColorsLines [[10]]];
```

Woods et al. J. Phys. D 20, 1130 (1987) find that the maximum yield increased from 0.7 to 0.9 for a surface bombarded with a fluence of $1.7E18 \text{ H}_2^+$ ions cm^2 . Deposition of Ni caused about the same increase in the maximum, although the maximum is shifted to higher energies.

The maximum yields are typical 1.3 at for Cu and 1.8 for Au.

■ Lin and Joy, Surface and Interface Analysis 37, 895 (2005).

These authors give a similar "universal law" for the relative δ along with tables of empirical constants for 44 elements. This compilation is said to be based on data compiled at <http://pciserver.bio.utk.edu/metrology/download/E-solid/database.doc>. I COULD NOT GET A RESPONSE.

These authors derive the following formula. They also obtain Monte Carlo solutions.

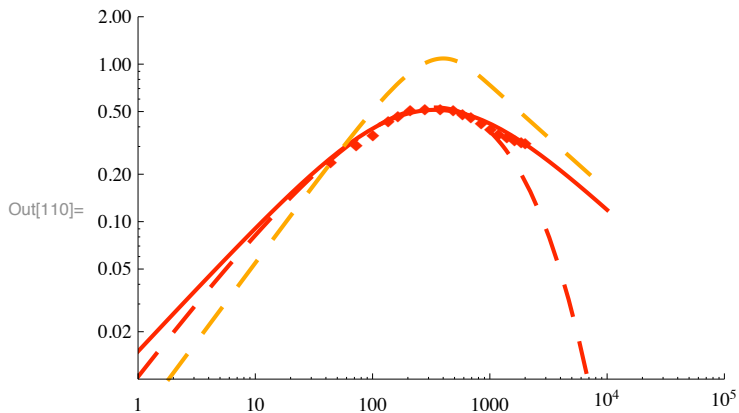
```
In[108]:= empiricalδLinJoy = δmax * 1.28 * (enp / enpmax) ^ -(2 / 3) (1 - Exp[-1.614 * (enp / enpmax) ^ (5 / 3)])
```

$$\text{Out[108]= } \frac{1.28 \left(1 - e^{-1.614 \left(\frac{\text{enp}}{\text{enpmax}}\right)^{5/3}}\right) \delta_{\text{max}}}{\left(\frac{\text{enp}}{\text{enpmax}}\right)^{2/3}}$$

For C (carbon), they give $\delta_{\text{max}} = 1.06$ and $\text{enpmax} = 400 \text{ eV}$.

```
In[109]:= empiricalδLinJoyPlot = LogLogPlot [(empiricalδLinJoy /. {δmax -> 1.06, enpmax -> 400}),
      {enp, 1, 10^4}, PlotRange -> {{1, 100 000}, {0.01, 2}}, PlotStyle -> plotColorsLines [[11]]];
```

```
In[110]:= Show[fitSecondaryPlot, empiricalfitPlot, woodsYieldPlot, empiricalδLinJoyPlot]
```



The fit of Lin & Joy's expression for C is poor for Poco graphite, although the relative decrease at high energies is about right..

Backscattered electrons η

A very interesting paper is that by G. Gergely, B. Gruzza, and M. Menyhárd, *Acta Physica Hungaricae* 48, 337 (1980)

Based on Sternglass (1954), the yield of backscattered electrons η integrated over product energy is often cited to be equal to 0.08 at low energies and to decrease slowly with energy above 3 keV. However, Verma, *J. Phys. D* 10, 1167 (1977), shows values for carbon at 2 keV ranging from 0.06 to 0.22 and decreasing by a factor of ~ 2 as the primary energy increases from 1 to 10 keV. Darlington and Cosslett, *J. Phys D* 5, 1969 (1972) found a large drop in η for carbon from 1 to 5 keV and a slight rise to 10 keV. Gergely et al found roughly an inverse energy dependence for η from 1 to 3 keV, but does not give a magnitude. I have not found data for pyrolytic graphite or Poco graphite.

I propose:

```
In[111]:= etaCarbon [enp_] = 0.08 / (1 + 1000 / enp)
```

$$\text{Out[111]} = \frac{0.08}{1 + \frac{1000}{\text{enp}}}$$

Distribution in energy of the secondary electrons

According to Sternglass (1954) the electron energy distributions for the higher energy product electrons for C are rather flat up to $\sim 70\%$ of the incident energy E_p and then decrease. For metals he found distributions are broadly peaked toward the primary energy, i.e., possibly elastic scattering with poor energy resolution. Darlington and Cosslett (1972) found distributions for carbon and for metals that increased roughly linearly from zero at $0.4 E_p$ to about 0.7 of E_p and then more slowly to a narrow elastic peak, but did not look at low product energies. Gergely's (1980) much higher energy resolution data show a rather flat distribution above 272 eV, the Auger threshold??, with the narrow elastic peak containing only a small fraction of the product electrons. The distribution in energy below the elastic peak is often discussed in terms of diffusion down in energy. To me this seems inconsistent with the sharp structures observed and attributed to plasmon and Auger excitation unless, for example, the diffusion occurs deep in the solid and the sharp excitation occurs near the surface for exiting electrons.

■ Energy independent assumption

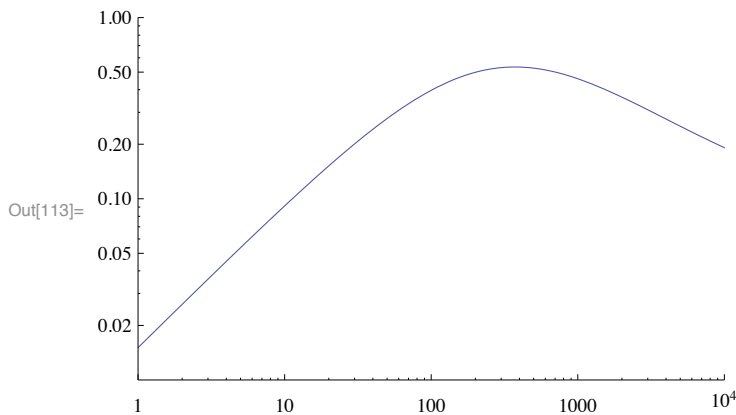
In view of the wide spread in experimental results, one assumption is that the exit energy distribution is independent of product electron energy and that it has a magnitude equal to the sum of the secondary and backscattered components.

Keep in mind that electron collisions with H2 at below 16.6 eV do not excite Halpha.

```
In[112]:= reflectedElectron [enp_] = fitSecondaryGraphite [enp] + etaCarbon [enp]
```

$$\text{Out[112]} = \frac{0.08}{1 + \frac{1000}{\text{enp}}} + \frac{0.0150713 \text{ enp}^{0.8}}{\left(1 + \frac{\text{enp}}{300}\right)^{1.5}}$$

```
In[113]:= LogLogPlot [%, {enp, 1, 10 000}, PlotRange -> {{1, 10 000}, {0.01, 1}}]
```



■ Chung and Everhardt (1974)

Chung and Everhardt, J. Appl. Phys. 45, 707 (1974) and Chung, JAP 46, 465 (1975) derive simple exit energy distributions based on an escape model with various assumptions as to the mean free path for escape. (It seems similar to McCracken's model for atom escape? CHECK)

```
In[114]:= fChung = aChung * en / (en + φ) ^ 4
```

$$\text{Out[114]= } \frac{aChung \, en}{(en + \phi)^4}$$

```
In[115]:= δChung = Integrate[fChung, {en, 0, Infinity}, Assumptions -> {φ > 0}]
```

$$\text{Out[115]= } \frac{aChung}{6 \, \phi^2}$$

Here I have replaced their $E-E_f-\phi$ by en and $E-E_f$ by $en+\phi$, where ϕ is the work function. We set $\deltaChung=empiricalfit\deltaGraphite$. We found in the literature (GOOGLE) that the photoelectric work function is $\phi = 4.6$ for pyrolytic graphite.

```
In[116]:= fChung1 = fChung /. {aChung -> 6 * φ ^ 2 * empiricalfitδGraphite, φ -> 4.6}
```

$$\text{Out[116]= } \frac{1.4642 \, e^{-0.108465 \, enp^{0.5}} \, en \, enp}{(4.6 + en)^4}$$

■ Analytic approach

■ Piecewise function

```
In[117]:= electronDist2 =
  Piecewise[{{fChung1, 0 < en < 50 && enp > 50}, {fChung1, 16.6 ≤ enp < 50 && 16.6 ≤ en ≤ enp},
    {10 * etaCarbon[enp] / enp, enp ≥ en ≥ 50 && enp > 50}}]
```

$$\text{Out[117]= } \begin{cases} \frac{1.4642 \, e^{-0.108465 \, enp^{0.5}} \, en \, enp}{(4.6+en)^4} & (0 < en < 50 \, \&\& \, enp > 50) \, || \, (16.6 \leq enp < 50 \, \&\& \, 16.6 \leq en \leq enp) \\ \frac{0.8}{\left(1 + \frac{1000}{enp}\right) \, enp} & enp \geq en \geq 50 \, \&\& \, enp > 50 \\ 0 & \text{True} \end{cases}$$

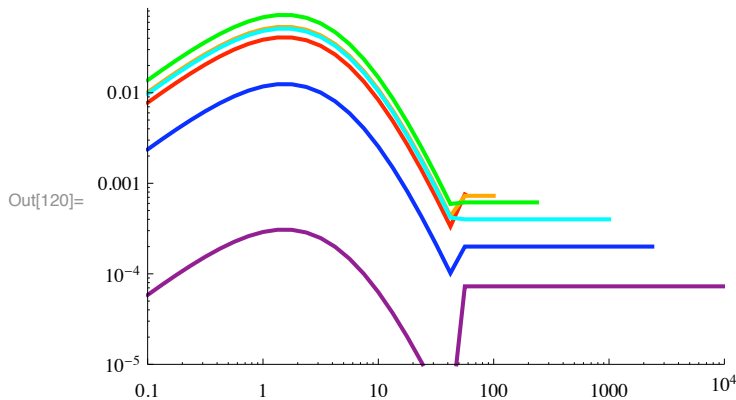
```
In[118]:= enpList = {60, 100, 300, 1000, 3000, 10 000}
```

```
Out[118]= {60, 100, 300, 1000, 3000, 10 000}
```

```
In[119]:= Do[
  electronDistTable[i] = Table[
    {0.1 * 10^((j - 1) / 8), electronDist2 /. {en -> 0.1 * 10^((j - 1) / 8), enp -> enpList[[i]]}},
    {j, 1, 41}];, {i, Length[enpList]}
```



```
In[120]:= ListLogLogPlot [Table [electronDistTable [i], {i, Length [enpList]}], Joined -> True,
  PlotRange -> {{0.1, 10 000}, {0.00001, All}}, PlotStyle -> plotColorsLines]
```



Note the unrealistic discontinuities at 50 eV.

- Combined distribution using a continuous function instead of the Mathematica's Piecewise function.

Combine Chung and Everhardt with Gergley, et al

- first trial

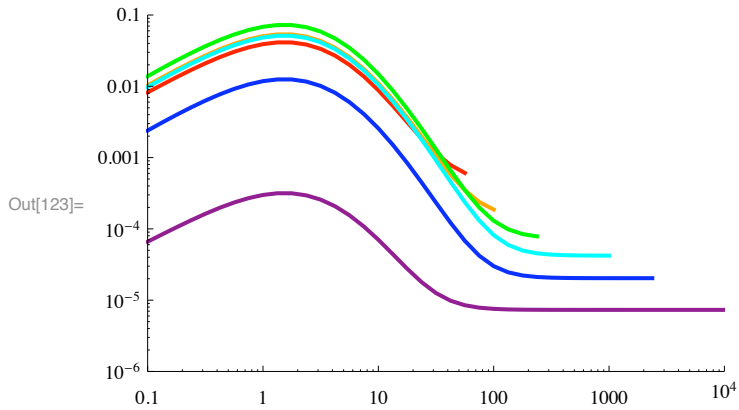
```
In[121]:= analyticDist1 = ((1.464 * en * enp) / (E ^ (0.1084 * enp ^ 0.5) *
  (4.6 + en) ^ 4) + 0.08 / (1 + 1000 / enp) / (enp - 50)) UnitStep [enp - en]
```

$$\text{Out[121]=} \left(\frac{0.08}{\left(1 + \frac{1000}{\text{enp}}\right) (-50 + \text{enp})} + \frac{1.464 e^{-0.1084 \text{enp}^{0.5}} \text{en enp}}{(4.6 + \text{en})^4} \right) \text{UnitStep}[-\text{en} + \text{enp}]$$

Note that I have effectively neglected the elastic scattering peak. Gergely et al (1980) find its integral is small. However, Fig. 7 of Furman and Pivi, Phys. Rev. Spec. Topics - Accelerators and Beams, 5, 124404 (2002) shows experimental (not theory) data for Cu at an incident energy of 10 eV for which the energy-integrated backscattered primaries roughly equals the intergrated lower energy electrons. Again, our excitation observations are not sensitive to such low energy electrons. At 30 eV the experimental backscattered component is ~ 20% of the total.

```
In[122]:= Do [
  electronDistTable2 [i] = Table [
    {0.1 * 10 ^ ((j - 1) / 8), analyticDist1 /. {en -> 0.1 * 10 ^ ((j - 1) / 8), enp -> enpList [[i]]},
    {j, 1, 41}];, {i, Length [enpList]}
```

```
In[123]:= ListLogLogPlot [Table[electronDistTable2 [i], {i, Length[enpList]}], Joined → True,
  PlotRange → {{0.1, 10 000}, {0.000001, 0.1}}, PlotStyle → plotColorsLines]
```



```
In[124]:= electronδTable1 = Table[{enpList[[j]],
  Integrate[(analyticDist1 /. enp -> enpList[[j]]), {en, 0, 50}]}, {j, Length[enpList]}];
```

```
In[125]:= electronηTable1 = Table[
  {enpList[[j]], Integrate[(analyticDist1 /. enp -> enpList[[j]]), {en, 50, enpList[[j]]}],
  {j, Length[enpList]}];
```

```
In[126]:= analyticδAndη =
  ListLogLogPlot[{electronδTable1, electronηTable1}, PlotRange → {{10, 10 000}, {0.01, 1}},
  PlotStyle → plotColorsLines[{{1, 5}}], Joined → True];
```

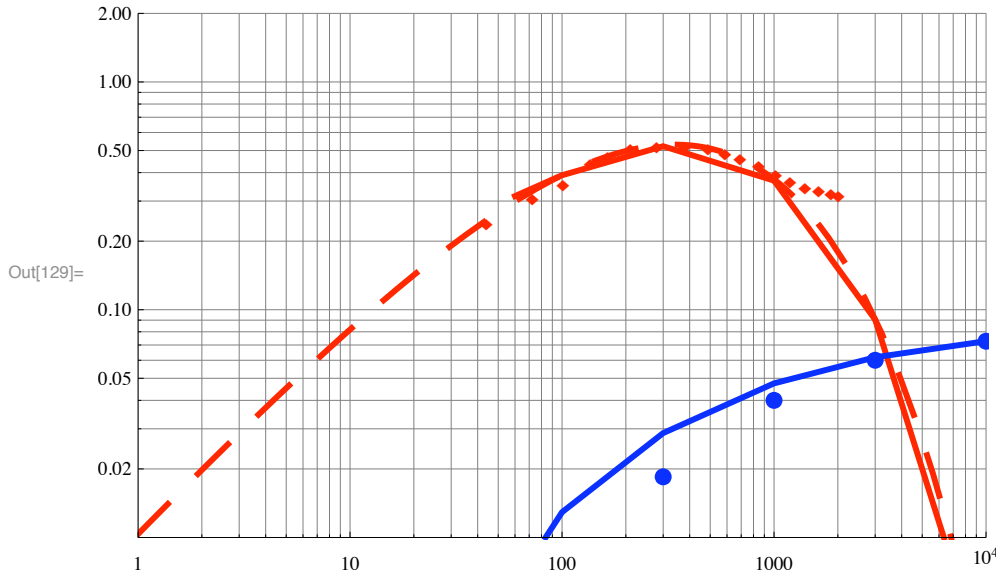
```
In[127]:= etaTable = Table[{enpList[[j]], etaCarbon[enpList[[j]]}], {j, Length[enpList]}
```

```
Out[127]= {{60, 0.0045283}, {100, 0.00727273},
  {300, 0.0184615}, {1000, 0.04}, {3000, 0.06}, {10 000, 0.0727273}}
```

```
In[128]:= etaPlot = ListLogLogPlot[etaTable,
  PlotRange → {{10, 10 000}, {0.01, 1}}, PlotStyle → plotColorsPoints[{{5}}];
```

```
In[129]:= Show[{woodsYieldPlot, analyticδAndη, etaPlot, empiricalfitPlot},
  PlotLabel -> "Secondary δ and backscattered η
    electron yield vs primary energy (eV): normal incidence"]
```

Secondary δ and backscattered η electron yield vs primary energy (eV): normal incidence



From these fits it would seem that our distributions are reasonable, but could be improved.

■ second trial

```
In[130]:= enpList = {30, 60, 100, 300, 1000, 3000, 10 000}
```

```
Out[130]= {30, 60, 100, 300, 1000, 3000, 10 000}
```

The backscattered (higher energy) component at low incident energies has been raised from initial trial.

```
In[131]:= analyticDist2 = ((1.464 * en * enp) / (E^(0.1084 * enp^0.5) *
  (4.6 + en)^4 / (1 + 10 / (enp)) + 0.08 / (enp) (* (1 + 1 / (enp)) *)) UnitStep[enp - en]
```

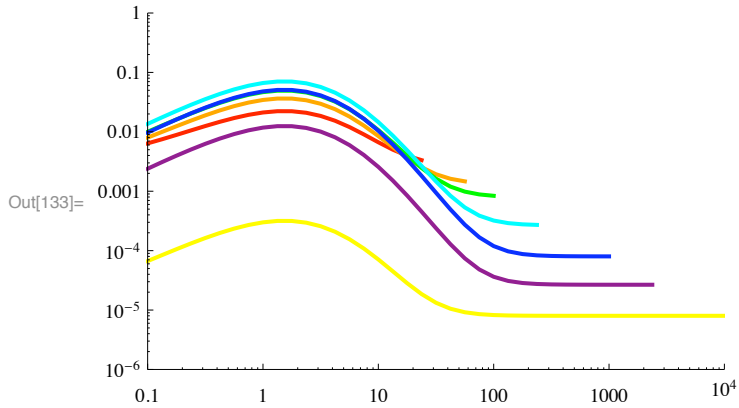
```
Out[131]= 
$$\left( \frac{0.08}{enp} + \frac{1.464 e^{-0.1084 enp^{0.5}} en enp}{(4.6 + en)^4 \left(1 + \frac{10}{enp}\right)} \right) \text{UnitStep}[-en + enp]$$

```

Note that I have effectively neglected the elastic scattering peak. Gergely et al (1980) find its integral is small. However, Fig. 7 of Furman and Pivi, Phys. Rev. Spec. Topics - Accelerators and Beams, 5, 124404 (2002) shows experimental (not theory) data for Cu at an incident energy of 10 eV for which the energy-integrated elastic backscattered primaries roughly equals the intergrated lower energy electrons. Again, our excitation observations are not sensitive to such low energy electrons. For 30 eV primaries, the experimental elastic backscattered component is ~ 20% of the total.

```
In[132]:= Do[
  electronDistTable2[i] = Table[
    {0.1 * 10^((j - 1) / 8), analyticDist2 /. {en -> 0.1 * 10^((j - 1) / 8), enp -> enpList[[i]]}},
    {j, 1, 41}];, {i, Length[enpList]}
```

```
In[133]:= analyticDist2LogPlot = ListLogLogPlot [Table [electronDistTable2 [i], {i, Length [enpList]}],
  Joined → True, PlotRange → {{0.1, 10 000}, {0.000001, 1}}, PlotStyle → plotColorsLines]
```



```
In[134]:= electronδTable2 = Table [{enpList [[j]],
  Integrate [(analyticDist2 /. enp -> enpList [[j]]), {en, 0, 50}], {j, Length [enpList]}}];
```

```
In[135]:= electronηTable2 = Table [
  {enpList [[j]], Integrate [(analyticDist2 /. enp -> enpList [[j]]), {en, 50, enpList [[j]]}],
  {j, Length [enpList]}}];
```

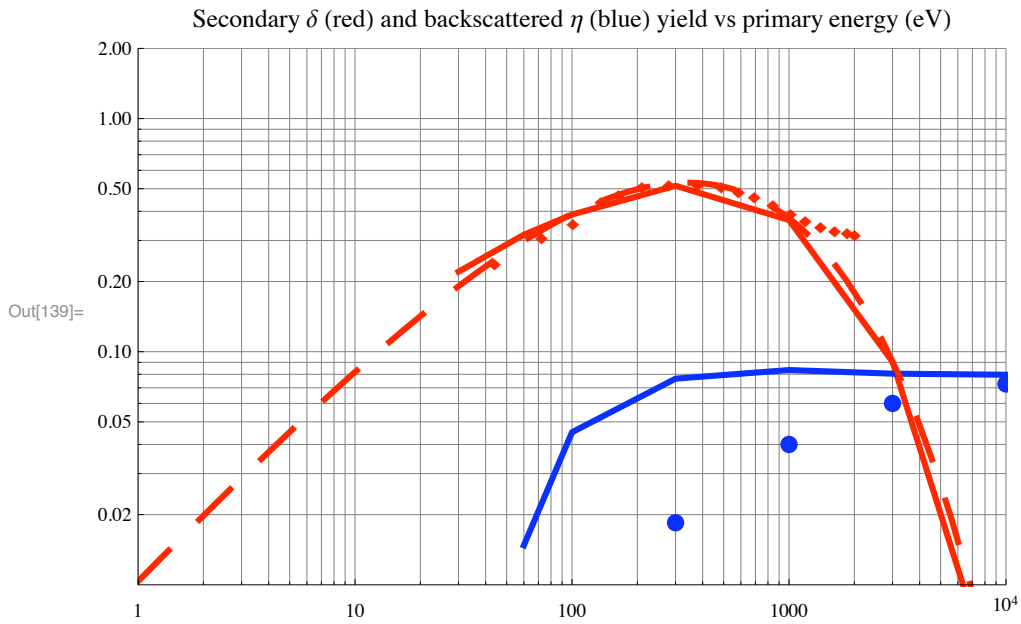
```
In[136]:= analyticδandηPlot =
  ListLogLogPlot [{electronδTable2, electronηTable2}, PlotRange → {{10, 10 000}, {0.01, 1}},
  PlotStyle → plotColorsLines [[{1, 5}]], Joined → True];
```

```
In[137]:= etaTable = Table [{enpList [[j]], etaCarbon [enpList [[j]]}], {j, Length [enpList]}
```

```
Out[137]= {{30, 0.0023301}, {60, 0.0045283}, {100, 0.00727273},
  {300, 0.0184615}, {1000, 0.04}, {3000, 0.06}, {10 000, 0.0727273}}
```

```
In[138]:= etaPlot = ListLogLogPlot [etaTable,
  PlotRange → {{10, 10 000}, {0.01, 1}}, PlotStyle → plotColorsPoints [[5]]];
```

```
In[139]:= Show[{woodsYieldPlot, analyticδandηPlot, etaPlot, empiricalfitPlot},
PlotLabel -> "Secondary δ (red) and backscattered η (blue) yield vs primary energy (eV)"]
```



This choice for the backscattered component (blue) is closer to the essentially constant value of Sternglass (1950), not Woods et al (1987).

On the question of the units of the electron energy distributions: We integrated over exit electron energy in eV (not delE) to get dimensionless reflection coefficients.

Electron scattering from metals

- Experiment - Knights and Coleman, Appl. Surf. Sci. 85, 43 (1995). Electron scattering by Ag.
- Experimental energy distributions

```
In[140]:= Import["knights&coleman95fig2applsrfsci.dat", "CSV"] // TableForm
```

```
Out[140]//TableForm=
```

-4.14819E+00	6.36308E-02
-2.67333E+00	4.55863E-02
-1.19879E+00	5.56446E-02
-9.22822E-01	1.02612E-01
-7.40084E-01	2.43213E-01
-5.61699E-01	7.67887E-01
-3.44877E-01	1.96705E+00
-1.77960E-01	3.50343E+00
-4.95867E-02	4.37468E+00
1.31665E-01	4.64643E+00
3.63140E-01	4.55286E+00
5.50656E-01	4.27192E+00
1.01701E+00	3.78502E+00
1.57754E+00	3.12018E+00
2.13945E+00	2.33356E+00
3.11674E+00	1.49092E+00
3.99752E+00	1.03232E+00
5.15372E+00	6.67519E-01
6.86176E+00	4.06024E-01
8.89152E+00	2.19621E-01
1.17036E+01	1.27262E-01
1.46073E+01	9.11509E-02
1.69578E+01	6.41489E-02
1.85706E+01	7.42719E-02
1.99532E+01	6.55518E-02

```
In[141]:= knights1000 = Import["knights&coleman95fig2applsrfsci.dat", "Table"];
```

The experimental data is multiplied by a scale factor that gives an eye-ball fit to the model.

```
In[142]:= knights1000Table = Table[{%[[j, 1]], %[j, 2]] * 0.12}, {j, Length[%]}];
```

```
In[143]:= knights1000LogPlot = ListLogLogPlot[knights1000Table,
PlotRange -> {{0.1, 10 000}, {0.000001, 1}}, PlotStyle -> plotColorsPoints[[5]]];
```

```
In[144]:= knights100 = Import["knights&coleman95fig3dapplsurfsci.dat", "Table"];
```

The experimental data is multiplied by a scale factor that is the same as for 1000 eV and gives an eye-ball fit to the model.

```
In[145]:= knights100Table = Table[{{%[[j, 1]], %[j, 2]] * 0.04}, {j, Length[%}}];
```

```
In[146]:= knights100LogPlot = ListLogLogPlot[knights100Table,
      PlotRange -> {{0.1, 10 000}, {0.000001, 1}}, PlotStyle -> plotColorsPoints[[3]]];
```

The authors claim an energy resolution of 0.5 eV, so we ignore data below about 1 eV.

■ Relative secondary electron yield δ for Ag from Knights and Coleman

```
In[147]:= Import["knights&coleman95fig5bapplsurfsci.dat", "CSV"] // TableForm
```

```
Out[147]//TableForm=
```

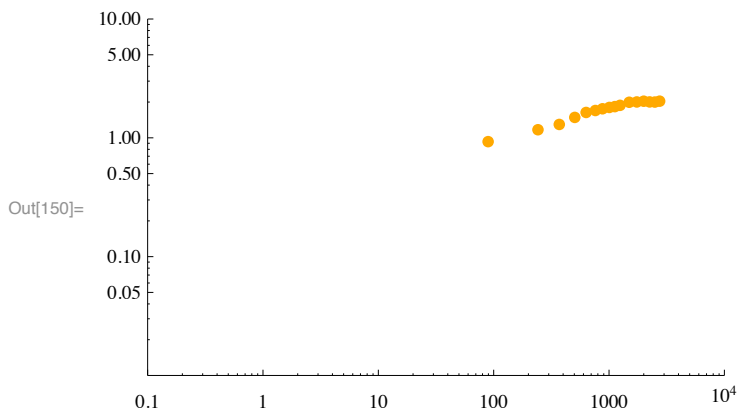
8.94783E+01	4.64286E-01
2.42033E+02	5.84805E-01
3.70378E+02	6.47989E-01
5.04686E+02	7.42699E-01
6.32971E+02	8.17344E-01
7.61481E+02	8.49010E-01
8.77752E+02	8.77797E-01
1.00631E+03	9.00867E-01
1.12265E+03	9.15327E-01
1.24508E+03	9.38390E-01
1.49601E+03	9.95984E-01
1.74107E+03	1.00200E+00
1.99835E+03	1.01662E+00
2.24965E+03	1.00258E+00
2.49476E+03	9.99994E-01
2.74589E+03	1.01747E+00

```
In[148]:= knights $\delta$  = Import["knights&coleman95fig5bapplsurfsci.dat", "Table"];
```

The experimental data is multiplied by a scale factor that gives an eye-ball fit to the model.

```
In[149]:= knights $\delta$ Table = Table[{{%[[j, 1]], %[j, 2]] * 2}, {j, Length[%}}];
```

```
In[150]:= knightsδLogPlot = ListLogLogPlot[knightsδTable,
      PlotRange → {{0.1, 10 000}, {0.01, 10}}, PlotStyle → plotColorsPoints[[2]]]
```



The values of δ seem unusual in that most published data for other materials are decreasing at 1000 eV. The magnitude at 300 eV seems typical.

■ **Fit of Chung and Everhardt to experiment for Ag. Work function = 4.73 eV**

```
In[151]:= enpList = {30, 60, 100, 300, 1000, 3000, 4000, 5000, 10 000}
```

```
Out[151]= {30, 60, 100, 300, 1000, 3000, 4000, 5000, 10 000}
```

We modify the formula used above so as to "fit" experiment.

```
In[152]:= analyticDist3 = ((0.4 * en * enp) / (E ^ (0.1084 * enp ^ 0.5) *
      (2.0 + en) ^ 4) / (1 + 1 / (enp)) * (1 + (enp / 500) ^ 1.4) + 0.27 / (enp) / (1 + 10 / enp))
      UnitStep[enp - en]
```

```
Out[152]= 
$$\left( \frac{0.27}{\left(1 + \frac{10}{\text{enp}}\right) \text{enp}} + \frac{0.4 e^{-0.1084 \text{enp}^{0.5}} \text{en enp} (1 + 0.000166511 \text{enp}^{1.4})}{(2. + \text{en})^4 \left(1 + \frac{1}{\text{enp}}\right)} \right) \text{UnitStep}[-\text{en} + \text{enp}]$$

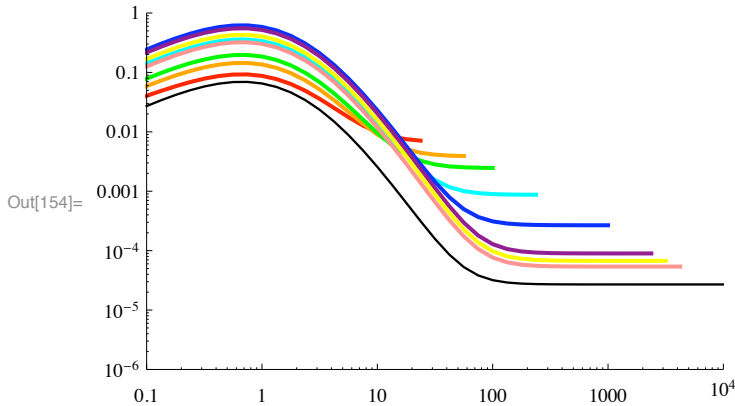
```

I am very surprised at the low apparent work function, 2 eV, in this formula. The low energies at the peaks compared to the theoretical values of ~ 5 eV could be an experimental artifact.

```
In[153]:= Do[
      electronDistTable3[i] = Table[
        {0.1 * 10 ^ ((j - 1) / 8), analyticDist3 /. {en -> 0.1 * 10 ^ ((j - 1) / 8), enp -> enpList[[i]]}},
        {j, 1, 41}];, {i, Length[enpList]}
```

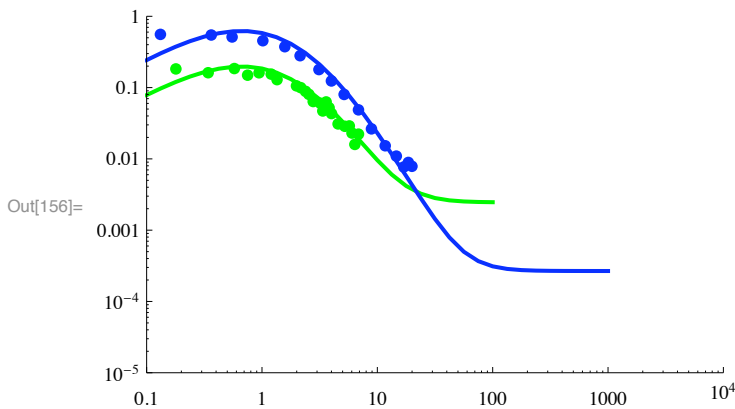


```
In[154]:= analyticDist3LogPlot = ListLogLogPlot [Table [electronDistTable3 [i], {i, Length [enpList]}],
  Joined → True, PlotRange → {{0.1, 10 000}, {0.000001, 1}}, PlotStyle → plotColorsLines]
```



```
In[155]:= analyticDist3LogPlot =
  ListLogLogPlot [{electronDistTable3 [3], electronDistTable3 [5]}, Joined → True,
  PlotRange → {{0.1, 10 000}, {0.00001, 1}}, PlotStyle → plotColorsLines [{3, 5}]]];
```

```
In[156]:= Show [analyticDist3LogPlot, knights1000LogPlot, knights100LogPlot]
```



Keep in mind that the magnitude factors applied to the above experimental points are arbitrary and are determined by fitting the secondary electron yields δ shown below. We have not found data for the backscattered yields η , i.e., the high energy tails. Again, the portions of these curves below the electron excitation thresholds and peaks of the cross sections are irrelevant in our model, i.e., the above fit is more for show than for its usefulness. The low energy electrons could dissociatively attach to H₂ or O₂.

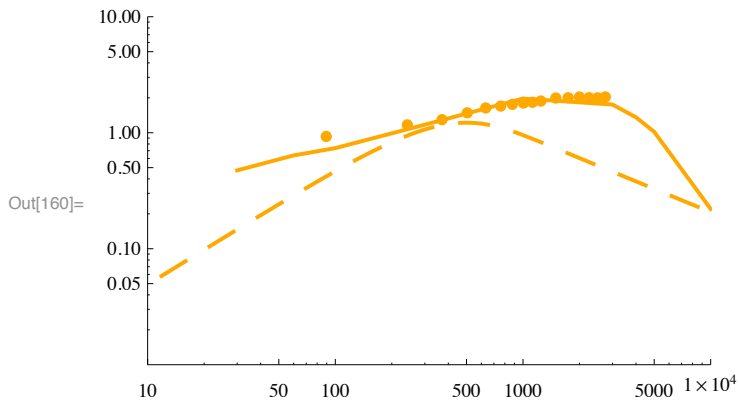
■ Secondary electron yields δ for Ni (assumed equivalent to stainless steel)

```
In[157]:= electronδTable3 = Table [{enpList [[j]],
  Integrate [(analyticDist3 /. enp -> enpList [[j]]), {en, 0, 50}], {j, Length [enpList]}];
```

```
In[158]:= analytic3δPlot = ListLogLogPlot [electronδTable3,
  PlotRange → {{10, 10 000}, {0.01, 10}}, PlotStyle → plotColorsLines [[2]], Joined → True];
```

```
In[159]:= empiricalδLinJoyPlot = LogLogPlot [(empiricalδLinJoy /. {δmax → 1.19, enpmax → 500}),
  {enp, 1, 10^4}, PlotRange -> {{1, 100 000}, {0.01, 2}}, PlotStyle → plotColorsLines [[11]]];
```

```
In[160]:= Show[analytic3δPlot, knightsδLogPlot, empiricalδLinJoyPlot]
```



From this comparison, the fit of the Lin and Joy (2005) empirical formula for δ is poor at primary energies above 500 eV for Ni.

■ Secondary electron yields δ for Ni (assumed equivalent to stainless steel)

```
In[161]:= electronηTable3 = Table [
  {enpList[[j]], Integrate[(analyticDist3 /. enp -> enpList[[j]]), {en, 50, enpList[[j]]}},
  {j, Length[enpList]};
```

```
In[162]:= analytic3ηPlot = ListLogLogPlot [electronηTable3,
  PlotRange -> {{10, 10 000}, {0.01, 10}}, PlotStyle -> plotColorsLines[[6]], Joined -> True];
```

```
In[163]:= Import["thomas85ORNL6088V3pD2.txt", "CSV"] // TableForm
```

Out[163]//TableForm=

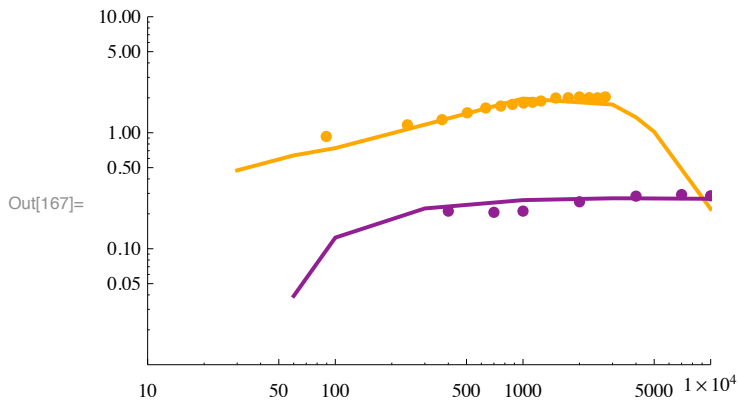
6.0E-02	1.00E-09	1.20E-01	1.00E-09	1.00E-09
1.0E-01	1.00E-09	1.78E-01	1.00E-09	1.00E-09
2.0E-01	1.23E-01	2.22E-01	1.00E-09	1.00E-09
4.0E-01	1.43E-01	2.31E-01	1.00E-09	2.11E-01
7.0E-01	1.49E-01	2.31E-01	1.00E-09	2.06E-01
1.0E+00	1.45E-01	2.31E-01	1.00E-09	2.11E-01
2.0E+00	1.20E-01	2.21E-01	1.00E-09	2.54E-01
4.0E+00	9.63E-02	1.96E-01	2.59E-01	2.84E-01
7.0E+00	8.16E-02	1.76E-01	2.62E-01	2.93E-01
1.0E+01	7.49E-02	1.65E-01	2.59E-01	2.86E-01
2.0E+01	6.43E-02	1.50E-01	2.52E-01	2.77E-01
4.0E+01	5.68E-02	2.40E-01	2.66E-01	1.00E-09
6.0E+01	5.39E-02	1.00E-09	1.00E-09	1.00E-09
Energy (keV)	C	Al	Ti	Fe
Backscattering Coefficient (electrons/electron)				
Thomas ORNL 6088/V3 (1985)p. D-2				

```
In[164]:= Drop[Drop[Import["thomas85ORNL6088V3pD2.txt", "Table"], 3], -5];
```

```
In[165]:= thomasηFe6088Table = Table[{{j, 1}} * 1000, %[[j, 5]]}, {j, Length[%]}];
```

```
In[166]:= thomasηFe6088Plot = ListLogLogPlot [thomasηFe6088Table,
  PlotRange -> {{10, 10 000}, {0.01, 10}}, PlotStyle -> plotColorsPoints[[6]]];
```

```
In[167]:= Show[analytic3δPlot, knightsδLogPlot, analytic3ηPlot, thomasηFe6088Plot]
```



It would appear that we have a reasonable fit to the δ and η experiments for Fe-Ag.

```
In[168]:= Quit[]
```

H (n = 3) produced at surface

The production of H (n = 3) at metal surfaces per incident H + and H₂ + by Baird, Zivitz, and Thomas, Phys. Rev. A 12, 876 (1975) was measured to be $\sim 1 \text{ E}^{-4}$.

```
In[75]:= a = 1;
In[76]:= ClearAll["Global`*"];
In[77]:= Remove["Global`*"];
In[78]:= startclock = SessionTime[];
In[79]:= Off[General::spell];
In[80]:= Off[General::spell1];
In[81]:= today = StringForm["`"/`/` ``:``:``", Date][[2]],
           Date][[3]], Date][[1]], Date][[4]], Date][[5]], N[Date][[6]], 2]]
Out[81]:= 9/16/2011 20:46:17.673419`2.
```

```
In[82]= SetDirectory [NotebookDirectory []]
```

```
Out[82]= C:\Users\avp\Documents\Mathbook\HYDROGEN\SurfaceEffects\SurfaceExcitation
```

```
In[83]= plotColorsLines = {
  (*1*) {Red, Thickness [0.007], Dashing [{}]},
  (*2*) {Hue [0.1], (*Orange,*) Thickness [0.007], Dashing [{}]},
  (*3*) {Green, Thickness [0.007], Dashing [{}]},
  (*4*) {Cyan, Thickness [0.007], Dashing [{}]},
  (*5*) {Blue, Thickness [0.007], Dashing [{}]},
  (*6*) {Purple, Thickness [0.007], Dashing [{}]},
  (*7*) {Yellow, Thickness [0.007], Dashing [{}]},
  (*8*) {Pink, Thickness [0.007], Dashing [{}]},
  (*9*) {Black, Thickness [0.004], Dashing [{}]},
  (*10-dash*) {Red, Thickness [0.007], Dashing [{0.05, 0.05}]},
  (*11-dash*) {Hue [0.1], Thickness [0.007], Dashing [{0.05, 0.05}]},
  (*12-dash*) {Green, Thickness [0.007], Dashing [{0.05, 0.05}]},
  (*13-dash*) {Cyan, Thickness [0.007], Dashing [{0.05, 0.05}]},
  (*14-dash*) {Blue, Thickness [0.007], Dashing [{0.05, 0.05}]},
  (*15-dash*) {Purple, Thickness [0.007], Dashing [{0.05, 0.05}]},
  (*16-dash*) {Yellow, Thickness [0.007], Dashing [{0.05, 0.05}]},
  (*17-dash*) {Pink, Thickness [0.007], Dashing [{0.02, 0.02}]},
  (*18-dash*) {Black, Thickness [0.007], Dashing [{0.02, 0.02}]}
};
```

```
In[84]= plotColorsPoints = {
  (*1*) {Red, PointSize [0.02]},
  (*2*) {Hue [0.1], PointSize [0.02]},
  (*3*) {Green, PointSize [0.02]},
  (*4*) {Cyan, PointSize [0.02]},
  (*5*) {Blue, PointSize [0.02]},
  (*6*) {Purple, PointSize [0.02]},
  (*7*) {Yellow, PointSize [0.02]},
  (*8*) {Pink, PointSize [0.02]},
  (*9*) {Black, PointSize [0.02]},
  (*10*) {Red, PointSize [0.014]},
  (*11*) {Hue [0.1], PointSize [0.014]},
  (*12*) {Green, PointSize [0.014]},
  (*13*) {Cyan, PointSize [0.014]},
  (*14*) {Blue, PointSize [0.014]},
  (*15*) {Purple, PointSize [0.014]},
  (*16*) {Yellow, PointSize [0.014]},
  (*17*) {Pink, PointSize [0.014]},
  (*18*) {Black, PointSize [0.014]}
};
```

■ Contribution of $H(n=3)$ produced at surface

In most of our modeling we have neglected the production of $H(n=3)$ at the surfaces because of the low yields per incident H^+ and H_2^+ found by Baird, Zivitz, and Thomas, Phys. Rev. A 12, 876 (1975), e.g., $\sim 1E-4$. This probability is to be compared with the probability of excitation in the volume caused by collisions of H with H_2 .

I do not understand the emission in the long wavelength wing found by Baird et al. In fact, McCracken and Erents, Phys. Lett. 31A, 429 (1970) had found rather different profiles for Lyman alpha and attribute the long wavelength wing to reflected light. Unfortunately, Baird et al (1975) do not give their spectral resolution or refer to McCracken and Erents (1970).

- **Rough estimate of relative integrated profiles from surface and from volume excitation**

We will assume the collisional excitation probability to given by the excitation cross section of $1\text{E-}21\text{ m}^2$ times the gas density of $5\text{E-}3\text{ Torr} \cdot 3.3\text{E}22 = 16.7\text{E}19\text{ m}^{-3}$ times an observation length of $\sim 2\text{E-}2\text{ m}$. This gives a probability of $3\text{E-}4$. This needs to be multiplied by the fraction of the incident flux that is reflected as fast H, e.g., ~ 0.1 . This number of $3\text{E-}5$ is smaller than the $\sim 1\text{E-}4$ for surface excitation. The surface excitation produces a negative shift and so tends to equalize the wing intensities.

Note that the length of the region from which emission is collected is important in the Kriptidis experiment.

An important contribution to the excitation is expected from electrons reflected from the wall anode. The secondary electron coefficient may well be larger than unity, so that the reflected electron flux may be larger than the primary electron flux.

- **Lyman alpha produced at surface from McCracken and Erents (1970)**

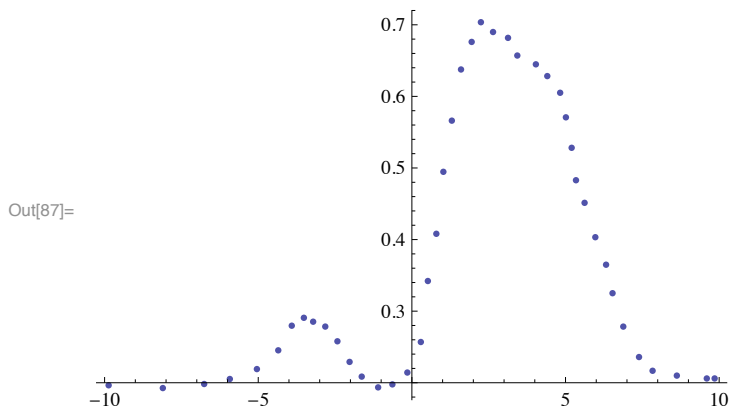
```
In[85]= TableForm[Import["mccracken&erents33kevcorrected.dat", "Table"],
  TableHeadings -> {None, {"Δλ (Å)", "Intensity"}}] // TableForm
```

Out[85]/TableForm=

$\Delta\lambda$ (Å)	Intensity
-9.86849	0.196447
-8.105	0.192568
-6.75951	0.198247
-5.92452	0.20523
-5.04339	0.219088
-4.34836	0.245282
-3.90887	0.279683
-3.51487	0.290726
-3.21304	0.285273
-2.81834	0.278459
-2.4231	0.257909
-2.02754	0.229117
-1.6323	0.208567
-1.09807	0.193531
-0.634199	0.197715
-0.147608	0.214265
0.291556	0.256908
0.520236	0.342104
0.796072	0.408076
1.0247	0.494646
1.30032	0.566113
1.59914	0.637582
1.94566	0.676091
2.24621	0.703605
2.64118	0.689923
3.12874	0.681748
3.43133	0.657065
4.03506	0.644785
4.40693	0.628353
4.82548	0.605058
5.01244	0.570744
5.19972	0.528187
5.34071	0.482877
5.62036	0.451322
5.97027	0.403293
6.31981	0.364879
6.53018	0.325073
6.88004	0.278418
7.39215	0.235906
7.83373	0.216735
8.62286	0.209976
9.5975	0.205989
9.85272	0.206024

In[86]:= Import["mccracken&erents33kevcorrected.dat", "Table"];

In[87]:= **ListPlot** [%]



The instrumental FWHM from the core profile is 0.6 Ang. The calculated maximum Doppler shift in nm is

In[88]:= **delLambdaLy** = **lambdaLy** / **c** * **Sqrt** [2 * **qe** * **en** / **mH**] /.
 {**lambdaLy** → 121.6, **qe** → 1.602 * 10⁻¹⁹, **mH** → 1.673 * 10⁻²⁷, **c** → 3 * 10⁸, **en** → 33 000} (*nm*)

Out[88]= 1.01898

McCracken and Erents say that the high energy falloff in their profile at energies below the energetic limit is caused by the decrease in the flux of H atom reflected from the surface.

Our original model does not take into account the relative decrease in reflected H with product energy that occurs at high incident energies. It assumes a uniform energy distribution and so does not account for the relative decrease in average energy of these H atoms as the energy of the incident particles increases.

One way to distinguish surface excitation from gas phase excitation is to look for the continuum peak at ~ 320 nm for Cu and ~ 350 nm for Mo.

Surface production of H-

```
In[1]:= a = 1;

In[2]:= ClearAll["Global`*"];

In[3]:= Remove["Global`*"];

In[4]:= startclock = SessionTime[];

In[5]:= Off[General::spell];

In[6]:= Off[General::spell1];

In[7]:= today = StringForm["`~/`~/`~ `~:``:``", Date][[2]],
      Date][[3]], Date][[1]], Date][[4]], Date][[5]], N[Date][[6]], 2]]

Out[7]= 9/18/2011 23:0:12.274913`2.

In[8]:= date = DateString[{"Month", "Day", "YearShort"}]

Out[8]= 091811

In[9]:= SetDirectory["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\H2cathodefall\\Boris_Wisc"]

Out[9]= c:\\users\\avp\\documents\\Mathbook\\hydrogen\\H2cathodefall\\Boris_Wisc

In[10]:= plotColorsLines = {
  (*1*) {Red, Thickness[0.007], Dashing[{}]},
  (*2*) {Hue[0.1], (*Orange,*)Thickness[0.007], Dashing[{}]},
  (*3*) {Green, Thickness[0.007], Dashing[{}]},
  (*4*) {Cyan, Thickness[0.007], Dashing[{}]},
  (*5*) {Blue, Thickness[0.007], Dashing[{}]},
  (*6*) {Purple, Thickness[0.007], Dashing[{}]},
  (*7*) {Yellow, Thickness[0.007], Dashing[{}]},
  (*8*) {Pink, Thickness[0.007], Dashing[{}]},
  (*9*) {Black, Thickness[0.004], Dashing[{}]},
  (*10-dash*) {Red, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*11-dash*) {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*12-dash*) {Green, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*13-dash*) {Cyan, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*14-dash*) {Blue, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*15-dash*) {Purple, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*16-dash*) {Yellow, Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*17-dash*) {Pink, Thickness[0.007], Dashing[{0.02, 0.02}]},
  (*18-dash*) {Black, Thickness[0.007], Dashing[{0.02, 0.02]}}
};
```

```
In[11]:= plotColorsPoints = {
  (*1*) {Red, PointSize[0.02]},
  (*2*) {Hue[0.1], PointSize[0.02]},
  (*3*) {Green, PointSize[0.02]},
  (*4*) {Cyan, PointSize[0.02]},
  (*5*) {Blue, PointSize[0.02]},
  (*6*) {Purple, PointSize[0.02]},
  (*7*) {Yellow, PointSize[0.02]},
  (*8*) {Pink, PointSize[0.02]},
  (*9*) {Black, PointSize[0.02]},
  (*10*) {Red, PointSize[0.014]},
  (*11*) {Hue[0.1], PointSize[0.014]},
  (*12*) {Green, PointSize[0.014]},
  (*13*) {Cyan, PointSize[0.014]},
  (*14*) {Blue, PointSize[0.014]},
  (*15*) {Purple, PointSize[0.014]},
  (*16*) {Yellow, PointSize[0.014]},
  (*17*) {Pink, PointSize[0.014]},
  (*18*) {Black, PointSize[0.014]}
};
```

This process is probably very important.

■ Surface production

In spite of considerable searching, I have not found really relevant data for the production of H⁻ at reasonably clean metallic and/or graphite surfaces.

1) For a polycrystalline diamond surface, Wurz et al, Surface Science 373, 56 (1997) give a total negative ion yield per reflected atom for incident H₂⁺ that decrease from 5.5 % to 3.5 % as the incident energy increases from 300 to 700 eV at 82 deg or perpendicular energies of 6 to 14 eV. They claim that the yield is independent of whether the incident particle is an ion or a neutral.

2) Verbeek, Eckstein, and Bhattacharya, Surface Science 95, 380 (1980) give values that peak at about 6% at half the incident energy of 5 keV/atom for H₂⁺ incident on Au. Their results show an approximate cos[theta] sin[theta] dependence on exit angle theta and are independent of energy for 5 and 10 keV. Eckstein and Matschke, Phys. Rev. B find no significant variation of the negative ion fraction for 2 keV H₂⁺ and 5 keV H⁺.

We chose a constant value of 4% for all metals and energies to be multiplied by the fast neutral flux. Obviously, this does not apply to cesiated, etc. surfaces.

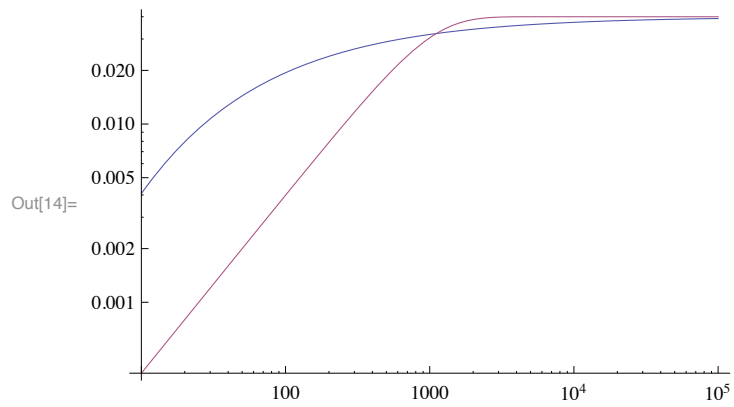
```
In[12]:= fneg = 0.04;
```

One should ask why the production of H⁻ is not subject to a low velocity cutoff since 1) dissociative attachment of electrons to H₂ is severely reduced by autodetachment and 2) the situation is similar to that for surface excitation of H α .

```
In[13]:= fneg = 0.04 * Exp[-vA / va] /.
  {va -> Sqrt[2 * qe * en / mH], vA -> 10^5, qe -> 1.602 * 10^-19, mH -> 1.673 * 10^-27}
```

```
Out[13]= 0.04 e $\frac{7.22606}{\sqrt{en}}$ 
```

```
In[14]:= LogLogPlot[{fneg, 0.04 * Tanh[en / 1000]}, {en, 10, 100 000}, PlotRange -> All]
```



The exponential does no help much.

Find and include Cartry data

Cross sections for e + H2 collisions

Setup notebook environment

```
In[1]:= a = 1;
```

```
In[2]:= ClearAll["Global`*"];
```

```
In[3]:= Remove["Global`*"];
```

```
In[4]:= startclock = SessionTime[];
```

```
In[5]:= Off[General::spell];
```

```
In[6]:= Off[General::spell1];
```

```
In[7]:= today = StringForm["`~/`~/` ` `:``:``", Date][[2]],  
Date][[3]], Date][[1]], Date][[4]], Date][[5]], Date][[6]]]
```

```
Out[7]= 1/16/2011 11:26:45.9504143`9.414864297864533
```

```
In[8]:= SetDirectory["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\h2electroncollisions "]
```

```
Out[8]= c:\users\avp\documents\Mathbook\hydrogen\h2electroncollisions
```

```
In[9]:= plotColorsLines = {
  (*1-red*) {Hue[0.0], Thickness[0.007], Dashing[{}]},
  (*2-orange*) {Hue[0.1], Thickness[0.007], Dashing[{}]},
  (*3-green*) {Hue[0.3], Thickness[0.007], Dashing[{}]},
  (*4-cyan*) {Hue[0.5], Thickness[0.007], Dashing[{}]},
  (*5-dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{}]},
  (*6-purple*) {Hue[0.8], Thickness[0.007], Dashing[{}]},
  (*7-black*) {Thickness[0.007], Dashing[{}]},
  (*8-dash red*) {Hue[0.0], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*9-dash orange*) {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*10-dash green*) {Hue[0.3], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*11-dash cyan*) {Hue[0.5], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*12-dash dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*13-dash purple*) {Hue[0.8], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*14-dash black*) {Thickness[0.007], Dashing[{0.02, 0.02}]}];
```

```
In[10]:= plotColorsPoints = {
  (*1-red*) {Hue[0.0], PointSize[0.02]},
  (*2-orange*) {Hue[0.1], PointSize[0.02]},
  (*3-green*) {Hue[0.3], PointSize[0.02]},
  (*4-cyan*) {Hue[0.5], PointSize[0.02]},
  (*5-dk blue*) {Hue[0.7], PointSize[0.02]},
  (*6-purple*) {Hue[0.8], PointSize[0.02]},
  (*7-black*) {PointSize[0.02]},
  (*8-dash red*) {Hue[0.0], PointSize[0.02]},
  (*9-dash orange*) {Hue[0.1], PointSize[0.02]},
  (*10-dash green*) {Hue[0.3], PointSize[0.02]},
  (*11-dash cyan*) {Hue[0.5], PointSize[0.02]},
  (*12-dash dk blue*) {Hue[0.7], PointSize[0.02]},
  (*13-dash purple*) {Hue[0.8], PointSize[0.02]},
  (*14-dash black*) {PointSize[0.02]}];
```

From MBCFElectron.nb

```
In[11]:= fac=10^20;
```

■ Ionization, energy loss, and excitation cross sections for electrons in H2.

From our Web site

```
In[12]:= Import["c:/users/avp/documents/mathbook/hydrogen/H2ElectronCollisions/h2emomtransq.txt",
  "CSV"] // TableForm
```

Out[12]/TableForm=

H2 MOMENTUM-TRANSFER CROSS SECTION

	ENERGY	Effective Qm - Defined in introduction
0.00001	6.4000	
0.0010	6.4000	
0.0020	6.5000	
0.0030	6.6000	
0.0050	6.8000	
0.0070	7.1000	
0.0085	7.2000	
0.0100	7.3000	
0.0150	7.7000	
0.0200	8.0000	
0.0300	8.5000	
0.0400	8.9600	
0.0500	9.2800	
0.0700	9.8500	
0.1000	10.5000	
0.1200	10.8500	
0.1500	11.4000	
0.1700	11.6000	
0.2000	12.0000	
0.2500	12.5000	
0.3000	13.0000	
0.3500	13.4500	
0.4000	13.9000	
0.5000	14.7000	
0.7000	16.3000	
1.0000	17.4000	
1.2000	17.8000	
1.3000	18.0000	
1.5000	18.2500	
1.7000	18.2500	
1.9000	18.1000	
2.1000	17.9000	
2.2000	17.7000	
2.5000	17.0000	
2.8000	16.4000	
3.0000	16.0000	
3.3000	15.6000	
3.6000	14.8000	
4.0000	14.0000	
4.5000	13.1000	
5.0000	12.2000	
6.0000	10.4000	

7.0000	8.9000
8.0000	7.8500
10.0000	6.0000
12.0000	5.2000
15.0000	4.5000
17.0000	4.2000
20.0000	3.9000
25.0000	3.6000
30.0000	3.4000
50.0000	2.9000
75.0000	2.6000
100.0000	2.3000
150.0000	1.9000
200.0000	1.6200
300.0000	1.2800
500.0000	0.9200
700.0000	0.7200
1000.0000	0.5400
1500.0000	0.3700
2000.0000	0.2900
3000.0000	0.2100
5000.0000	0.1400
7000.0000	0.1040
10000.0000	0.0770

```
In[13]:= Drop[Import["c:/users/avp/documents/mathbook/hydrogen/H2ElectronCollisions/h2emomtransq.txt"]
```

```
In[14]:= h2Qm = ListLogLogPlot[%, GridLines -> Automatic, Joined -> True,
  PlotRange -> {{.1, 10 000}, {10^20 * 0.99 * 10^-23, 10^20 * 2.01 * 10^-19}},
  ImageSize -> 400, PlotStyle -> plotColorsLines[[6]]];
```

The following are from H2Nonequ092605.nb

- **Electron impact ionization of H2 to form H2+ - this is an empirical quasi-steady-state or local-field equilibrium formula ?FROM WHERE?**

```
In[15]:= qes2[we_] := UnitStep[we-15.4]*8.5 10^-21*2*(we-15.4)/(40-15.4)/((we/40)^1.78+1)+1.*10^(-30)
```

For the present we take the cross section for the production of H+ in e + H2 collisions as 5% of that for production of H2+.

```
In[16]:= qes1[we_] := 0.05*UnitStep[we-15.4]*8.5 10^-21*2*(we-15.4)/(40-15.4)/((we/40)^1.78+1)+1.*10^(-30)
```

- **Electron energy loss**

Electron energy loss to vibrational excitation at low energy plus high energy loss to dissociation and ionization. At 100 eV to 10 keV the following results are in reasonable agreement with Cravens, Victor, and Dalgarno, Planet. Space Sci. 23, 1059 (1975) and for 10 to 1000 eV with Dalgarno et al, Ap. J. Supp. 125, 237 (1999)..

```
In[17]:= lein[we_] := UnitStep[we-0.54]*1.7*10^-21*((we-.54)/(3-.54))^2/((we+3)/6)^4 + UnitStep[we-8]
  8.7*10^-21*(we-8)/((we+50)/100)^1.8 + 1.*10^-30
```

For case 41, increasing the second term by a factor of 10 increased the slope of the decay of emission with distance to roughly experiment, but did not help increase the magnitude. A factor of 3 made little difference.

From Munoz et al Chem. Phys. Lett. 433, 253 (2007), their experimental mass stopping power leads to the following inelastic energy loss

```
In[18]:= Import["c:\\users\\avp\\documents\\mathbook\\hydrogen\\H2ElectronCollisions\\
Munoz07ChemPhysLettTable2.txt", "CSV"] // TableForm
```

```
Out[18]/TableForm=
```

Energy (eV)	Total σ ($\text{a}0^2$)	Elastic/total η	Mass stopping power ($1\text{E}8 \text{ eV cm}^2/\text{g}$)
5	54.2	1	0
7.5	45.7	1	0
10	38.4	1	0
15	28.8	0.848	423.9
20	23.2	0.732	703.5
30	17.4	0.595	910.7
40	14.5	0.514	995.2
50	13.2	0.458	1037
75	10.6	0.373	1065
100	9.08	0.322	1054
150	7.05	0.261	891.1
200	5.9	0.226	781.9
300	4.4	0.183	614.9
400	3.57	0.158	514.2
500	2.99	0.141	439.4
750	2.19	0.115	331.8
1000	1.76	0.0992	271.4
1500	1.28	0.0806	201.4
2000	1.02	0.0696	162.4
3000	0.735	0.0566	118.7
4000	0.579	0.0488	94.26
5000	0.481	0.0436	78.74

```
In[19]:= munozData=Drop[Import["c:\\users\\avp\\documents\\mathbook\\hydrogen\\H2ElectronCollisions\\
```

```
In[20]:= munozEnergyLoss=Table[{#[[j,1]],#[[j,4]]*2/(6.022*10^23)*100},{j,Length[%]}];
```

```
In[21]:= MunozEnergyLossPlot=ListLogLogPlot[Table[{#[[j,1]],#[[j,2]]fac},{j,Length[%]}], PlotRange->{
ImageSize->400,PlotStyle->plotColorsPoints[[4]], PlotLabel-> "Cross sections for e + H2 (10
```

■ Electron excitation of near uv

```
In[22]:= qeuv[we_] := 5.*10^-21*UnitStep[we-11.8]*((1/((we/11.8)^2.8+1)-1/((we/11.8)^9+1))) + 1.*10^-
```

■ Electron excitation of Halpha

```
In[23]:= qeHa[we_] := UnitStep[we-17.]* (8.5*10^-23.*2*(we-17)/(50-17)/
((we/50)^1.9+1)+(5.2*10^-23/((we/30)^4+1))+1.*10^-30
```

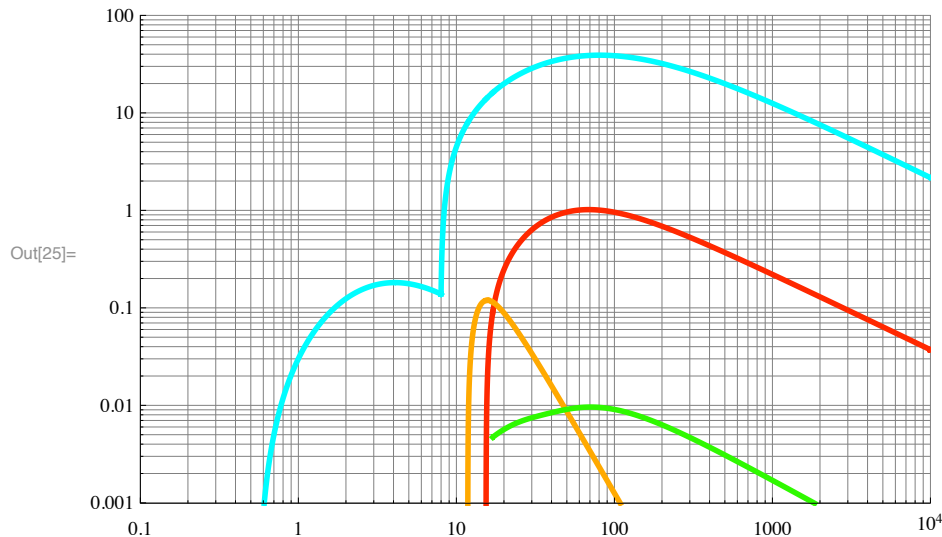
We have not listed a cross section for production of the Lymanalpha line. According to Fujimoto et al (1989) it peaks at $1.2\text{E}-1 \text{ Pi } \text{a}0^2 = 1.06\text{E}-17 \text{ cm}^2$ at about 100 eV.

```
In[24]:= fac=10^20;
```



```
In[25]:= h2inelasticQs = LogLogPlot[{fac * qes2[we], fac * qeuv[we], fac * qeha[we], fac * lein[we]},
  {we, .1, 10 000}, PlotPoints -> 10 000, GridLines -> Automatic,
  PlotRange -> {{.1, 10 000}, {fac * 0.99 * 10^-23, fac * 1.01 * 10^-18}},
  ImageSize -> 400, PlotStyle -> plotColorsLines,
  PlotLabel -> "Cross sections for e + H2 (10^-20 m^2) vs energy (eV)"]
```

Cross sections for e + H2 (10^{-20} m^2) vs energy (eV)



Here we have divided the energy loss function `lein[we]` by 10 for ease of plotting.

```
In[26]:= Show[h2inelasticQs, h2Qm, MunozEnergyLossPlot, DisplayFunction->$DisplayFunction];
```

The very recent Munoz et al recommendation is about 30% lower than our choice at energies above 100 eV.

■ Ionization in e + H2 collisions

Recent papers have attempted to define an accurate set of electron induced ionization cross section for H2. Lui and Shemansky, Ap. J. 614, 1132 (2004) use a combination of theory and experiment to derive cross sections for the formation of H2+ and H+. They recommend the experimental data tabulated by Lindsay and Mangan, in Landolt-Bornstein, vol I/17C, ed by Itikawa, (Springer, Berlin, 2003). Since it is very difficult for CU to get a copy of this, I will use Table 1 and Fig. 2 of Lui and Shemansky.

```
In[27]:= Import["Liu&ShemanskyH2pb.txt", "Table"];
```

```
In[28]:= Table[#[[j, 1]], {j, Length[%]}];
```

```
In[29]:= Flatten[Drop[Import["Liu&ShemanskyH2pc.txt", "Table"], 1]];
```

```
In[30]:= ionizationQH2p=Table[{#[[j]], #[[j]]*10^-17*fac/10^4}, {j, Length[%]}];
```

```
In[31]:= ionizationQH2p // TableForm
```

Out[31]/TableForm=

16	0.01
17	0.059
18	0.122
19	0.181
20	0.235
22.5	0.355
25	0.457
27.5	0.544
30	0.617
32.5	0.676
35	0.728
40	0.801
45	0.846
50	0.871
55	0.883
60	0.886
65	0.884
70	0.877
75	0.869
80	0.859
85	0.849
90	0.838
95	0.827
100	0.816
105	0.805
110	0.794
115	0.784
120	0.773
125	0.763
130	0.752
135	0.742
140	0.732
145	0.722
150	0.713
155	0.703
160	0.694
165	0.684
170	0.675
175	0.666
180	0.657
190	0.64
200	0.623
225	0.584
250	0.549

```

275 0.517
300 0.489
350 0.44
400 0.4
408 0.395
450 0.367
500 0.34
545 0.319
550 0.316
600 0.296
650 0.279
700 0.263
750 0.25
800 0.238
817 0.234
850 0.227
900 0.217
950 0.208
1000 0.2
1089 0.187
1200 0.173
1362 0.156
1400 0.153
1500 0.144
1600 0.137
1638 0.135
1800 0.125
1906 0.119
2000 0.114
2200 0.106
2400 0.0986
2500 0.0953
2600 0.0923
3000 0.082

```

```

In[32]:= h2pionizationQ = ListLogLogPlot [ionizationQH2p, GridLines -> Automatic,
      PlotRange -> {{.1, 10 000}, {fac * 0.99 * 10^-23, fac * 1.01 * 10^-18}},
      ImageSize -> 400, PlotStyle -> plotColorsPoints [[2]],
      PlotLabel -> "Cross section for e + H2 -> H2+ (10^-20 m^2) vs energy (eV)"];

```

```

In[33]:= qes2[we_] := UnitStep[we-15.4]*1.7*10^-20*(we-15.4)/(40-15.4)/((we/37)^1.78+1)+1.*10^(-30)

```

```

In[34]:= h2ionizationFitQ =
      LogLogPlot [fac * qes2[we], {we, .1, 10 000}, PlotPoints -> 10 000, GridLines -> Automatic,
      PlotRange -> {{10, 10 000}, {fac * 0.99 * 10^-23, fac * 1.01 * 10^-20}},
      PlotPoints -> 500, ImageSize -> 400, PlotStyle -> plotColorsLines,
      PlotLabel -> "Cross section for e + H2 -> H2+ (10^-20 m^2) vs energy (eV)"];

```

```

In[35]:= Show[h2ionizationFitQ, h2pionizationQ, PlotLabel-> "Cross section for e + H2 -> H2+ (10^-20 m^2) vs energy (eV)"];

```

Liu and Shemansky for e + H2 -> H+

```
In[36]:= Import["LiuShemanskyHp.dat", "CSV"] // TableForm
```

```
Out[36]/TableForm=
```

2.09820E+01	4.06714E-18
2.97385E+01	2.48023E-17
3.67621E+01	6.63161E-17
4.02952E+01	1.16153E-16
4.55950E+01	1.90909E-16
4.91312E+01	2.44900E-16
5.61792E+01	3.19648E-16
5.97185E+01	3.77793E-16
6.67604E+01	4.44233E-16
7.02936E+01	4.94070E-16
7.55841E+01	5.56363E-16
7.73568E+01	5.89590E-16
8.26352E+01	6.35265E-16
8.96618E+01	6.80933E-16
9.14376E+01	7.18315E-16
1.00203E+02	7.51513E-16
1.08993E+02	8.17945E-16
1.19520E+02	8.67753E-16
1.38799E+02	9.34142E-16
1.59839E+02	1.01714E-15
1.79104E+02	1.06276E-15
1.98353E+02	1.08760E-15
2.26358E+02	1.13318E-15
2.50824E+02	1.12062E-15
2.75306E+02	1.12883E-15
2.99812E+02	1.17027E-15
3.50520E+02	1.18252E-15
3.99462E+02	1.16985E-15
4.50158E+02	1.16549E-15
5.00882E+02	1.19851E-15
5.49799E+02	1.15261E-15
6.00513E+02	1.17317E-15
6.51210E+02	1.16881E-15
7.00176E+02	1.18938E-15
7.50872E+02	1.18501E-15
8.01571E+02	1.18480E-15
8.52249E+02	1.15551E-15
8.99488E+02	1.20517E-15
9.51917E+02	1.18002E-15
9.99107E+02	1.16321E-15

```
In[37]:= Import["LiuShemanskyHp.dat", "Table"]; (*Omega in cm^2 eV*)
```

Collision strengths are usually related to cross sections using Eq. (7-2-8) from McDaniel, Atomic Collisions: Electron and Photon Projectiles (Wiley, New York, 1989), i.e., $Q = \Omega/g_i/(en_{rel}/Ry)$. From the units, apparently Liu and Shemansky omit the Rydberg normalization. Assume $g_i = 1$.

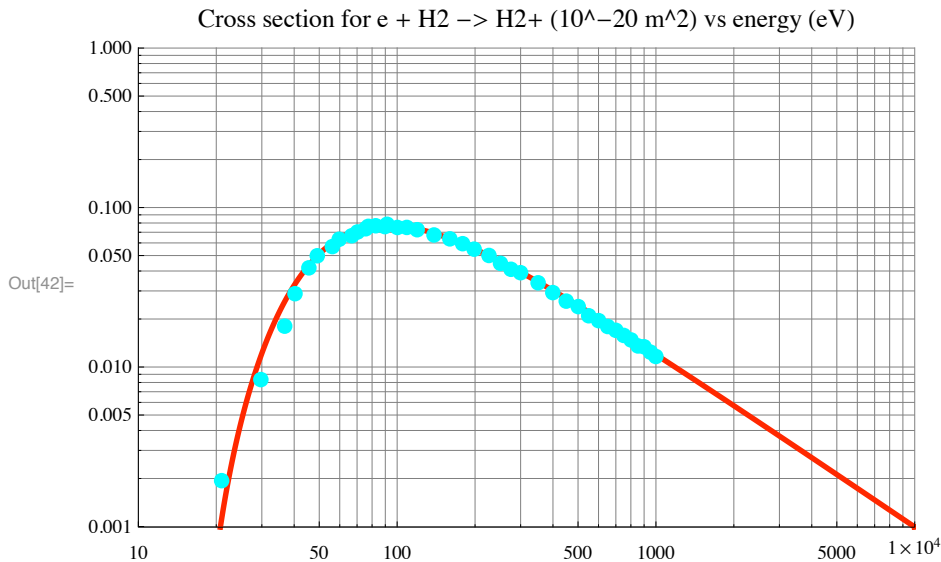
```
In[38]:= ionizationQHp=Table[{{j,1}},%[[j,2]]/%[[j,1]]*fac/10^4},{j,Length[%]}];
```

```
In[39]:= hpionizationQ = ListLogLogPlot [ionizationQHp, GridLines -> Automatic,
PlotRange -> {{.1, 10 000}, {fac * 0.99 * 10^-23, fac * 1.01 * 10^-18}},
ImageSize -> 400, PlotStyle -> plotColorsPoints [[4]],
PlotLabel -> "Cross section for e + H2 -> H+ (10^-20 m^2) vs energy (eV)"]; 
```

```
In[40]:= qes1[we_] := UnitStep[we-15.4]*1.17*10^-25*(we-15.4)^3.0/((we/35)^2.05+1)^2+1.*10^(-30)
```

```
In[41]:= hpionizationFitQ =
  LogLogPlot[fac * qes1[we], {we, .1, 10 000}, PlotPoints -> 10 000, GridLines -> Automatic,
  PlotRange -> {{10, 10 000}, {fac * 0.99 * 10^-23, fac * 1.01 * 10^-20}},
  PlotPoints -> 500, ImageSize -> 400, PlotStyle -> plotColorsLines];
```

```
In[42]:= Show[hpionizationFitQ, hpionizationQ, PlotLabel-> "Cross section for e + H2 -> H2+ (10^-20 m^
```



■ Differential scattering cross sections for e + H2

■ Theory

A summary of their approximate fits to differential cross section data for electron collisions with H2 is given by Heaps and Green, *J. Appl. Phys.* 46, 4718 (1975). For elastic scattering, they use the momentum transfer cross section. For triplet state excitation, they assume isotropic scattering. For singlet state excitation, they refer to Green and Dutta, *J. Geophys. Res.* 72, 3933 (1967). This paper uses the first term of an exponential series for the generalized oscillator strength. This approximation seems rather different than the power-law, e.g., (momentum change)⁻¹² derived by Mott and Massey, "Theory of Atomic Collisions, 3rd Ed, (Oxford, Clarendon, 1965), Sec 7. Green and Dutta, Eq. (10), give an expansion for the generalized oscillator strength that they say is qualitatively different from Eq. (116) of Mott and Massey. Both references cite experiment to justify their approximation for 2¹S and 2¹P electron excitation of He.

We note that the differential cross section does not appear in most of the papers on energy loss in H2 because they are not concerned with electron transport, but only with energy loss by electrons with an isotropic velocity distribution. These papers do emphasize the importance of adding cross sections to represent the excitation of high lying excited states. See for example, Dalgarno, Yan, and Liu, *Ap. J. Supp.* 125, 237 (1999).

The normalized momentum change $\text{normx} = x/xt = (a_0 \cdot K)^2 \cdot \text{Re}/W$ is related to the polar scattering angle θ and the normalized energy $\text{enorm} = E/W$, where $xt = W/\text{Re}$ by

```
In[43]:= normx:=2*enorm*(1-(1-1/enorm)^0.5*Cos[theta]-1/(2*enorm))
```

```
In[44]:= LogLogPlot[{normx /. enorm->1, normx /. enorm->10, normx /. enorm->100}, {theta, 0.01, Pi}, PlotStyle
  PlotLabel-> "Normalized momentum change versus angle";
```

```
In[45]:= LogLogPlot[{normx /.theta->0.1,normx /.theta->0.01,normx /.theta->0.001},{enorm,1,100}, Plot
PlotLabel-> "Normalized momentum change versus normalized energy"];
```

```
In[46]:= solTheta=Solve[x/xt==normx,theta][[2]];
```

Solve::ifun :

Inverse functions are being used by Solve, so some solutions may not be found; use Reduce for complete solution information. >>

```
In[47]:= thetal:=theta/.solTheta
```

We are interested primarily in small angles and enorm > 10. There does not seem to be any simple approximation to normx versus theta for these parameters.

```
In[48]:= thetal/.{enorm->10,x->0.1*xt}
```

```
Out[48]= 0.0881482
```

■ Experiment

```
In[49]:= a0=0.529*10^-10;
Ry=13.61;
W=12.;
```

From Khakoo and Trajmar, Phys. Rev. A 34, 146 (1986) the differential cross section are

```
In[52]:= Import["khakoo&trajmar_B1Sigma.txt", "CSV"] // TableForm
```

```
Out[52]/TableForm=
```

Khakoo&Trajmar (1986) - 1E-18 cm ² /sr B ¹ Sigma				
angle	20 eV	30 eV	40 eV	60 eV
10	18.6	41.8	66.8	86.3
20	8.99	10.7	19.8	7.22
30	4.26	3.61	5.02	1.86
40	2.77	2.23	1.83	0.888
50	2.05	1.59	0.918	0.564
60	1.55	1.15	0.644	0.424
70	1.20	0.920	0.545	0.218
80	0.927	0.755	0.433	0.204
90	0.783	0.623	0.350	0.133
100	0.621	0.504	0.252	0.110
110	0.508	0.372	0.197	0.100
120	0.490	0.316	0.151	0.093

```
In[53]:= Take[Import["khakoo&trajmar_B1Sigma.txt", "Table"],2]
```

```
Out[53]= {{Khakoo&Trajmar, (1986), -, 1. × 10-18, cm2/sr, B1Sigma},
{angle, 20, eV, 30, eV, 40, eV, 60, eV}}
```

```
In[54]:= Drop[Drop[Import["khakoo&trajmar_B1Sigma.txt", "Table"],2],-2];
```

For 60 eV

```
In[55]:= IthetaB1SigmaData=Table[{#[[j,1]],#[[j,5]]*10^-22},{j,Length[%]}];
```

```
In[56]:= IthetaB1SigmaPlot=ListLinearLogPlot[IthetaB1SigmaData,PlotRange->{{0,180.01},{0.99*10^-24,1.},
PlotStyle->plotColorsPoints[[1]], PlotLabel-> "I(theta) (m2/sr) versus theta (deg)"];
```

We wish to plot the GOS versus $(Ka_0)^2 = x$.

```
In[57]:= normx
Out[57]= 2 enorm  $\left( 1 - \frac{1}{2 \text{enorm}} - \left( 1 - \frac{1}{\text{enorm}} \right)^{0.5} \text{Cos}[\text{theta}] \right)$ 
In[58]:= KhakooGOSB1Sigma=Table[{(normx*xt//.{theta->IthetaB1SigmaData[[j,1]]*Pi/180,xt->12/13.6,enorm
((IthetaB1SigmaData[[j,2]]/(4*a0^2*Ry/W*(1-1/enorm)^0.5/(normx*xt)))/.
{theta->IthetaB1SigmaData[[j,1]]*Pi/180,xt->12/13.6,enorm->60/12})},{j,Length[IthetaB1SigmaD
In[59]:= ListPlot[%,PlotStyle->plotColorsPoints[[5]],PlotLabel->"GOS versus (K*a0)^2",
TextStyle->{FontFamily->"Helvetica",FontSize->12}];
```

From Khare, Phys. Rev. A 149,33 (1966) we get the differential cross section measured by Geiger, Z. Physik 181, 413 (1964) in units of a_0^2 versus Ka_0 .

```
In[60]:= Import["khare66Fig1.dat", "CSV"] // TableForm
```

```
Out[60]/TableForm=
3.28742E-02 2.32175E+03
4.25826E-02 1.48554E+03
6.17599E-02 7.06103E+02
8.39914E-02 4.68652E+02
1.23738E-01 1.53788E+02
1.52687E-01 1.06006E+02
2.00897E-01 4.68258E+01
2.96085E-01 1.99140E+01
3.95963E-01 9.12726E+00
6.21933E-01 1.78233E+00
8.05051E-01 7.31186E-01
9.45475E-01 3.00198E-01
1.26268E+00 5.65635E-02
```

```
In[61]:= khareDataFig1=Import["khare66Fig1.dat", "Table"];
```

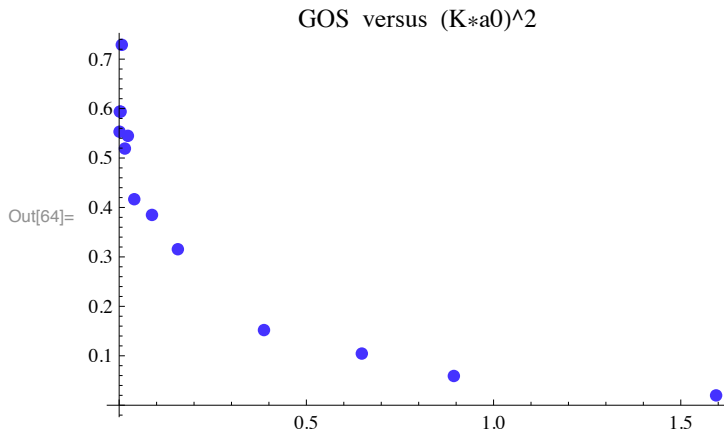
We convert this to $I[\text{theta}]$ in m^2/sr versus angle in degrees

```
In[62]:= khareDataI=Table[{(180/Pi*theta1/.{enorm->25000/12,x->(%[[j,1]])^2,xt->12/13.6}),%[[j,2]]*(.
```

Alternatively, we convert this to the generalized oscillator strength versus angle in momentum change Ka_0 , where Heaps and Dalgarno (1975) Eq. (1) give the generalized oscillator strength $GOS = f(x)$ in terms of differential cross section in m^2 units by $I[\text{theta}] = 4*a_0^2Ry/W*(1-W/en)^{0.5}*f(x)/x$. Note that in the Kahre plot the differential cross section was in a_0^2 units versus Ka_0 .

```
In[63]:= KhareGOS=Table[{(khareDataFig1[[j,1]])^2, ((khareDataFig1[[j,2]]/(4*Ry/W*(1-W/en)^0.5)*(khare
{j,Length[khareDataFig1]});
```

```
In[64]:= ListPlot[%,PlotStyle->plotColorsPoints[[5]], PlotLabel-> "GOS versus (K*a0)^2"]
```



```
In[65]:= Import["khare66Fig2exp.dat", "CSV"] // TableForm
```

Out[65]/TableForm=

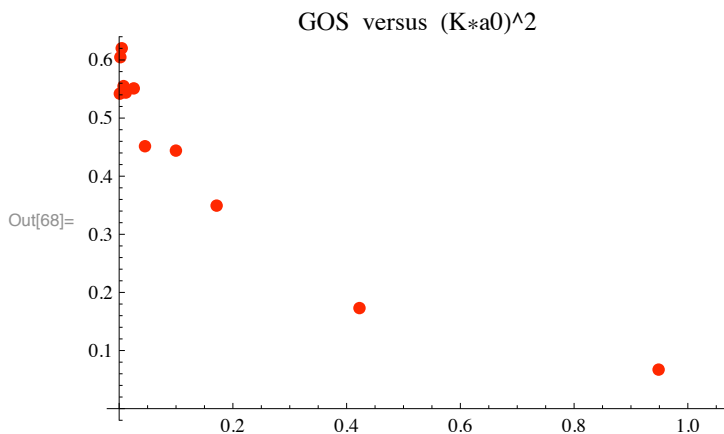
-6.71917E+00	5.42034E-01
-6.17422E+00	6.04775E-01
-5.40345E+00	6.20161E-01
-4.86475E+00	5.55029E-01
-4.44842E+00	5.43895E-01
-3.66226E+00	5.51097E-01
-3.09157E+00	4.51564E-01
-2.30442E+00	4.44013E-01
-1.76373E+00	3.49374E-01
-8.61350E-01	1.73065E-01
-5.27504E-02	6.71699E-02
4.99578E-01	2.00816E-02

```
In[66]:= Import["khare66Fig2exp.dat", "Table"];
```

In Fig. 2, Kahre plots Geiger's values for the GOS for the sum of the B and C states versus $\ln[K^2a_0^2]$.

```
In[67]:= khareDataFig2=Table[{(Exp[%[[j,1]]),%[[j,2]]},{j,Length[%]}];
```

```
In[68]:= ListPlot[%,PlotStyle->plotColorsPoints[[1]], PlotLabel-> "GOS versus (K*a0)^2"]
```



These values for the sum of the B and C state excitation in H2 by 25000 eV electrons are roughly twice the values for He(1¹P) excitation by 500 eV electrons in Fig. 67 of Mott and Massey (1965).

Dissociative attachment

Import the dissociative attachment cross section from Joon et al, J. Phys. Chem. Ref Data 37, 913 (2008). This does not include the formation of H2- proposed recently.

```
In[69]:= Import["Yoon08DiscAtt.txt", "CSV"] // TableForm
```

```
Out[69]/TableForm=
```

3.56	9.70E-07
3.63	1.90E-06
3.69	8.09E-06
3.75	1.80E-05
3.76	2.07E-05
3.81	1.94E-05
3.88	1.29E-05
3.94	8.38E-06
4	6.21E-06
4.06	3.88E-06
4.13	2.80E-06
4.25	2.00E-06
4.375	9.70E-07
7.50	1E-07
7.67	1.94E-05
7.84	2.64E-05
8.08	3.76E-05
8.3	4.90E-05
8.59	6.51E-05
8.87	8.15E-05
9.17	9.74E-05
9.48	1.10E-04
9.78	1.19E-04
9.99	1.22E-04
10.2	1.23E-04
10.4	1.23E-04
10.6	1.20E-04
10.8	1.16E-04
11	1.12E-04
11.2	1.08E-04
11.4	1.02E-04
11.6	9.29E-05
11.8	8.27E-05
12.1	6.80E-05
12.4	5.57E-05
12.6	5.17E-05

```

12.9 5.01E-05
13.2 6.92E-05
13.3 9.03E-05
13.5 1.48E-04
13.7 1.80E-04
13.8 1.95E-04
13.9 1.95E-04
14 1.89E-04
14.1 1.72E-04
14.2 1.55E-04
14.3 1.39E-04
14.4 1.26E-04
14.5 1.12E-04
14.6 1.02E-04
14.7 9.33E-05
14.8 8.88E-05
14.9 8.31E-05
15.2 8.03E-05
15.4 7.89E-05
15.5 7.85E-05
15.6 7.86E-05
15.9 7.97E-05
16.4 8.29E-05
16.9 8.70E-05
17.4 9.41E-05
18 1.00E-04

```

```
In[70]:= yoonDiscAttData = Drop[Import["Yoon08DiscAtt.txt", "Table"], -2];
```

```
In[71]:= yoonDiscAttPlot = ListLogLogPlot[yoonDiscAttData,
PlotRange -> {{.1, 10000}, {fac * 0.99 * 10^-26, fac * 1.01 * 10^-21}},
Joined -> True, ImageSize -> 400, PlotStyle -> plotColorsLines,
PlotLabel -> "Cross sections for e + H2 -> H- (10^-20 m^2) vs energy (eV)"];

```

Fit experiment

```
In[72]:= dissocAttFit[we_] = UnitStep[we - 8.5] * 1. * 10^-24 / (1 + we / 50)^2 + 1. * 10^-30
```

```
Out[72]= 1. * 10^-30 +  $\frac{1. \times 10^{-24} \text{UnitStep}[-8.5 + \text{we}]}{\left(1 + \frac{\text{we}}{50}\right)^2}$ 
```

```
In[73]:= dissocAttFit[we_] = UnitStep[we - 2.2] * 4. * 10^-24 * (we / 8)^4 * Exp[-we / 4] + 1. * 10^-30
```

```
Out[73]= 1. * 10^-30 + 9.76563 * 10^-28 e^-we/4 we^4 UnitStep[-2.2 + we]
```

```
In[74]:= dissocAttFit[we_] =
UnitStep[we - 7] * 5. * 10^-24 / (1 + 1 / (we - 8)) / (1 + (we / 10)^4) + 1. * 10^-30
```

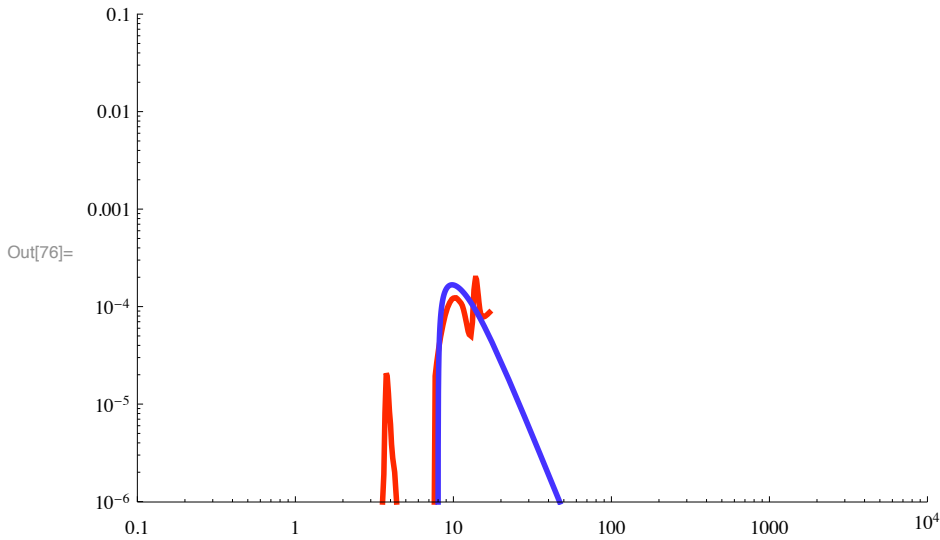
```
Out[74]= 1. * 10^-30 +  $\frac{5. \times 10^{-24} \text{UnitStep}[-7 + \text{we}]}{\left(1 + \frac{1}{-8 + \text{we}}\right) \left(1 + \frac{\text{we}^4}{10000}\right)}$ 
```

```
In[75]:= dissocAttFitPlot = LogLogPlot[fac * dissocAttFit[we], {we, 0.1, 10^4},
PlotRange -> {{.1, 10000}, {fac * 0.99 * 10^-26, fac * 1.01 * 10^-21}},
PlotStyle -> plotColorsLines[[5]]];

```

In[76]:= Show[yoonDiscAttPlot, dissocAttFitPlot]

Cross sections for e + H2 -> H- (10^-20 m^2) vs energy (eV)



This should give a reasonable first estimate of the dissociative attachment for our relatively high energy electrons.

■ Ionization in limit of free fall of electrons

In[77]:= qes2Best[we_] = Piecewise[
 {{1.7 * 10^-20 * (we - 15.4) / (40 - 15.4) / ((we / 37)^1.78 + 1), we > 15.4}, {0, we <= 15.4}}]

Out[77]=
$$\begin{cases} \frac{6.91057 \times 10^{-22} (-15.4 + we)}{1 + 0.00161659 we^{1.78}} & we > 15.4 \\ 0 & True \end{cases}$$

Mathematica cannot handle the preceding approximation. The following approximation will fall off too fast at high we and high E/N.

In[78]:= qes2[we_] = Piecewise[
 {{1.7 * 10^-20 * (we - 15.4) / (40 - 15.4) / ((we / 37)^2 + 1), we > 15.4}, {0, we <= 15.4}}]

Out[78]=
$$\begin{cases} \frac{6.91057 \times 10^{-22} (-15.4 + we)}{1 + \frac{we^2}{1369}} & we > 15.4 \\ 0 & True \end{cases}$$

qes2[we] = Piecewise[{{1.7 * 10^-20 * (we - 15.4) / (40 - 15.4), we > 15.4}, {0, we <= 15.4}}]

In the limit of zero pressure, the Bennet model gives the ionization as

I am disappointed that these do not agree better at high E/N. The usual definition of an alpha coefficient is the integral of the reaction frequency over the distribution function divided by the drift velocity. If the distribution function is a beam at the local available energy, then this prescription gives the cross section at the local energy, i.e., the cyan curve for a representative nd value. However, our fit to experiment is the green curve.

```
In[85]:= Quit[]
```

■ Attempt at solution of energy balance equations for single beam

```
Clear[ques2]
```

At high energies

```
ques2Best[we_] = 1.7 * 10^-20 * (we - 15.4) / (40 - 15.4) / ((we / 37)^1.78 + 1)
```

At very high energies Eq. (6) of Phelps et al (1987) gives

```
energyBalance = D[en[nz], nz] == qe * eon - en[nz] * ques2[en];
```

Since I have been unable to get a general solution for an arbitrary energy dependence of the ionization cross section, let us try a perturbation approach. The zero order solution is

```
en0 := eon * qe * nz
```

So that the perturbation solution is

```
en[nz_] := en0 + p * enp[nz]
```

```
energyBalance =
```

```
D[en[nz], nz] == qe * eon - (en[nz] * ques2[en[nz]] /. ques2[en[nz]] -> ques2Best[en[nz]])
```

Keeping only the terms to first order in p

```
energyBalancep =
```

```
p * enp'[nz] == -Series[(eon * nz * qe) * ques2[en[nz]] /. ques2[en[nz]] -> ques2Best[en[nz]], {p, 0, 1}]
```

```
DSolve[{energyBalancep}, enp[nz], nz]
```

```
Quit[]
```

InverseFunction[f] represents the inverse of the function f , defined so that InverseFunction[f][y] gives the value of x for which $f[x]$ is equal to y . In the following $-nz \rightarrow x$, $en \rightarrow y$.

```
in1 = en[nz] /. %[[1]] /. C[1] -> 0
```

```
in2 = in1 /. {eon -> 1. * 10^-20, qe -> 1, aa -> 1. * 10^-21, en1 -> 100}
```

```
in3 = in2 /. nz -> -10^20
```

```
Solve[in2 == en, nz]
```

```
nz3 = nz /. %[[1]]
```

```
nz3 /. en -> 1
```

This is garbage for reasistic en

```
Plot[Evaluate[nz3], {en, -100, 100}, PlotRange -> {{-100, 100}, All}]
```

What I really want is $\text{alphon} = D[\text{ne}[\text{nz}], \text{nz}] / \text{ne}[\text{nz}] == (\text{qes2}[\text{en}] * \text{ne}[\text{nz}] - D[\text{ne}[\text{nz}], \text{en}]) / \text{ne}[\text{nz}]$

```
alphon = ((qes2[en] * ne[nz] /. qes2[en] -> aa * en[nz]) - D[ne[nz], en]) / ne[nz]
```

Try a velocity solution where $w^2 = en = m * u^2 / (2 * qe)$ or $w = \text{Sqrt}[m / (2 * qe)] * u$

```
energyBalance1 = D[(w[nz])^2, nz] == qe * eon - (w[nz])^2 * qes2 /. qes2 -> bb * (w[nz])^2
```

Try a constant ionization cross section, i.e., cc

```
energyBalance1 =
```

```
D[(w[nz])^2, nz] == qe * eon - (w[nz])^2 * Piecewise[{{cc, w[nz] > wi}, {0, w[nz] < wi}}]
```

```
DSolve[energyBalance1, w[nz], nz]
```

```
w1 = w[nz] /. %[[1]] /. C[1] -> 0
```

```
in = w1 /. {eon -> 1. * 10^-20, qe -> 1, cc -> 1. * 10^-21, wi -> 15.4}
```

```
N[in /. nz -> 10^20]
```

```
N[Evaluate[in /. nz -> 1. * 10^20]]
```

```
LogLogPlot[Evaluate[nz /. {eon -> 10^-20, qe -> 1, cc -> 10^-21, wi -> 15.4}], {w1, 10, 1000}]
```

```
LogLogPlot[Evaluate[w1 /. {eon -> 10^-20, qe -> 1, bb -> 10^-21, wi -> 15.4}], {nz, 10^16, 10^24}]
```

in the following the $\text{Sqrt}[2 * qe / m]$ on each side of equation cancel

```
particleBalance = D[w[nz] * ne[nz], nz] == w[nz] * ne[nz]
```

```
DSolve[%, ne[nz], nz]
```

```
ne1 = ne[nz] /. %[[1]]
```

```
Solve[(ne1 /. nz -> 0) == 1, C[1]]
```

What I really want is

```
ne1 = ne1 /. %[[1]]
```

```
alphon = (D[ne1, nz] / ne1) /. {w[nz] -> w1, w'[nz] -> D[w1, nz]} // Simplify
```

```
LogLogPlot[(1 - %) /. {eon -> 10^-20, qe -> 1, cc -> 10^-21, wi -> 15.4}, {nz, 10^16, 10^24}]
```

what does all this mean?

```
Quit[]
```

Swarm coefficients for e + H2 collisions

Setup notebook environment

```
In[1]:= a = 1;
In[2]:= ClearAll["Global`*"];
In[3]:= Remove["Global`*"];
In[4]:= startclock = SessionTime[];
In[5]:= Off[General::spell];
In[6]:= Off[General::spell1];
In[7]:= today = StringForm["`"/`"/` `:`:`:", Date][[2]],  
         Date][[3]], Date][[1]], Date][[4]], Date][[5]], Date][[6]]
Out[7]= 1/4/2011 17:0:51.1801524`9.461676424815021
```

```

In[8]:= SetDirectory["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\h2electroncollisions"]
Out[8]:= c:\users\avp\documents\Mathbook\hydrogen\h2electroncollisions

In[9]:= plotColorsLines = {
  (*1-red*) {Hue[0.0], Thickness[0.007], Dashing[{}]},
  (*2-orange*) {Hue[0.1], Thickness[0.007], Dashing[{}]},
  (*3-green*) {Hue[0.3], Thickness[0.007], Dashing[{}]},
  (*4-cyan*) {Hue[0.5], Thickness[0.007], Dashing[{}]},
  (*5-dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{}]},
  (*6-purple*) {Hue[0.8], Thickness[0.007], Dashing[{}]},
  (*7-black*) {Thickness[0.007], Dashing[{}]},
  (*8-dash red*) {Hue[0.0], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*9-dash orange*) {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*10-dash green*) {Hue[0.3], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*11-dash cyan*) {Hue[0.5], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*12-dash dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*13-dash purple*) {Hue[0.8], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*14-dash black*) {Thickness[0.007], Dashing[{0.02, 0.02}]}];

In[10]:= plotColorsPoints = {
  (*1-red*) {Hue[0.0], PointSize[0.02]},
  (*2-orange*) {Hue[0.1], PointSize[0.02]},
  (*3-green*) {Hue[0.3], PointSize[0.02]},
  (*4-cyan*) {Hue[0.5], PointSize[0.02]},
  (*5-dk blue*) {Hue[0.7], PointSize[0.02]},
  (*6-purple*) {Hue[0.8], PointSize[0.02]},
  (*7-black*) {PointSize[0.02]}}];

In[11]:= loglogPlotRange={ {9.9, 101000}, {0.99*10^-24, 4.01*10^-20}};

```

■ H2 excited state kinetics

Here we review the collisional kinetics for the $c3\Pi_u$ and $a3\Sigma_g^+$ excited states of H2.

■ $c3\Pi_u$ state

Tischer and Phelps, Chem. Phys. Lett. 117, 550 (1985) and Wedding and Phelps, J. Chem. Phys. 89, 2965 (1988) find that the quenching rate coefficient for the various rotational and vibrational levels of the $c3\Pi_u$ state is $1.9E-15$ m³/s for pressure from 0.2 to 0.9 Torr and that radiative loss is negligible. This large rate coefficient corresponds roughly to quenching by the first collision of a molecule in the $c3\Pi_u$ state with H2. The products of the quenching are unknown, but appear to be of no interest here. Electron induced quenching is calculated to be completely negligible for drift tube conditions. The question is whether one can neglect collisional mixing with the $a3\Sigma_g^+$ state.

■ $a3\Sigma_g^+$ state

Wedding and Phelps, J. Chem. Phys. 89, 2965 (1988) find that the quenching rate coefficient for the various rotational and vibrational levels of the $a3\Sigma_g^+$ state is $1.E-16$ m³/s for pressure from 1.3 to 4 Torr and that radiative loss is dominant. This small product of the quenching rate coefficient and radiative lifetime is consistent with our conclusion above that one can forget quenching at our pressures. The products of the quenching appears to be the $c3\Pi_u$ state, which is very rapidly quenched. Electron induced quenching is presumably completely negligible for drift tube conditions. The question is whether one can neglect collisional mixing with the $c3\Pi_u$ state.

Can one neglect excitation to all states besides $a3\Sigma_g^+$? How about $d3\Pi_u$? Presumably it is rapidly quenched, i.e., like $c3\Pi_u$. Only $?3\Pi_u$ states would seem to have the right symmetry to radiate to the $a3\Sigma_g^+$.

■ Can one neglect $c3\Pi_u$ collisional excitation to the $a3\Sigma_g^+$?

From Wedding and Phelps (1988) Eqs. (4) and (5) the rate equations for the density of $a3\Sigma_g^+$ state n_a and $c3\Pi_u$ state n_c excited H2 molecules are:

$$\text{In[12]:= } \text{dncodt} = k_{ec} n_{H2} n_e + k_{ac} n_{H2} n_a - (k_{qc} + k_{ca}) n_{H2} n_c$$

and

$$\text{In[13]:= } \text{dnaodt} = k_{ea} n_{H2} n_e + k_{ca} n_{H2} n_c - (A_{ab} + k_{qa} n_{H2} + k_{ac} n_{H2}) n_a$$

We are interested in the steady state solutions for n_a and n_c

In[14]:= **Solve**[{**dncodt**==0,**dnaodt**==0},**na**,**nc**]

$$\text{Out[14]} = \left\{ \left\{ \text{na} \rightarrow \frac{(kca \text{ kea } ne + kca \text{ kec } ne + \text{ kea } kqc \text{ ne}) nH2}{Aab \text{ kca} + Aab \text{ kqc} + kca \text{ kqa } nH2 + kac \text{ kqc } nH2 + kqa \text{ kqc } nH2} \right\} \right\}$$

In[15]:= **na=na/.%[[1]]//Simplify**

$$\text{Out[15]} = \frac{(kca (kea + kec) + \text{ kea } kqc) \text{ ne } nH2}{Aab (kca + kqc) + (kca \text{ kqa} + (kac + kqa) \text{ kqc}) \text{ nH2}}$$

We want the ratio of the continuum emission originating with the $c3\Pi_u$ to that originating with the $a3\Sigma_g^+$ state. This equal to the ratio of the kea term to the kec term in na .

In[16]:= **ratio=Coefficient**[%,**kec**]***kec**/**(Coefficient**[%,**kea**]***kea**)

$$\text{Out[16]} = \frac{kca \text{ kec}}{kea (kca + kqc)}$$

At $E/N=300$ Td

In[17]:= **kec=1.157*10^-15 (*m^3/s*)**;
kea=8.04*10^-16;
kqc=1.88*10^-15;
kqa=1.*10^-15;
kac=3.*10^-16;
kca=1.8*10^-16;
Aab=9.3*10^8; (*s^-1*)

In[24]:= **ratio**

Out[24]= 0.125743

We looked at the contribution of diffusion and free-fall to the loss of $c3\Pi_u$ and concluded it was negligible for our drift tube and pressures. Unfortunately, the calculations were lost.

We still have not accounted for cascading effects from levels with $n \Rightarrow 3$. According to Fig. 2 of Wedding and Phelps (1988), cascading to the $a3\Sigma_g^+$ state can occur from the $d3\Pi_u$ state and to the $c3\Pi_u$ state from the $i3\Pi_g$ state. The contribution of the latter is limited by branching to the $b3\Sigma_u^+$ state and by the rapid quenching of the $c3\Pi_u$ state and so should be negligible. Agello and Shemansky, Ap. J. 407, 820 (1993) cite data estimating sum of the the cascade contributions of the $d3\Pi_u$ and $e3\Sigma_u^+$ states to be 1/3 of the $a3\Sigma_g^+$ cross section. This estimate does not take into account the larger collisional quenching of the higher states in our experiments.

- **H2 near uv continuum excitation by electrons**
- **Lunt, Meek, and Smith, Proc. Roy. Soc. (London) 158A, 729 (1937)**

Figure 1 compares a smooth calculated curve with relative measurements for the near uv excitation efficiency.

```
In[25]:= Import["H2ContinuumLunt.txt", "CSV"] // TableForm
```

```
Out[25]//TableForm=
```

```
H2 electron excitation of continuum
E/p      eta
25.5     4.4
29       4.0
30.5     4.4
35.5     5.4
42       5.0
48.5     5.4
51       5.0
138      1.8
92       3.0
97       2.6
119      2.2
145      1.6
235      1.2
247      0.9
```

```
In[26]:= Drop[Drop[Import["H2ContinuumLunt.txt", "Table"], 2], -1];
```

```
In[27]:= luntUVContinuum = Table[{{#[[j, 1]] / 0.346, #[[j, 2]] * 10^-2}, {j, Length[#]}}];
```

We now need use power input $eon \cdot efficiency = \epsilon \cdot \alpha_{phaxon}$. From my Web site for electrons in H2 the E/N (Td) - drift velocity (m/s) table is:

```
In[28]:= wvseon = Transpose[{{20, 40, 70, 100, 200, 300, 500, 1000, 2000},
  {28809, 47910, 87265, 132240, 289650, 446860, 725560, 1258100, 2121200}}];
```

```
In[29]:= w = Interpolation[wvseon]
```

```
Out[29]= InterpolatingFunction[{{20, 2000}}, <>]
```

```
In[30]:= epsilonx = 8;
```

```
In[31]:= alphaxonTable =
  Table[{{#[[j, 1]], #[[j, 1]] * 10^-21 * #[[j, 2]] / epsilonx}, {j, Length[#]}} & [luntUVContinuum];
```

```
In[32]:= luntuvPlot = ListLogLogPlot[alphaxonTable, PlotRange -> loglogPlotRange,
  ImageSize -> 400, PlotStyle -> plotColorsPoints[[3]], GridLines -> Automatic,
  PlotLabel -> "Spatial reaction coefficients for e + H2 (m^2)-> uv vs E/N (Td)"];

```

```
In[33]:= Export["alphaxonLunt.txt", alphaxonTable, "Table"]
```

```
Out[33]= alphaxonLunt.txt
```

■ Empirical curve from Phelps' notes. Revised 11/05/10

Electron impact excitation of uv - this is an empirical quasi-steady-state or local-field equilibrium fit to the sum of the a, c, and d state excitation coefficients. Calc of 12/23/94 givig E/N in Td and α/N in m^2 .

```
In[34]:= boltzmannCalcNearUVTable =
  {{40, 4.23 * 10^-23}, {70, 8.04 * 10^-22}, {100, 1.687 * 10^-21}, {200, 3.11 * 10^-21},
  {300, 3.47 * 10^-21}, {500, 3.22 * 10^-21}, {1000, 2.11 * 10^-21}, {2000, 9.22 * 10^-22},
  {3000, 4.43 * 10^-22}, {5000, 1.482 * 10^-22}} // TableForm
```

```
Out[34]//TableForm=
```

```
40    4.23 × 10-23
70    8.04 × 10-22
100   1.687 × 10-21
200   3.11 × 10-21
300   3.47 × 10-21
500   3.22 × 10-21
1000  2.11 × 10-21
2000  9.22 × 10-22
3000  4.43 × 10-22
5000  1.482 × 10-22
```

```
In[35]:= boltzmannCalcNearUVTable = {{40, 4.23 * 10^-23}, {70, 8.04 * 10^-22},
  {100, 1.687 * 10^-21}, {200, 3.11 * 10^-21}, {300, 3.47 * 10^-21}, {500, 3.22 * 10^-21},
  {1000, 2.11 * 10^-21}, {2000, 9.22 * 10^-22}, {3000, 4.43 * 10^-22}, {5000, 1.482 * 10^-22}};
```

```
In[36]:= boltzCalcNearUVPlot = ListLogLogPlot[boltzmannCalcNearUVTable,
      PlotRange -> loglogPlotRange, PlotStyle -> plotColorsPoints[[1]]];
```

The following formula in the spreadsheet HALPHAEX.WQ1 probably fits the a state excitation, not the a plus c state excitation.

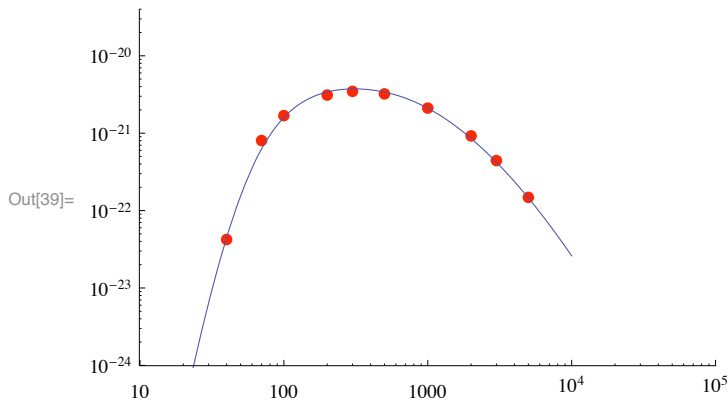
$$\text{alH2uv}[\text{eonTd}_] := 1.6 * 10^{-20} * \text{Exp}[-115 / \text{eonTd}] - 1.4 * 10^{-20} * \text{Exp}[-(600 / \text{eonTd})] + 10^{-30}$$

The following formula in the spreadsheet HALPHAEX.WQ1 fits the a + c + higher state excitation.

```
In[37]:= alH2uv[eonTd_] := 5 * 10^{-21} / (1 + (50 / eonTd)^2)^5 / (1 + (eonTd / 900)^1.7) / (1 + (eonTd / 6000)^1.5)
```

```
In[38]:= uvBoltzFitPlot = LogLogPlot[{alH2uv[eonTd]}, {eonTd, 10, 10000} (*,
      PlotRange->loglogPlotRange, ImageSize->400, PlotStyle->plotColorsLines[[1]]*)];
```

```
In[39]:= Show[boltzCalcNearUVPlot, uvBoltzFitPlot]
```



From the Boltzmann calculations of 12/23/94 with spatial growth included

```
In[40]:= h2eBoltzmann=Drop[Import["c:/users/avp/documents/mathbook/hydrogen/H2ElectronCollisions/H2eBoltzmann
```

The last point probably should be dropped as being too low. These values are significantly lower than the values plotted by Stokic et al (1992) and are outside the scatter in the experimental values of Stokic et al.

These values are an order of magnitude below those in JILA Rept. 27 for the sum of the higher triplet states, but is about right for the c3Sigma state!!!

For reasons I do not recall, I decided to fit an empirical curve to these Boltzmann results and then construct a table of values to be used later, rather than using the original table.

Plotting vs the reciprocal of E/N in Td.

```
In[41]:= astateElectronExcitCalc1=Table[{1/h2eBoltzmann[[j,1]],h2eBoltzmann[[j,6]]},{j,Length[h2eBoltzmann]-1}
```

```
In[42]:= astateElectronExcitCalc1Plot=ListLogPlot[astateElectronExcitCalc1,PlotRange->{{0.,0.03},{10^{-23},2.*10^{-22}},
      ImageSize->400, PlotStyle->plotColorsPoints[[7]](*, DisplayFunction->Identity*)];
```

Plotting versus E/N.

```
In[43]:= astateElectronExcitCalc=Table[{h2eBoltzmann[[j,1]],h2eBoltzmann[[j,6]]},{j,Length[h2eBoltzmann]-1}];
```

```
In[44]:= astateElectronExcitCalcPlot=ListLogLogPlot[astateElectronExcitCalc,PlotRange->{{10,10000},{10^{-23},10^{-22}},
      ImageSize->400, PlotStyle->plotColorsPoints[[7]](*, DisplayFunction->Identity*)];
```

Break up the fit into regions above and below 300 Td

For E/N <= 300 Td

```
In[45]:= astateExcitationCalcFit1= If[eonTd<=300,33*10^{-20}*Exp[-330/eonTd]/(1+(eonTd/25)^1)^2*(1+(eonTd/315)^1.5)*10^{-22}/(1+(eonTd/800)^3)^0.5]
```

$$\text{Out[45]= If} \left[\text{eonTd} \leq 300, \frac{33 \text{Exp} \left[-\frac{330}{\text{eonTd}} \right] \left(1 + \left(\frac{\text{eonTd}}{315} \right)^1 \right)}{10^{20} \left(1 + \left(\frac{\text{eonTd}}{25} \right)^1 \right)^2}, \frac{13.5}{10^{22} \left(1 + \left(\frac{\text{eonTd}}{800} \right)^3 \right)^{0.5}} \right]$$

Express the same fit in terms of reciprocal of eonTd so as to emphasize the low E/N

```
In[46]:= astateExcitationCalcFit2= astateExcitationCalcFit1/. eonTd->1/reonTd
```

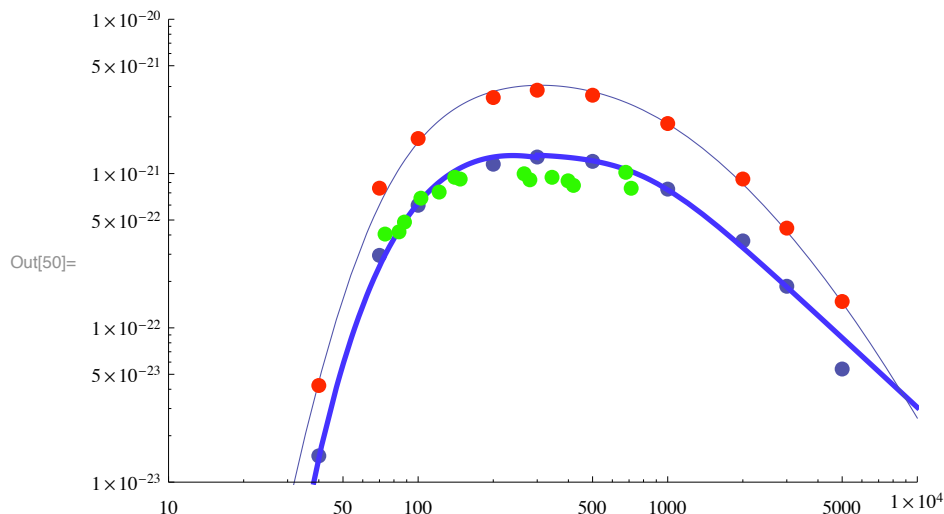
$$\text{Out[46]= If}\left[\frac{1}{\text{reonTd}} \leq 300, \frac{33 \text{Exp}\left[-\frac{330}{\text{reonTd}}\right] \left(1 + \left(\frac{1}{\text{reonTd} 315}\right)^1\right)}{10^{20} \left(1 + \left(\frac{1}{\text{reonTd} 25}\right)^1\right)^2}, \frac{13.5}{10^{22} \left(1 + \left(\frac{1}{\text{reonTd} 800}\right)^3\right)^{0.5}}\right]$$

```
In[47]:= astateExcitationCalcFit2Plot=LogPlot[astateExcitationCalcFit2,{reonTd,0.0,0.025}, ImageSize->400,
PlotStyle->plotColorsPoints[[1]], PlotRange->{{0,0.025},{10^-23,10^-20}}, DisplayFunction->Identity]
```

```
In[48]:= Show[astateElectronExcitCalc1Plot,astateExcitationCalcFit2Plot];
```

```
In[49]:= astateExcitationCalcFit1Plot=LogLogPlot[astateExcitationCalcFit1,{eonTd,10,10000}, ImageSize->400,
PlotStyle->plotColorsLines[[5]], PlotRange->{{10,10000},{10^-23,10^-20}}];
```

```
In[50]:= Show[astateElectronExcitCalcPlot, astateExcitationCalcFit1Plot, luntuvPlot, uvBoltFitPlot,boltCalcNe
```



```
In[51]:= astateFit2006=Table[{10.*10^(j/8),1.*astateExcitationCalcFit1/.eonTd->10*10^(j/8)},{j,0,24}];
```

```
In[52]:= Export["PhelpsUV06.dat",astateFit2006,"Table"];
```

```
In[53]:= alH2uv[eonTd_]:=astateExcitationCalcFit1
```

```
In[54]:= uvFitPlot = LogLogPlot[alH2uv[eonTd], {eonTd, 10, 10 000}, PlotRange -> loglogPlotRange,
PlotPoints -> 500, ImageSize -> 400, PlotStyle -> plotColorsLines[[1]], GridLines -> Automatic,
PlotLabel -> "Spatial reaction coefficients for e + H2 (m^2)-> uv vs E/N (Td)"];
```

```
In[55]:= astateElectronExcitCalc=Table[{h2eBoltzmann[[j,1]],h2eBoltzmann[[j,6]]},{j,Length[h2eBoltzmann]}];
```

```
In[56]:= astateElectronExcitCalcPlot=ListLogLogPlot[astateElectronExcitCalc, PlotRange->loglogPlotRange,
ImageSize->400, Joined->True, PlotStyle->plotColorsLines[[2]], DisplayFunction->Identity];
```

Here we have dropped the 5 kTd point because of its sudden departure from a smooth curve.

```
Show>(*maxuvElectronExcitCalcPlot,*)uvFitPlot, astateElectronExcitCalcPlot, DisplayFunction->$Displa
```

a state excitation coefficients calculated using Ajello and Shemansky (1993) cross sections and using BOLSIGPLUS give

```
bolsigplusOutput=Import["C:\\users\\avp\\documents\\DATABASE\\BOLSIGPLUS\\H2Output051406.dat", "Table",
Position[%,11.8]
```

```
In[57]:= bolsigplusastate=Take[Import["C:\\users\\avp\\documents\\DATABASE\\BOLSIGPLUS\\H2Output051406.dat", '
```

```
In[58]:= bolsigplusastatePlot=ListLogLogPlot[bolsigplusastate,PlotRange->loglogPlotRange, ImageSize->400,
PlotStyle->plotColorsLines[[14]], Joined->True];
```

H2Bolsigplusastate5.dat is for shared energy and spatial growth, H2Bolsigplusastate4.dat is for one electron energy loss and spatial growth, H2Bolsigplusastate3.dat is for shared energy and temporal growth

■ Stojanovic et al experiment

From Fig. 4 of the unpublished report by Stojanovic, Bozin, Stokic, Petrovoc, and Jelenkovic we get the experimental excitation coefficients.

```
In[59]:= Import["stojanovicvexpt.dat", "CSV"]//TableForm
```

```
Out[59]//TableForm=
```

1.90725E+02	8.18152E-18
4.86867E+02	1.27335E-17
9.50536E+02	9.42873E-18
1.35123E+03	6.55649E-18
1.59919E+03	5.93226E-18
1.92095E+03	5.08317E-18
2.85511E+03	3.17009E-18
3.55053E+03	2.54916E-18
4.66317E+03	2.36956E-18
5.02283E+03	2.14436E-18
5.77024E+03	1.87121E-18
5.85616E+03	1.60391E-18

```
In[60]:= Import["stojanovicvexpt.dat", "Table"];
```

```
In[61]:= stojanovicvexptPlot=ListLogLogPlot[%,PlotRange->loglogPlotRange, ImageSize->400, PlotStyle->plotCol
```

■ Tisher and Phelps - relative values

From an unpublished graph by Tischer and Phelps, we get the relative experimental excitation coefficients.

```
In[62]:= Import["tischercontinuum.dat", "CSV"]//TableForm
```

```
Out[62]//TableForm=
```

5.18744E+01	1.71133E+00
5.71491E+01	3.37731E+00
6.09602E+01	4.02496E+00
6.50256E+01	5.17948E+00
6.86197E+01	6.24077E+00
7.39876E+01	7.35642E+00
7.72415E+01	8.29942E+00
8.15108E+01	9.06031E+00
9.07703E+01	1.07978E+01
9.78711E+01	1.21819E+01
1.06669E+02	1.35936E+01
1.11360E+02	1.46780E+01

```
In[63]:= Import["tischercontinuum.dat", "Table"];
```

```
In[64]:= Table[{{%[[j,1]],%[[j,2]]*4.*10^-23},{j,Length[%]}}];
```

```
In[65]:= tischerDataPlot=ListLogLogPlot[%,PlotRange->loglogPlotRange, ImageSize->400, PlotStyle->plotColorsPc
```

■ Buckman and Phelps? - Boltzmann calc

From Fig. 4 of the unpublished report by Stojanovic, Bozin, Stokic, Petrovoc, and Jelenkovic we get the calculated excitation coefficients said to be from Buckman and Phelps. Actually, these coefficients are much closer to those from the 12/23/94 Boltzmann results than to JILA information Report No. 27 and the Web.

```
In[66]:= Import["stojanovicvtheory.dat", "CSV"]//TableForm
```

```
Out[66]//TableForm=
```

```
1.01681E+02    6.28415E-22
1.43488E+02    8.59429E-22
1.89427E+02    1.12884E-21
2.57118E+02    1.32680E-21
3.26492E+02    1.35388E-21
4.10003E+02    1.30027E-21
5.65867E+02    1.14030E-21
7.68076E+02    8.94857E-22
1.21125E+03    5.91467E-22
1.97486E+03    3.42837E-22
```

```
In[67]:= Import["stojanovicvtheory.dat", "Table"];
```

```
In[68]:= stojanovicvtheoryPlot=ListLogLogPlot[%,PlotRange->loglogPlotRange, Joined->True, ImageSize->400];
```

From our Web site and file ELETRANS.TXT and JILA Information Center Report No. 27, we get Boltzmann results using the cross sections listed in the report.

```
In[69]:= Drop[Import["H2EleTransastate.txt", "Table"], 2];
```

```
In[70]:= boltzHUVWeb=Table[{%[[1,j]],%[[2,j]]},{j,Length[%[[1]]}];
```

```
In[71]:= webastatePlot=ListLogLogPlot[%,PlotRange->loglogPlotRange, Joined->True, ImageSize->400];
```

■ Halpha excitation by electrons

This is an empirical quasi-steady-state or local-field equilibrium formula

```
In[72]:= alHalpHa[eonTd_] := + 2.1 * 10^-22 * Exp[- 400 / eonTd] - 1. * 10^-22 * Exp[- (2000 / eonTd) ^ 2] + 10^-30
```

This is taken from the spreadsheet HALPHAEX.WQ1 and is listed for $100 < E/N < 2000$ Td.

This seems somewhat high, but the E/N extends beyond the range of validity of the two-term Boltzmann solutions.

■ From Stokic et al

From Fig. 6 of Stokic, Fraga, Bozin, Stojanovic, Petrovic, and Jelenkovic, Phys. Rev. A 45, 7463 (1992), we get experiment and their theory

```
In[73]:= Import["stokichaexpt1.dat", "CSV"]//TableForm
```

```
Out[73]//TableForm=
```

```
1.97123E+02    2.52859E-23
2.18701E+02    4.39223E-23
2.63665E+02    5.01463E-23
3.38317E+02    5.85309E-23
3.52670E+02    7.71420E-23
4.31109E+02    8.42673E-23
5.38056E+02    9.41069E-23
7.24687E+02    1.11061E-22
8.32340E+02    1.18670E-22
1.28758E+03    1.41605E-22
1.79529E+03    1.59896E-22
1.89756E+03    1.54685E-22
```

```
In[74]:= Import["stokichaexpt1.dat", "Table"];
```

```
In[75]:= stokichaexpt1Plot=ListLogLogPlot[%,PlotRange->loglogPlotRange, ImageSize->400, PlotStyle->plotColors
```

The following plot appears to be the deuterium data in Fig. 6.

```
In[76]:= Import["stokichaexpt2.dat", "CSV"] // TableForm
```

```
Out[76]//TableForm=
```

```
2.15692E+02    2.47335E-23
3.38317E+02    5.24113E-23
6.22279E+02    8.90513E-23
2.45174E+03    1.28208E-22
```

```
In[77]:= Import["stokichaexpt2.dat", "Table"];
```

```
In[78]:= stokichaexpt2Plot=ListLogLogPlot[%,PlotRange->loglogPlotRange, ImageSize->400, PlotStyle->plotColors
```

```
In[79]:= Import["stokichatheor.dat", "CSV"] // TableForm
```

```
Out[79]//TableForm=
```

```
2.06914E+02    3.64042E-23
2.96606E+02    5.35818E-23
3.80584E+02    6.90763E-23
4.91733E+02    8.71060E-23
6.44203E+02    1.07442E-22
9.49388E+02    1.31071E-22
1.22665E+03    1.43178E-22
1.53096E+03    1.51306E-22
2.04776E+03    1.63466E-22
```

```
In[80]:= Import["stokichatheor.dat", "Table"];
```

```
In[81]:= stokichatheorPlot=ListLogLogPlot[%,PlotRange->loglogPlotRange, Joined-> True, ImageSize->400];
```

■ From Nygaard, Apl. Sci Res. B 12, 91 (1965) one gets alpha/p vs E/p values for Halpha excitation by electrons

```
In[82]:= Import["nygaard65fig2halpha.dat", "CSV"] // TableForm
```

```
Out[82]//TableForm=
```

```
6.43356E+01    2.32788E-02
7.99160E+01    2.93481E-02
9.93081E+01    3.28089E-02
1.49355E+02    5.52069E-02
1.99473E+02    8.11643E-02
2.49605E+02    1.07769E-01
```

```
In[83]:= Import["nygaard65fig2halpha.dat", "Table"];
```

```
In[84]:= nygaardHalpHaExpt = Table[{#[[j, 1]] / 0.33, #[[j, 2]] * 100 / (3.3 * 10^22)}, {j, Length[%]}];
```

```
In[85]:= nygaardHalpHaPlot=ListLogLogPlot[nygaardHalpHaExpt,PlotRange->loglogPlotRange,
ImageSize->400, PlotStyle->plotColorsPoints[[3]](*, DisplayFunction->Identity*);
```

■ Empirical expressions

In MultiBeamSpatial041706.nb, we used the fit cited at the beginning of this section.

```
In[86]:= alHalpHa[eonTd_] := +2.1 * 10^-22 * Exp[-400 / eonTd] - 1. * 10^-22 * Exp[-(2000 / eonTd)^2] + 10^-30
```

```
In[87]:= alHalpHa[500]
```

```
Out[87]= 9.43591 × 10-23
```

On 050407 we modified this to drop more rapidly at high E/N so as to reflect the drop below theory found from the experimental current growth.

```
In[88]:= alHalpHa1[eonTd_] := +2.1 * 10^-22 * Exp[-400 / eonTd] - 2.08 * 10^-22 * Exp[-(3500 / eonTd)]
```

On 080907? I lowered alpha/N for Halpha at 1 kTd to give a better fit to experiment. This lowered the 10 kTd value even more, but we hope this will not be noticed.

```
In[89]:= alHalpHa1[eonTd_] := +2.1 * 10^-22 * Exp[-400 / eonTd] - 2.08 * 10^-22 * Exp[-(1500 / eonTd)]
```

On 091508 I adopted the following so as to fit better Halpha at 45 kTd

```
In[90]:= alHalpHa[eonTd_] :=
+1.25 * (2.2 * 10^-22 * Exp[-400 / eonTd] - 1.5 * 10^-22 * Exp[-(800 / eonTd)]) + 1. * 10^-30
```

```
In[91]:= alHalpahl[500]
```

```
Out[91]:= 8.40034 × 10-23
```

```
In[92]:= alHalpahlFitPlot=LogLogPlot[alHalpahl[eonTd],{eonTd,10,10000},PlotRange->loglogPlotRange,
PlotStyle->plotColorsLines[[1]]];
```

From the Boltzmann calculations of 12/23/94 with spatial growth included

```
In[93]:= Import["c:/users/avp/documents/mathbook/hydrogen/H2ElectronCollisions/H2eBoltzmann.txt","CSV"]//Tabl
```

```
Out[93]//TableForm=
```

40	4.45E-25	5.69E-27	6.8E-29	2.68E-22	1.48E-23
70	5.21E-23	8.86E-25	4.42E-27	2.96E-21	2.95E-22
100	2.51E-22	4.34E-24	1.798E-26	5.14E-21	6.23E-22
200	1.638E-21	2.46E-23	1.132E-25	7.89E-21	1.15E-21
300	3.46E-21	4.59E-23	2.43E-25	8.37E-21	1.28E-21
500	6.92E-21	8.01E-23	4.71E-25	7.58E-21	1.20E-21
1000	1.27E-20	1.31E-22	7.36E-25	4.91E-21	7.93e-22
2000	1.674E-20	1.608E-22	7.61E-25	2.25E-21	3.66E-22
3000	1.666E-20	1.524E-22	6.51E-25	1.156E-21	1.86e-22
5000	1.15E-20	9.7E-23	3.9E-25	3.4E-22	5.41E-23

Bolt. calc. of 12/23/94 pure H2

ioniz.	H alpha	H2 1G	H2sum trip	H2 a state
E/n	alpha/n	alpha/n	alpha/n	alpha/n
Td	m ²	m ²	m ²	m ²

```
In[94]:= Drop[Import["c:/users/avp/documents/mathbook/hydrogen/H2ElectronCollisions/H2eBoltzmann.txt","Table'
```

```
In[95]:= halpahl22394=Table[{{[[j,1]],%[[j,3]]},{j,Length[%]-1}}];
```

```
In[96]:= halpahl22394Plot=ListLogLogPlot[halpahl22394,PlotRange->loglogPlotRange, ImageSize->400, Joined->Tru
```

Here we have dropped the 5 kTd point because of its sudden departure from a smooth curve.

From our Web site and file ELETRANS.TXT and JILA Information Center Report No. 27, we get Boltzmann results using the cross sections listed in the report.

```
In[97]:= Import["H2EleTranshalpahl.txt","CSV"]//TableForm
```

```
Out[97]//TableForm=
```

Halpahl from Web							
E/N (Td = 1E-21 Vm ²)	alpha/N (m ²)						
40	70	100	200	300	500	1000	2000
5.66E-27	8.86E-25	4.43E-24	2.66E-23	5.12E-23	9.06E-23	1.42E-22	1.39e-22

```
In[98]:= Drop[Import["H2EleTranshalpahl.txt","Table"],2];
```

```
In[99]:= boltzHalpahlWeb=Table[{{[[1,j]],%[[2,j]]},{j,Length[%[[1]]}}];
```

```
In[100]:= webhalpahlPlot=ListLogLogPlot[%,PlotRange->loglogPlotRange, Joined->True, ImageSize->400];
```

This red curve shows that our Web site gives higher values than the preceding fit to experiment by ~ 50% at E/n = 1000 Td.


```
In[101]:= bolsigplusHalpHa=Take[Import["C:\\users\\avp\\documents\\DATABASE\\BOLSIGPLUS\\H2Output051406.dat",  
{1123,1145}]]//TableForm
```

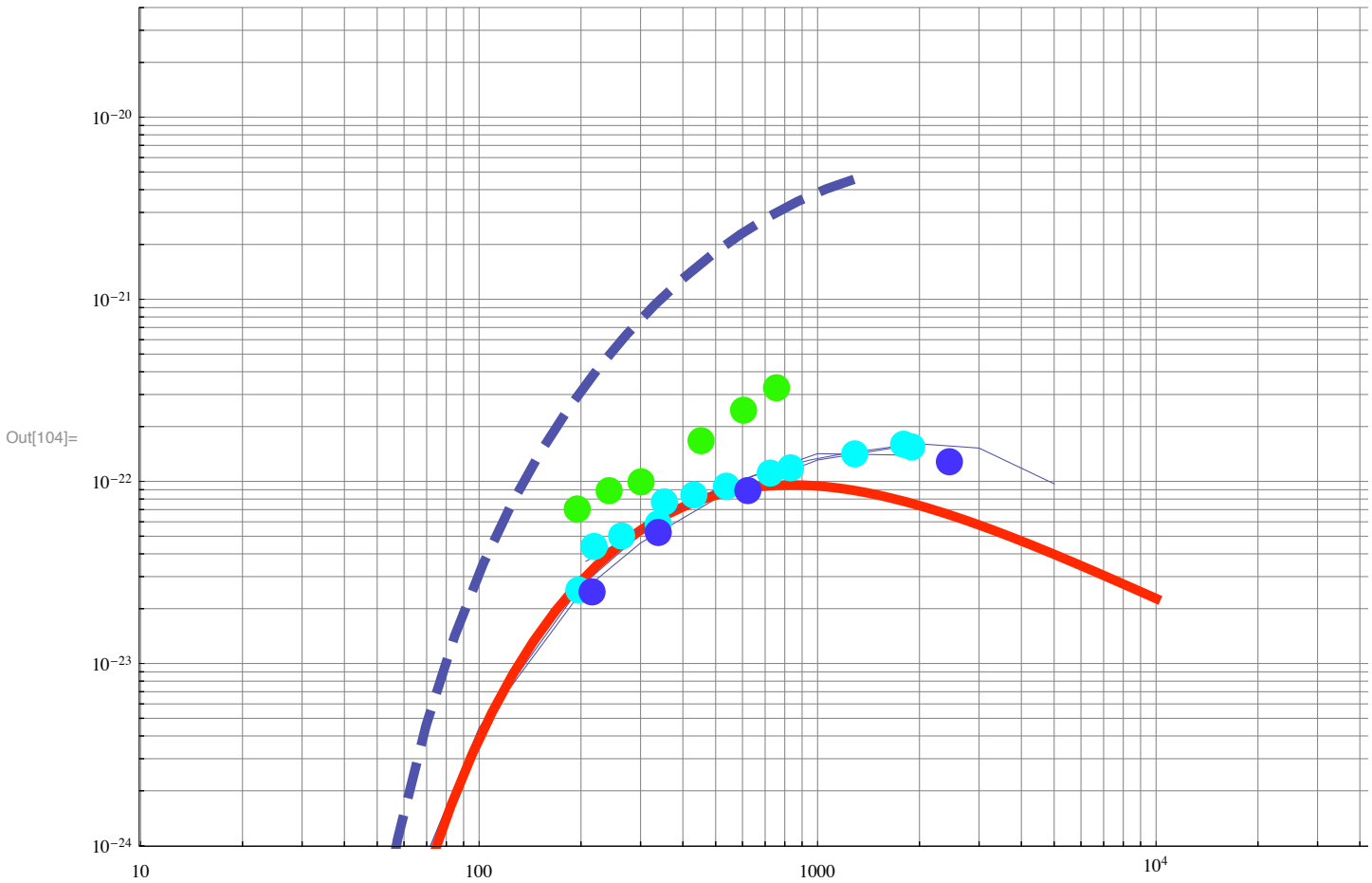
```
Out[101]/TableForm=
```

17.91	0.000
21.75	0.7609E-32
26.42	0.3136E-29
32.09	0.3508E-27
38.97	0.1188E-25
47.32	0.1600E-24
57.47	0.1088E-23
69.80	0.4601E-23
84.77	0.1421E-22
102.9	0.3542E-22
125.0	0.7578E-22
151.8	0.1449E-21
184.4	0.2536E-21
224.0	0.4140E-21
272.0	0.6370E-21
330.3	0.9322E-21
401.2	0.1305E-20
487.2	0.1753E-20
591.7	0.2271E-20
718.6	0.2844E-20
872.7	0.3444E-20
1060.	0.4034E-20
1287.	0.4571E-20

```
In[102]:= bolsigplusHalpHa=Take[Import["C:\\users\\avp\\documents\\DATABASE\\BOLSIGPLUS\\H2Output051406.dat",  
{1123,1145}]];
```

```
In[103]:= bolsigplusHalpHaPlot=ListLogLogPlot[bolsigplusHalpHa,PlotRange->loglogPlotRange, ImageSize->400, Gr.  
PlotStyle->plotColorsLines[[14]], Joined->True];
```

```
In[104]= Show[bolsigplusHalpPlot,webhalpPlot, halp122394Plot, alHalpFitPlot, stochatheorPlot, stok.
stokichaexpt2Plot,nygaardHalpPlot, ImageSize->700]
```



black dash - BOLSIGPLUS; blue curve - Web/AVP; red curve - fit; cyan points - Stokic expt H2; orange curve - Boltz94; blue points - ???; cyan dash - Stokic expt D2;

In the write-up of the Halp experiments, I decided to show the Stokic experiments for H2 and the Boltzmann results labeled alHalpFit-Plot (red curve). These Boltzmann excitation coefficients are the closest I can find to what Zoran probably used to calibrate his Halp data. Apparently I used an approximately 20% smaller value in my recent scaling of Zoran's data in the MultiBeam... files. See also, Mathbook/Hydrogen/SpatialExpt/H2Calib1.qpw.

■ H2 ionization by electrons

■ Electron impact ionization of H2 to form H2+ - this is an emperical quasi-steady-state or local-field equilibrium formula

```
In[105]= alion[eonTd_] := 1.4*10^-20*Exp[-405/eonTd]/((1+(eonTd/10000)^1.5)^.5)+10^-30
```

or an apparently older form that gives ~ 20% lower values around E/N of 1 to 5 kTd.

```
alion1[eonTd_] := 1.6*10^-20*Exp[-400/eonTd]-6.5*10^-21*Exp[-750/eonTd]
```

From H2CurrentGrowth120706.nb our fits to the transient current growth data give effective ionization coefficients versus E/N of

```
In[106]:= growthData={{500, 5.7*^-21}, {1000, 7.*10^-21}, {3000, 5.5*^-21}, {10000, 4.*^-21}, {45000, 1.5*10^-21}}
Out[106]= {{500, 5.7 × 10-21}, {1000, 7. × 10-21}, {3000, 5.5 × 10-21}, {10000, 4. × 10-21}, {45000, 1.5 × 10-21}}
In[107]:= currentGrowthIonizationPlot=ListLogLogPlot[%,PlotRange->loglogPlotRange, ImageSize->400,
PlotStyle->plotColorsPoints[[7]]];
```

This data requires a change in the empirical fit of the ionization coefficient data

```
In[108]:= alion1[eonTd_] = 1.4*10^-20*Exp[-405/eonTd]/((1+(eonTd/550)^3)^.145)+1.*10^-30;
In[109]:= ionizationFitGrowthPlot=LogLogPlot[{alion1[eonTd],0.84*alion1[eonTd]},{eonTd,10,100000}, PlotRange->
ImageSize->400, PlotStyle->plotColorsLines[[7]]];
In[110]:= growthIonizationPlot=Show[ionizationFitGrowthPlot, currentGrowthIonizationPlot, DisplayFunction->$D;
```

In MultiBeamSpatial041706.nb we used the fit

```
In[111]:= alion3[eonTd_] := 0.8*1.4*10^-20*Exp[-405/eonTd]/(((eonTd/10000)^1.5+1)^.5)+10^-30
In[112]:= alion3[1000]
Out[112]= 7.35476 × 10-21
In[113]:= alion3[350]
Out[113]= 3.50962 × 10-21
```

This is good at 350 Td, but is a poor fit at high E/N. Try

```
In[114]:= alion3[eonTd_] := 1.2*10^-20*Exp[-405/eonTd]/(((eonTd/2000)^1.5+1)^.5)+10^-30
In[115]:= alion3[1000]
Out[115]= 6.87946 × 10-21
In[116]:= alion3[350]
Out[116]= 3.64165 × 10-21
In[117]:= ionizationFitPlot=LogLogPlot[alion3[eonTd]},{eonTd,10,10000},PlotRange->loglogPlotRange, ImageSize->
PlotStyle->plotColorsLines[[1]]];
```

This fit, without the 0.84 factor, is designated as fit#2 on the spreadsheet C:\H2DATA\H2Q\EMPIRICAL.WQ1 dated 3/10/96. This is a better fit to what is listed as "experimental" data in the same table. The source of the experimental data is not given. It appears to be a compromise between the low values from Belgrade drift tube experiments similar to the present ones and the higher values of Rose as obtained using the Townsend current growth method. alion3 fits better Zoran's 350 Td spatial scan.

From our Web site and file ELETRANS.TXT and JILA Information Center Report No. 27, we get Boltzmann results using the cross sections listed in the report.

```
In[118]:= Import["H2EleTransIonization.txt", "CSV"] // TableForm
Out[118]/TableForm=
ionization from Web
E/N (Td = 1E-21 Vm2) alpha/N (m^2)
40      70      100      200      300      500      1000      2000
4.42E-25 5.21E-23 2.56E-22 1.79E-21 3.93E-21 8.04E-21 1.39E-20 1.47E-20
In[119]:= Drop[Import["H2EleTransIonization.txt", "Table"], 2];
In[120]:= boltzIonizWeb=Table[{{%[[1,j]],%[[2,j]]},{j,Length[%[[1]]}}];
In[121]:= webIonizationPlot=ListLogLogPlot[%,PlotRange->loglogPlotRange, Joined->True, ImageSize->400,
PlotStyle->plotColorsLines[[5]]];
```

This red curve shows that our Web site gives higher values than the preceding fit to experiment by ~ 50% at E/n = 1000 Td.

Ionization coefficients calculated using our Web cross sections, but using BOLSIGPLUS give

```
In[122]:= Import["C:\\users\\avp\\documents\\DATABASE\\BOLSIGPLUS\\H2Output051406.dat", "CSV"] // TableForm
```

Out[122]/TableForm=

Angular field frequency / N (m3/s)	0.000
Gas temperature (K)	300.0
Ionization degree	0.000
Electron density (1/m3)	0.1000E+19
Energy sharing	1.000
Growth model	1.000
Maxwellian mean energy (eV)	0.000
# of grid points	50.00
Grid type	3.000
Precision	0.1000E-09
Convergence	0.1000E-03
Maximum # of iterations	100.0
Mole fraction H2	1.000

E/N (Td)	Electric field / N (Td)
10.00	10.00
12.14	12.14
14.75	14.75
17.91	17.91
21.75	21.75
26.42	26.42
32.09	32.09
38.97	38.97
47.32	47.32
57.47	57.47
69.80	69.80
84.77	84.77
102.9	102.9
125.0	125.0
151.8	151.8
184.4	184.4
224.0	224.0
272.0	272.0
330.3	330.3
401.2	401.2
487.2	487.2
591.7	591.7
718.6	718.6
872.7	872.7
1060.	1060.
1287.	1287.
1563.	1563.
1898.	1898.
2306.	2306.
2800.	2800.

E/N (Td)	Maximum energy
10.00	5.177
12.14	6.202
14.75	7.646
17.91	14.66
21.75	19.70
26.42	19.33
32.09	28.61

38.97	34.30
47.32	38.38
57.47	42.05
69.80	45.88
84.77	50.72
102.9	56.67
125.0	64.98
151.8	79.62
184.4	94.90
224.0	115.9
272.0	145.3
330.3	177.3
401.2	219.8
487.2	297.8
591.7	366.5
718.6	493.8
872.7	686.2
1060.	1367.
1287.	2041.
1563.	2909.
1898.	3269.
2306.	5141.
2800.	8415.

E/N (Td)	Mean energy (eV)
10.00	0.5947
12.14	0.6694
14.75	0.7545
17.91	0.8531
21.75	0.9722
26.42	1.127
32.09	1.350
38.97	1.700
47.32	2.201
57.47	2.786
69.80	3.371
84.77	3.922
102.9	4.452
125.0	4.992
151.8	5.571
184.4	6.225
224.0	6.989
272.0	7.912
330.3	9.049
401.2	10.46
487.2	12.23
591.7	14.46
718.6	17.30
872.7	20.95
1060.	25.71
1287.	32.00
1563.	40.50
1898.	52.23
2306.	68.78
2800.	92.77

E/N (Td)	Mobility x N (1/m/V/s)
10.00	0.1854E+25
12.14	0.1702E+25
14.75	0.1567E+25
17.91	0.1445E+25
21.75	0.1338E+25
26.42	0.1245E+25
32.09	0.1164E+25
38.97	0.1104E+25
47.32	0.1073E+25
57.47	0.1071E+25
69.80	0.1085E+25
84.77	0.1103E+25
102.9	0.1121E+25
125.0	0.1138E+25
151.8	0.1149E+25
184.4	0.1155E+25
224.0	0.1154E+25
272.0	0.1145E+25
330.3	0.1127E+25
401.2	0.1101E+25
487.2	0.1063E+25
591.7	0.1016E+25
718.6	0.9600E+24
872.7	0.9007E+24
1060.	0.8398E+24
1287.	0.7799E+24
1563.	0.7259E+24
1898.	0.6793E+24
2306.	0.6406E+24
2800.	0.6112E+24

E/N (Td)	Diffusion coefficient x N (1/m/s)
10.00	0.9353E+24
12.14	0.9661E+24
14.75	0.9998E+24
17.91	0.1038E+25
21.75	0.1083E+25
26.42	0.1144E+25
32.09	0.1242E+25
38.97	0.1422E+25
47.32	0.1716E+25
57.47	0.2097E+25
69.80	0.2508E+25
84.77	0.2921E+25
102.9	0.3335E+25
125.0	0.3768E+25
151.8	0.4236E+25
184.4	0.4759E+25
224.0	0.5356E+25
272.0	0.6046E+25
330.3	0.6853E+25
401.2	0.7790E+25
487.2	0.8878E+25
591.7	0.1014E+26

718.6	0.1161E+26
872.7	0.1336E+26
1060.	0.1548E+26
1287.	0.1813E+26
1563.	0.2162E+26
1898.	0.2641E+26
2306.	0.3331E+26
2800.	0.4381E+26

E/N (Td)	Energy mobility x N (1/m/V/s)
10.00	0.2775E+25
12.14	0.2561E+25
14.75	0.2370E+25
17.91	0.2199E+25
21.75	0.2047E+25
26.42	0.1915E+25
32.09	0.1811E+25
38.97	0.1762E+25
47.32	0.1780E+25
57.47	0.1832E+25
69.80	0.1886E+25
84.77	0.1928E+25
102.9	0.1959E+25
125.0	0.1975E+25
151.8	0.1979E+25
184.4	0.1967E+25
224.0	0.1938E+25
272.0	0.1892E+25
330.3	0.1830E+25
401.2	0.1752E+25
487.2	0.1661E+25
591.7	0.1559E+25
718.6	0.1455E+25
872.7	0.1353E+25
1060.	0.1258E+25
1287.	0.1174E+25
1563.	0.1105E+25
1898.	0.1051E+25
2306.	0.1017E+25
2800.	0.1005E+25

E/N (Td)	Energy diffusion coef. x N (1/m/s)
10.00	0.1031E+25
12.14	0.1066E+25
14.75	0.1107E+25
17.91	0.1157E+25
21.75	0.1222E+25
26.42	0.1324E+25
32.09	0.1538E+25
38.97	0.1979E+25
47.32	0.2643E+25
57.47	0.3365E+25
69.80	0.4045E+25
84.77	0.4681E+25
102.9	0.5310E+25

125.0	0.5968E+25
151.8	0.6685E+25
184.4	0.7481E+25
224.0	0.8379E+25
272.0	0.9395E+25
330.3	0.1055E+26
401.2	0.1187E+26
487.2	0.1340E+26
591.7	0.1519E+26
718.6	0.1737E+26
872.7	0.2013E+26
1060.	0.2383E+26
1287.	0.2894E+26
1563.	0.3642E+26
1898.	0.4773E+26
2306.	0.6633E+26
2800.	0.9875E+26

E/N (Td)	Imaginary mobility x N (1/m/V/s)
----------	----------------------------------

10.00	0.000
12.14	0.000
14.75	0.000
17.91	0.000
21.75	0.000
26.42	0.000
32.09	0.000
38.97	0.000
47.32	0.000
57.47	0.000
69.80	0.000
84.77	0.000
102.9	0.000
125.0	0.000
151.8	0.000
184.4	0.000
224.0	0.000
272.0	0.000
330.3	0.000
401.2	0.000
487.2	0.000
591.7	0.000
718.6	0.000
872.7	0.000
1060.	0.000
1287.	0.000
1563.	0.000
1898.	0.000
2306.	0.000
2800.	0.000

E/N (Td)	Cross-B diffusion coef. x N (1/m/s)
----------	-------------------------------------

10.00	0.9353E+24
12.14	0.9661E+24
14.75	0.9998E+24
17.91	0.1038E+25

21.75	0.1083E+25
26.42	0.1144E+25
32.09	0.1242E+25
38.97	0.1422E+25
47.32	0.1716E+25
57.47	0.2097E+25
69.80	0.2508E+25
84.77	0.2921E+25
102.9	0.3335E+25
125.0	0.3768E+25
151.8	0.4236E+25
184.4	0.4759E+25
224.0	0.5356E+25
272.0	0.6046E+25
330.3	0.6853E+25
401.2	0.7790E+25
487.2	0.8878E+25
591.7	0.1014E+26
718.6	0.1161E+26
872.7	0.1336E+26
1060.	0.1548E+26
1287.	0.1813E+26
1563.	0.2162E+26
1898.	0.2641E+26
2306.	0.3331E+26
2800.	0.4381E+26

E/N (Td)	Total collision freq. / N (m3/s)
10.00	0.6912E-13
12.14	0.7529E-13
14.75	0.8194E-13
17.91	0.8910E-13
21.75	0.9693E-13
26.42	0.1057E-12
32.09	0.1155E-12
38.97	0.1263E-12
47.32	0.1365E-12
57.47	0.1444E-12
69.80	0.1496E-12
84.77	0.1526E-12
102.9	0.1542E-12
125.0	0.1550E-12
151.8	0.1552E-12
184.4	0.1551E-12
224.0	0.1549E-12
272.0	0.1547E-12
330.3	0.1549E-12
401.2	0.1557E-12
487.2	0.1572E-12
591.7	0.1598E-12
718.6	0.1638E-12
872.7	0.1692E-12
1060.	0.1763E-12
1287.	0.1847E-12
1563.	0.1945E-12
1898.	0.2052E-12

2306.	0.2160E-12
2800.	0.2263E-12

E/N (Td)	Effect. momentum freq. / N (m3/s)
10.00	0.9485E-13
12.14	0.1033E-12
14.75	0.1123E-12
17.91	0.1217E-12
21.75	0.1314E-12
26.42	0.1413E-12
32.09	0.1511E-12
38.97	0.1593E-12
47.32	0.1639E-12
57.47	0.1642E-12
69.80	0.1622E-12
84.77	0.1594E-12
102.9	0.1568E-12
125.0	0.1546E-12
151.8	0.1530E-12
184.4	0.1523E-12
224.0	0.1525E-12
272.0	0.1537E-12
330.3	0.1560E-12
401.2	0.1598E-12
487.2	0.1654E-12
591.7	0.1732E-12
718.6	0.1832E-12
872.7	0.1953E-12
1060.	0.2094E-12
1287.	0.2255E-12
1563.	0.2423E-12
1898.	0.2589E-12
2306.	0.2746E-12
2800.	0.2878E-12

E/N (Td)	Effect. mom. transfer fraction
10.00	1.000
12.14	1.000
14.75	1.000
17.91	1.000
21.75	1.000
26.42	1.000
32.09	1.000
38.97	1.000
47.32	1.000
57.47	1.000
69.80	1.000
84.77	1.000
102.9	1.000
125.0	1.000
151.8	1.000
184.4	1.000
224.0	1.000
272.0	1.000
330.3	1.000

401.2	1.000
487.2	1.000
591.7	1.000
718.6	1.000
872.7	1.000
1060.	1.000
1287.	1.000
1563.	1.000
1898.	1.000
2306.	1.000
2800.	1.000

E/N (Td)	Temporal growth coef. (m3/s)
10.00	0.000
12.14	0.000
14.75	0.000
17.91	0.000
21.75	0.3688E-26
26.42	0.1357E-23
32.09	0.1392E-21
38.97	0.4577E-20
47.32	0.6311E-19
57.47	0.4610E-18
69.80	0.2168E-17
84.77	0.7599E-17
102.9	0.2177E-16
125.0	0.5401E-16
151.8	0.1204E-15
184.4	0.2461E-15
224.0	0.4697E-15
272.0	0.8446E-15
330.3	0.1443E-14
401.2	0.2351E-14
487.2	0.3661E-14
591.7	0.5462E-14
718.6	0.7830E-14
872.7	0.1082E-13
1060.	0.1443E-13
1287.	0.1860E-13
1563.	0.2326E-13
1898.	0.2827E-13
2306.	0.3337E-13
2800.	0.3829E-13

E/N (Td)	Spatial growth coef. (m2)
10.00	0.000
12.14	0.000
14.75	0.000
17.91	0.000
21.75	0.1267E-30
26.42	0.4128E-28
32.09	0.3728E-26
38.97	0.1064E-24
47.32	0.1242E-23
57.47	0.7489E-23

69.80	0.2864E-22
84.77	0.8127E-22
102.9	0.1886E-21
125.0	0.3797E-21
151.8	0.6897E-21
184.4	0.1156E-20
224.0	0.1818E-20
272.0	0.2713E-20
330.3	0.3875E-20
401.2	0.5325E-20
487.2	0.7068E-20
591.7	0.9090E-20
718.6	0.1135E-19
872.7	0.1377E-19
1060.	0.1621E-19
1287.	0.1853E-19
1563.	0.2050E-19
1898.	0.2192E-19
2306.	0.2259E-19
2800.	0.2237E-19

E/N (Td)	Power / N (eV m3/s)
----------	---------------------

10.00	0.1875E-15
12.14	0.2533E-15
14.75	0.3433E-15
17.91	0.4664E-15
21.75	0.6361E-15
26.42	0.8716E-15
32.09	0.1201E-14
38.97	0.1679E-14
47.32	0.2407E-14
57.47	0.3540E-14
69.80	0.5288E-14
84.77	0.7929E-14
102.9	0.1189E-13
125.0	0.1779E-13
151.8	0.2650E-13
184.4	0.3928E-13
224.0	0.5786E-13
272.0	0.8468E-13
330.3	0.1230E-12
401.2	0.1771E-12
487.2	0.2523E-12
591.7	0.3555E-12
718.6	0.4957E-12
872.7	0.6859E-12
1060.	0.9433E-12
1287.	0.1292E-11
1563.	0.1774E-11
1898.	0.2448E-11
2306.	0.3405E-11
2800.	0.4792E-11

E/N (Td)	Elastic power loss / N (eV m3/s)
----------	----------------------------------

10.00	0.2746E-16
-------	------------

12.14	0.3343E-16
14.75	0.4067E-16
17.91	0.4957E-16
21.75	0.6084E-16
26.42	0.7587E-16
32.09	0.9770E-16
38.97	0.1304E-15
47.32	0.1739E-15
57.47	0.2211E-15
69.80	0.2647E-15
84.77	0.3027E-15
102.9	0.3365E-15
125.0	0.3688E-15
151.8	0.4014E-15
184.4	0.4370E-15
224.0	0.4778E-15
272.0	0.5271E-15
330.3	0.5888E-15
401.2	0.6677E-15
487.2	0.7708E-15
591.7	0.9069E-15
718.6	0.1089E-14
872.7	0.1337E-14
1060.	0.1679E-14
1287.	0.2145E-14
1563.	0.2789E-14
1898.	0.3675E-14
2306.	0.4922E-14
2800.	0.6676E-14

E/N (Td)	Inelastic power loss / N (eV m ³ /s)
10.00	0.1600E-15
12.14	0.2198E-15
14.75	0.3025E-15
17.91	0.4164E-15
21.75	0.5746E-15
26.42	0.7952E-15
32.09	0.1103E-14
38.97	0.1548E-14
47.32	0.2233E-14
57.47	0.3317E-14
69.80	0.5015E-14
84.77	0.7597E-14
102.9	0.1145E-13
125.0	0.1715E-13
151.8	0.2543E-13
184.4	0.3730E-13
224.0	0.5411E-13
272.0	0.7745E-13
330.3	0.1094E-12
401.2	0.1518E-12
487.2	0.2068E-12
591.7	0.2756E-12
718.6	0.3591E-12
872.7	0.4579E-12
1060.	0.5708E-12

1287.	0.6953E-12
1563.	0.8290E-12
1898.	0.9686E-12
2306.	0.1107E-11
2800.	0.1237E-11

E/N (Td)	# of iterations
10.00	6.000
12.14	6.000
14.75	5.000
17.91	6.000
21.75	6.000
26.42	5.000
32.09	5.000
38.97	5.000
47.32	5.000
57.47	5.000
69.80	5.000
84.77	5.000
102.9	4.000
125.0	4.000
151.8	4.000
184.4	4.000
224.0	5.000
272.0	6.000
330.3	6.000
401.2	6.000
487.2	8.000
591.7	8.000
718.6	8.000
872.7	9.000
1060.	9.000
1287.	10.00
1563.	10.00
1898.	10.00
2306.	10.00
2800.	10.00

E/N (Td)	# of grid trials
10.00	2.000
12.14	2.000
14.75	2.000
17.91	3.000
21.75	3.000
26.42	2.000
32.09	2.000
38.97	2.000
47.32	2.000
57.47	2.000
69.80	2.000
84.77	2.000
102.9	2.000
125.0	2.000
151.8	2.000
184.4	2.000

224.0	2.000
272.0	2.000
330.3	2.000
401.2	2.000
487.2	2.000
591.7	2.000
718.6	2.000
872.7	2.000
1060.	3.000
1287.	3.000
1563.	3.000
1898.	2.000
2306.	2.000
2800.	2.000

E/N (Td)	Error code
10.00	0.000
12.14	0.000
14.75	0.000
17.91	0.000
21.75	0.000
26.42	0.000
32.09	0.000
38.97	0.000
47.32	0.000
57.47	0.000
69.80	0.000
84.77	0.000
102.9	0.000
125.0	0.000
151.8	0.000
184.4	0.000
224.0	0.000
272.0	0.000
330.3	0.000
401.2	0.000
487.2	0.000
591.7	0.000
718.6	0.000
872.7	0.000
1060.	0.000
1287.	0.000
1563.	0.000
1898.	0.000
2306.	0.000
2800.	0.000

C1	H2	Elastic
E/N (Td)		Townsend coefficient / N (m2)
10.00		0.3654E-17
12.14		0.3560E-17
14.75		0.3453E-17
17.91		0.3337E-17
21.75		0.3211E-17
26.42		0.3078E-17

32.09	0.2937E-17
38.97	0.2757E-17
47.32	0.2495E-17
57.47	0.2157E-17
69.80	0.1800E-17
84.77	0.1476E-17
102.9	0.1200E-17
125.0	0.9721E-18
151.8	0.7870E-18
184.4	0.6384E-18
224.0	0.5195E-18
272.0	0.4244E-18
330.3	0.3486E-18
401.2	0.2884E-18
487.2	0.2411E-18
591.7	0.2042E-18
718.6	0.1753E-18
872.7	0.1523E-18
1060.	0.1340E-18
1287.	0.1191E-18
1563.	0.1063E-18
1898.	0.9482E-19
2306.	0.8413E-19
2800.	0.7379E-19

C2	H2	Excitation	0.04 eV
E/N (Td)		Townsend coefficient	/ N (m2)
10.00		0.2372E-19	
12.14		0.2587E-19	
14.75		0.2819E-19	
17.91		0.3075E-19	
21.75		0.3370E-19	
26.42		0.3732E-19	
32.09		0.4189E-19	
38.97		0.4696E-19	
47.32		0.5029E-19	
57.47		0.4980E-19	
69.80		0.4598E-19	
84.77		0.4061E-19	
102.9		0.3496E-19	
125.0		0.2971E-19	
151.8		0.2508E-19	
184.4		0.2113E-19	
224.0		0.1780E-19	
272.0		0.1503E-19	
330.3		0.1272E-19	
401.2		0.1079E-19	
487.2		0.9205E-20	
591.7		0.7887E-20	
718.6		0.6785E-20	
872.7		0.5840E-20	
1060.		0.5023E-20	
1287.		0.4310E-20	
1563.		0.3666E-20	
1898.		0.3082E-20	
2306.		0.2557E-20	

2800. 0.2087E-20

C3	H2	Excitation	0.07 eV
E/N (Td)		Townsend coefficient	/ N (m2)
10.00		0.4103E-19	
12.14		0.4472E-19	
14.75		0.4868E-19	
17.91		0.5309E-19	
21.75		0.5828E-19	
26.42		0.6477E-19	
32.09		0.7315E-19	
38.97		0.8263E-19	
47.32		0.8913E-19	
57.47		0.8876E-19	
69.80		0.8228E-19	
84.77		0.7286E-19	
102.9		0.6285E-19	
125.0		0.5349E-19	
151.8		0.4520E-19	
184.4		0.3812E-19	
224.0		0.3215E-19	
272.0		0.2716E-19	
330.3		0.2300E-19	
401.2		0.1953E-19	
487.2		0.1666E-19	
591.7		0.1428E-19	
718.6		0.1228E-19	
872.7		0.1058E-19	
1060.		0.9101E-20	
1287.		0.7811E-20	
1563.		0.6642E-20	
1898.		0.5579E-20	
2306.		0.4621E-20	
2800.		0.3759E-20	

C4	H2	Excitation	0.52 eV
E/N (Td)		Townsend coefficient	/ N (m2)
10.00		0.8811E-20	
12.14		0.1188E-19	
14.75		0.1566E-19	
17.91		0.2024E-19	
21.75		0.2573E-19	
26.42		0.3216E-19	
32.09		0.3924E-19	
38.97		0.4557E-19	
47.32		0.4832E-19	
57.47		0.4613E-19	
69.80		0.4066E-19	
84.77		0.3420E-19	
102.9		0.2802E-19	
125.0		0.2262E-19	
151.8		0.1808E-19	
184.4		0.1435E-19	
224.0		0.1133E-19	
272.0		0.8894E-20	

330.3	0.6938E-20
401.2	0.5382E-20
487.2	0.4157E-20
591.7	0.3203E-20
718.6	0.2462E-20
872.7	0.1886E-20
1060.	0.1442E-20
1287.	0.1106E-20
1563.	0.8494E-21
1898.	0.6544E-21
2306.	0.5107E-21
2800.	0.4085E-21

C5	H2	Excitation	1.00 eV
E/N (Td)		Townsend coefficient	/ N (m2)
10.00		0.4110E-22	
12.14		0.9539E-22	
14.75		0.1965E-21	
17.91		0.3691E-21	
21.75		0.6466E-21	
26.42		0.1069E-20	
32.09		0.1667E-20	
38.97		0.2386E-20	
47.32		0.2974E-20	
57.47		0.3183E-20	
69.80		0.3036E-20	
84.77		0.2700E-20	
102.9		0.2305E-20	
125.0		0.1920E-20	
151.8		0.1573E-20	
184.4		0.1274E-20	
224.0		0.1021E-20	
272.0		0.8108E-21	
330.3		0.6367E-21	
401.2		0.4941E-21	
487.2		0.3792E-21	
591.7		0.2876E-21	
718.6		0.2152E-21	
872.7		0.1582E-21	
1060.		0.1140E-21	
1287.		0.8072E-22	
1563.		0.5563E-22	
1898.		0.3697E-22	
2306.		0.2367E-22	
2800.		0.1473E-22	

C6	H2	Excitation	1.50 eV
E/N (Td)		Townsend coefficient	/ N (m2)
10.00		0.1317E-23	
12.14		0.4217E-23	
14.75		0.1118E-22	
17.91		0.2538E-22	
21.75		0.5112E-22	
26.42		0.9336E-22	
32.09		0.1555E-21	

38.97	0.2310E-21
47.32	0.2924E-21
57.47	0.3138E-21
69.80	0.2987E-21
84.77	0.2644E-21
102.9	0.2244E-21
125.0	0.1858E-21
151.8	0.1513E-21
184.4	0.1217E-21
224.0	0.9694E-22
272.0	0.7642E-22
330.3	0.5959E-22
401.2	0.4592E-22
487.2	0.3498E-22
591.7	0.2634E-22
718.6	0.1959E-22
872.7	0.1431E-22
1060.	0.1025E-22
1287.	0.7220E-23
1563.	0.4954E-23
1898.	0.3279E-23
2306.	0.2091E-23
2800.	0.1299E-23

C7	H2	Excitation	8.90 eV
E/N (Td)		Townsend coefficient / N (m2)	
10.00		0.000	
12.14		0.000	
14.75		0.000	
17.91		0.1514E-27	
21.75		0.2367E-25	
26.42		0.1068E-23	
32.09		0.1824E-22	
38.97		0.1347E-21	
47.32		0.5107E-21	
57.47		0.1190E-20	
69.80		0.2032E-20	
84.77		0.2879E-20	
102.9		0.3654E-20	
125.0		0.4336E-20	
151.8		0.4914E-20	
184.4		0.5383E-20	
224.0		0.5747E-20	
272.0		0.5988E-20	
330.3		0.6107E-20	
401.2		0.6086E-20	
487.2		0.5928E-20	
591.7		0.5631E-20	
718.6		0.5207E-20	
872.7		0.4668E-20	
1060.		0.4051E-20	
1287.		0.3385E-20	
1563.		0.2709E-20	
1898.		0.2068E-20	
2306.		0.1505E-20	
2800.		0.1034E-20	

C8	H2	Excitation	11.30 eV
E/N (Td)		Townsend coefficient	/ N (m2)
10.00		0.000	
12.14		0.000	
14.75		0.000	
17.91		0.3056E-29	
21.75		0.8683E-27	
26.42		0.6178E-25	
32.09		0.1512E-23	
38.97		0.1496E-22	
47.32		0.7245E-22	
57.47		0.2086E-21	
69.80		0.4293E-21	
84.77		0.7218E-21	
102.9		0.1076E-20	
125.0		0.1489E-20	
151.8		0.1966E-20	
184.4		0.2510E-20	
224.0		0.3131E-20	
272.0		0.3831E-20	
330.3		0.4615E-20	
401.2		0.5473E-20	
487.2		0.6391E-20	
591.7		0.7345E-20	
718.6		0.8298E-20	
872.7		0.9197E-20	
1060.		0.9987E-20	
1287.		0.1061E-19	
1563.		0.1098E-19	
1898.		0.1107E-19	
2306.		0.1084E-19	
2800.		0.1028E-19	

C9	H2	Excitation	11.75 eV
E/N (Td)		Townsend coefficient	/ N (m2)
10.00		0.000	
12.14		0.000	
14.75		0.000	
17.91		0.1763E-29	
21.75		0.5823E-27	
26.42		0.4664E-25	
32.09		0.1251E-23	
38.97		0.1324E-22	
47.32		0.6722E-22	
57.47		0.1988E-21	
69.80		0.4124E-21	
84.77		0.6859E-21	
102.9		0.9918E-21	
125.0		0.1306E-20	
151.8		0.1608E-20	
184.4		0.1878E-20	
224.0		0.2103E-20	
272.0		0.2267E-20	
330.3		0.2366E-20	

401.2	0.2391E-20
487.2	0.2345E-20
591.7	0.2234E-20
718.6	0.2064E-20
872.7	0.1845E-20
1060.	0.1597E-20
1287.	0.1331E-20
1563.	0.1064E-20
1898.	0.8128E-21
2306.	0.5931E-21
2800.	0.4095E-21

C10 H2 Excitation 11.80 eV
E/N (Td) Townsend coefficient / N (m2)

10.00	0.000
12.14	0.000
14.75	0.000
17.91	0.6268E-30
21.75	0.2349E-27
26.42	0.2091E-25
32.09	0.6149E-24
38.97	0.6997E-23
47.32	0.3759E-22
57.47	0.1163E-21
69.80	0.2493E-21
84.77	0.4250E-21
102.9	0.6266E-21
125.0	0.8376E-21
151.8	0.1044E-20
184.4	0.1233E-20
224.0	0.1394E-20
272.0	0.1518E-20
330.3	0.1600E-20
401.2	0.1634E-20
487.2	0.1621E-20
591.7	0.1562E-20
718.6	0.1459E-20
872.7	0.1317E-20
1060.	0.1149E-20
1287.	0.9630E-21
1563.	0.7718E-21
1898.	0.5890E-21
2306.	0.4279E-21
2800.	0.2932E-21

C11 H2 Excitation 12.40 eV
E/N (Td) Townsend coefficient / N (m2)

10.00	0.000
12.14	0.000
14.75	0.000
17.91	0.1005E-30
21.75	0.5107E-28
26.42	0.5851E-26
32.09	0.2160E-24
38.97	0.3002E-23

47.32	0.1931E-22
57.47	0.7055E-22
69.80	0.1768E-21
84.77	0.3496E-21
102.9	0.5953E-21
125.0	0.9176E-21
151.8	0.1320E-20
184.4	0.1803E-20
224.0	0.2369E-20
272.0	0.3012E-20
330.3	0.3731E-20
401.2	0.4513E-20
487.2	0.5342E-20
591.7	0.6202E-20
718.6	0.7064E-20
872.7	0.7891E-20
1060.	0.8641E-20
1287.	0.9261E-20
1563.	0.9683E-20
1898.	0.9860E-20
2306.	0.9746E-20
2800.	0.9319E-20

C12	H2	Excitation	14.00 eV
E/N (Td)		Townsend coefficient	/ N (m2)
10.00		0.000	
12.14		0.000	
14.75		0.000	
17.91		0.6297E-33	
21.75		0.9753E-30	
26.42		0.1856E-27	
32.09		0.1035E-25	
38.97		0.1966E-24	
47.32		0.1604E-23	
57.47		0.6991E-23	
69.80		0.1987E-22	
84.77		0.4270E-22	
102.9		0.7624E-22	
125.0		0.1194E-21	
151.8		0.1700E-21	
184.4		0.2244E-21	
224.0		0.2785E-21	
272.0		0.3280E-21	
330.3		0.3691E-21	
401.2		0.3981E-21	
487.2		0.4129E-21	
591.7		0.4128E-21	
718.6		0.3978E-21	
872.7		0.3689E-21	
1060.		0.3295E-21	
1287.		0.2822E-21	
1563.		0.2309E-21	
1898.		0.1801E-21	
2306.		0.1336E-21	
2800.		0.9368E-22	

C13	H2	Excitation	15.00 eV
E/N (Td)		Townsend coefficient	/ N (m2)
10.00		0.000	
12.14		0.000	
14.75		0.000	
17.91		0.000	
21.75		0.1022E-32	
26.42		0.5971E-30	
32.09		0.9250E-28	
38.97		0.3964E-26	
47.32		0.6403E-25	
57.47		0.4998E-24	
69.80		0.2338E-23	
84.77		0.7740E-23	
102.9		0.2015E-22	
125.0		0.4410E-22	
151.8		0.8495E-22	
184.4		0.1481E-21	
224.0		0.2392E-21	
272.0		0.3627E-21	
330.3		0.5226E-21	
401.2		0.7213E-21	
487.2		0.9585E-21	
591.7		0.1232E-20	
718.6		0.1537E-20	
872.7		0.1861E-20	
1060.		0.2189E-20	
1287.		0.2499E-20	
1563.		0.2760E-20	
1898.		0.2944E-20	
2306.		0.3022E-20	
2800.		0.2976E-20	

C14	H2	Excitation	15.20 eV
E/N (Td)		Townsend coefficient	/ N (m2)
10.00		0.000	
12.14		0.000	
14.75		0.000	
17.91		0.000	
21.75		0.7609E-32	
26.42		0.3136E-29	
32.09		0.3508E-27	
38.97		0.1188E-25	
47.32		0.1600E-24	
57.47		0.1088E-23	
69.80		0.4601E-23	
84.77		0.1421E-22	
102.9		0.3542E-22	
125.0		0.7578E-22	
151.8		0.1449E-21	
184.4		0.2536E-21	
224.0		0.4140E-21	
272.0		0.6370E-21	
330.3		0.9322E-21	
401.2		0.1305E-20	

487.2	0.1753E-20
591.7	0.2271E-20
718.6	0.2844E-20
872.7	0.3444E-20
1060.	0.4034E-20
1287.	0.4571E-20
1563.	0.4998E-20
1898.	0.5269E-20
2306.	0.5342E-20
2800.	0.5198E-20

C15 H2 Ionization 15.40 eV
E/N (Td) Townsend coefficient / N (m2)

10.00	0.000
12.14	0.000
14.75	0.000
17.91	0.000
21.75	0.1267E-30
26.42	0.4127E-28
32.09	0.3728E-26
38.97	0.1064E-24
47.32	0.1242E-23
57.47	0.7489E-23
69.80	0.2864E-22
84.77	0.8127E-22
102.9	0.1886E-21
125.0	0.3797E-21
151.8	0.6897E-21
184.4	0.1155E-20
224.0	0.1818E-20
272.0	0.2713E-20
330.3	0.3875E-20
401.2	0.5325E-20
487.2	0.7068E-20
591.7	0.9090E-20
718.6	0.1135E-19
872.7	0.1377E-19
1060.	0.1621E-19
1287.	0.1853E-19
1563.	0.2050E-19
1898.	0.2192E-19
2306.	0.2259E-19
2800.	0.2237E-19

C16 H2 Excitation 16.60 eV
E/N (Td) Townsend coefficient / N (m2)

10.00	0.000
12.14	0.000
14.75	0.000
17.91	0.000
21.75	0.4704E-33
26.42	0.2350E-30
32.09	0.3031E-28
38.97	0.1126E-26
47.32	0.1599E-25


```

57.47    0.1109E-24
69.80    0.4650E-24
84.77    0.1391E-23
102.9    0.3296E-23
125.0    0.6601E-23
151.8    0.1168E-22
184.4    0.1878E-22
224.0    0.2806E-22
272.0    0.3950E-22
330.3    0.5308E-22
401.2    0.6871E-22
487.2    0.8626E-22
591.7    0.1056E-21
718.6    0.1264E-21
872.7    0.1479E-21
1060.    0.1692E-21
1287.    0.1887E-21
1563.    0.2042E-21
1898.    0.2139E-21
2306.    0.2156E-21
2800.    0.2083E-21

```

```
In[123]:= bolsigplusionization=Take[Import["C:\\users\\avp\\documents\\DATABASE\\BOLSIGPLUS\\H2Output051406.d
{1089,1113}]];
```

```
In[124]:= bolsigplusIonizationPlot=ListLogLogPlot[%,PlotRange->loglogPlotRange, ImageSize->400, PlotStyle->pl
Joined->True];
```

From Zoran's exponential fits to experimental Halpha emission versus position data, he derived the following apparent ionization coefficients. We drop the very low value at 800 Td and the highest pressure, because there is no clear exponential.

```
In[125]:= Import["ExptIonCoef.txt", "CSV"]//TableForm
```

```
Out[125]//TableForm=
```

D	A	E	B	F	C
500		4.99E-21	800	7.78E-21	1000 7.03E-21
500		4.59E-21	800	5.98E-21	1000 6.26E-21
500		5.89E-21	800	7.28E-21	1000 7.26E-21
500		4.81E-21	800	6.15E-21	1000 7.1E-21
500		4.87E-21	800	1.14E-21	1000 6.36E-21
500		4.59E-21	800	6.06E-21	1000 6.93E-21

```
In[126]:= Drop[Import["ExptIonCoef.txt", "Table"], 1];
```

```
In[127]:= Drop[Partition[Flatten[%, 2], 2], {-5}];
```

```
In[128]:= halphaIonizationZoranPlot=ListLogLogPlot[%,PlotRange->loglogPlotRange, ImageSize->400, PlotStyle->p
```

From Zoran's exponential fits to the H2 uv continuum data, he derived the following apparent ionization coefficients. We drop the values for 10 and 20 kTd because there is no clear exponential growth.

```
In[129]:= Import["H2Continuum2.txt", "CSV"] // TableForm
```

```
Out[129]/TableForm=
```

E/N (Td)	p (Torr)	alpha _i	alpha _{ion}	anode	no quench	quench	norm fact
300	0.95	1.116	3.57E-21	1.31E-21	6.15E+10	4.90E+00	4.36E-33
300	0.95	1.112	3.55E-21	1.30E-21	6.09E+10	4.90E+00	4.36E-33
300	0.95	1.131	3.61E-21	1.31E-21	8.21E+11	4.90E+00	3.26E-34
500	0.47	0.89	5.75E-21	9.89E-22	2.55E+10	8.86E+00	4.36E-33
500	0.47	0.949	6.13E-21	9.80E-22	3.38E+11	8.87E+00	3.26E-34
800	0.305	0.85	8.46E-21	7.24E-22	1.26E+10	1.31E+01	4.36E-33
800	0.305	0.868	8.64E-21	7.32E-22	1.28E+10	1.31E+01	4.36E-33
800	0.305	1.033	1.03E-20	7.41E-22	1.73E+11	1.31E+01	3.26E-34
1000	0.267	0.897	1.02E-20	7.03E-22	1.09E+10	1.49E+01	4.35E-33
1000	0.267	1.006	1.14E-20	6.81E-22	1.41E+11	1.49E+01	3.26E-34
3000	0.185	0.964	2.58E-20	6.01E-22	6.60E+09	2.10E+01	4.36E-34
3000	0.185	0.84	1.38E-20	5.48E-22	8.01E+10	2.10E+01	3.26E-34
3000	0.185	0.737	1.21E-20	5.57E-22	8.14E+10	2.10E+01	3.26E-34
10000	0.144	-0.1517	-3.20E-21	4.89E-22	3.85E+09	2.67E+01	4.36E-33
10000	0.144	0.075	1.58E-21	4.69E-22	5.39E+10	2.67E+01	3.26E-34
20000	0.117	-0.255	-6.62E-21	5.19E-22	4.88E+10	3.26E+01	3.26E-34
20000	0.117	-0.1024	-2.66E-21	5.70E-22	5.35E+10	3.26E+01	3.26E-34

```
In[130]:= Drop[Drop[Import["H2Continuum2.txt", "Table"], 2], -4];
```

```
In[131]:= Table[{{[[j, 1]], {{[[j, 4]]}}, {j, Length[%]}}];
```

```
In[132]:= continuumIonizationZoranPlot=ListLogLogPlot[%, PlotRange->loglogPlotRange, ImageSize->400, PlotStyle->plotColorsPoints[[6]]];
```

From the Boltzmann calculations of 12/23/94 with spatial growth included

```
In[133]:= Import["c:/users/avp/documents/mathbook/hydrogen/H2ElectronCollisions/H2eBoltzmann.txt", "CSV"] // TableForm
```

```
Out[133]/TableForm=
```

40	4.45E-25	5.69E-27	6.8E-29	2.68E-22	1.48E-23
70	5.21E-23	8.86E-25	4.42E-27	2.96E-21	2.95E-22
100	2.51E-22	4.34E-24	1.798E-26	5.14E-21	6.23E-22
200	1.638E-21	2.46E-23	1.132E-25	7.89E-21	1.15E-21
300	3.46E-21	4.59E-23	2.43E-25	8.37E-21	1.28E-21
500	6.92E-21	8.01E-23	4.71E-25	7.58E-21	1.20E-21
1000	1.27E-20	1.31E-22	7.36E-25	4.91E-21	7.93E-22
2000	1.674E-20	1.608E-22	7.61E-25	2.25E-21	3.66E-22
3000	1.666E-20	1.524E-22	6.51E-25	1.156E-21	1.86E-22
5000	1.15E-20	9.7E-23	3.9E-25	3.4E-22	5.41E-23

Bolt. calc. of 12/23/94 pure H2

E/n	ioniz.	H alpha	H2 1G	H2sum trip	H2 a state
Td	alpha _i /n	alpha _x /n	alpha _x /n	alpha _x /n	alpha _x /n
	m ²	m ²	m ²	m ²	m ²

```
In[134]:= Drop[Import["c:/users/avp/documents/mathbook/hydrogen/H2ElectronCollisions/H2eBoltzmann.txt", "Table
```

```
In[135]:= ionization122394=Table[{{[[j, 1]], {{[[j, 2]]}}, {j, Length[%]-1}}];
```

```
In[136]:= ionization122394Plot=ListLogLogPlot[ionization122394, PlotRange->loglogPlotRange, ImageSize->400, Join PlotStyle->plotColorsLines[[2]]];
```

Here we have dropped the 5 kTd point because of its sudden departure from a smooth curve.

```
In[137]:= Export["electronBoltIoniz.txt", ionization122394, "Table"]
```

```
Out[137]= electronBoltIoniz.txt
```

Published experimental and Boltzmann data are

```
In[138]:= Import["stokicionbolt.dat", "CSV"]//TableForm
```

```
Out[138]//TableForm=
```

1.00071E+02	2.63026E-22
1.42453E+02	7.47527E-22
1.94611E+02	1.71020E-21
2.61511E+02	3.27608E-21
3.66073E+02	5.57387E-21
5.60778E+02	9.47963E-21
9.02242E+02	1.40390E-20
1.40457E+03	1.64090E-20
1.99790E+03	1.67108E-20

```
In[139]:= Import["stokicionbolt.dat", "Table"];
```

```
In[140]:= stokicionBoltPlot=ListLogLogPlot[%,PlotRange->loglogPlotRange, ImageSize->400, Joined-> True, PlotStyle->plotColorsLines[[1]]];
```

```
In[141]:= Import["stokicionfolkard.dat", "CSV"]//TableForm
```

```
Out[141]//TableForm=
```

1.52126E+02	9.10372E-22
3.05588E+02	3.61344E-21
4.56729E+02	5.67958E-21
6.08470E+02	6.13857E-21
7.65468E+02	7.04111E-21
9.09228E+02	7.31917E-21
1.22120E+03	7.30995E-21
1.53614E+03	7.30276E-21

```
In[142]:= Import["stokicionfolkard.dat", "Table"];
```

```
In[143]:= stokicionFolkardPlot=ListLogLogPlot[%,PlotRange->loglogPlotRange, ImageSize->400, PlotStyle->plotColorsPoints[[3]], DisplayFunction->Identity];
```

```
In[144]:= Import["stokicionrose.dat", "CSV"]//TableForm
```

```
Out[144]//TableForm=
```

1.06859E+02	2.90225E-22
1.21874E+02	4.75089E-22
1.37853E+02	7.04652E-22
1.53384E+02	9.65870E-22
1.83744E+02	1.48989E-21
2.12995E+02	2.04183E-21
2.42880E+02	2.63758E-21
2.72444E+02	3.21149E-21
3.81350E+02	4.95052E-21
4.56743E+02	5.90823E-21
5.29394E+02	6.91442E-21
6.08559E+02	7.47793E-21
7.65580E+02	8.57736E-21
9.16896E+02	9.64823E-21
1.22154E+03	1.06358E-20
1.52411E+03	1.14986E-20
1.81038E+03	1.21910E-20
2.41177E+03	1.26662E-20
3.03384E+03	1.31632E-20

```
In[145]:= Import["stokicionrose.dat", "Table"];
```

```
In[146]:= stokicionRosePlot=ListLogLogPlot[%,PlotRange->loglogPlotRange, ImageSize->400, PlotStyle->plotColorsPoints[[4]], DisplayFunction->Identity];
```

```
In[147]:= Import["stokicionstokic.dat", "CSV"]//TableForm
```

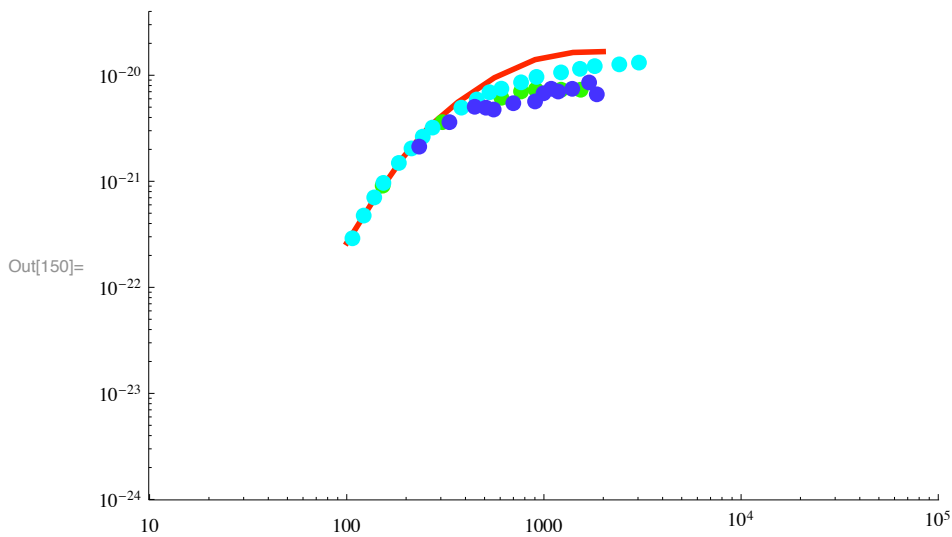
```
Out[147]//TableForm=
```

2.33093E+02	2.12322E-21
3.31684E+02	3.61217E-21
4.45600E+02	5.04583E-21
5.08016E+02	4.94446E-21
5.55918E+02	4.75125E-21
6.99357E+02	5.44979E-21
9.01637E+02	5.66304E-21
9.94932E+02	6.76098E-21
1.08886E+03	7.45930E-21
1.18179E+03	7.02801E-21
1.39230E+03	7.45147E-21
1.69506E+03	8.54821E-21
1.85459E+03	6.61117E-21

```
In[148]:= Import["stokicionstokic.dat", "Table"];
```

```
In[149]:= stokicionStokicPlot=ListLogLogPlot[%,PlotRange->loglogPlotRange, ImageSize->400,
PlotStyle->plotColorsPoints[[5]], DisplayFunction->Identity];
```

```
In[150]:= Show[stokicionBoltPlot, stokicionFolkardPlot, stokicionRosePlot, stokicionStokicPlot]
```



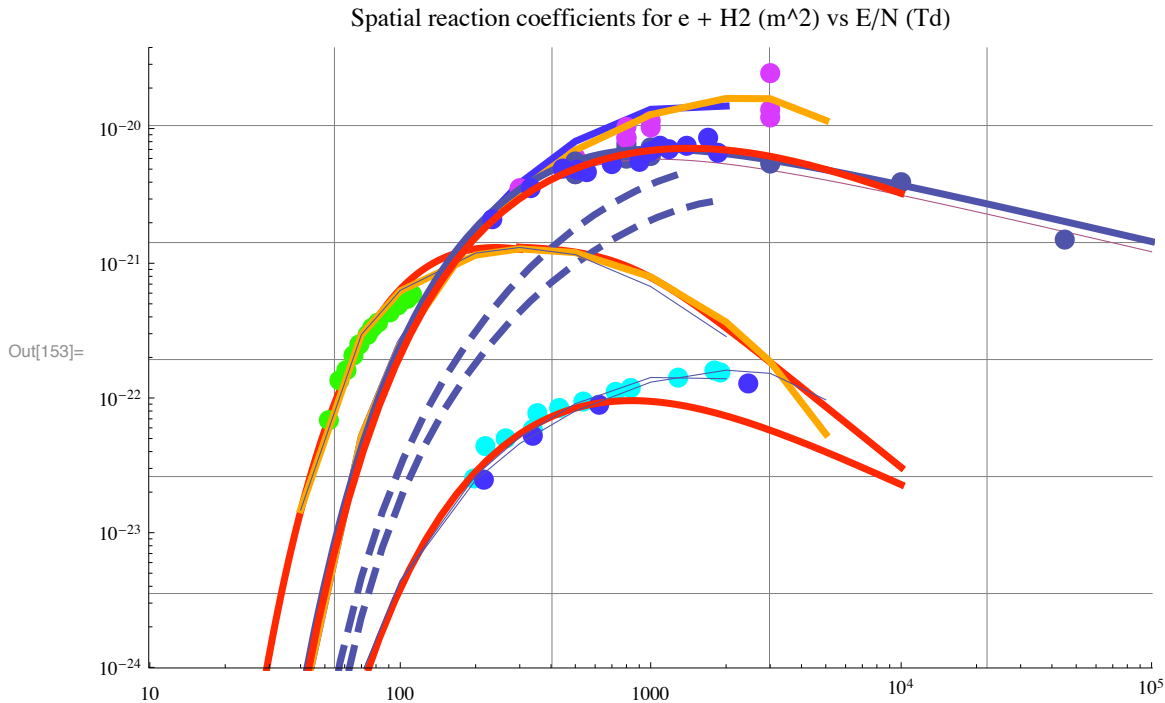
```
In[151]:= boltzAlphaWeb = Table[{boltzIonizWeb[[j, 1]], boltzIonizWeb[[j, 2]],
boltzHalpaweb[[j, 2]], boltzHUVweb[[j, 2]]}, {j, Length[boltzIonizWeb]}];
```

```
In[152]:= Export["alphaBoltzWeb.dat", boltzAlphaWeb, "Table"]
```

```
Out[152]= alphaBoltzWeb.dat
```

■ Summary plot

```
In[153]:= Show[stojanovicuexptPlot, (*stojanovicvtheoryPlot,*) stokichaexpt1Plot, stokichaexpt2Plot, (*stokicl
(*maxuvElectronExcitCalcPlot,*)webIonizationPlot, alHalpfitPlot, halpfitIonizationZoranPlot, conti
tischerDataPlot, bolsigplusIonizationPlot, bolsigplusastatePlot, bolsigplusHalpfitPlot, astateElectr
ionization122394Plot, halpfit122394Plot, webhalpfitPlot, webastatePlot, growthIonizationPlot, stokioc
ionizationFitPlot, GridLines->Automatic, PlotLabel-> "Spatial reaction coefficients for e + H2 (m^2
ImageSize->500]
```



The blue curves are from the BACKPRO calculation as given on the Web. The orange curves are from BACKPRO calculations of 12/23/94. The black dashed curves are from BOLSIGPLUS calculations of 5/14/06. The red curves are our empirical fits. The empirical fit for ionization was chosen to fit the Belgrade experimental ionization coefficients rather than the BACKPRO results or Rose's Townsend type experimental results. The points are experimental data, although the green points at $E/N < 120$ Td are only relative values from Tisher and Phelps that have been scaled to fit theory at one E/N .

The hard thing to rationalize is the divergence between the BOLSIGPLUS and BACKPRO α_{HAI}/n result for increasing E/N . We find that the BOLSIGPLUS results at 1 kTd are independent of the number of grid points used in BOLSIGPLUS when $\# \geq 50$. The black dashed curve shows that the a-state excitation peaks higher and drops lower at high E/N when the ionization energy loss is all to one product electron. When the cross section for Halpfit is added to BOLSIG.SEC very little changes.

11/09/07 There seems to be no basis for lowering the ionization coefficients below our fit for 350 Td as seems to be needed to fit Zoran's data for run h2350s3.091. Zoran give $\alpha_{\text{HAI}}/N = 3.75\text{E-}21$ m²

```
In[154]:= Quit[]
```

Cross sections for e + H3+ collisions

Setup notebook environment

```
In[1]:= a = 1;
```

```
In[2]:= ClearAll["Global`*"];
```

```
In[3]:= Remove["Global`*"];
```

```
In[4]:= startclock = SessionTime[];
```

```
In[5]:= Off[General::spell];
```

```
In[6]:= Off[General::spell1];
```

```
In[7]:= today = StringForm["`"/`"/` `:`:``", Date][[2]],  
Date][[3]], Date][[1]], Date][[4]], Date][[5]], Date][[6]]]
```

```
Out[7]= 9/15/2011 22:57:44.5227935`9.40115727466699
```

```
In[8]:= SetDirectory[NotebookDirectory[]]
```

```
Out[8]= C:\Users\avp\Documents\Mathbook\HYDROGEN\H3pElectronCollisions
```

```
In[9]:= plotColorsLines = {  
  (*1-red*) {Hue[0.0], Thickness[0.007], Dashing[{}]},  
  (*2-orange*) {Hue[0.1], Thickness[0.007], Dashing[{}]},  
  (*3-green*) {Hue[0.3], Thickness[0.007], Dashing[{}]},  
  (*4-cyan*) {Hue[0.5], Thickness[0.007], Dashing[{}]},  
  (*5-dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{}]},  
  (*6-purple*) {Hue[0.8], Thickness[0.007], Dashing[{}]},  
  (*7-black*) {Thickness[0.007], Dashing[{}]},  
  (*8-dash red*) {Hue[0.0], Thickness[0.007], Dashing[{0.05, 0.05}]},  
  (*9-dash orange*) {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05}]},  
  (*10-dash green*) {Hue[0.3], Thickness[0.007], Dashing[{0.05, 0.05}]},  
  (*11-dash cyan*) {Hue[0.5], Thickness[0.007], Dashing[{0.05, 0.05}]},  
  (*12-dash dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{0.05, 0.05}]},  
  (*13-dash purple*) {Hue[0.8], Thickness[0.007], Dashing[{0.05, 0.05}]},  
  (*14-dash black*) {Thickness[0.007], Dashing[{0.02, 0.02}]}];
```

```

In[10]:= plotColorsPoints = {
  (*1-red*) {Hue[0.0], PointSize[0.02]},
  (*2-orange*) {Hue[0.1], PointSize[0.02]},
  (*3-green*) {Hue[0.3], PointSize[0.02]},
  (*4-cyan*) {Hue[0.5], PointSize[0.02]},
  (*5-dk blue*) {Hue[0.7], PointSize[0.02]},
  (*6-purple*) {Hue[0.8], PointSize[0.02]},
  (*7-black*) {PointSize[0.02]},
  (*8-dash red*) {Hue[0.0], PointSize[0.02]},
  (*9-dash orange*) {Hue[0.1], PointSize[0.02]},
  (*10-dash green*) {Hue[0.3], PointSize[0.02]},
  (*11-dash cyan*) {Hue[0.5], PointSize[0.02]},
  (*12-dash dk blue*) {Hue[0.7], PointSize[0.02]},
  (*13-dash purple*) {Hue[0.8], PointSize[0.02]},
  (*14-dash black*) {PointSize[0.02]};

```

Electron recombination with H3+

From Glosik et al, Phys. Rev. A 79, 052707 (2009)

```

In[11]:= recombTheory = Import["Glosik09PRATheory.dat"];

```

```

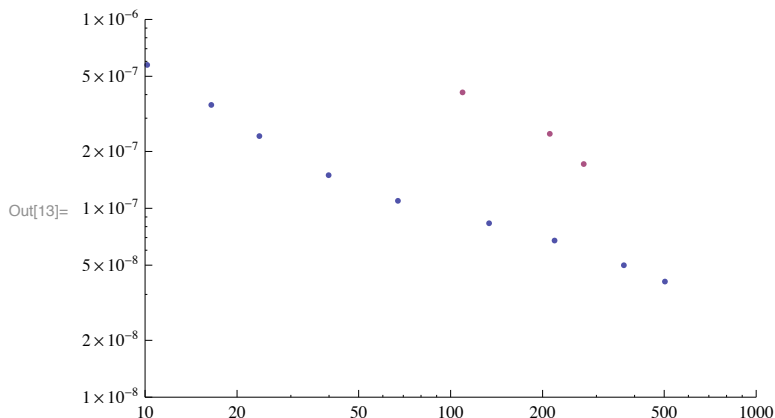
In[12]:= amanoExpt = Import["Glosik09PRAAmano.dat"];

```

```

In[13]:= ListLogLogPlot[{recombTheory, amanoExpt}, PlotRange -> {{10, 1000}, {10^-8, 10^-6}}]

```



```

In[14]:= beamExpt = Import["kreckel10PRAfig7.dat"];

```

```

In[15]:= kreckelPlot = ListLogLogPlot[{beamExpt}, PlotRange -> {{10^-2, 100}, {10^-10, 10^-6}}];

```

```

In[16]:= qe3[enrel_] = 4.5 * 10^-9 / enrel^0.7 / (1 + (enrel / 0.25)^4)^0.42 *
  (1 + (enrel / 1.65)^2)^2.55 / (1 + (enrel / 10)^4)^1

```

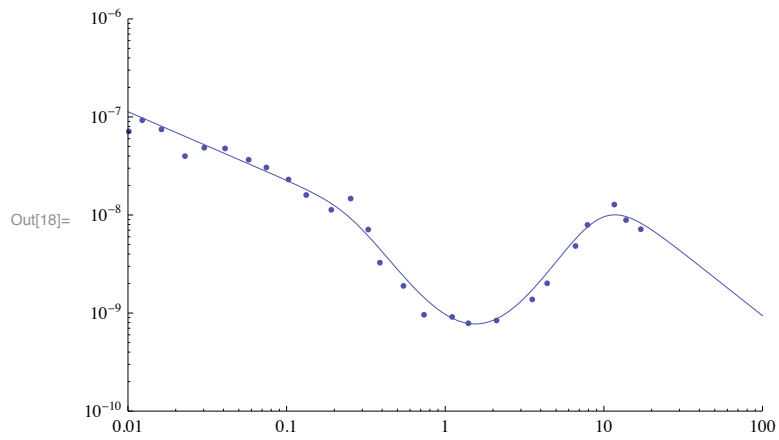
Out[16]=
$$\left(4.5 \times 10^{-9} \left(1 + 0.367309 \text{enrel}^2\right)^{2.55}\right) / \left(\text{enrel}^{0.7} \left(1 + \frac{\text{enrel}^4}{10000}\right) \left(1 + 256. \text{enrel}^4\right)^{0.42}\right)$$

```

In[17]:= fitPlot = LogLogPlot[{qe3[enrel]},
  {enrel, 10^-2, 100}, PlotRange -> {{10^-2, 100}, {10^-10, 10^-6}}];

```

```
In[18]:= Show[fitPlot, kreckelPlot]
```



These units are cm³/s.

```
In[19]:= Quit[]
```


9 Summary

Cross sections for multi-beam model of H2 at high E/N including neutrals

The cells to be transferred when the package H2CROSSSECTIONS.m (made from H2CROSSSECTIONS.nb - this notebook - by using SAVE, should be marked as initialization cells using CELL/CELL PROPERTIES/INITIALIZATION CELL.

All cross sections should be a function of LABoratory energy!

Setup notebook environment

```
In[95]:= a = 1;
In[96]:= ClearAll["Global`*"];
In[97]:= Remove["Global`*"];
In[98]:= startclock = SessionTime[];
In[99]:= Off[General::spell];
In[100]:= Off[General::spell1];
In[101]:= today = DateList[]
Out[101]= {2011, 9, 15, 23, 15, 43.8015247}
```

```
In[102]:= SetDirectory["c:\users\avp\documents\Mathbook\hydrogen\h2lowcurrent\spatialmodel"]
```

```
Out[102]= c:\users\avp\documents\Mathbook\hydrogen\h2lowcurrent\spatialmodel
```

```
In[103]:= plotColorsLines = {
  (*1-red*) {Hue[0.0], Thickness[0.007], Dashing[{}]},
  (*2-orange*) {Hue[0.1], Thickness[0.007], Dashing[{}]},
  (*3-green*) {Hue[0.3], Thickness[0.007], Dashing[{}]},
  (*4-cyan*) {Hue[0.5], Thickness[0.007], Dashing[{}]},
  (*5-dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{}]},
  (*6-purple*) {Hue[0.8], Thickness[0.007], Dashing[{}]},
  (*7-yellow*) {Hue[0.2], Thickness[0.007], Dashing[{}]},
  (*8-pink*) {Hue[0.9], Thickness[0.007], Dashing[{}]},
  (*9-black*) {Thickness[0.007], Dashing[{}]},
  (*10-dash red*) {Hue[0.0], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*11-dash orange*) {Hue[0.1], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*12-dash green*) {Hue[0.3], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*13-dash cyan*) {Hue[0.5], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*14-dash dk blue*) {Hue[0.7], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*15-dash purple*) {Hue[0.8], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*16-dash yellow*) {Hue[0.2], Thickness[0.007], Dashing[{0.05, 0.05}]},
  (*17-dash pink*) {Hue[0.9], Thickness[0.007], Dashing[{0.02, 0.02}]},
  (*18-dash black*) {Thickness[0.007], Dashing[{0.02, 0.02}]}
};
```

```
In[104]:= plotColorsPoints = {
  (*1-red*) {Hue[0.0], PointSize[0.02]},
  (*2-orange*) {Hue[0.1], PointSize[0.02]},
  (*3-green*) {Hue[0.3], PointSize[0.02]},
  (*4-cyan*) {Hue[0.5], PointSize[0.02]},
  (*5-dk blue*) {Hue[0.7], PointSize[0.02]},
  (*6-purple*) {Hue[0.8], PointSize[0.02]},
  (*7-yellow*) {Hue[0.2], PointSize[0.02]},
  (*9-pink*) {Hue[0.9], PointSize[0.02]},
  (*8-black*) {PointSize[0.02]}
};
```

```
In[105]:= plotColorsLines[{{1, 2}}]
```

```
Out[105]= {{Hue[0.], Thickness[0.007], Dashing[{}]}, {Hue[0.1], Thickness[0.007], Dashing[{}]}}
```

```
In[106]:= Precision[0. * i]
```

```
Out[106]= MachinePrecision
```

```
In[107]:= Precision[Re[0. * i] - 0]
```

```
Out[107]= ∞
```

```
In[108]:= $MachinePrecision
```

```
Out[108]= 15.9546
```

■ Cross sections and reflection coefficients for H+ ions

See H2HpQdata_7.nb

```
In[109]:= fac=10^20;
```

Define a factor multiplying H+ destruction cross sections

```
In[110]:= g1=1;
```

■ H+ balmer alpha excitation

H+ balmer alpha excitation from Phelps (1990)

```
In[111]:= q1ha1[w1_] = (2.2*10^-25*w1/((w1/1000)^4+1)^.5 + (1.*10^-25*w1))*UnitStep[w1-20];
```

This did not have a threshold, so I arbitrarily added one.

This is assumed to produce a fast H atom excited to the n= 3 state and emitting Balmer alpha in small angle scattering, i.e., it does not contribute significantly to energy loss compared to the elastic scattering energy loss. This assumption is based on Williams, Geddes, and Gilbody (1982) measurements of Doppler shifted and unshifted H α emission using beam techniques at energies ≥ 1.5 keV. See Fig. 1 of Van Zyl, Gealy, and Neuman, Phys. Rev. A 40, 1664 (1989) for ratio for Lyman alpha.

By scaling the Lyman alpha data of Van Zyl et al (1989) and fitting to the energy dependence of Hess (1974), we estimate the H α excitation as follows:

```
In[112]:= q1ha[w1_] = 6.*10^-28*UnitStep[w1-50] (w1-50)^2 / (1+(w1/700)^4)^0.5*(1+(w1/3000)^4)^0.25;
```

I have not added an effect of electronic excitation, e.g., Lyman series or Balmer series or triplet excitation, to the effective momentum transfer cross section. The Lyman and Balmer series cross sections are small below 1000 eV, while the triplet excitation of H₂ by H⁺ is unknown. Judging from our H + H₂ cross section, the triplet excitation for H⁺ + H₂ could be large at low energies.

■ Lyman alpha excitation by H+

A fit to Lyman alpha excitation by H⁺ from Van Zyl et al (1989) is

```
In[113]:= q1Lya[w1_] :=
  4.5 * 10^-27 * UnitStep[w1 - 50] (w1 - 50)^2 / (1 + (w1 / 700)^4)^0.5 * (1 + (w1 / 3000)^4)^0.25
```

■ Ionization in H+ + H₂ -> e + 2 H⁺ + H from Phelps (1990). Actually total electron production. Products could be e + H⁺ + H₂⁺. Not used in most calculations.

```
In[114]:= q1e1[w1_] := 5.7 * 10^-26 * (w1 - 30)^1.25 * UnitStep[w1 - 30]
```

■ H+ + H₂ -> slow H₂⁺ + fast H by charge transfer

From Heim and Stori

```
q1s2Heim[w1_] := 5.*10^-20*UnitStep[w1-2.]
```

This is assumed to produce a fast H and a H2+ ion at zero energy.

From Phelps (1990)

```
q1s2Phelps[w1_] := UnitStep[w1-2.7]*((4.5 10^-20*(2*w1/(1000+w1))^1.7/((w1/25000)+1)+
(5.5*10^-21/((w1+0.04)/10)^.5))+1.*10^(-30)
```

This cross section is much smaller than that of Heim and Stori at energies of interest to us. We had to modify the square root term because *Mathematica* was unhappy with $(0)^{0.5}$. Our choice of $w1 + 0.04$ is because $w1 = 0.04$ eV is the average energy for thermal ions and neutrals. Until 9/5/06, I was using the wrong threshold for this process in this program.

We did use

```
q1s2[w1_] := UnitStep[w1-2.7]*((4.5 10^-20*(2*w1/(1000+w1))^1.7/((w1/25000)+1)+
(5.5*10^-21/((w1+0.04)/10)^.5))+1.*10^(-30)
```

but the following fits better near threshold

```
In[115]:= q1s2[w1_] := g1*2.* 10^-20*UnitStep[w1-2.700001]/(1+1/(w1-2.7))^0.5/(1+(w1/1))^0.5*
(1+(w1/110)^2.1)/(1+(w1/1450)^1.8);
```

The following is a test of the TeX cross section used at one time, but no longer applies.

```
q1s2T[w1_] := UnitStep[w1-1.](1.46*10^-19(1+1000/w1)^-1.7/((w1/25000)+1)
+(5.5*10^-21/((w1+0.04)/10)^0.5))+1.*10^(-30)
```

■ reduced energy H production in H+ + H2 -> H2+ + fast H

We assume that momentum transfer during this charge transfer collision results in a significant loss of energy, as in elastic scattering, and that the cross section is given by $q1s2*fitQmoQtDiff$. Here $fitQmoQtDiff$ is a rough estimate of the fractional momentum transfer estimated from the theory for vibrational excitation by Krstic and Schultz. This cannot be added to the effective momentum transfer cross section because it is a reaction collision.

```
In[116]:= qlfA[w1_] := qls2[w1] * fitQmoQtDiff /. enLab -> w1
```

11/14/07 and 04/04/08 Tests using this to calculate the initial energy distribution of the fast H produced by $H + H_2 \rightarrow f H + H_2^+$, showed very little change in the spatially dependent Halpha at 350 Td or 10 kTd or in the Halpha profile at 10 kTd. When FitQmoQtDiff[enLab] was changed to a constant 0.55, there was a significant drop in the heavy particle component of Halpha excitation at 350 Td and a small drop at 10 kTd.

Because this estimated cross section makes so little difference, we simplify things by essentially setting it to zero.

```
In[117]:= qlfA[w1_] := qls2[w1] * 10^-9
```

Note that Heckman et al (1984) seem to find much larger H atom scattering at large reduced angles than do Payne and Riviere (1972) at low keV energies.

Is this reasonable????? See Rice data!!!

■ Rotational excitation

```
In[118]:= Clear[enLab]
```

From the file HpH2Qdata101507.nb my fit to the cross section in 10^{-20} m^2 for the $J=0 \rightarrow J=2$ rotational transition is:

```
In[119]:= fitRotation02[enLab_] = UnitStep[enLab - 0.066] * 17 / (1 + (0.04 / (enLab - 0.066))^4) * (1 + (enLab / 0.3)^1) / (1 + (enLab / 27)^1.8)^1.4
```

```
Out[119]= 
$$\frac{17 (1 + 3.33333 \text{ enLab}) \text{ UnitStep}[-0.066 + \text{enLab}]}{\left(1 + \frac{2.56 \times 10^{-6}}{(-0.066 + \text{enLab})^4}\right) (1 + 0.588235 \text{ enLab})^2 (1 + 0.00265183 \text{ enLab}^{1.8})^{1.4}}$$

```

I will take the total rotational excitation cross section as 5/3 of this equation at energies well above threshold. Based on Linder (1980). Engelhardt et al got a similar ratio from statistical weights.

I now assume that the contribution of rotational excitation to the momentum transfer cross section has the same ratio to the total rotational excitation cross section as found from Krstic and Schultz (1999) for vibrational excitation.

```
In[120]:= fitQmoQtDiff := 0.55 / (1 + (enRel / 4)^4)^0.4 /. enRel -> 2/3 * enLab
```

so that

```
In[121]:= fitQmRot[enLab_]=10^-20*5./3.*fitRotation02[enLab]*fitQmoQtDiff
```

$$\text{Out[121]} = \frac{1.55833 \times 10^{-19} (1 + 3.33333 \text{ enLab}) \text{UnitStep}[-0.066 + \text{enLab}]}{\left(1 + \frac{2.56 \times 10^{-6}}{(-0.066 + \text{enLab})^4}\right) (1 + 0.588235 \text{ enLab})^2 (1 + 0.00265183 \text{ enLab}^{1.8})^{1.4} \left(1 + \frac{\text{enLab}^4}{1296}\right)^{0.4}}$$

Because of the small energy loss, the principle effect of rotational excitation in our multibeam model is to add to the effective momentum transfer cross section.

I decided not to use this addition to Qm.

■ H+ + H2 -> H- + ?(2H+)?

From Barnett et al, Red Book, Table A.4.4 and H2HpQs110207_7.nb

```
In[122]:= q1N1[w1_] := 1.3 * 10^-23 *
  ((w1 - 30) / 1000.)^1.5 / (1 + (w1 / 25000.)^4 + (w1 / 33000.)^8.5) UnitStep[w1 - 30];
```

Fournier, et al, J. Phys. B 5, L58 (1972) claim that at their 4 keV, the H- occurs via a two step process involving H+ + H2 -> H + H2+ and H + H2 -> H- + H2+.

■ Vibrational excitation

From H2HpQdata.nb a fit to Krstic and Schultz (1999) vibrational excitation for the sum of the transitions from v=0 is

```
In[123]:= fitVibrationTotal=(UnitStep[enLab-3/2*0.52]*20/(1+(1.5/(enLab-3/2*0.52))^1)/(1+(enLab/2.8)^2
  (1+(enLab/5.1)^3.9)^1.2/ (1+(enLab/10)^1.2)^2.1/ (1+(enLab/150)^2.2)^0.3)
```

$$\text{Out[123]} = \frac{20 (1 + 0.00173971 \text{ enLab}^{3.9})^{1.2} \text{UnitStep}[-0.78 + \text{enLab}]}{\left(1 + \frac{1.5}{-0.78 + \text{enLab}}\right) (1 + 0.0630957 \text{ enLab}^{1.2})^{2.1} (1 + 0.0000163155 \text{ enLab}^{2.2})^{0.3} (1 + 0.084493 \text{ enLab}^{2.4})}$$

Because of the small energy loss, the principle effect of vibrational excitation in our multibeam model is to add to the effective momentum transfer cross section. Presumably this is included in the cross section theory of Krstic and Schultz (1999).

■ Inelastic scattering of H+ by H2

From H2HpQdata.nb a fit to our L(inelastic) function in 1985 revision of Table 2 of JPCRD 1990 is

```
In[124]:= l1in[enLab_] = 2*8.0*10^-20*(1+(enLab/450)^4)^0.16;
```

Theory says this is too low at high energies. This partially justifies applying factor of 2. See Fig. 1 of 1991 erratum to Phelps 1990. The Halpha spatial distributions are insensitive to multiplying this by factors of 0.1 and 10 at E/N = 10 kTd. At 300 Td a factor of 10 almost eliminates the Halpha. Try adding the following step function to see where the increase is in l1in[w1] needed.

$$\text{l1in}[w1_] = 10^{-20} * 30 * (\text{UnitStep}[w1 - 10] - \text{UnitStep}[w1 - 300]) + 8.0 * 10^{-20} * (1 + (w1/450)^4)^{0.16};$$

This step function shows that a factor of 5 increase in the loss function for H+ in H2 for energies between 10 and 300 eV reduces the Halpha at E/N ~ 300 Td to give reasonable agreement with experiment. This is a much less drastic increase in the loss function than that needed for H3+ to accomplish the same reduction in Halpha.

I modified the l1in[enLab] on about 9/16/06 so as to drop the elastic recoil contribution at low energies. I did not try to follow the detail of the rotational and vibrational contributions given in Phelps (1990). We continue to use the higher theoretical value at high energies.

```
ln[125]:= l1in[enLab_] = 1.2*10^-20*enLab^0.45*(1+(enLab/350)^4)^0.02;
```

Using the first form of l1in[w1] rather than the form immediately above reduces the Halpha signal at 350 Td, especially for m = 97. It has little effect at 10 kTd. Adding a UnitStep[enLab-0.54*3/2] made little difference at 350 Td. Not tested at 10 kTd.

10/28/07 I need to update this by including the rotational and vibrational excitation contributions.

```
l1in2[enLab_]= 1.2*10^-20*enLab^0.45*(1+(enLab/350)^4)^0.02+ 0.044*5/3*10^-20*fitRotation02[
0.52*10^-20*fitVibrationTotal];
```

This algebra formula is too complex, so we approximate it by

```
ln[126]:= l1in[enLab_] = 2 * (0.5 * (1.2 * 10^-20 * enLab^0.45 * (1 + (enLab / 350)^4)^0.02) +
4. * 10^-20 / (1 + 0.1 / (enLab - 0.066)) * UnitStep[enLab - 0.066]);
```

This gives a pretty good fit, but it should be lowered slightly. Try the following:

```
ln[127]:= l1in[enLab_] = 2. * (0.5 * (1.2 * 10^-20 * enLab^0.45 * (1 + (enLab / 350)^4)^0.02) +
4. * 10^-20 / (1 + 0.1 / (enLab - 0.066)) * UnitStep[enLab - 0.066]);
```

Here we add a bump in the energy loss near 150 eV. The following is the result of numerous trials. It still needs raising at low energies and lowering of the bump magnitude.

```
l1in[enLab_] =
(2 * 0.5 * (1.2 * 10^-20 * enLab^0.45 * (1 + (enLab / 350)^4)^0.02) / (1 + (enLab / 200)) *
(1 + (enLab / 800))^2. / (1 + (enLab / 10 000))^1 +
4. * 10^-20 / (1 + 0.1 / (enLab - 0.066)) * UnitStep[enLab - 0.066] +
9 * 10^-20 * ((enLab - 10) / 10)^2 / (1 + (enLab / 50)^5) * UnitStep[enLab - 10];
```

■ Momentum transfer scattering of H+ by H2

From our 1990 compilation, the momentum transfer cross section for elastic scattering of H+ by H2 is approximately the momentum loss function from NONEQUIL.NB/energy. The momentum loss function is

```
ln[128]:= l1 := (3.5*10^-19*(u1[z]^2/(10*u1[z]+2))^0.4*(100/(u1[z]+50))^1.4)
```

Comparison with Eq. (5) of Phelps et al, Phys. Rev. A 36, 5327 (1987) shows that the momentum transfer cross section is

```
ln[129]:= qmHpH2Phelps[w1_] := l1/u1[z] /. u1[z] -> w1
```

The following, along with a reduced l1in[] gave improved convergence and a fit to Halpha at 350 Td on 08/26/09. From our TeX file this should be equivalent to

```
q1f1[w1_] := 1.674 * 10^-16 / ((w1 + 0.04)^0.2 * (50 + w1)^1.4 * (1 + 5 * w1)^0.4)
```

The following is out of date

```
q1f1[w1_] = 3.5*10^-19*(w1^2/(10*w1+2))^0.4/w1*(100/(w1+50))^1.4//PowerExpand//FullSimplify
```

The high energy portion of this is based on my extrapolation and interpolation of the differential scattering data from Stebbings et al.

```
ln[130]:= q1mRice = {{500, 2.4*10^-22}, {1500, 3.8*10^-23}};
```

If we adopt the Krstic and Schultz (1998) cross sections for H+ + H2 elastic scattering for relative energies up to 100 eV, including the effects of vibrational excitation, an approximate fit is

```
In[131]:= qmHpH2Krstic [w1_] = 1.5 * 10^-19 * (enrel + 0.04)^-0.5 *
  ((enrel / 0.1)^2 + 1)^0.15 / (1 + (enrel / 2.)^2)^0.75 /. enrel -> 2 / 3 * w1;
```

Here the 0.04 is used to avoid a singularity that upsets *Mathematica*. Its value is chosen to represent thermal motion.

We do not use the following cross section of K&S that one downloads from the ORNL website, because it does not include the effects of vibrational excitation.

```
In[132]:= Drop[Import["C:\\users\\avp\\documents\\mathbook\\hydrogen\\h2hpcollisions\\krsticElasticQm.
```

Convert to LAB energy

```
In[133]:= Table[%[[j,1]]*3/2,%[[j,2]]*fac},{j,Length[%]}];
```

Our approximation to Krstic and Schultz (1998) is much smaller than Phelps (1990) at high energies. K&S (1999) is supposed to include the contribution of vibrational excitation to the momentum transfer cross section. As of 10/28/07, I have added my estimated contribution of rotational excitation to Qm. See H2HpQdata101507.nb for its derivation in which one assumes that the principle effect of rotational excitation is to increase the momentum transfer cross section.

Krstic and Schulz plus rotation does not help. Therefore, we add something peaking at ~ 100 eV

```
q1f1 [w1_] :=
  1.5 * 10^-19 * (2 * w1 / 3 + 0.04)^-0.5 * ((2 * w1 / 3 / 0.1)^2 + 1)^0.15 / (1 + (w1 / 3.)^2)^0.75 +
  15. * 10^-21 * UnitStep [w1 - 0.1] * (w1 - 0.1) / (1 + (w1 / 25)^2)^2 / (1 + (w1 / 250)^4)
```

This improves the agreement of the calculated and measured H+ energy distributions at 2 kTd, but completely suppresses heavy particle excitation of Halpha at 350 Td. Without the last term, this gives too much heavy particle excitation at 350 Td. With it there is no heavy particle excitation at 350 Td.

```
q1f1 [w1_] := 1.5 * 10^-19 * (2 * w1 / 3 + 0.04)^-0.5 *
  ((2 * w1 / 3 / 0.1)^2 + 1)^0.15 / (1 + (w1 / 3.)^2)^0.75 * (1 + (w1 / 40)^2) / (1 + (w1 / 120)^2.3)
```

Because of the apparent success of the high section momentum transfer cross for H3+ + H2, I feel obligated to try a similar increase for H+ + H2 and H + H2. The following choice fits our 1990 Qm at high energies. It also is expected to approach the Rice result. **As of 07/31/09 the following, along with the full I1in[], was replaced by my old Qm from above, along with a reduced I1in[].**

```
In[134]:= q1f1 [w1_] = 1.5 * 10^-19 * (2 * w1 / 3 + 0.04)^-0.5 *
  ((2 * w1 / 3 / 0.1)^2 + 1)^0.15 / (1 + (w1 / 3.)^2)^0.75 *
  (1 + enrel / 140)^1.5 / (1 + enrel / 1000)^2.3 /. enrel -> 2 / 3 * w1;
```

This reduces heavy particle Halpha at 350 Td, but not enough.

Krstic and Schultz (1999) modified to enLab.

```
q1f1 [w1_] := 1.5 * 10^-19 * (2 * w1 / 3 + 0.04)^-0.5 *
  ((2 * w1 / 3 / 0.1)^2 + 1)^0.15 / (1 + (w1 / 3.)^2)^0.75 (**fitQmRot [w1] *)
```

A first estimate of a large q1f1 is to scale the proposed q3f3 used to fit the H3+ energy distribution.

```
q1f1 [w1_] := 22 * 10^-20 / (enrel + 0.04)^0.5 / (1 + (enrel / 19)^2)^0.25 *
  (1 + (enrel / 43)^2)^1.3 / (1 + enrel / 250)^2.6 /. enrel -> 2 / 3 * w1
```


The fractional energy loss on elastic collision is $2*mM/(m+M)^2*(1-\text{Cos}[\text{theta}]) = 4/9*(1-\text{Cos}[\text{theta}])$. Because we use the diffusion (momentum transfer) cross section q_m , the $(1-\text{Cos}[\text{theta}])$ is included in the q_m .

■ 3-body formation of H3+

We should include the three-body destruction of H+ to form H3+. The only rate coefficient we have is the 300 K value of $3.2\text{E}-29 \text{ cm}^6/\text{s} = 3.2\text{E}-41 \text{ m}^6/\text{s}$ from Miller et al, Phys. Rev. 173, 115 (1968) and $3.0\text{E}-41 \text{ m}^6/\text{s}$ from Johnsen and Biondi (1976). I assume it to decrease as $1/\text{enlab}^{0.5}$, as discussed by Johnsen and Biondi, J. Chem. Phys. 65, 1539 (1976). This reaction occurs primarily with H+ in the lowest energy bin. It is assumed to produce zero energy H3+. From the file H2HpTransport.nb the ion drift velocity versus ion temperature in eV is $4620 \sqrt{kT_{\text{ion}}}$. Therefore the effective 3-body reaction coefficient is roughly

```
In[135]:= q1s3[kTion_] := g1*3.2*10^-41*(0.026/(kTion+0.026))^0.5*n/(4620*(kTion+0.026))
```

Corrected 05/23/08

■ reflection of H+ as fast H

In Petrovic et al, Phys. Rev. Lett., 68, 325 (1992) for an AuPd cathode, we assumed the reflection of fast H+ as fast H with an energy of $2/3$ of the incident H+ energy and 60% of the number, i.e., $R_N = 0.6$. The mean energy of the reflected atoms is $2/3 = R_E/R_N$.

Assume reflection is independent of energy and neglect diffuse scattering

$$r1A[m_, q_] := 0.5 * j1[m, q]$$

Production of a reflected fast H atom from H+ ($j1$) incident on cathode. In order to partially take into account the spread in energies of the reflected atoms, we will take the mean energy of the reflected atoms as $2/3$ of the available energy, i.e., $2/3$ of the incident ion energy. In units of q this is $2/3*k$ in the summation. We also must take into account the atoms lost, i.e., assume 50% reflected.

$$r1A[m_, q_] = 0.5 * \text{If}[1 <= q <= m, \text{Sum}[\text{If}[\text{Round}[2/3*k] == q, (j1[m, k]), 0], \{k, q+1, m\}], 0];$$

This assumption corresponds to $R_N = 0.5$ and $R_E = 0.33$. I do not find data for H on Au in Eckstein and Vereek, J. Plasma Phys. and Nuclear Fusion: Special Issue 1984, p. 12. These values are in the general region shown for other surfaces.

The following input values of R_E and R_N come from the NIFS data Web site under the category CURVES, in which one enters the incident atom mass, the target atom mass, and the angle of incidence (0 deg) and get a plot of their empirical fit to Monte Carlo calculations of the backscattering coefficients R_N and R_E . I then digitized the curves and fitted them as given below. They do not give data for incident molecules, so I will take them to be the same as for atoms of the same energy per atom.

```
In[136]:= rEmodel=Import["c:\\users\\avp\\documents\\mathbook\\hydrogen\\SurfaceEffects\\HAtomReflecti
```

```
In[137]:= rEmodelPlot =
```

$$\text{ListLogLogPlot}[rEmodel, \text{PlotRange} \rightarrow \left\{ \left\{ 1, 10^5 \right\}, \left\{ \frac{1}{10^3}, 1 \right\} \right\}, \text{PlotStyle} \rightarrow \text{plotColorsPoints}[\{1\}];$$

```
In[138]:= fitModelRE=0.5/(1+(enlab/7500)^(0.5))^2.8;
```

```
In[139]:= fitModelREPlot=LogLogPlot[fitModelRE, {enlab, 1, 10^5}, PlotRange->{{1, 10^5}, {10^-3, 1}}, PlotSty
```

This R_E seems high compared to the $1/3$ we assumed above.

```

ln[140]:= rNmodel=Import["c:\\users\\avp\\documents\\mathbook\\hydrogen\\SurfaceEffects\\HAtomReflecti
Out[140]:= {{2.28179, 0.556887}, {39.1022, 0.553411}, {381.634, 0.449483}, {1625.67, 0.322163},
           {8264.37, 0.179092}, {27748.5, 0.0855769}, {58042.8, 0.0453073}, {100000., 0.0252457}}
ln[141]:= rNmodelPlot=LogLogListPlot[rNmodel, PlotRange->{{1, 10^5}, {10^-3, 1}}, PlotStyle->plotColorsPoir
ln[142]:= fitModelRN=0.6/(1+(enlab/30000)^(0.5))^3.0;

```

The following formula was replaced by formulas based on Eckstein and Biersack (1985) as of 05/03/07

```

ln[143]:= fitRN[enlab_]=0.6/(1+(enlab/30000)^(0.5))^3.0;
ln[144]:= fitModelRNPlot=LogLogPlot[fitModelRN, {enlab, 1, 10^5}, PlotRange->{{1, 10^5}, {10^-3, 1}}, PlotSty
ln[145]:= avgEnModelPlot=LogLogPlot[fitModelRE/fitModelRN, {enlab, 1, 10^5}, PlotRange->{{1, 10^5}, {10^-3, 1}}
          Show[rEmodelPlot, rNmodelPlot, fitModelRNPlot, fitModelREPlot, avgEnModelPlot, ImageSize->500, Gr
          DisplayFunction->$DisplayFunction, PlotLabel-> "Backscattering coefficients for H on Au vs I

```

In the following fitModelRN replaces the RN = 1/2, fitModelRE replaces the RE = 1/3, and fitModelRE/fitModelRN replaces the RE/RN = 2/3.

```

r1A[m_, q_]=If[1<=q<=m, (fitModelRN/.enlab->q*delE)* Sum[If[Round[((fitModelRE/fitModelRN)/.en.
(j1[m, k]), 0], {k, q+1, m}], 0];

```

Revision of 04/05/06. See notebook AtomReflection030906.nb. Here fitRE/fitRN = 1/2 because of uniform distribution, i.e., we do not have a choice for RE/RN. A further revision of 03/23/10 is

Here division by k spreads the reflected flux uniformly in energy (or velocity for velocity grid).

```

ln[146]:= r1A[q_]:=Sum[fitRN[(k-1)*delE]/k*j1[m, k], {k, q, mh-mo}]*reflectionFactor;

```

As of 05/03/07, we have adopted fits to the H atom reflection based on Eckstein and Biersack, Appl. Phys. A 38, 123 (1985) rather than on Eckstein and Verbeek (1984). The formulas are rather different for a heavy metal and for carbon. For Au we use a formula scaled in energy by 1.08 from calculations for W. See Eckstein and Verbeek (1984).

```

ln[147]:= fitRNAu[enlab_]:=0.95/(1+(0.4/(1+1.08*enlab))^2)/(1+((1.08*enlab/7))^0.15/
          (1+((1.08*enlab)/30000))^1.35*UnitStep[1 - enrel];

```

For graphite, we use results based on calculations by Eckstein and Biersack (1985) for amorphous carbon.

```

ln[148]:= fitRNC[enlab_]:=0.8/(1+(1.4/(1+enlab))^4)/(1+(enlab/5))^0.35/(1+(enlab/3000))^1.15*
          UnitStep[1 - enrel];

```

We will use a fit to Eckstein and Biersack (1985) to represent the behavior of stainless steel.

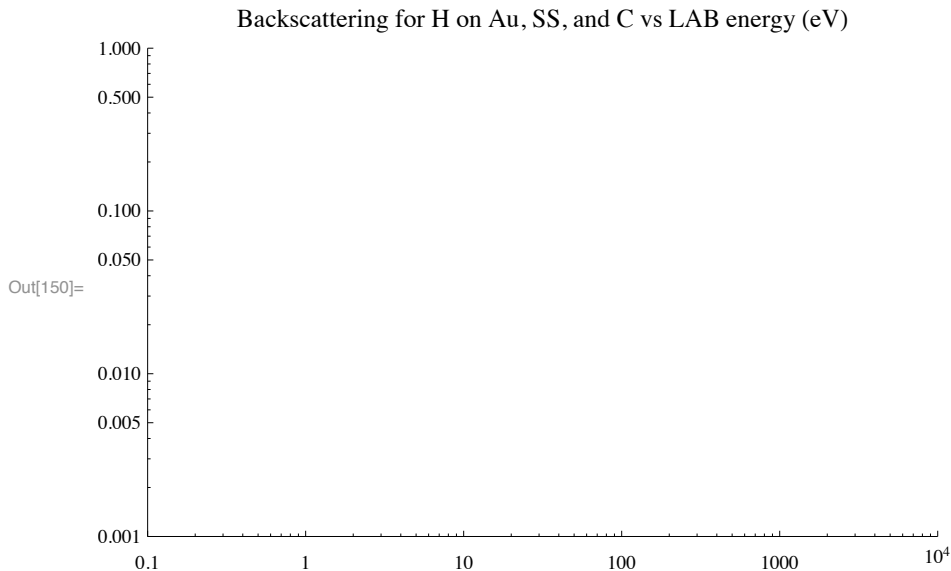
```

ln[149]:= fitRNSS[enlab_] := 0.95 / (1 + (0.6 / (1 + enlab))^2.5) / (1 + (enlab / 10))^0.23 /
          (1 + (enlab / 30000))^1.27 * UnitStep[1 - enrel]

```

Note that I have modified the fits at energies near and below 1 eV so as to remain finite at zero energy.

```
In[150]:= LogLogPlot[{fitRNAu[enlab], fitRNC[enlab], fitRNSS[enlab]}, {enlab, 0.1, 10^4}, PlotRange -> {{0.1, 10},
PlotStyle -> plotColorsLines, Ticks -> Automatic, ImageSize -> 400,
PlotLabel -> "Backscattering for H on Au, SS, and C vs LAB energy (eV)"]
```



■ Revised reflection of H+ as H - 05/16/2010

We wish to revise the reflection coefficient to approximate the distribution in energy of the reflected H atoms for SS with that for Ni. Until now, we have used a uniform distribution. See notebook FitAtomReflection051610_7.nb. The proposed distribution from this notebook is

```
phelpsFit1ASS := 0.52 * enrel ^ 0.4 * (1 + (900 / (en0 + 30)) * (enrel) ^ (17.9 / en0 ^ 0.3)) /
(1 + (8 * 10 ^ -8 * en0 ^ 2) * (enrel) ^ 1.5) (1 - enrel / 0.95) / (1 - enrel / 1.02)
```

Add cutoff at enrel = 0.95

```
In[151]:= PhelpsFit1ASS := 0.52 * enrel ^ 0.4 * (1 + (900 / (en0 + 30)) * (enrel) ^ (17.9 / en0 ^ 0.3)) /
(1 + (8 * 10 ^ -8 * en0 ^ 2) * (enrel) ^ 1.5) (1 - enrel / 0.95) / (1 - enrel / 1.05) *
UnitStep[0.95 - enrel]
```

The last factor is used to keep the fit less than unity as enrel decreases.

A test distribution is

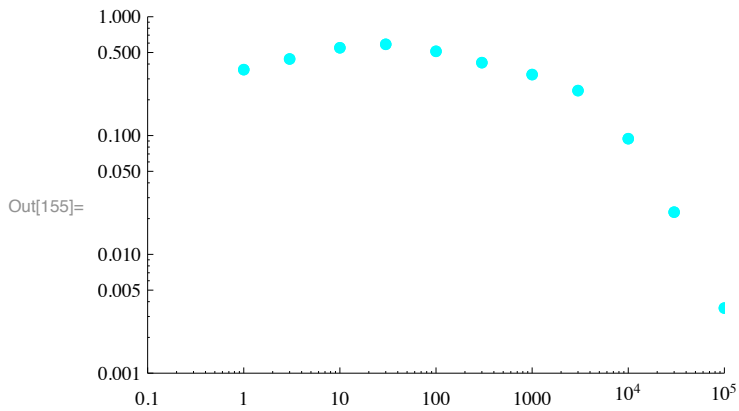
```
In[152]:= PhelpsFitTest := 0.5 * UnitStep[1 - enrel]
```

```
PhelpsFit1ASS = PhelpsFitTest
```

```
In[153]:= PhelpsFitReflectionFraction =
Table[{#[[j]], NIntegrate[(PhelpsFit1ASS / en0 -> #[[j]]], {enrel, 0, 0.95}]},
{j, Length[#]}] &[{{1, 3, 10, 30, 100, 300, 1000, 3000, 10000, 30000, 100000}}];
```

```
In[154]:= PhelpsFitRNPlot = ListLogLogPlot[%,
PlotRange -> {{0.1, 10^5}, {10^-3, 1}}, PlotStyle -> plotColorsPoints[[4]]];
```

In[155]:= Show[%, helpsFitRNPlot]



■ Excited H produced as backscattered H leaves surface

We adopt the view that there is a probability of H atom excitation at the surface that is proportional to the probability of escape multiplied by a survival factor. See, for example, Leung et al, Phys. Rev. A 18, 447 (1978). They give a survival constant of $1.6E8 \text{ cm/s} = 1.6E6 \text{ m/s}$. Kato et al, J. Nuclear Mat. 498-501, 390 (2009) do not discuss a survival effect, but do find a cuoff at low exit energies. They find a few percent probability of excitation of the H(n=3) that varies slowly with incident energy.

```
In[156]:= photonFit1XSS = excitationFrac * phelpsFit1ASS * Exp[-aa / vsX] /.
{aa -> 1.6 * 10^6, vsX -> Sqrt[2 * qe * enrel * en0 / mH + 10^5], qe -> 1.602 * 10^-19,
mH -> 1.67 * 10^-27}
```

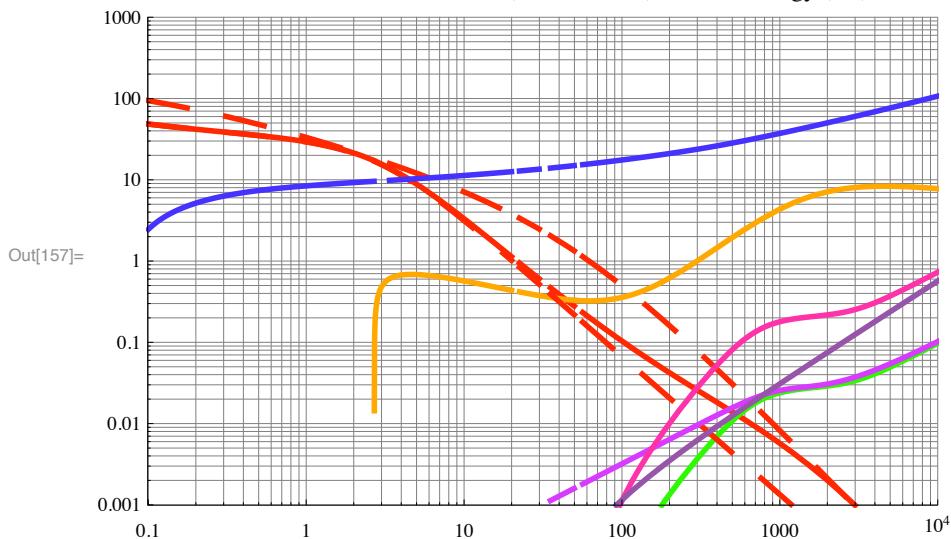
```
Out[156]= 
$$\left( 0.52 e^{-\frac{1.6 \times 10^6}{\sqrt{100000 + 1.91856 \times 10^8 \text{enrel}}}} (1 - 1.05263 \text{enrel}) \text{enrel}^{0.4} \left( 1 + \frac{900 \text{enrel}^{\frac{17.9}{\text{en0}^{0.3}}}}{30 + \text{en0}} \right) \right. \\ \left. \text{excitationFrac UnitStep}[0.95 - \text{enrel}] \right) / \left( (1 - 0.952381 \text{enrel}) \left( 1 + \frac{\text{en0}^2 \text{enrel}^{1.5}}{12500000} \right) \right)$$

```

■ Plot cross sections used

```
In[157]:= LogLogPlot[{fac * qlf1[w1], fac * qls2[w1], fac * qlha[w1], fac * qmHpH2Phelps[w1],
fac * qmHpH2Krstic[w1], fac * llin[w1], fac * qlha1[w1], fac * qlfA[w1], fac * qlLya[w1],
fac * qlel[w1] (*, fac * qlf1A[w1] *) (*, fac * llinB[w1], fac * llinC[w1] *)}, {w1, .1, 10000},
Ticks -> Automatic, PlotRange -> {{.099, 10000}, {fac * 0.099 * 10^-22, fac * 1.01 * 10^-17}},
PlotStyle -> plotColorsLines[{{1, 2, 3, 10, 10, 5, 6, 7, 8, 9}}],
ImageSize -> 400, GridLines -> Automatic,
PlotLabel -> "Cross sections for H+ + H2 (10^-20 m^2) vs LAB energy (eV)"]
```

Cross sections for H+ + H2 (10⁻²⁰ m²) vs LAB energy (eV)



```
In[158]:= xsecH2Hp = Table[{#, fac * qlf1[#[#], fac * qls2[#[#], fac * qlha[#[#],
fac * qmHpH2Phelps[#[#], fac * qmHpH2Krstic[#[#], fac * llin[#[#], fac * qlha1[#[#],
fac * qlfA[#[#], fac * qlLya[#[#]] &[0.1 * 10^(j / 10)], {j, 0, 5 * 10}];
```

```
In[159]:= Export["H2HpCrossSections.txt", xsecH2Hp, "Table"]
```

```
Out[159]= H2HpCrossSections.txt
```

■ Cross sections and reflection coefficients for H2+ ions

See H2H2pCrossSections_7.nb

H2+ breakup option

We introduce a factor that can effectively stop H2+ breakup in collisions.

```
In[160]:= g2=1.;
```

- **H2+ + H2 -> Halpha**

From H2H2PCROSSSECTIONS.xls and Phelps, J. Phys. Chem. Ref. Data 19, 653 (1990).

```
In[161]:= Drop[Import["H2H2pExcitation.txt", "Table"], 1];
```

```
In[162]:= Table[{#[[j, 1]], #[[j, 3]]}, {j, Length[#]}];
```

A fit to this data is

$$q2ha[w2_] := 0.7 * 10^{-26} * \text{UnitStep}[w2-20] * (w2-20)^{1.5} / (1+(w2/2000.)^4)^{.22}$$

As of 07/29/07, we replace this with an expression based on the high threshold found by Van Zyl for H+ + H2 ->. Lyman alpha.

Below 1 keV, the following is a fit to data scaled from the Lyman alpha excitation and then shifted to higher energies. We also fit the shape from Hess.

```
In[163]:= q2ha[w2_] := 4.*10^{-28}*UnitStep[w2-100] (w2-100)^2 / (1+(w2/1050)^4)^0.2 / (1+(w2/4000))^1.1
```

From our TeX file

$$q2haT[w2_] := 0.7 * 10^{-26} * \text{UnitStep}[w2-20] (w2-20)^{1.5} / (1+(w2/2000.)^4)^{0.22}$$

- **Ionization in H2+ + H2 -> e + H+ + H2+ + H. Actually total electron production from Phelps (1990). Product ions could be 2 H2+, so I split the cross section.**

```
In[164]:= q2e1[w2_] := 0.5*6.5*10^{-25}*UnitStep[w2-20] * (w2-20)^{1.1} / (1+w2/8000)^{0.3}
```

```
In[165]:= q2e2[w2_] := 0.5*6.5*10^{-25}*UnitStep[w2-20] * (w2-20)^{1.1} / (1+w2/8000)^{0.3}
```

- **H2+ + H2 -> slow H2+ + fast H2 by symmetric charge transfer**

```
In[166]:= q2s2Heim[w2_] := 5. * 10^{-19} * 1^w2
```

This produces a H2+ ion at zero energy.

Charge transfer cross section from Phelps' H2NONEQUI.NB.

```
In[167]:= q2s2Phelps1 := 0.83*10^{-19}*1^w2;
```

From the notebook H2H2PCROSSSECTIONS.nb and Phelps, J. Phys. Chem. Ref. Data 19, 653 (1990).

```
In[168]:= h2h2pPhelps2[w2_] = 1.45*10^{-20}*enlab^0.8*(1+(enlab/1.9)^4.5)^{(1/4)} / (1+(enlab/4.5)^4.1)^{(0.5)}
```

The following cross section follows more closely the data of Rothwell, Van Zyl, and Amme, J. Chem. Phys. 61, 3851 (1974).

```
ln[169]:= h2h2pPhelps3[w2_]=1.45*10^-20*enlab^0.8*(1+(enlab/1.9)^4.5)^(1/4)/(1+(enlab/4.5)^3.1)^(0.5)/
```

We use it in the form

```
ln[170]:= q2s2[w2_]= 1.45*10^-20*enlab^0.8*(1+(enlab/1.9)^4.5)^(1/4)/(1+(enlab/4.5)^3.1)^(0.5)/
(1+(enlab/16)^2)^(0.56)* (1+(enlab/325))^1.3/(1+(enlab/2000))^(0.2) /.enlab->w2;
```

From the TeX file

```
q2s2T[w2_] :=
1.45*10^-20*w2^0.8*(1+(w2/1.9)^4.5)^(1/4)/(1+(w2/4.5)^4.1)^0.5*(1+(w2/2500.)^4)^0.07
```

■ Inelastic scattering of H2+ by H2

In the file H2H2pCrossSections.nb we fit L[inelastic] data from H2pH2Q88.WK1

```
ln[171]:= l2in[enLab_]=0.0007*10^-20*enLab^2.9/(1+(enLab/10)^2)^1.5*(1+(enLab/120)^3)^0.6/
(1+(enLab/700)^3)^0.28;
```

Because we get too much heavy particle excitation of Halpha at 350 Td, we tried the same formula as for H+ + H2.

```
l2in[enLab_] =8.0*10^-20*(1+(enLab/450)^4)^0.16;
```

This does not help even when multiplied by 100, so we go back the fit from H2pH2Q88.WK1. Likewise reduction by 100 has little effect, even on the H2+ flux energy distribution.

11/19/08 Because l2in is so small compared to enlab*q2f2, I have not modified l2in at high energies to approach independent atom value of 2*Iin(w2/Sqrt[2]).

■ H2+ + H2 -> slow H+ + H2 + H by dissociative charge transfer

```
ln[172]:= q2s1Heim[w2_] := g2 * 5. * 10^-20 * 4 / 5 * UnitStep[w2 - 2]
```

This produces a H+ ion at zero energy.

From the notebook H2H2PCROSSSECTIONS.nb and Phelps, J. Phys. Chem. Ref. Data 19, 653 (1990). We do not know whether this cross section corresponds to fast H+ or to slow H+.

```
ln[173]:= h2h2pToHpFit[w2_] :=1.*10^-20*UnitStep[enlab-6]*(enlab-6)^0.501/(1+(enlab/6.5)^4)^(0.44)* (1-
```

Reduced q2s1 as of 05/22/08 to keep total as 1990 review.

We use

```
ln[174]:= q2s1[w2_] := 0.5*g2*1.*10^-20*UnitStep[enlab-6]*(enlab-6)^0.501/(1+(enlab/6.5)^4)^(0.44)*
(1+(enlab/20)^4+(enlab/50)^4.9)^(0.355) /. enlab->w2
```

Making this very small reduces the Halpha by about 30% at E/N = 350 Td. Cutting this and q2f1[enlab] off at 100 eV adds a small high enrgy tail to the f[enlab] for H2+.

From our TeX file

```
q2s1T[w2_] := 1.*10^-20*UnitStep[w2-6](w2-6)^0.501/(1+(w2/6.5)^4)^0.44*(1+(w2/20)^4+(w2/50)^4
```

H2+ + H2 -> H- + ?(H+ +H2+)?

Since I cannot find data for this H- process assume

```
ln[175]:= q2N1[w1_] := q1N1[w1];
```

■ **H2+ + H2 -> fast H+ + H2 + H by collision induced dissociation**

```
ln[176]:= q2f1Heim[w2_] := g2 * 5. * 10^-20 * 1 / 5 * UnitStep[w2 - 2.2]
```

This produces a H+ ion at 1/2*w2. Here I assume that the scattering angle is small, so that no energy is lost to the target H2 and the incident energy goes half with H+ and half with H.

From the notebook H2H2PCROSSSECTIONS.nb and Phelps, J. Phys. Chem. Ref. Data 19, 653 (1990). We do not know whether this cross section corresponds to fast H+ or to slow H+.

```
ln[177]:= h2h2pToHpFit[w2_] := 1.*10^-20*UnitStep[enlab-6] * (enlab-6)^0.501 / (1+(enlab/6.5)^4)^(0.44) * (1+
```

Reduced q2f1 as of 05/22/08 to keep total as of 1990 review.

We use

```
ln[178]:= q2f1[w2_] := 0.5*g2*1.*10^-20*UnitStep[enlab-6] * (enlab-6)^0.501 / (1+(enlab/6.5)^4)^(0.44) * (1+(enlab/20)^4+(enlab/50)^4.9)^(0.355) /. enlab->w2
```

This reduces the Halpha by about 10% at E/N = 350 Td.

From our TeX file

```
q2f1T[w2_] := 1.*10^-20*UnitStep[w2-6] (w2-6)^0.501 / (1+(w2/6.5)^4)^(0.44) (1+(w2/20)^4+(w2/50)^4.
```

■ **H2+ + H2 -> slow H3+ + H by proton transfer**

```
ln[179]:= q2s3Heim[w2_] := (1.5 * 10^-19 * (UnitStep[w2] - UnitStep[w2 - 4]) + 5. * 10^-20)
```

We assume that this produces a H3+ ion and an H atom at zero energy.

From the notebook H2H2PCROSSSECTIONS.nb and Phelps, J. Phys. Chem. Ref. Data 19, 653 (1990).

```
ln[180]:= h2h2pToH3pPhelps[w2_] := 25.2*10^-20*(enlab+0.04)^-0.5 / (1+(enlab/13)^1+(enlab/4)^3.)^(0.9) /. e
```

Here the 0.04 = 3kTg/2 limits the low energy singularity resulting from our lack of thermal motion of the gas.

We use

```
ln[181]:= q2s3[w2_] := 25.2*10^-20*(enlab+0.04)^-0.5 / (1+(enlab/13)^1+(enlab/4)^3.)^(0.9) /. enlab->w2
```

We rewrite this as a rate coefficient

```
ln[182]:= k2s3[w2_] :=
  q2s3[w2] * Sqrt[2 * qe * (w2 + 0.04) / (2 * mH)] /. {qe -> 1.602 * 10^-19, mH -> 1.673 * 10^-27}
  LogLogPlot[%, {w2, 0.1, 100}]
```

From the TeX file


```
q2s3T[w2_] := 25.2*10^-20*(w2+0.04)^-0.5/(1+(w2/13)+(w2/4)^3)^0.9
```

The following is a test cross section. It is normally not used.

```
q2s3[w2_] := 100*10^-20*UnitStep[w2-15]
```

We need to take into account the singular nature of q2s3 in the lowest energy bin. We do this by defining an average cross section given by

```
In[183]:= q2s3Avg:= NIntegrate[q2s3[w2], {w2, 0, delE/2}]/(delE/2)
```

Fortunately, this integral is finite.

```
In[184]:= q2s3z[w2_] := If[w2 == 0, q2s3Avg, Sum[j2[p, k] * q2s3z[delE * (k - 1)] * n * delx, {k, 2, mc}]]
```

```
In[185]:= delE = 1000;
```

```
In[186]:= q2s3Avg
```

```
Out[186]= 1.85843 × 10-21
```

```
In[187]:= q2s3z[0]
```

```
Out[187]= 1.85843 × 10-21
```

```
In[188]:= Clear[delE]
```

■ reflection of H2+ as fast H

In Petrovic et al, Phys. Rev. Lett., 68, 325 (1992) for an AuPd cathode, we assumed the reflection of fast H2+ as fast H with an energy of 2/3 of the incident H2+ energy and 120% of the number, i.e., RN = 1.2. Note that if RN = 2, the maximum energy per atom is 50% of the incident energy. From Babkina et al (2005) the reflection of H2+ as H2+ is undetectable.

We need to take into account the likely loss of energy in this process. Temporarily, we do this by using a lower reflection coefficient. Assume constant, neglect energy loss, and neglect diffuse scattering

```
In[189]:= r2A[m_, q_] = 2 * 0.5 * j2[m, q];
```

Production of fast reflected two H atoms at 1/2 initial energy of H2+ from j2 incident on cathode.

Production of three fast reflected H atoms from H2+ (j2) incident on cathode. In order to partially take into account the spread in energies of the reflected atoms, we will take the mean energy of the reflected atoms as 2/3 of the available energy, i.e., 2/3*1/2 of the incident ion energy. We assume that both product atoms have the same energy. We also must take into account the atoms lost, i.e., assume 50% reflected.

```
r2A[m_, q_] = 0.5 * 2 * If[1 <= q <= m, Sum[If[Round[2/3 * 1/2 * k] == q, (j2[m, k]), 0], {k, q+1, m}], 0];
```

This assumption corresponds to RN = 0.5 and RE = 0.33. I do not find data for H2+ on Au in Eckstein and Vereek. These values are the same as assumed for H on Au, as would be appropriate for an independent atom model.

For a uniform distribution of H atom energies between zero and 1/2 of the H2+ ion initial energy. Here k-1 represents the initial energy of the H2+ and 0 to (k-1)/2 is the range of energies of the two product H atoms.

```
r2A[q_] := (Sum[If[OddQ[k], 4 * fitRN[(k-1) * delE] / (k-1) * j2[m, k], 0] + If[EvenQ[k], 4 * fitRN[(k-1) * delE] * reflectionFactor, 0]] * reflectionFactor;
```

This was revised on 04/05/06. See notebook AtomReflection030906.nb. I will not try the variable probability cases.

This is a further revision and simplification as of 07/28/06. See CASE=16. Corrected 05/05/07. See tests in TestSum.nb

The following contains two terms to account for odd and even upper energy bins and a factor of 2 for two atoms from dissociation of the H2+.

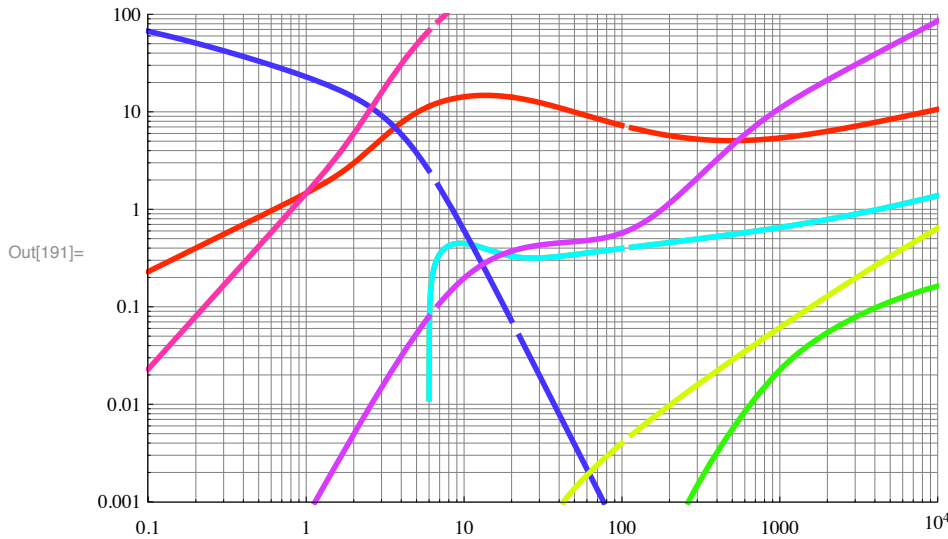
We assume fitRN[enlab] is the same as for H+ with an energy of the separate atoms, i.e., $(k-1)/2 \cdot \text{delE}$. We also assume that the 2 product atoms are spread uniformly over the available $k/2$ energy bins.

```
In[190]:= r2A[q_]:= (Sum[2*fitRN[(k-1)/2*delE]/k*j^2[m,k], {k, 2*q-1, m}] +
Sum[2*fitRN[(k-1)/2*delE]/k*j^2[m,k], {k, 2*q, m}]) * reflectionFactor;
```

■ Plot cross sections used

```
In[191]:= LogLogPlot[{fac * q2s2[w2], fac * q2s1[w2], fac * q2ha[w2], (*1.2**) fac * q2f1[w2],
fac * q2s3[w2], fac * l2in[w2], fac * q2e1[w2], w2 * fac * q2s2[w2]}, {w2, .1, 10 000},
PlotRange -> {{0.099, 10 000}, {fac * 0.99 * 10^-23, fac * 1.01 * 10^-18}}, ImageSize -> 400,
GridLines -> Automatic, Ticks -> Automatic, PlotStyle -> plotColorsLines,
PlotLabel -> "Cross sections for H2+ + H2 (10^-20 m^2) vs LAB energy (eV)"]
```

Cross sections for H2+ + H2 (10^{-20} m^2) vs LAB energy (eV)



```
In[192]:= Clear[g]
```

```
In[193]:= xsech2H2p =
Table[{#, fac * q2s2[##], fac * q2s1[##], fac * q2ha[##], (*1.2**) fac * q2f1[##], fac * q2s3[##],
fac * l2in[##]} &[0.1 * 10^(j / 10)], {j, 0, 5 * 10}];
```

```
In[194]:= Export["H2H2pCrossSections.txt", xsech2H2p, "Table"]
```

```
Out[194]= H2H2pCrossSections.txt
```

■ Cross sections and reflection coefficients for H3+ ions

See H2H3pQdata100910_7.nb

H3+ breakup option

We introduce a scale factor that can be used to essentially prevent H3+ breakup collisions.

```
In[195]:= g3=1.;
```

Apparently, the g3 values in the case cell is the one that counts in the solution.

■ Vibrational Relaxation

According to the ion-cyclotron resonance experiments of Kim et al, Int. J. Mass Spectrom. and Ion Phys. **15**, 223 (1974) the rate constant for the loss in collisions with H2 of highly excited (> 0.5 eV) H3+ formed from H2+ is $\sim 3E10^{-10}$ cm³/s. They used reactions of H3+ with various molecules to determine the presence of excited H3+. These authors found that their reaction rate coefficients are independent of the degree excitation of the H3+. At our typical H2 density of 10E16 cm⁻³, this corresponds to a relaxation time of 1 μ s. It is generally less than the H3+ transit time,[cite{PET07c}](#) but is comparable with reaction times.

Blakley et al J. Chem. Phys. 66, 2392 (1977) conclude from the evidence for vibrationally excited H₃⁺ in a supersonic beam used as an ion source for H₃⁺ + H₂ scattering experiments, that the relaxation of H₃⁺ levels with 3 quanta of excitation occurs with a rate coefficient of $\sim 10^{-11}$ cm³/s. For the lowest vibrational levels, they recommend $\sim 10^{-12}$ cm³/s. At our typical H₂ density, the latter corresponds to 100 μ s for the H₃⁺ relaxation and is long compared to the duration of our experiment.[cite{PET07c}](#)

Some authors propose that the vibrational relaxation occurs via proton transfer. See below for the energy dependent proton transfer cross section.

These rate coefficients correspond to roughly 10 collisions at low energies and mean that many of the reactions in our experiments involve excited H3+.

■ Excitation of Balmer alpha

From Phelps' H2H3pQdata.NB

H3+ + H2 -> excitation of balmer alpha

```
q3ha[w3_] := 1. * 10^-20 * (0.0027 * UnitStep[enrel - 18.3] *
enrel^0.47 / (1 + (5 / (enrel - 18.3)^1)) / (1 + (enrel / 70000)^2.)) /. enrel -> 2 / 5 * w3;
```

In an effort to reduce this cross section at low energies with out too much reduction at high energies we modify the H2+ + H2 -> Halpha cross section and try

```
In[196]:= q3haT[w3_] := 0.7*10^-26*UnitStep[w3-45.8] * (w3-45.8)^1.5 / (1+(w3/2000.)^4)^.26 /
(1+(w3/250000)^1)^0.5
```

This is similar to that for H2+ at low energies.

From our TeX file

```
q3haT[w3_] := 7. * 10^-27 * UnitStep[w3 - 45.8] * (w3 - 45.8)^1.5 / (1 + (w3 / 2000.)^4)^0.26 / (1 + (w3 / 250000)^1)^0.5
```

■ **H3+ + H2 -> slow H3+ + H2+ + e by target ionization.**

This is based on the total electron production. From H2H3PQDATA.nb

```
In[197]:= q3e2[w3_] = 6 * 10^-24 * UnitStep[w3 - 15.6] w3^0.9 / (1 + (5 / (w3 - 15.6)^1)) /
(1 + (w3 / 42000)^1.5);
```

■ **H3+ + H2 -> slow H2+ + H2 + H by dissociative charge transfer**

```
In[198]:= q3s2Heim[w3_] := 3. * 10^-20 * UnitStep[w3 - 2]
```

This produces a H+ ion at zero energy, but we do not know the energy distribution among the H and the H2. It seems to be the only H3+ reaction allowed by Heim and Stori experimental data.

```
In[199]:= q3s2Phelps[w3_] = 1. * 10^-20 * (0.3 * UnitStep[enrel - 6.2] / (1 + (5 / (enrel - 6.2)^2)) *
(1 + (enrel / 10)^2)^0.12 / (1 + (enrel / 2000)^1) + 1. * 10^-10) /. enrel -> 2 / 5 * w3;
```

We use Phelps' fit

```
In[200]:= q3s2[w3_] := (1. * 10^-20 * (0.3 * UnitStep[enrel - 6.2] / (1 + (5 / (enrel - 6.2)^2)) *
(1 + (enrel / 10)^2)^0.12 / (1 + (enrel / 2000)^1) + 1. * 10^-10)
/. enrel -> 2 / 5 * w3);
```

We modify the true cross section to take into account the possibility of a large energy grid spacing at low energies. Note that if $\text{delE}/2$ is less than the threshold we still get a zero entry.

```
In[201]:= q3s2Avg := NIntegrate[q3s2[w3], {w3, 0, delE / 2}] / (delE / 2)
```

```
In[202]:= q3s2z[w3_] := g3 * If[w3 == 0, q3s2Avg, q3s2[w3]];
```

```
In[203]:= delE = 1000
```

```
Out[203]= 1000
```

```
In[204]:= q3s2Avg
```

```
Out[204]= 4.60902 × 10-21
```

```
In[205]:= q3s2z[0]
```

```
Out[205]= 4.60902 × 10-21
```

```
In[206]:= Clear[delE]
```

From H2H3pCollisions.nb, we fitted Simko et al (1997) with simkoS2fit

```
q3s2[w3_] := (*g3*) (1. * 10^-20 * 0.3 * UnitStep[enrel - 6.2] / (1 + (70 / (enrel - 6.2)^2)) * (1 + (enrel / 10)^2)^
```

■ **H3+ + H2 -> fast H2+ + H2 + H by collision induced dissociation**

```
In[207]:= q3f2Heim[w3_] := 1. * 10^-22
```

This would produce a H₂⁺ ion at 2/3*w3. Heim and Stori say their results show that this cross section is negligible, so we use a small and constant cross section for their value.

```
ln[208]:= q3f2Phelps[w3_] :=
  1. * 10^-20 * (1.3 * UnitStep[enrel - 6.2] * enrel^0.6 / (1 + (25 / (enrel - 6.2)^1.1)) /
    (1 + (enrel / 15)^5.5)^1.0 * (1 + (enrel / 27)^5.5)^0.9 / (1 + (enrel / 210)^4.5)^0.4 *
    (1 + (enrel / 480)^2.8) / (1 + (enrel / 12000)^2) + 1. * 10^-10) /. enrel -> 2 / 5 * w3;
```

We use Phelps' fit

```
ln[209]:= q3f2[w3_] := g3*(1.*10^-20*(1.3*UnitStep[enrel-6.2]*enrel^0.6/(1+(25/
(enrel-6.2)^1.1))/(1+(enrel/15)^5.5)^1.0*(1+(enrel/27)^5.5)^0.9/
(1+(enrel/210)^4.5)^0.4*(1+(enrel/480)^2.8)/(1+(enrel/12000)^2)+1.*10^-10)
/.enrel->2/5*w3)
```

From our TeX file

```
q3f2T[w3_] := 1.3*10^-20*UnitStep[w3 - 15.5](0.4w3)^0.6/(1+(62.5/(w3-15.5)^1.1))/(1 + (w3/37.5
(1 + (w3/67.5)^5.5)^0.9/(1 + (w3/525)^4.5)^0.4(1 + (w3/1200)^2.8)/(1 + (w3/30000)^2)
```

From H2H3pCollisions.nb, we fitted Simko et al (1997) with simkoF2fit

```
q3f2[w3_] := (*g3*)(1.*10^-20*0.37*UnitStep[enrel-6.2]/(1+(130/(enrel-6.2)^2))/(1+(enrel/150)^
```

■ H₃⁺ + H₂ -> fast H⁺ + fast H₂ +slow H₂ by collision induced dissociation of the projectile

This would produce a H⁺ ion at (1/3)*w3 and a fast H₂ with (2/3)*w3.

```
ln[210]:= q3f1Heim[w3_] := 1.0 * 10^-22
```

Heim and Stori say the cross section is negligible, so we used a small cross section for their assumption.

```
ln[211]:= q3f1Phelps[w3_] := 1. * 10^-20 * (UnitStep[enrel - 4.4] *
  11 / Sqrt[enrel + 0.0001] / (1 + (12 / (enrel - 4.4))^2) / (1 + (enrel / 300)^3) *
  (1 + (enrel / 550)^4.5) / (1 + (enrel / 20000)^2.5) + 1. * 10^-10) /. enrel -> 2 / 5 * w3;
```

We use

```
ln[212]:= q3f1[w3_] := g3*(1.*10^-20*(UnitStep[enrel-4.4]*11/Sqrt[enrel+0.0001]/
(1+(12/(enrel-4.4))^2)/(1+(enrel/300)^3)*(1+(enrel/550)^4.5)/
(1+(enrel/20000)^2.5)(+ 1.*10^-10*))/enrel->2/5*w3)
```

The contribution of this process to the Halpha signal seems comparable with that of q3s1.

From our TeX file

```
q3f1T[w3_] := 1.1*10^-19*UnitStep[w3-11.]/Sqrt[0.4w3 + 0.0001]/(1 + (30/(w3 - 11.))^2) / (1 +
(1 + (w3/1375)^4.5)/(1 + (w3/50000)^2.5)
```

From H2H3pCollisions.nb, we fitted Simko et al (1997) with simkoF1fit

```
q3f1[w3_] := g3*(2.2*10^-20*UnitStep[enrel-4.4]/(1+(75/(enrel-4.4)^2))/
(1+(enrel/28)^2)^0.27(1+(enrel/280)^2)^0.29)/enrel->2*w3/5
```

■ H3+ + H2 -> slow H+ + 2*H2 by charge transfer induced dissociation

H3+ + H2 -> H+ + H2 + H2

The fits attributed to Phelps are from H2H3pData.nb and are based on Peko, Champion, and Wang, J. Chem. Phys. 104, 6149 (1997). At higher energies we use primarily McClure (1963). The energies in the original formulas are CM and are transformed to LAB energies.

```
ln[213]:= q3s1Phelps[w3_] :=
  1. * 10^-20 * (1.3 * UnitStep[enrel - 4.4] * enrel^0.6 / (1 + (2 / (enrel - 4.4)^1.1)) /
    (1 + (enrel / 8.)^4.05)^1.0 * (1 + (enrel / 21.)^4)^0.9 * (1 + (enrel / 120)^3.5)^0.4 /
    (1 + (enrel / 350)^1.9)^2 + 1. * 10^-10) /. enrel -> 2 / 5 * w3;
```

We use the Phelps fit

```
ln[214]:= q3s1[w3_] := g3 * (1. * 10^-20 * (1.3 * UnitStep[enrel - 4.4] * enrel^0.6 / (1 + (2 / (enrel - 4.4)^1.1)) /
  (1 + (enrel / 8.)^4.05)^1.0 * (1 + (enrel / 21.)^4)^0.9 * (1 + (enrel / 120)^3.5)^0.4 /
  (1 + (enrel / 350)^1.9)^2 + 1. * 10^-10) /. enrel -> 2 / 5 * w3)
```

From our TeX file

```
q3s1T[w3_] := 7.5 * 10^-21 * UnitStep[w3 - 11.] * w3^0.6 / (1 + (5 / (w3 - 11.)^1.1)) / (1 + (w3 / 20.)^4.05) *
  (1 + (w3 / 52.5)^4)^0.9 * (1 + (w3 / 300)^3.5)^0.4 / (1 + (w3 / 875)^1.9)^2
```

From H2H3pCollisions.nb, we fitted Simko et al (1997) with simkoS1fit

```
q3s1[w3_] := g3 * (1. * 10^-20 * 0.14 * UnitStep[enrel - 30] / (1 + (70 / (enrel - 30)^2)) *
  (1 + (enrel / 10)^2)^0.05) /. enrel -> 2 * w3 / 5
```

■ Elastic scattering of H3+ by H2

From our file H2H3pQdata.nb, we take the momentum transfer cross section in COM energy for elastic scattering of H3+ by H2 as

```
ln[215]:= qmH3pH2[w3_] := 22 / enrel^0.5 / (1 + (enrel / 0.4)^4) * 1. * 10^-20 /. enrel -> 2 / 5 * w3
```

This results in an energy loss of $2*2*3/(2+3)^2*(1-\text{Cos}[\text{theta}]) = 12/25*(1-\text{Cos}[\text{theta}])$. For 180 deg scattering this is 24/25, but the (1-Cos[]) is included in the momentum transfer cross section. We will assume an energy loss of 50% to simplify the calculation.

Proton transfer results in energy loss as fast H3+ + H2 -> slow H3+ + fast H2. From Phelps' H2NONEQU.NB and Peko and Champion, the fractional energy loss is 5/9.

```
ln[216]:= q3PT[w3_] := 1. * 10^-20 * (10 * UnitStep[enrel - 0.31] * (enrel + 0.00001)^-0.5 / (1 + (0.6 / (enrel - 0.31))^2) /
  (1 + (enrel / 6.2)^3.95) + 1. * 10^-10) /. enrel -> 2 / 5 * w3
```

Even though this cross section falls off rapidly with increasing energy, it is important at a few eV. Because of the similar energy losses we add the cross sections in the present model. Note the factor of two multiplying qPT to account for backward scattering in COM and to convert qPT to a momentum transfer cross section.

In view of the disagreement of the high energy tail of the calculated energy distribution for E/N < 1 kTd compared to the experimental results of Rao et al and Bretagne et al, we try a much larger momentum transfer cross section at high energies.

A polarization estimate with a roll-off at high energies at values larger than for H+ is

```
ln[217]:= q3f3C[w3_] := 22 * 10^-20 / (enrel + 0.04)^0.5 / (1 + (enrel / 2000)^2) /. enrel -> 2 / 5 * w3
```

The following is based on the statement by Krstic and Schultz that the momentum transfer cross sections for H+, D+, and T+ on H2 versus relative energy is independent of mass. Here $w1 = 3/2$ $enrel1 = 3/2$ $enrel3 = 3/2 * 2/5$ $w3 = 3/5$ $w3$

```
ln[218]:= q3f3[w3_] = 0.5 q1f1[w1] /. w1 -> 3 / 5 w3;
```

Factor of 0.5 added 08/26/09 to agree with publication.

As of 03/12/08, the following trial and error effective momentum transfer cross section gives a reasonably good fit to the H3+ energy distributions at 1 kTd. The H2+ fit is also good, but the H+ fit is poor.

```
ln[219]:= q3f3B[w3_] := 22 * 10^-20 / (enrel + 0.04)^0.5 / (1 + (enrel / 19)^2)^0.25 *
(1 + (enrel / 43)^2)^1.3 / (1 + enrel / 100)^3 /. enrel -> 2 / 5 * w3
```

As of 10/07/08 this gives too much energy loss so we reduce it at energies above ~ 100 eV.

```
ln[220]:= q3f3A[w3_] := 22 * 10^-20 / (enrel + 0.04)^0.5 / (1 + (enrel / 5)^2)^0.25 *
(1 + (enrel / 30)^2)^1.3 / (1 + enrel / 150)^3 /. enrel -> 2 / 5 * w3
```

This large cross section at high energies implies a large contribution of inelastic scattering to the momentum transfer cross section. This cross section is completely undetermined above 1 keV, but presumably drops reasonably rapidly.

As of about 05/23/08, we give up on trying to fit the ion flux energy distributions for H3+ and H+.

As of 10/09/08 we go back to the scaled Qm and try adding the excess energy loss to L3in.

■ Inelastic scattering of H3+ by H2

We use a fit derived in H2H2pQdata.nb to our L(inelastic) function in H2PH2Q88.WK1. This does not include rotational excitation.

```
l3in[enLab_] = 0.0007 * 10^-20 * enLab^2.9 / (1 + (enLab/10)^2)^1.5 * (1 + (enLab/120)^3)^0.6 /
(1 + (enLab/700)^3)^0.28;
```

This energy loss function appears to be much too small. Using the next formula give a much better fit at 350 Td.

From the file c:\spreadsheets\hydrogen\H2LowCurrent\H2EMPIRICALQs.qpw

```
l3in2[w3_] = 3. * 10^-19 * w3^0.5 / (w3/90)^1.2 + (6.5 * 10^-21 * w3^0.5);
```

This file appears to have been created on 02/19/03, presumably at the time of revision of the H3+ + H2 cross section set. Looking at the plot of this function, it must include elastic scattering. I wonder if it also includes reactions to form H+ and H2+. All of these are treated separately in our model and should not be in l3in[w3]. However, if I subtract the sum of the reactions times their energy loss, I get negative values above 200 eV.

```
ln[221]:= l3in1[w3_] = l3in[w3] - 5/9 * w3 * q3f3[w3] (* -w3 * q3s2[w3] - 1/3 * w3 * q3f2[w3] - w3 * q3s1[w3] - 2/3 * q3f1[w3] *)
```

A plot shows that this function still contains a large loss at low energies, which seems wrong!!

As of 071407, we use an energy loss equal to 40% of that for H+.

```
l3in[w3_] = 0.4 * l1in[w3];
```

A fit to the energy loss for Lyalpha, Halpha, and ionization follows. It does not include the reaction collisions as the only the energy of the product ion matters.

```
l3in2[w3_] = 10^-20 * (0.04 * UnitStep[3 * w3 / 5 - 15.6]) * (3 * w3 / 5 - 15.6)^0.9 / (1 + (3 * w3 / 5 / 300)^4)^0.14 * (1 +
```

At one time we added a large energy loss peaking near 50 eV. This added term has been dropped to zero. The high energy portion of the following was obtained by adding the inelastic contributions from Phelps (1990) and doubling to allow for other excited states.

$$l3[enrel_]= 16.4*lymanFit +18.3*halphaFit + 15.6*ionizationFit$$

As of 081407 we use the following. It also works well with the largest q3f3[w3].

$$ln[222]= 13in[w3_]=(1.20*^{-20}*w3^{0.45}/(1 + w3/30) + 3.5*10^{-22}*(w3-39)^{0.9}*(1 + 7.7*^{-15}*w3^4)^{0.12}*UnitStep[w3-39]/(1 + 3.2*^{-12}*w3^4)^{0.14} +$$

As of 02/19/08, we try adding a peak to the energy loss centered about 30 eV instead of such a large momentum transfer cross section. As of 02/20/08, I increased the high energy tail so as to lower the calculated H3+ temperature at 10 kTd.

$$13in[w3_]= 1.20*^{-20} * w3^{0.45} / (1 + w3 / 30) + 3.5 * 10^{-22} * (w3 - 39)^{0.9} * (1 + 7.7*^{-15} * w3^4)^{0.12} * UnitStep[w3 - 39] / (1 + 3.2*^{-12} * w3^4)^{0.14} + 2. * 10^{-18} / (1 + 10 / (w3 - 10)) / (1 + w3 / 50)^1 * UnitStep[w3 - 10];$$

This trial showed that using both the large momentum transfer cross section and/or the large continuous energy loss resulted in the observed Halpha for E/N = 350 Td and 10 kTd. Thus, experiment seems to require that the model eliminate H3+ as a source of H+ and subsequent Halpha excitation. This energy loss along with the q3f3 based on q1f1 give the right calculated temperature for T(H3+) at 1 kTd, but is much too high at 10 kTd. We therefore add a high energy energy loss

$$13in[w3_]= 1.20*^{-20} * w3^{0.45} / (1 + w3 / 30) + 3.5 * 10^{-22} * (w3 - 39)^{0.9} * (1 + 7.7*^{-15} * w3^4)^{0.12} * UnitStep[w3 - 39] / (1 + 3.2*^{-12} * w3^4)^{0.14} + (*2. *10^{-18} / (1+10 / (w3-10)) / (1+w3/50)^1*UnitStep[w3-10]**) 10. * 10^{-18} / (1 + 100 / (w3 - 100)) / (1 + w3 / 5000)^1 * UnitStep[w3 - 100];$$

02/20/08 By adding an energy loss function that is present only at energies above 100 eV we got rough agreement with the energy distribution for both 1 and 10 kTd. See preceding formula. The Halpha is very good at 10 kTd and good at 350 Td. The reflected component of the Doppler profile at 10 kTd is too weak relative to the core and approaching components.

$$13in[w3_]= 1.20*^{-20} * w3^{0.45} (* (1 + (w3/1)^{1.5})^{1/2} / (1 + (w3/10)^{1.5})^{1/2} * (1 + (w3 / 50)^2) / (1 + (w3 / 300)^2));$$

$$13in[w3_]= 1.20*^{-20} * w3^{0.5} * (1 + (w3 / 30)^4) / (1 + (w3 / 72)^4.5) / (1 + (w3 / 5000))^2;$$

As of 10/09/08 we try adding the excess from q3f3 times w3 to l3in

$$13in[w3_]= (1.20*^{-20} * w3^{0.45} / (1 + w3 / 30) + 3.5 * 10^{-22} * (w3 - 39)^{0.9} * (1 + 7.7*^{-15} * w3^4)^{0.12} * UnitStep[w3 - 39] / (1 + 3.2*^{-12} * w3^4)^{0.14} (*3*11in[w3/Sqrt[w3]] / (1 + (3000/w3)^2) *);$$

As of 11/19/08 I increased l3in at energies above about 1000 eV so as to approach the effect of three separate H atoms at constant velocity. See Ray et al, Nuclear Instr. Methods B69, 133 (1992) for measurements in solids.

$$ln[223]= 13in[w3_]=(1.20*^{-20}*w3^{0.45}/(1 + w3/30) + 3.5*10^{-22}*(w3-39)^{0.9}*(1 + 7.7*^{-15}*w3^4)^{0.12}*UnitStep[w3-39]/(1 + 3.2*^{-12}*w3^4)^{0.14} + 3*11in[w3/Sqrt[3]] / (1 + (3000/w3)^2));$$

In order to check high energy extrapolation using theoretical scaling evaluate the following:

$$ln[224]= 13in[10000]$$

$$Out[224]= 2.80719 \times 10^{-18}$$

If we assume that the energy loss at high energy scales as appropriate for three H⁺ ions at constant velocity the exped

```
In[225]:= 3 * 11 in [10 000 / Sqrt [3]]
```

```
Out[225]= 2.45993 × 10-18
```

This shows that our energy loss function for H₃⁺ is ~ 4 times too small at high energies.

■ **Trial 13in[w3] using tabular input - an unsuccessful attempt at covering a wide range of E/N. Try adjusting q3f3[w3]**

The following worked well at 10 kTd and was used as a starting list for 1kTd. It did not work well at 1 kTd.

```
trialTable = {{0.1, 4.3 * 10-21}, {0.316, 7.9 * 10-21}, {1., 1.98 * 10-20},
  {3.16, 7.7 * 10-20}, {10., 2.8 * 10-19}, {31.6, 7.4 * 10-19}, {100., 2. * 10-18},
  {150, 6.5 * 10-18}, {316, 7.6 * 10-18}, {500, 7.2 * 10-18}, {1000., 3. * 10-18},
  {1500, 1.5 * 10-18}, {3160., 8. * 10-19}, {10000., 3. * 10-19}};
```

The following worked well at 1 kTd and at 10 eV, but is very bad at 2 kTd, where the calculation shows a sharp break at 100eV.

```
trialTable = {{0.1, 4.3 * 10-21}, {0.316, 7.9 * 10-21},
  {1., 1.98 * 10-20}, {3.16, 7.7 * 10-20}, {5.5, 2. * 10-19}, {10., 4. * 10-19},
  {15, 6. * 10-19}, {31.6, 8. * 10-19}, {55.0, 8. * 10-19}, {100., 1. * 10-18},
  {150, 6.5 * 10-18}, {316, 7.6 * 10-18}, {500, 7.2 * 10-18}, {1000., 3. * 10-18},
  {1500, 1.5 * 10-18}, {3160., 8. * 10-19}, {10000., 3. * 10-19}};
```

```
13inFcn = Interpolation [trialTable, InterpolationOrder -> 1]
```

```
13in [w3_] = 13inFcn [w3]
```

■ **reflection of H₃⁺ as fast H.**

In Petrovic et al, Phys. Rev. Lett., 68, 325 (1992) for an AuPd cathode, we assumed the reflection of fast H₃⁺ as fast H with an energy of 2/3 of the incident H₃⁺ energy and 120% of the number, i.e., RN = 1.2. Note that if RN = 3, the maximum energy per atom is 33% of the incident energy. From Babkina et al (2005) the reflection of H₃⁺ as H₃⁺, H₂⁺, or H₂ is undetectable.

We need to take into account the likely loss of energy in this process. Temporarily, we do this by using a lower reflection coefficient. Assume constant, neglect energy loss, and neglect diffuse scattering.

```
In[226]:= r3A [m_, q_] = 3 * 0.4 * j3 [m, q];
```

Production of three fast reflected H atoms from H₃⁺ (j₃) incident on cathode. In order to partially take into account the spread in energies of the reflected atoms, we will take the mean energy of the reflected atoms as 2/3 of the available energy, i.e., 2/3*1/3 of the incident ion energy. We assume that all three product atoms have the same energy. We also must take into account the atoms lost, i.e., assume 50% reflected.

```
r3A [m_, q_] = 0.5 * 3 * If [1 <= q <= m, Sum [If [Round [2/3 * 1/3 * k] == q, (j3 [m, k]), 0], {k, q+1, m}], 0];
```

This assumption corresponds to RN = 0.5 and RE = 0.33. I do not find data for H₃⁺ on Au in Eckstein and Vereek. These values are the same as assumed for H on Au, as would be appropriate for an independent atom model.

For a uniform distribution of H atom energies. See notebook AtomReflection030906.nb for an early version. I will not try the variable probability cases. This is a further revision and simplification as of 07/28/06. See CASE=16. Corrected 05/05/07.

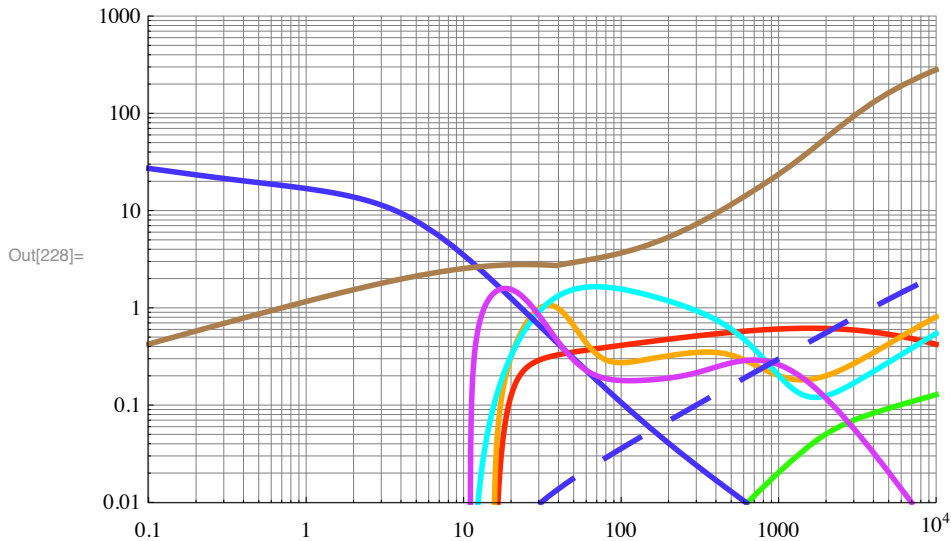
where we assume fitRN[enlab] is the same as for H⁺ with an energy of the separate atoms, i.e., (k-1)/3*delE. We also assume that the atoms are spread uniformly over the available k/3 energy bins.

```
In[227]:= r3A[q_]:= (Sum[3*fitRN[(k-1)/3*delE]/k*j3[m,k], {k,3*q-2,m}]+
Sum[3*fitRN[(k-1)/3*delE]/k*j3[m,k], {k,3*q-1,m}] +
Sum[3*fitRN[(k-1)/3*delE]/k*j3[m,k], {k,3*q,m}])*reflectionFactor;
```

■ Plot cross sections used

```
In[228]:= LogLogPlot[{fac * q3s2[w3] /. delE -> 100, fac * q3f2[w3], fac * q3ha[w3], fac * q3f1[w3],
fac * q3f3[w3], fac * q3s1[w3], fac * l3in[w3], fac * q3e2[w3]}, {w3, .1, 10 000},
PlotRange -> {{.099, 10 000}, {fac * 0.99 * 10^-22, fac * 1.01 * 10^-17}},
ImageSize -> 400, PlotStyle -> plotColorsLines[{{1, 2, 3, 4, 5, 6, 9, 14}}],
GridLines -> Automatic, Ticks -> Automatic, BaseStyle -> {FontSize -> 10},
PlotLabel -> "Cross sections for H3+ + H2 (10^-20 m^2) vs LAB energy (eV)"]
```

Cross sections for H3+ + H2 (10⁻²⁰ m²) vs LAB energy (eV)



blue - momentum transfer; red - slow H2+; orange - fast H2+; green - Halpha; cyan - fast H+; purple - slow H+; yellow - energy loss; pink - old energy loss.

```
In[229]:= xsech2H3p = Table[{#, fac * q3f3[#[#], fac * q3s2[#[#] /. delE -> 100, fac * q3f2[#[#], fac * q3s1[#[#],
fac * q3f1[#[#], fac * q3ha[#[#], fac * l3in[#[#]] &[0.1 * 10^(j / 10)], {j, 0, 5 * 10}];
```

```
In[230]:= Export["H2H3pCrossSections.txt", xsech2H3p, "Table"]
```

```
Out[230]= H2H3pCrossSections.txt
```

■ Plot of TeX formulas

```
In[231]:= Clear[b]
```

■ Cross sections and reflection coefficients for fast H atoms in H2

See H2HCrossSections103110_7.nb

- fast H + H2 -> fast H(n=3) + H2 by small-angle (long range) collisional excitation - Balmer alpha excitation.

```
In[232]:= qAxB[wA_] := UnitStep[wA - 26.] * (1.77 * 10^-27. * (wA - 26.)^3 / (wA / 230. + 1)^4 +
(5.5 * 10^-26. * wA))
```

The following two entries are trial cross sections.

```
qAxB[wA_] := 1. * 10^-30;
```

```
qAxB[wA_] :=
(UnitStep[wA - 250.] * (1.77 * 10^-27. * (wA - 26.)^3 / (wA / 230. + 1)^4 + (5.5 * 10^-26. * wA))) +
1. * 10^(-30)
```

This is assumed to produce a fast H atom excited to the n=3 state and emitting Balmer alpha in small angle scattering, i.e., it does not contribute significantly to energy loss compared to the elastic scattering energy loss. This assumption is based on Williams, Geddes, and Gilbody (1982) measurements of Doppler shifted and unshifted H α emission using beam techniques at energies ≥ 2 keV.

From TEX file

```
qAxBT[wA_] := UnitStep[wA - 26.](1.77*10^-27(wA - 26.)^3/(wA/230. +1)^4 + (5.5*10^-26*wA))
```

We need to assume the fractional excitation that results in dissociative excitation leading to H α with only a small Doppler shift.

We disable the following to allow its variation in the various case notebooks. It would be better to set up two different types of H α excitation cross sections - projectile & target.

```
fracDissoc=0.1;
```

- fast H + H2 -> H2 uV continuum excitation.

We initially proposed the following which looks something like the other excitation cross sections

```
qAuv[wA_] := UnitStep[wA - 26.](3*10^-27(wA - 26.)^3/(wA/300. +1)^4 + (5.5*10^-26*wA))
```

At 300 Td, this gives almost no uv excitation compared to electron excitation. This gives about the right H atom excitation at E/N = 10 kTd. We therefore try something that peaks closer to threshold and falls off at ~ 500 eV, at the mean energies found for E/N = 10 kTd.

```
qAuv[wA_] := UnitStep[wA - 20.]*1.*10^-20/(1+30/(wA-20.))/(1+wA/100)
```

As of 081107 I raised the threshold so as to reduce the continuum emission at 300 Td.

```
In[233]:= qAuv2[wA_] := UnitStep[wA - 40.00001] * 1. * 10^-20 / (1 + 50 / (wA - 40.)) / (1 + wA / 100)
```

On 08/25/08, qAuv[wA] was lowered near threshold in order to improve agreement with experiment at low E/N. We have not included this in the flux equations as a separate fixed energy loss, because it is implicitly included in I $A_{in}[w3]$.

```
In[234]:= qAuv[wA_] := UnitStep[wA - 40.00001]*1.3*10^-20/(1+(100/(wA-40.))^1.3)/(1+wA/100)
```

fast H + H2 -> fast H(n=2) + H2 - Lyman alpha excitation plus H2 uV excitation.

This enters our model only as an energy loss. We arbitrarily increase the cross section of van Zyl, Gealy, and Neumann (1989) by a factor of 2 to allow for other states. We should be able to do better when we evaluate the continuum excitation data. Note that setting the energy loss to \sim vertical energy transition in H2 assumes no angular scattering of the H atom during excitation.

```
In[235]:= qALy[wA_] := 0. * 2.0 * 10^-23 * UnitStep[wA - 18.0] * (wA - 18.0)^1.45 / (1 + (wA/50.)^2)^.45 /
(1 + (wA/700)^1)^1.25 * (1 + wA/15000)
```

We have not included this in the flux equations as a fixed energy loss, because it should be included in l3in[w3].

```
In[236]:= delELy=20.;
```

From TEX file

```
qALyT[wA_] := 2.0 * 10^-23 * UnitStep[wA - 18.0] * (wA - 18.0)^1.45 / (1 + (wA/50.)^2)^0.45 / (1 + (wA/700)^1)^1.2
```

■ **fast H + H2 -> fast H+ + e + H2 .**

```
In[237]:= qAe1[enLab_] := 8. * 10^-26 * (enLab - 32)^1.55 * UnitStep[enLab - 32] /
(1 + (enLab/3000)^3) * (1 + (enLab/6500)^3)^0.67;
```

■ **fast H + H2 -> slow H2+ + e + fast H.**

```
In[238]:= qAe2[wA_] := UnitStep[wA - 25.] * 2.1 * 10^-26 * wA^1.5 / (wA/8000 + 1)
```

- fast H + H2 -> fast H- + slow H2+.

```
qAN2[wA_] := UnitStep[wA - 23.] * (3.5*10^-24.*(wA-23.)/((wA-70.)/120)^2+1)
+(3.9*10^-31.*wA^3/(wA/4000.+1)^4));
```

or

```
In[239]:= qAN2[enLab_] := 3.*10^-22/(1+250/(enLab-27)^1.55)*UnitStep[enLab-27]/(1+(enLab/350)^3)^0.55+
3.*10^-28*(enLab-450)^1.98*UnitStep[enLab-450]/(1+(enLab/5000)^2)^1.4;
```

- fast H + H2 -> fast H- + slow H+ + H.

```
In[240]:= qAN1[enLab_] := 1.*10^-22/(1+300/(enLab-32)^1.55)*UnitStep[enLab-32]/
(1+(enLab/350)^3)^0.55+
1.*10^-28*(enLab-450)^1.98*UnitStep[enLab-450]/(1+(enLab/5000)^2)^1.4
```

- fast H + H2 -> e + fast H3+ from Brehm et al (1995). A resonance!

```
In[241]:= qAe3[enLab_] := 1.7*10^-21*Exp[-((enLab-19.1)/2)^2]+1.*10^-30;
```

Because the narrow Gaussian-like cross section may well be missed with our coarse energy grid, we have integrated the cross section over energy and will attempt to use it in our model.

```
intQAe3 = Integrate[qAe3[enLab], {enLab, 10, 30}];
```

```
In[242]:= intQAe3 = 6.026 * 10^-21
```

Out[242]= 6.026 × 10⁻²¹

When using this it should be divided by delE

- Inelastic scattering of H by H2

From H2HQdata.nb a fit to our L(inelastic+elastic) function in Table 9 of JPCRD 1990

```
In[243]:= lAin2[enLab_] := 3.4*10^-20*enLab^0.7/(1+(enLab/4)^1.5)^.3*(1+(enLab/1900)^2)^.6/(1+(enLab/3
```

Multiplying this by 0.1 or 10 does not change the fit at 350 Td much. A factor of 100 give a reasonable fit, but changes the shape of Halpha at ~ 300 Td. Multiplying by 10E-6 or 10 makes the fit at 10kTd only slightly worse, but multiplying by 100 makes the calculation significantly too small.

From H2HQdata.nb a fit to +- 20% of our L(inelastic) function in Table 9 of JPCRD 1990

```
In[244]:= lAin[enLab_] := 5.2*10^-21*enLab^0.625; (*eV m^2*)
```

This estimate includes the contributions of rotational and vibrational excitation. Does the vibrational estimate need to be changed because of the lower peak vibrational excitation cross section? I conclude that the change in vibrational excitation cross section at energies (~ 1 eV) where it is important to the energy loss function are small. At higher energies (~ 100 eV) the change in vibrational excitation is a factor ~ 2 , but the contribution to the energy loss function is small. Therefore, I have made no changes in my model.

Using the previous $lAin[enLab]$ instead of this one does not help decrease the $H\alpha$ at 10 kTd and only makes a small reduction at 350 Td. We tried the following option.

```
lAin[wA_]:=lAinFactor*10^-20*UnitStep[wA-15.6]/(1 + (200/(wA -15.6)^2))/(1+wA/500)^2 +lAin2[
lAinFactor= 1;
```

It takes factor of 1000 step function from 10 to 1000 eV to give an approximate fit to $H\alpha$ at ~ 300 Td. It was difficult to correlate the beginning and end energies with the effects produced. This factor of 1000 step function improves the fit to $H\alpha$ at 10 kTd by decreasing the signal slightly.

■ Momentum transfer scattering of H by H₂

Elastic scattering is neglected by Heim and Stori.

From our file HH2Q88A.WK1, we take the momentum transfer cross section for elastic scattering in COM?? as

```
ln[245]= qmHH2Phelps[wA_] :=(7.*10^-20/(.001+wA)^.33/(wA/10+1)^.67/(wA/150+1)^.7)
```

The Krstic and Schultz (1998) cross sections for H + H₂ elastic scattering for energies up to 100 eV, including the effects of vibrational excitation, an approximate fit are

```
ln[246]= qmHH2Krstic[wA_] :=9.*10^-20/(.001+wA)^.33/(1+(wA/.9)^3)^.238
```

The approximate agreement of the results obtained using this cross section with the data of Konjevic et al suggests the H($n=3$) excitation raises the question of whether excitation of H to $n \geq 2$ leads to large angle scattering and therefore to significantly larger energy loss than just excitation.

Next we give the result of a fit to the sum of K&S (1999) and my estimate of the contribution of rotational excitation

```
qAsA[wA_] :=(9.*10^-20/enLab^0.42/(1+(enLab/15))^0.7/(1+(enLab/200))^0.8)/.enLab->wA
```

If we go back to $qmHH2Phelps[wA]$.

```
qAsA[wA_] :=(7.*10^-20/(.001+wA)^.33/(wA/10+1)^.67/(wA/150+1)^.7);
```

As of 02/18/08 we use Krstic and Schultz (1999), modified at high energies to agree with Rice data as analyzed by Phelps(1990).

```
ln[247]= qAsA[wA_] :=9.*10^-20/(.001+wA)^.33/(1+(wA/.9)^3)^.238*(1+enrel/120)^1.5/
(1+enrel/400)^2.6* // . enrel->2/3*wA
```

From TEX file

```
qAsAT[wA_] := 7.*10^-20/(.001+wA)^0.33/(wA/10+1)^0.67/(wA/150+1)^0.7
```

To be consistent, this cross section should have been labeled $qAfA[wA]$, not $qAsA[wA]$.

reflection of fast H as fast H

In Petrovic et al, Phys. Rev. Lett., 68, 325 (1992) for an AuPd cathode, we assumed the reflection of fast H as fast H with an energy of 2/3 of the incident H energy and 60% of the number, i.e., $RN = 0.6$.

Assume constant, neglect energy loss, and neglect diffuse scattering

$$rAA[m_, q_] = 0.5 * jA[m, q];$$

Production of a reflected fast H atom from H (jA) incident on cathode. In order to partially take into account the spread in energies of the reflected atoms, we will take the mean energy of the reflected atoms as 2/3 of the available energy, i.e., 2/3 of the incident ion energy. We also must take into account the atoms lost, i.e., assume 50% reflected.

$$rAA[m_, q_] = 0.5 * If[1 <= q <= m, Sum[If[Round[2/3 * k] == q, (jA[m, k]), 0], {k, q+1, m}], 0];$$

This assumption corresponds to $RN = 0.5$ and $RE = 0.33$. I do not find data for H on Au in Eckstein and Vereek, J. Plasma Phys. and Nuclear Fusion: Special Issue 1984, p. 12. These values are in the general region shown for other surfaces.

For a uniform distribution of backscattered energies, the following is copied from the H+ -> surface -> H entry.

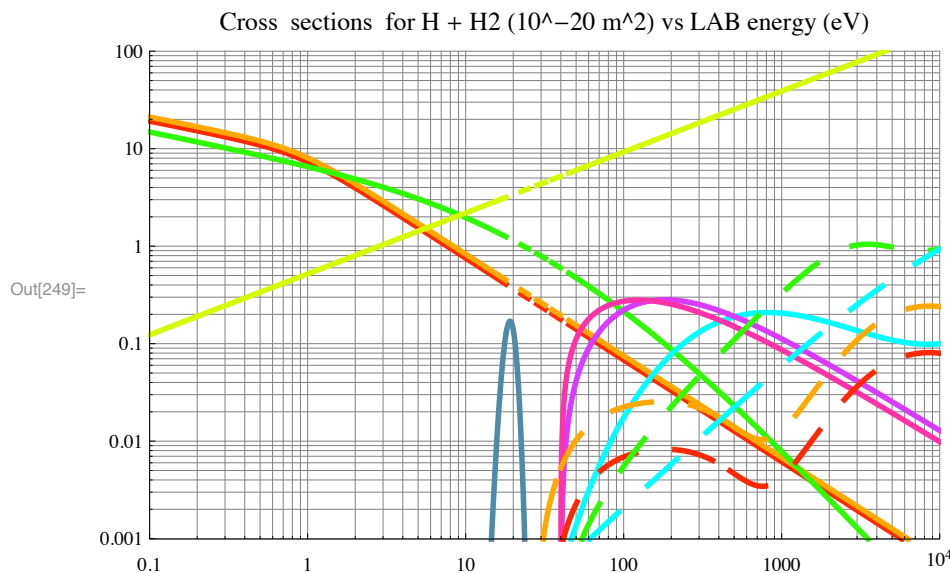
This was revised on 04/05/06. See notebook AtomReflection030906.nb. I will not try to fit the variable probability cases-. Revised to add p index rather than assume m - 03/18/10

```
In[248]:= rAA[q_] := Sum[fitRN[(k-1)*delE]/k*jA[m,k], {k,q,m}]*reflectionFactor;
```

■ Plot cross sections used

qmHH2Kristic is multiplied by 1.1 to separate it from qAsA

```
In[249]:= LogLogPlot[{fac * qAsA[wA], 1.1 * fac * qmHH2Kristic[wA], fac * qmHH2Phelps[wA], fac * qAxB[wA],
  fac * qALy[wA], fac * qAuv[wA], fac * lAin[wA], fac * qAuv2[wA], fac * qAe3[wA],
  fac * qAN1[wA], fac * qAN2[wA], fac * qAe1[wA], fac * qAe2[wA]}, {wA, .1, 10 000},
  GridLines -> Automatic, PlotRange -> {{.1, 10 000}, {fac * 0.99 * 10^-23, fac * 1.01 * 10^-18}},
  ImageSize -> 400, PlotStyle -> plotColorsLines,
  PlotLabel -> "Cross sections for H + H2 (10^-20 m^2) vs LAB energy (eV)"]
```



red - Phelps' elastic Qm; orange - H alpha; purple - Ly alpha; green - H+ production; cyan - H2+ production; yellow - energy loss; dashed orange - Krstic and Schultz's Qm

Note that qALy[wA] has been multiplied by zero earlier to simplify plot.

```
In[250]:= xsech2H = Table[{#, fac * qAsA[#, fac * qAxB[#,
    fac * qAf1[#, fac * qAs2[#, fac * qALy[#, fac * qAuv[#, fac * lAin[#,
    fac * qmHH2Krstic[#, fac * qmHH2Phelps[#]} &[0.1 * 10^(j / 10)], {j, 0, 5 * 10}];
In[251]:= Export["H2HCrossSections.txt", xsech2H, "Table"]
Out[251]= H2HCrossSections.txt
```

Note that the Qm for H + H2 from Phelps (1990) and that from K&S (1999) with the added Qm contribution of rotational excitation differ so little, especially at energies above the excitation threshold, that the calculated Halpha spatial profiles using these Qm are negligibly different.

Note that it was necessary to use 10000 points to get a decent plot of the various cross sections.

- Plot of TeX formulas
- Cross sections and reflection coefficients for fast H2 molecules

See H2H2Qs110205_7.nb

- - Balmer alpha excitation. in fast H2 + H2 -> fast H(n=3) + H2 +H by small-angle (long range) collisional excitation

This produces a fast H atom excited to the n= 3 state and emitting Balmer alpha or Lyman beta. We assume that this results in small angle scattering and that this inelastic process does not contribute significantly compared to the elastic scattering energy loss. See Williams, Geddes, and Gilbody, J. Phys. B 16, L765 (1983). This means that the kinetic energies of the product H(n=3) and H(n=0) are each one half that of the incident H2.

Our pre-11/02/05 expression gives a large cross section at low energies and is

$$qMxB[wM_] := \text{UnitStep}[wM - 18.] * 1. * 10^{-22} * wM^{0.23} / ((15 / (wM - 18.))^{0.8} + 1)^{1.25}$$

This gives a large contribution to the approaching profile and apparent core. The core portion could be balanced out by reducing the dissociation in H + H2 -> Halpha.

Fitting the high energy experiment and raising the threshold energy gives

```
In[252]:= qMxB[wM_] := 0.7 * 10^{-24} * UnitStep[wM - 45.8] *
    (wM - 45.8)^{1.11} / (1 + (wM / 200.)^4)^{.2} / (1 + (wM / 250000)^1)^{0.5}
```

We use a constant cross section to test our scheme for solving the jX equation

$$qMxB[wM_] := 5. * 10^{-22} * \text{UnitStep}[wM - 200.]$$

This seems like a good compromise.

Alternatively, one can extrapolate the high energy data of Williams et al (1983) with a minimal cross section based on H+ + H2 data of

$$qMxB[wM_] := 1.1 * 10^{-25} * \text{UnitStep}[wM - 45.8] * (wM - 45.8)^{1.11} / (1 + (wM / 2000.)^4)^{.2} / (1 + (wM / 250000)^1)^{.5}$$

This guess gives very little excitation from fast H2.

We try the following cross section for H atoms $q_{AxB}[wA]$ from Van Zyl et al (198?) as a trial

$$q_{MxB}[wM_] := 0.25 * (\text{UnitStep}[wM - 26.] * (1.77 * 10^{-27} * (wM - 26.)^3 / (wM / 230. + 1)^4 + (5.5 * 10^{-26} * wM))) +$$

Compared to our first guess, this has a smaller cross section near threshold, but a larger cross section at intermediate energies. At 10 kTd, it results in a predicted spatial scan that is too large by about 40% and an approaching magnitude at small wavelength shifts that is comparably large. A factor of 4 reduction makes the contribution to the spatial scan small, but leaves some contribution to the approaching part of the Doppler profile. At 350 Td, excitation of H α by H2 is negligible.

From TEX file

$$q_{MxBT}[wM_] := 1.1 * 10^{-25} * \text{UnitStep}[wM - 45.8] * (wM - 45.8)^{1.11} / (1 + (wM / 2000.)^4)^{0.2} / (1 + (wM / 250000)^1)$$

■ Inelastic scattering of H2 by H2

For the lack of anything better, we use a fit from H2HpQdata.nb a fit to our L(inelastic) function in 1985 revision of Table 2 of JPCRD 1990

$$l_{\text{Min}}[enLab_] = 8.0 * 10^{-20} * (1 + (enLab / 450)^4)^{0.16};$$

Increasing this by 100 seems to make little difference in the fit to experiment at 350 Td or at 10 kTd.

From Phelps, 1990 we get

$$\ln[253] := l_{\text{Min}}[wM_] = 1.9 * 10^{-20} * (wM)^{0.625}; \quad (*eV \ m^2*)$$

■ fast H2 + H2 -> H + H + H2 - Added to some models beginning 04/10/09 - Q from Phelps (1990)

In my 1990 paper, I have misinterpreted McClure (1964) and the dissociation cross section for H2 at 10 keV. The cross section shown is that for the production of fast atoms. The cross section should be decreased by 2.14 to represent destruction of H2 by dissociation to produce the fast atoms. However, Williams et al (1984) says McClure (1964) is low by just this factor.

$$\ln[254] := q_{MfA}[wM_] := \text{UnitStep}[wM - 18.] * 3. * 10^{-21} * wM^{0.23} / ((200 / (wM - 18.)^1) + 1)^{1.25} + 1. * 10^{-30};$$

On 04/15/09 I raised the threshold and reduced the magnitude by arbitrary amounts similar to the changes for H α excitation, so as to reduce the destruction of H2 via H formation..

$$q_{MfA}[wM_] = \text{UnitStep}[wM - 38.] * 1. * 10^{-21} * wM^{0.23} / ((200 / (wM - 38.)^1) + 1)^{1.25} + 1. * 10^{-30};$$

We raise the threshold and delay the approach to the high energy limit, while retaining the 10 keV point.

$$\ln[255] := q_{MfA}[wM_] = \text{UnitStep}[wM - 46.] * 3. * 10^{-21} * wM^{0.23} / ((500 / (wM - 46.)^1) + 1)^{1.25} (*+1.*10^{-30}*) ;$$

We use a constant cross section to test our scheme for solving the jX equation

$$q_{MfA}[wM_] = \text{UnitStep}[wM - 200.] * 10. * 10^{-21} + 1. * 10^{-30};$$

■ **fast H2 + H2 -> H+ + e +H + H2.**

From H2H2Qs110205_7

```
In[256]:= qMe1[wM_] := UnitStep[wM - 60.1] * 7. * 10^-27 * (wM - 60)^1.45;
```

```
In[257]:= qMe1[0]
```

```
Out[257]= 0
```

```
In[258]:= qeM1[wM_] := Piecewise[{{0, wM ≤ 60}, {7. * 10^-27 * (wM - 60)^1.45, wM > 60}}]
```

```
In[259]:= qeM1[0]
```

```
Out[259]= 0
```

```
In[260]:= qMe1[30]
```

```
Out[260]= 0
```

```
In[261]:= qMe1[60]
```

```
Out[261]= 0
```

■ **fast H2 + H2 -> H2+ + e (not H-) + H2.**

From H2H2Qs110205_7

```
In[262]:= qMe2[wM_] := UnitStep[wM - 35] * 1.5 * 10^-25 * (wM - 35)^2 * (1 + (wM / 100)^3.3)^-0.5;
```

```
In[263]:= qMe2[0]
```

```
Out[263]= 0
```

■ **Elastic scattering of H2 by H2**

From our H2 cross section review, we take the momentum transfer cross section for elastic scattering in H2H2COLLISIONS.NB.

```
In[264]:= qmH2H2Phelps[wM_] := (4.5*10^-19 / (wM / .001 + 1)^.17 / (wM / 9 + 1)^1. / (wM / 650 + 1)^1.3) (*m^2*)
```

The energy loss in elastic scattering is $2*2*2/(2+2)^2*(1-\text{Cos}[\text{theta}])=1/2(1-\text{Cos}[\text{theta}])$. Again, we assume that the $(1-\text{Cos}[\text{theta}])$ is accounted for by using the momentum transfer cross section.

As discussed by Phelps et al (2000), at the higher collision energies the scattering is peaked in the forward direction and $q_v = 3/2*q_m$. This and our delta function model for the differential scattering cross section leads to $q_b = -q_m/4$, which does not make sense. Presumably, this means that the assumption that $q_v = 3/2*q_m$ is inconsistent with our delta function model. When we do not include the energy loss associated with perpendicular scattering we under estimate the energy loss. We neglect this effect.

Judging from Krstic and Schultz's results for H+ + H2, this cross section is probably too large at high energies.

Try

```
In[265]:= qMsM[wM_] = (4.5 * 10^-19 / (wM / .001 + 1)^.17 / (wM / 9 + 1)^1. / (wM / 650 + 1)^1.3);
```

From TEX file

$$qMsMT[wM_] := 4.5 * 10^{-19} / (wM / .001 + 1)^{0.17} / (wM / 9 + 1) / (wM / 650 + 1)^{1.3}$$

■ Ion pair formation $H_2 + H_2 \rightarrow H^- + ?(H^+ + H_2)?$

S. Hayakawa, M. Kogo, A. Matsumoto, and T. Sugiura, In. J. Mass Spectrom. and Ion Processes 84, 113 (1988).

```
In[266]:= qM1N[enLab_] :=
  9. * 10^{-24} * ((enLab - 30) / 1000)^{1.5} / (1 + enLab / 30000)^2 * UnitStep[enLab - 30];
```

■ reflection of fast H2 as fast H

Based on the absence of fast reflected H2 from Babkina et al, Europhysics Lett. 72, 235 (2005) for an stainless steel cathode, we assumed the reflection of fast H2 as fast H with an energy of 1/2 of the incident H energy and 60% of the number, i.e., RN = 0.6. These authors give calculated and measured energy distributions of H backscattered normal to the surface.

Assume constant and neglect energy loss.

```
In[267]:= rMA[m_, q_] = 2 * 0.6 * jM[m, q];
```

Production of two reflected fast H atoms from H2 (jM) incident on cathode. In order to partially take into account the spread in energies of the reflected atoms, we will take the mean energy of the reflected atoms as 2/3 of the available energy, i.e., 1/2*2/3 of the incident ion energy. We also must take into account the atoms lost, i.e., assume 50% reflected.

$$rMA[m_, q_] = 0.5 * 2 * \text{If}[1 \leq q \leq m, \text{Sum}[\text{If}[\text{Round}[2/3 * 1/2 * k] == q, (jM[m, k]), 0], \{k, q+1, m\}], 0];$$

It is necessary to add a small number to the reflection to avoid a zero in the log plot to follow.

This assumption corresponds to RN = 0.5 and RE = 0.33. I do not find data for H2 on Au in Eckstein and Vereek. These values are the same as assumed for H on Au as would be appropriate for an independent atom model.

The following is borrowed from H2+ + surface $\rightarrow 2 H$.

$$rMA[q_] := (\text{Sum}[\text{If}[\text{OddQ}[k], 4 * \text{fitRN}[(k-1) * \text{delE}] / (k-1) * jM[m, k], 0] + \text{If}[\text{EvenQ}[k], 4 * \text{fitRN}[(k-1) * \text{delE}]] * \text{If}[q == 1, 2 * jM[m, q], 0]);$$

This was revised on 04/05/06. See notebook AtomReflection030906.nb. I will not try the variable probability cases.

This is a further revision and simplification as of 07/28/06. Corrected 05/05/07.

```
In[268]:= rMA[q_] := (Sum[2 * fitRN[(k-1)/2 * delE] / k * jM[m, k], {k, 2 * q - 1, m}] +
  Sum[2 * fitRN[(k-1)/2 * delE] / k * jM[m, k], {k, 2 * q, m}]) * reflectionFactor;
```

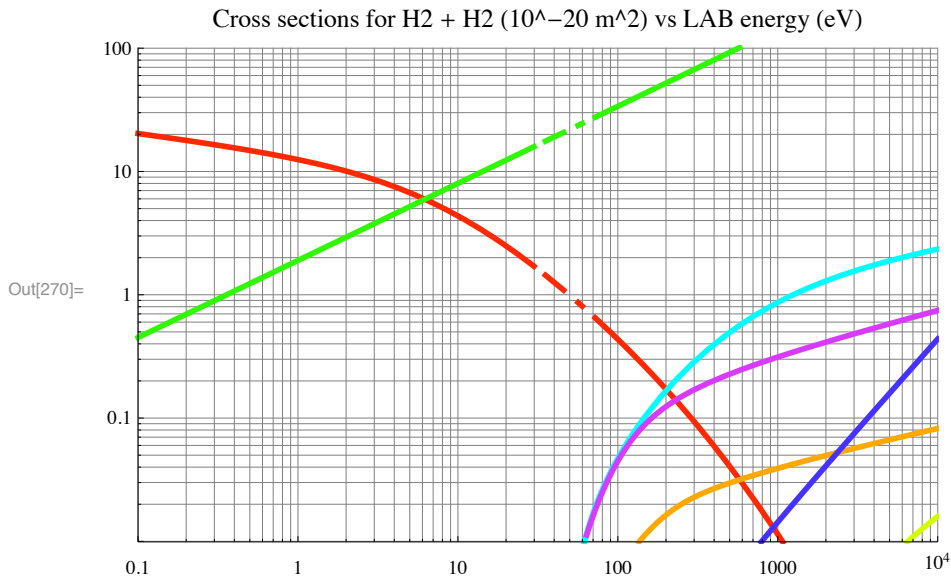
■ reflection of fast H2 as fast H2

Based on Babkina et al (2005), we assume negligible backscattering scattering of H2. Probably reflection is typical RN=0.5 and RE=0.33, but H2 flux is small in Babkina et al.

```
In[269]:= rMM[q_] := 0.000001 * rMA[q];
```

■ Summary plot for fast H2 cross sections

```
In[270]:= LogLogPlot[{fac * qMsM[wM], fac * qMxB[wM], fac * lMin[wM], fac * qMfA[wM], fac * qMe1[wM],
  fac * qMe2[wM], fac * qM1N[wM] (*, qmH2H2Kristic[wM], qmH2H2Phelps[wM] *)}, {wM, .1, 10 000},
  GridLines -> Automatic, PlotRange -> {{.1, 10 000}, {fac * 0.99 * 10^-22, fac * 1.01 * 10^-18}},
  ImageSize -> 400, Ticks -> Automatic, PlotStyle -> plotColorsLines,
  PlotLabel -> "Cross sections for H2 + H2 (10^-20 m^2) vs LAB energy (eV)"]
```



```
In[271]:= xsech2H2 = Table[{#, fac * qMsM[#[#], fac * qMxB[#[#], fac * qMfA[#[#], fac * lMin[#[#]] &[
  0.1 * 10^(j / 10)], {j, 0, 5 * 10}}];
```

```
In[272]:= Export["H2H2CrossSections.txt", xsech2H2, "Table"]
```

```
Out[272]= H2H2CrossSections.txt
```

■ Collisions of H- with H2

See H2HnCrossSections_7.nb

■ Collisional detachment

This is the same as in Phelps, J. Phys. Chem. Ref. Data 19, 656 (1990).

```
In[273]:= qNeA[wN_] := UnitStep[wN - 2.2] * 5. *
  10^-20 / (1 + 4.5 / (wN - 2.2)) * (1 + (wN / 170)^2)^0.25 / (1 + (wN / 1000)^2)^0.25
```

■ Momentum transfer

This is the same as in Phelps, J. Phys. Chem. Ref. Data 19, 656 (1990).

```
In[274]:= qNm[wN_] := 10 / fac / Sqrt[wN] / (1 + wN / 50)^1.2
```

■ Energy loss function

We know nothing about inelastic collisions of H⁻ with H₂ and will neglect them

■ Charge transfer

Charge transfer to form H₂⁻ is unlikely and will be neglected. Note that many processes besides H⁻ + H₂ → H₂⁻ + H are listed in the literature as charge transfer.

■ Halpna production

From H2HnCollisions.nb a cross section consistent with Geddes et al is

```
In[275]:= qNha[wN_] := 6. * 10^-28 * UnitStep[wN - 50]
           (wN - 50)^2 / (1 + (wN / 700)^4)^0.5 / (1 + (wN / 3000)^4)^0.04 (* (1 + (wN/30000)^3)^0.4 *)
```

A maximum cross section consistent with Geddes et al is NOT USED

```
qNha[wN_] := 2.1 * 10^-21 *
             UnitStep[wN - 50] / (1 + 100 / (wN - 50)^1) / (1 + (wN / 200))^0.5 * (1 + (wN / 16000)^3)^0.48
```

```
In[276]:= qNha[wN]
```

```
Out[276]= 
$$\frac{6. \times 10^{-28} (-50 + wN)^2 \text{UnitStep}[-50 + wN]}{\left(1 + \frac{wN^4}{81000000000000}\right)^{0.04} \left(1 + \frac{wN^4}{240100000000}\right)^{0.5}}$$

```

■ Fast H atom production

We assume that this is the same as collisional detachment, although it might not be the same, i.e., qNeA[wN].

■ Surface production

This process is probably very important for negative ions.

From H2HnCollisions.nb we assume that the fraction of the fast atoms leaving the cathode as negative ions is constant and is typically

```
In[277]:= fneg = 0.04;
```

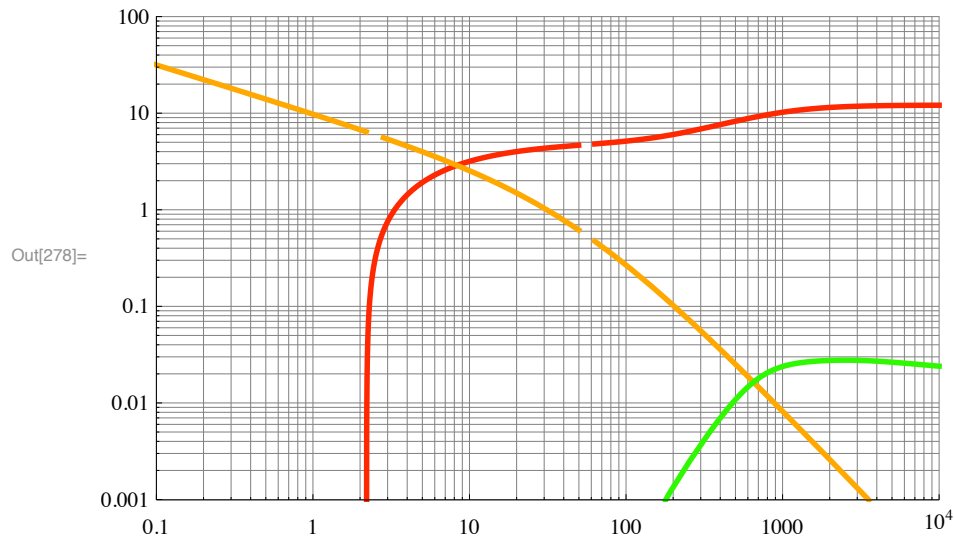
■ Surface destruction of the H- and reflection as H atoms

We probably have no information on this process. We assume destruction of the H- and its reflection as for H+.

■ Summary plot

```
In[278]:= LogLogPlot [{fac * qNeA[wN], fac * qNm[wN], fac * qNha[wN]},
  {wN, .01, 10 000}, GridLines -> Automatic,
  PlotRange -> {{0.1, 10 000}, {fac * 0.99 * 10^-23, fac * 1.01 * 10^-18}}, ImageSize -> 400,
  PlotStyle -> plotColorsLines, BaseStyle -> FontSize -> 10, Ticks -> Automatic,
  PlotLabel -> "Cross sections for H- + H2 (10^-20 m^2) vs LAB energy (eV)"]
```

Cross sections for H- + H2 (10^{-20} m²) vs LAB energy (eV)



```
In[279]:= negIonQTable = Table [{#, qNeA [#], qNm [#], qNha [#]}, {j, 8 * 4}] & [10^(j / 8.)];
```

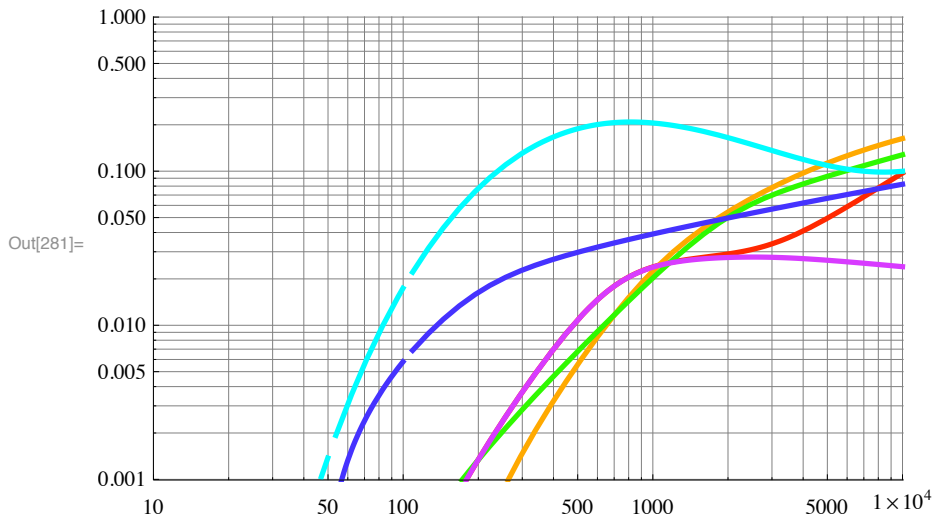
```
In[280]:= Export["NegIonQs.txt", negIonQTable, "Table"]
```

```
Out[280]= NegIonQs.txt
```

■ Comparison of Halpha cross sections.

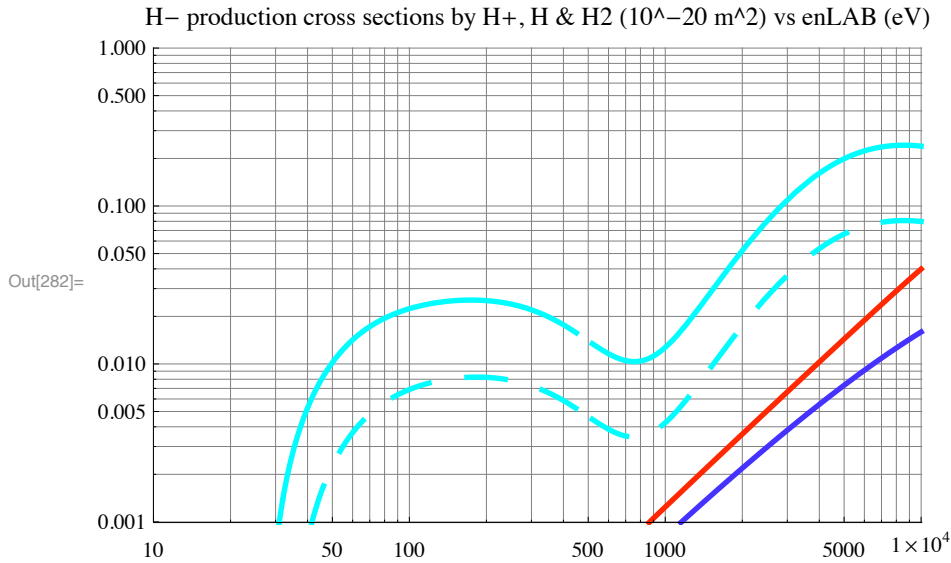
```
In[281]:= LogLogPlot[{fac * q1ha[enlab], fac * q2ha[enlab], fac * q3ha[enlab], fac * qAxB[enlab],
  fac * qMxB[enlab], fac * qNha[enlab]}, {enlab, 10, 10000}, GridLines -> Automatic,
  PlotRange -> {{9.99, 10100}, {fac * 0.99 * 10^-23, fac * 1.01 * 10^-20}},
  ImageSize -> 400, PlotStyle -> plotColorsLines, BaseStyle -> FontSize -> 10,
  PlotLabel -> "Halpha cross sections H+, H2+, H3+, H-, H & H2 (10^-20 m^2) vs enLAB (eV)"]
```

Halpha cross sections H+, H2+, H3+, H-, H & H2 (10^{-20} m^2) vs enLAB (eV)



■ Comparison of H- formation cross sections.

```
In[282]:= LogLogPlot[{fac * q1N1[enlab], (*fac*q2N1[enlab],*) fac * qAN2[enlab],
  fac * qAN1[enlab], fac * qM1N[enlab]}, {enlab, 10, 10000}, GridLines -> Automatic,
  PlotRange -> {{9.99, 10100}, {fac * 0.99 * 10^-23, fac * 1.01 * 10^-20}}, ImageSize -> 400,
  PlotStyle -> plotColorsLines[{{1, 4, 13, 5}}], BaseStyle -> FontSize -> 10,
  PlotLabel -> "H- production cross sections by H+, H & H2 (10^-20 m^2) vs enLAB (eV)"]
```



```
In[283]:= pairTable = Table[{#, q1N1[#, qAN2[#, qAN1[#, qM1N[#]}, {j, 8 * 4}] & [10^(j / 8.)];
```

```
In[284]:= Export["PairFormationQs.txt", pairTable, "Table"]
```

```
Out[284]= PairFormationQs.txt
```

Spatial ionization and excitation coefficients for electrons in H2.

See H2ElectronSwarmData_7.nb

- Electron impact ionization of H2 to form H2+ - this is an empirical quasi-steady-state or local-field equilibrium formula ?FROM WHERE?

We reduce this by $\times 0.8$ to give a better fit to the experimental spatial distributions.

```
In[285]:= alion1[eonTd_] := 0.8 * 1.4 * 10^-20 * Exp[-405/eonTd] / (((eonTd/10000)^1.5 + 1)^.5)
```

or an apparently older form that gives $\sim 20\%$ lower values around E/N of 1 to 5 kTd.

```
alion1[eonTd_] := 1.6 * 10^-20 * Exp[-400/eonTd] - 6.5 * 10^-21 * Exp[-750/eonTd]
```

```
alion1Plot = LogLogPlot[alion1[eonTd] / 0.8, {eonTd, 99, 100000}, PlotRange -> {{99, 100000}, {0.99 * 10^-
```

This fit is said to be to Brana's data in EH2IONIZ.WQ1

Note that our Web site gives higher values by $\sim 50\%$ at E/n = 1000 Td.

From H2ElectronSwarmData.nb a fit to our transient current growth data gives somewhat lower values at very high E/N, but values that are expected to be $\sim 20\%$ too high at moderate E/N.

The following was chosen to "fit" the upper limit to the transient data so as to increase α/N at high E/N

```
In[286]:= alion[eonTd_] = 0.84 * 1.4 * 10^-20 * Exp[-405 / eonTd] / ((1 + (eonTd / 1000)^3)^.145);
```

The following was chosen to fit Mokrov and Raizer (2008) and to drop at very high E/N


```

In[287]:= alion1[eonTd_] = 0.84 * 1.4 * 10^-20 * Exp[-400 / eonTd] *
          (1 + eonTd / 1500)^0.5 / ((1 + (eonTd / 2000)^2) * (1 + (eonTd / 4000)));
In[288]:= alion2[eonTd_] = 0.84 * 1.4 * 10^-20 * Exp[-400 / eonTd] *
          (1 + eonTd / 3000)^0.5 / ((1 + (eonTd / 2700)^2) * (1 + (eonTd / 4000)));
In[289]:= alionPlot=LogLogPlot[{alion[eonTd], alion1[eonTd], alion2[eonTd]}, {eonTd, 99, 100000}, PlotRange

```

Our current growth fits to the transient data give the following alion[eonTd] values

```

In[290]:= currentGrowthIonizationTable =
          Import["c:\\users\\avp\\documents\\Mathbook\\hydrogen\\h2lowcurrent\\H2transients\\
          ionizationCoeffTrans.txt", "Table"];
In[291]:= fitParamAlionPlot=ListLogLogPlot[currentGrowthIonizationTable, PlotRange->{{99,100000},{0.99

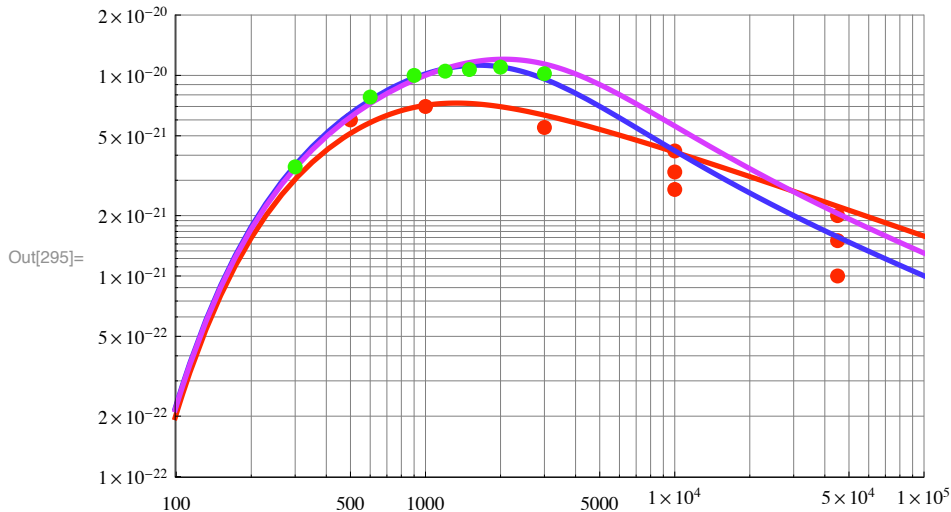
```

Mokrov and Raizer (2008) give

```

In[292]:= monteCarloIonizData = Drop[Import[
          "c:\\users\\avp\\documents\\Mathbook\\hydrogen\\h2electroncollisions\\mokrov&raizer.
          xls", "XLS"][[1]], 4];
In[293]:= monteCarloIonizTable = Table[{%[[j, 1]], %[j, 2]}, {j, 7}];
In[294]:= monteCarloIonizPlot=ListLogLogPlot[%, PlotRange->{{99,100000},{0.99*10^-22,2.01*10^-20}}, In
In[295]:= Show[fitParamAlionPlot, alionPlot, monteCarloIonizPlot, DisplayFunction->$DisplayFunction]

```



■ electron impact excitation of H alpha - this is an empirical quasi-steady-state or local-field equilibrium formula

On 050407 we modified this to drop more rapidly at high E/N so as to reflect the drop below theory found from the experimental current growth. See ElectronSwarmData.nb. On 080907 I reduced the Halpha production at 500 Td and above, but I reduced it too much at

```

In[296]:= alHalpaha2[eonTd_] := +(2.1*10^-22*Exp[-400/eonTd]-1.*10^-22*Exp[-(1000/eonTd)])
In[297]:= alHalpaha1[eonTd_] :=+2.1*10^-22*Exp[-400/eonTd]
In[298]:= alHalpaha3[eonTd_] := +(2.1 * 10^-22 * Exp[-400 / eonTd] - 1. * 10^-22 * Exp[-(1000 / eonTd)]) /
          (1 + (eonTd / 8000)^4)^0.25

```

This extends beyond the range of validity of the two-term Boltzmann solutions and the Belgrade experiments. It is subject to considerable uncertainty at high E/N. It gave poor results at 500 Td to 3 kTd.

On 08/25/08, I attempted to improve the fit of the model to experiment at 1 kTd by reducing alpha/N for Halpha by 20%. It turned out to be important to keep the high values at high E/N.

```
In[299]:= alHalpha [eonTd_] :=  
+ 1.25 * (2.2 * 10^-22 * Exp[-400 / eonTd] - 1.5 * 10^-22 * Exp[-(800 / eonTd)])
```

■ **electron impact excitation of uv - this is an empirical quasi-steady-state or local-field equilibrium formula**

```
alH2uv1 [eonTd_] := 1.6 * 10^-21 * Exp[-115 / eonTd] - 1.4 * 10^-21 * Exp[-(600 / eonTd)]
```

alH2uv updated 05/16/06. See c:\Mathbook\hydrogen\H2ElectronCollisions\H2ElectronSwarmData.nd

```
In[300]:= alH2uv2 [eonTd_] :=  
If [eonTd <= 300, 33 * 10^-20 * Exp[-330 / eonTd] / (1 + (eonTd / 25)^1)^2 * (1 + (eonTd / 315)^1)  
( * / (1 + (eonTd / 270)^4)^0.25 * ), 13.5 * 10^-22 / (1 + (eonTd / 800)^3)^0.5]
```

This is based on the spreadsheet HALPHAEX.WQ1 as listed for $100 < E/N < 2000$ Td. Note the the values are an order of magnitude smaller than those given for the maximum vuv excitation in the file ELECTTRANS.TXT on the Web site.

As of 09/22/08 we need to lower the near uv excitation by electrons at 800 Td by 30-50 %, while keepng the excitation at 300 TD the same or raising it slightly.

```
alH2uv [eonTd_] :=  
If [eonTd <= 300, 33 * 10^-20 * Exp[-330 / eonTd] / (1 + (eonTd / 25)^1)^2 * (1 + (eonTd / 315)^1),  
13.5 * 10^-22 / (1 + (eonTd / 500)^3)^0.5]
```

This fit is about 70% of Stojanovic et al. (unpublished) and about 40% of the 1994 Boltzamann results.

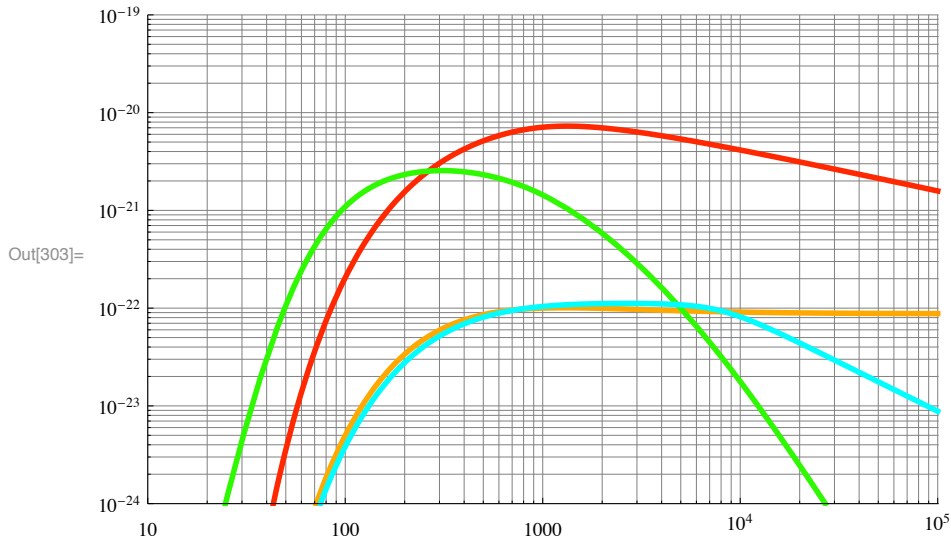
As of 5/6/11 the following from H2ElectronSwarmData_7.nb was changed to fit the changes in cross sections discussed below, i.e., the BKP5C (1949) results were multiplied by 0.683

```
In[301]:= alH2uv [eonTd_] :=  
0.683 * 5 * 10^-21 / (1 + (50 / eonTd)^2)^5 / (1 + (eonTd / 900)^1.7) / (1 + (eonTd / 6000)^1.5)
```

```
In[302]:= alH2uv [500]
```

```
Out[302]= 2.31912 × 10-21
```

```
In[303]:= LogLogPlot[{alIon[eonTd], alHalpHa[eonTd], alH2uv[eonTd], alHalpHa3[eonTd](*,
  alH2uv2[eonTd]*)}, {eonTd, 10, 100 000}, PlotRange -> {{10, 101 000}, {10^-24, 10^-19}},
  ImageSize -> 400, PlotStyle -> plotColorsLines, Ticks -> Automatic,
  GridLines -> Automatic, PlotLabel -> "Spatial reaction coefficients (m^2) vs E/N (Td)"]
```

Spatial reaction coefficients (m²) vs E/N (Td)

```
Out[303]=
In[304]:= alphaH2e = Table[{#, alIon[#], alHalpHa[#], alH2uv[#](*, alHalpHa1[#], alHalpHa2[#]*)} & [
  10. * 10^(j / 10)], {j, 0, 4 * 10}];
```

```
In[305]:= Export["electronAlphaModel.txt", alphaH2e, "Table"]
```

```
Out[305]= electronAlphaModel.txt
```

■ Nonequilibrium effects near the cathode

We will try to include nonequilibrium effects by using the approximation in which the onset of ionization is delayed by a distance d_{i0} or the corresponding voltage v_{i0} . There must also be a delay in the onset of excitation. Our H2CurrentGrowth analyses at high E/N gave $v_{i0} = 50$ eV. However, our low E/N spatial distributions require $v_{i0} \rightarrow v_{x0}$. Assume

$$v_{i0} = ((50-15) * \text{Exp}[-1000/eonA] + 15);$$

and based on the present spatial distribution data

$$v_{x0} = 15;$$

The 50 V value for v_{i0} is about twice the $E/N * d_0$ value from Folkhard and Haydon, Australian J. Phys. 24, 527 (1970), i.e., it is about equal to their $E/N * Nd_0'$ value of 55 V for 250 Td.

These v_{i0} values are also much larger than those I infer from Mohrov and Raizer, Tech. Phys. 53, 436 (2008). A fit to their data is;

```
In[306]:= vi0 = -11 * (1 - Exp[-(500 / eona) ^ 2]) + 26;
```

We note that the threshold for HalpHa excitation by electrons is higher than the ionization potential, so we try

```
In[307]:= vx0 = 18;
```

■ Ionization, energy loss, and excitation cross sections for electrons in H2.

See H2ElectronCrossSections_7.nb

From our Web site the momentum transfer cross section is

```
In[308]:= Drop[Import["c:/users/avp/documents/mathbook/hydrogen/H2ElectronCollisions/h2emomtransq.txt"]
```

```
In[309]:= qem[we_]=10.*10^-20*(1+we)/(1+(we/2.5)^2)*(1+(we/18)^4)^0.21/(1+(we/140)^2)^0.32;
```

The following are from H2Nonequ092605.nb

■ Electron impact ionization of H2 to form H2+ and H+

Recent papers have attempted to define an accurate set of electron induced ionization cross section for H2. Liu and Shemansky, Ap. J. 614, 1132 (2004) use a combination of theory and experiment to derive cross sections for the formation of H2+ and H+. They recommend the experimental data tabulated by Lindsay and Mangan, in Landolt-Bornstein, vol I/17C, ed by Itikawa, (Springer,Berlin, 2003). Since it is very difficult for CU to get a copy of this, I will use Liu and Shemansky's Table 1 and my understanding of Fig. 2. See H2ElectronCrossSections.nb for the accuracy of our fits.

For the production of H2+

```
ln[310]:= qes2[we_] := UnitStep[we-15.41]*1.7*10^-20*(we-15.4)/(40-15.4)/((we/37)^1.78+1)
```

For the production of H+

```
ln[311]:= qes1[we_] := UnitStep[we-15.41]*1.17*10^-25*(we-15.4)^3.0/((we/35)^2.05+1)^2
```

■ Energy loss function

Electron energy loss to vibrational excitation at low energy plus high energy loss to dissociation and ionization. At 100 eV to 10 keV the following results are in reasonable agreement with Cravens, Victor, and Dalgarno, Planet. Space Sci. 23, 1059 (1975) and for 10 to 1000 eV with Dalgarno et al, Ap. J. Supp. 125, 237 (1999)..

```
ln[312]:= lein[we_] := UnitStep[we-0.541]*1.7*10^-21*((we-.54)/(3-.54))^2/((we+3)/6)^4 +
UnitStep[we-8]*8.7*10^-21*(we-8)/((we+50)/100)^1.8
```

For case 41, increasing the second term by a factor of 10 increased the slope of the decay of emission with distance to roughly experiment, but did not increase the magnitude. A factor of 3 increase made little difference.

■ Electron excitation of near uv

From Ajello and Shemansky, Ap. J. 407, 820 (1993) the peak cross section for near UV production occurs at 15.5 eV and, in the absence of quenching and including cascading for the a + d + e states, is $(1.73+0.42+0.33)E-21 = 2.48E-21$ m². This is to be compared to a sum for the a + d + e states of $(0.2+0.122+0.041)E-20=3.63E-21$ used in BKP5C (1994). Note that this omits "cascading" from te c state, which Weding and Phelps say does not transfer to the a state. As a result the excitation coefficients from BKP5C (1949) and in this file need to be reduced by $2.48/3.63=0.683$. The qeuv[we] values below are multiplied by 2.12 to scale them to Ajello and Shemansky (1993).

According to Tisher and Phelps (unpublished) the effective quenching rate coefficient is $9E-16$ m³/s. See also Wedding and Phelps, J. Chem. Phys. 89, 2965 (1988).

```
ln[313]:= qeuv[we_] := 2.12*5.*10^-21*UnitStep[we-11.8]*((1/((we/11.8)^2.8+1))-1/((we/11.8)^9+1))
```

```
In[314]:= FindMaximum[qeuv[we], {we, 15.}]
```

```
FindMaximum::fmgz :
```

Encountered a gradient that is effectively zero. The result returned may not be a maximum; it may be a minimum or a saddle point. >>

```
Out[314]= {2.48717 × 10-21, {we → 15.}}
```

■ Electron excitation of Halpha

```
In[315]:= qeha[we_] := UnitStep[we-17.]* (8.5*10^-23.*2*(we-17)/(50-17)/
((we/50)^1.9+1)+(5.2*10^-23/((we/30)^4+1)))
```

We have not listed a cross section for production of the Lyman alpha line. According to Fujimoto et al (1989) it peaks at $1.2E-17 \text{ cm}^2$ at about 100 eV.

■ Dissociative attachment

We need some kind of estimate of the dissociative attachment cross section. Based on Yoon et al, J. Phys. Chem. Ref. Data 37, 913 (2008). We neglect the 4 eV resonance contribution. At energies above 18 eV, we have no information. If this give a significant negative ion production, we will need to refine it. This will be too small to show on our summary plot.

```
In[316]:= qeneg[we_] := UnitStep[we - 8.01] * 5. * 10^-24 / (1 + 1 / (we - 8)) / (1 + (we / 10)^4)
```

The following would be an upper limit to the high energy attachment.

```
qeneg[we_] = UnitStep[we - 8.5] * 1. * 10^-24 / (1 + we / 500);
```

For the high voltage experiments, such as Kipritidis, we want the average cross section over the lowest energy bin. Here we say that integration to infinity is the same as integration over any realistic ΔE , because of the low energy of the resonant attachment cross section.

```
qesN = Integrate[qeneg[we], {we, 8.0, Infinity}] / delE
```

This gives

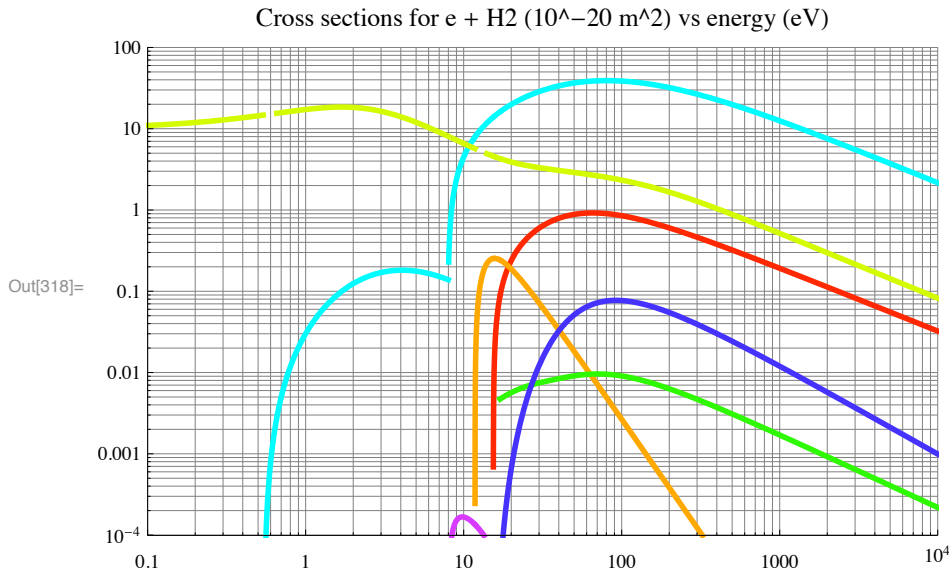
```
In[317]:= qesN = 1.28 * 10^-23 / deIE
```

```
Out[317]= 
$$\frac{1.28 \times 10^{-23}}{\text{deIE}}$$

```

■ Summary plot for electrons

```
In[318]:= LogLogPlot[{fac * qes2[we], fac * qeuv[we], fac * qeha[we], fac * lein[we], fac * qes1[we],
  fac * qeneg[we], fac * qem[we]}, {we, .1, 10000}, GridLines -> Automatic,
  PlotRange -> {{.1, 10000}, {fac * 0.99 * 10^-24, fac * 1.01 * 10^-18}},
  ImageSize -> 400, Ticks -> Automatic, PlotStyle -> plotColorsLines,
  PlotLabel -> "Cross sections for e + H2 (10^-20 m^2) vs energy (eV)"]
```



Here we have divided the energy loss function `lein[we]` by 10 for ease of plotting.

```
In[319]:= h2inelasticQs =
  Table[{#, qes2[#, qes1[#, qeuv[#, qeha[#, lein[#, qeneg[#,] & [10 * 10^(j / 10)],
    {j, 0, 4 * 10}];
```

```
In[320]:= Export["electronh2inelQs.txt", h2inelasticQs, "Table"]
```

```
Out[320]= electronh2inelQs.txt
```

■ Dissociative electron ion recombination

In file `H3pElectronCrossSection_7.nb` we have fitted the following expression to the data of Kreckel et al, Phys. Rev. A 82, 042715 (2001). We assume that the H3⁺ is not in an excited state. The rate coefficient units in Kreckel are cm³/s, so the we need to multiply by 10E-6.

```
In[321]:= ke3[enrel_] = 10^-6 * 4.5 * 10^-9 / (enrel + 0.001)^0.7 / (1 + (enrel / 0.25)^4)^0.42 *
  (1 + (enrel / 1.65)^2)^2.55 / (1 + (enrel / 10)^4)^1
```

```
Out[321]= 
$$\frac{4.5 \times 10^{-15} (1 + 0.367309 \text{enrel}^2)^{2.55}}{(0.001 + \text{enrel})^{0.7} \left(1 + \frac{\text{enrel}^4}{10000}\right) (1 + 256 \cdot \text{enrel}^4)^{0.42}}$$

```

Cross sections and transition probabilities for fast excited H(n=3) atoms in H2

- fast H (n=3) + H2 -> fast H(n=1) + H2 quenching of Balmer alpha excitation.

We assume a constant quenching rate coefficient from the file H2QUENCHHALPHA.NB

```
In[322]:= kquench := 7.5 * 10^-15 (*m^3/s*)
```

```
In[323]:= aX=0.98*10^8;
```

- Scaling factors for Petrovic data files

```
In[324]:= scalePhelps = 1.; (*an alternative used until 09/01/08 was 0.8*)
```

```
In[325]:= EmitSound [Sound [ {Play [Sin [440 * 2 * Pi * t] * Sin [2 Pi * t]^2, {t, 0, 0.5}]]]
```

```
In[326]:= Quit[]
```


Collisions of H+ with H2: differential cross sections

This notebook reviews the theory and experimental concerned with differential cross sections for collisions of H+ with H2 and attempts to derive an analytical expression fitting the available data from 0.1 to 3333 eV (COM).

Setup notebook enviroment

```
In[981]:= a = 1.;
```

```
In[982]:= ClearAll["Global`*"];
```

```
In[983]:= Remove["Global`*"];
```

```
In[984]:= startclock = SessionTime[];
```

```
In[985]:= Off[General::spell];
```

```
In[986]:= Off[General::spell1];
```

```
In[987]:= SetDirectory[NotebookDirectory[]]
```

```
Out[987]= C:\Users\avp\Documents\Mathbook\HYDROGEN\H2HpCollisions
```

```
SetDirectory["c:\\users\\avp\\documents\\Mathbook\\Hydrogen\\H2HpCollisions"]
```

```
In[988]:= plotColorsLines = {
  (*1*) {Red, Thickness[0.007], Dashing[{}]},
  (*2*) {Hue[0.1], (*Orange,*)Thickness[0.007], Dashing[{}]},
  (*3*) {Green, Thickness[0.007], Dashing[{}]},
  (*4*) {Cyan, Thickness[0.007], Dashing[{}]},
  (*5*) {Blue, Thickness[0.007], Dashing[{}]},
  (*6*) {Magenta, Thickness[0.007], Dashing[{}]},
  (*7*) {Yellow, Thickness[0.007], Dashing[{}]},
  (*8*) {Pink, Thickness[0.007], Dashing[{}]},
  (*9*) {Black, Thickness[0.004], Dashing[{}]},
  (*10-dash*) {Red, Thickness[0.007], Dashing[{0.03, 0.03}]},
  (*11-dash*) {Hue[0.1], Thickness[0.007], Dashing[{0.03, 0.03}]},
  (*12-dash*) {Green, Thickness[0.007], Dashing[{0.03, 0.03}]},
  (*13-dash*) {Cyan, Thickness[0.007], Dashing[{0.03, 0.03}]},
  (*14-dash*) {Blue, Thickness[0.007], Dashing[{0.03, 0.03}]},
  (*15-dash*) {Magenta, Thickness[0.007], Dashing[{0.03, 0.03}]},
  (*16-dash*) {Yellow, Thickness[0.007], Dashing[{0.03, 0.03}]},
  (*17-dash*) {Pink, Thickness[0.007], Dashing[{0.02, 0.02}]},
  (*18-dash*) {Black, Thickness[0.007], Dashing[{0.02, 0.02]}}
};
```

```
In[989]:= plotColorsPoints = {
  (*1*) {Red, PointSize[0.015]},
  (*2*) {Hue[0.1], PointSize[0.015]},
  (*3*) {Green, PointSize[0.015]},
  (*4*) {Cyan, PointSize[0.015]},
  (*5*) {Blue, PointSize[0.015]},
  (*6*) {Magenta, PointSize[0.015]},
  (*7*) {Yellow, PointSize[0.015]},
  (*8*) {Pink, PointSize[0.015]},
  (*9*) {Black, PointSize[0.015]},
  (*10*) {Red, PointSize[0.01]},
  (*11*) {Hue[0.1], PointSize[0.01]},
  (*12*) {Green, PointSize[0.01]},
  (*13*) {Cyan, PointSize[0.01]},
  (*14*) {Blue, PointSize[0.01]},
  (*15*) {Magenta, PointSize[0.01]},
  (*16*) {Yellow, PointSize[0.01]},
  (*17*) {Pink, PointSize[0.01]},
  (*18*) {Black, PointSize[0.01]}
};
```

In this notebook the energies are relative energies appropriate to COM collisions and cross sections are in atomic units of ao^2 .

```
In[990]:= startTime = TimeUsed[]
```

```
Out[990]= 608.742
```

In the following, setting `calcAll=0` allows one to skip the slower forms of the calculation of the cumulative probability.

```
In[991]:= calcAll = 0;
```

Polarization potential scattering

```
In[992]:= polDispatch = Dispatch[{mroma -> 1.008 * 2.016 / (1.008 + 2.016),
  mr -> mroma * 1.661 * 10^-27,
  qe -> 1.602 * 10^-19,
  alphaMcDaniel -> 0.808 * 10^-30,      (*m^3 from McDaniel (1993)*)
  epsilon0 -> 8.85 * 10^-12,
  ao -> 0.529 * 10^-10,      (*m*)
  me -> 9.11 * 10^-31, (*kgm*)
  ry -> 27.211 / 2 (*eV*)}]
```

```
Out[992]= Dispatch[{mroma -> 0.672, mr -> 1.661 * 10^-27 mroma,
  qe -> 1.602 * 10^-19, alphaMcDaniel -> 8.08 * 10^-31, epsilon0 -> 8.85 * 10^-12,
  ao -> 5.29 * 10^-11, me -> 9.11 * 10^-31, ry -> 13.6055}, -DispatchTables -]
```

From Lieberman and Lichtenberg (1994), Eq. (3.3.17). Their alphaR is given in terms of McDaniel and Mason's alpha by

```
In[993]:= alphaau = alphaMcDaniel / ao^3 /. polDispatch
```

```
Out[993]= 5.45814
```

```
In[994]:= kLLieberman = 8.99 * 10^-16 * (alphaau / mroma)^0.5 /. polDispatch
```

```
Out[994]= 2.56211 * 10^-15
```

In atomic units, the potential is

```
In[995]:= polarizationPotential = -1 / 2 * alphaau * rau^-4
```

```
Out[995]= - 2.72907
          rau^4
```

■ Langevin cross section

```
In[996]:= langevinQ = 2 * Pi (**ao^2*) * (13.6 / enrel * alphaau)^0.5
```

```
Out[996]= 54.1342 ( 1 / enrel )^0.5
```

The cross section used by Mason et al in thermal mobility calculations appears to be that for a polarization attraction with a rigid core (?at the spiraling radius?) and is larger than the Langevin cross section by $6.95/(2\text{Pi})=1.124$

```
In[997]:= masonPolarQ := 6.95 * langevinQ / (2 * Pi) (*m^2*)
```

```
In[998]:= masonPolarQ /. enrel -> {0.1, 100}
```

```
Out[998]= {189.355, 5.98793}
```

■ Total cross section

See McDaniel, Mitchell, and Rudd, "Atomic Collisions: Heavy Particle Projectiles" (Wiley, 1993, New York) p. 69 -72.

For a polarization potential

```
In[999]:= n = 4;
```

The Landau-Lifshitz formula for gammaLL is

```
In[1000]:= fn = Pi / 4;
```

```
In[1001]:= gammaLL = N[Pi^2 * (2 fn)^(2 / (n - 1)) * Csc[Pi / (n - 1)] / Gamma[2 / (n - 1)]]
```

```
Out[1001]= 11.3726
```

Note that the gammaLL formula is different than that given in Massey, Burhop, and Gilbody (1971) or in McDaniel, Mitchell, and Rudd (1993), but gives numbers in exact agreement with Massey et al Table 16.2.

```
In[1002]:= qtotalLL :=
  gammaLL(**ao^2*) * alphaau^(2 / 3) * (mr / me / 4 * ry / enrel)^(1 / 3) // PowerExpand
```

```
In[1003]:= qtotalLL
```

```
Out[1003]= 
$$\frac{22.2093 \text{mr}^{1/3} \text{ry}^{1/3}}{\text{enrel}^{1/3} \text{me}^{1/3}}$$

```

In ao² units this gives

```
In[1004]:= qtotalLL /. polDispatch /. enrel -> {0.1, 100, 3333}
```

```
Out[1004]= {1222.31, 122.231, 37.9812}
```

The value for a relative energy of 3333 equal to 38 ao² is much smaller than I get below from the screened Coulomb fit.

Differential cross section formulas

```
In[1005]:= Clear[ry, alphaau, enrel, theta0, ao]
```

■ Small angle formula

The small angle scattering formula for a polarization potential from McDaniel et al (1993) in Eq. (1-15-36) is that $d\sigma/d\Omega$ equals

```
In[1006]:= ismallPol := (3 * Pi) ^ (1 / 2) / 8 * (ry * alphaau * ao^4 / (enrel * theta0)) ^ (2 / 4) /
            (theta0 * Sin[theta0]) / (ao^2) /.
            enrel -> enrelau * 2 * ry // PowerExpand // Simplify;
```

where $d\sigma/d\theta = d\sigma/d\Omega * 2 \pi \sin\theta$

```
In[1007]:= ismallPol//PowerExpand //Cancel
```

$$\text{Out[1007]= } \frac{\sqrt{\text{alphaau}} \sqrt{\frac{3\pi}{2}} \text{Csc}[\text{theta0}]}{8 \sqrt{\text{enrelau}} \text{theta0}^{3/2}}$$

The total cross section in this approximation is

```
In[1008]:= qTotalIsmallPol:=2*Pi*Integrate[ismallPol*Sin[theta0],{theta0,theta1,Pi},
Assumptions->{ry>0,alphaau>0,ao>0,enrelau>0,theta0>0,theta1>0,theta1<Pi}]
```

I really should find an empirical expression for theta1.

```
In[1009]:= qTotalIsmallPol
```

$$\text{Out[1009]= } \frac{1}{2} \sqrt{\frac{3}{2}} \pi \left(\sqrt{\pi} - \sqrt{\text{theta1}} \right) \sqrt{\frac{\text{alphaau}}{\text{enrelau} \text{theta1}}}$$

The cumulative scattering probability used in Monte Carlo calculations is

```
In[1010]:= cumulativeIsmallPol:=2*Pi*Integrate[ismallPol*Sin[theta0],{theta0,theta1,thetaCum},
Assumptions->{ry>0,alphaau>0,ao>0,enrelau>0,theta0>0,thetaCum>theta1>0,theta1<Pi,thetaCum<Pi}]
```

```
In[1011]:= cumulativeIsmallPol/.cSmall->0//PowerExpand//Cancel
```

$$\text{Out[1011]= } -\frac{\sqrt{\pi} \left(\sqrt{\text{theta1}} - \sqrt{\text{thetaCum}} \right)}{\left(\sqrt{\pi} - \sqrt{\text{theta1}} \right) \sqrt{\text{thetaCum}}}$$

```
In[1012]:= Series[cumulativeIsmallPol,{thetaCum,theta1,1},Assumptions->{Pi>theta1>0,alphaau>0,enrelau>0,cSmall->0}]
```

$$\text{Out[1012]= } \left(\sqrt{\frac{\text{alphaau}}{\text{enrelau}}} \text{enrelau} \sqrt{\pi} \sqrt{\frac{\text{alphaau}}{\text{enrelau} \text{theta1}}} (\text{thetaCum} - \text{theta1}) \right) / \left(2 \text{alphaau} \left(\sqrt{\pi} - \sqrt{\text{theta1}} \right) \sqrt{\text{theta1}} \right) + O[\text{thetaCum} - \text{theta1}]^2$$

```
In[1013]:= Limit[cumulativeIsmallPol,thetaCum->Pi,Assumptions->{Pi>theta1>0,alphaau>0,enrelau>0,cSmall->0}]
```

Out[1013]= 1

■ Modified small angle formula

We modify this small angle formula by adding a constant `cSmall`. We also divide by a factor $(1+(\text{thetaD}/\text{theta0})^{5/2})$ that causes the differential cross section to become constant for $\text{theta0} \ll \text{thetaD}$, the angle below which diffraction effects become important.

```
In[1014]:= ismall := (3 * Pi) ^ (1 / 2) / 8 * (ry * alphaau * ao ^ 4 / (enrel * theta0)) ^ (2 / 4) /
            (theta0 * Sin[theta0]) / (ao ^ 2) / (1 + (thetaD / theta0) ^ (5 / 2)) //.
            enrel -> enrelau * 2 * ry // PowerExpand // Simplify;
```

where $d\sigma/d\theta = d\sigma/d\Omega * 2 \pi \sin\theta$

```
In[1015]:= ismall
```

$$\text{Out[1015]= } \frac{\sqrt{\text{alphaau}} \sqrt{\frac{3\pi}{2}} \text{theta0 Csc[theta0]}}{8 \sqrt{\text{enrelau}} (\text{theta0}^{5/2} + \text{thetaD}^{5/2})}$$

Find the cross section from this formula at $\text{theta0} = 0$.

```
In[1016]:= limitingI = Limit[ismall, theta0 -> 0]
```

$$\text{Out[1016]= } \frac{\sqrt{\text{alphaau}} \sqrt{\frac{3\pi}{2}}}{8 \sqrt{\text{enrelau}} \text{thetaD}^{5/2}}$$

We can either use $\text{thetaD} = \pi/(k*a)$, where a is the hard sphere radius from Massey and Mohr or the Q for $\text{theta0} = 0$ for a polarization potential from Massey and Mohr (1934) as modified by Landau and Lifshitz (1965) as described above.

The following was modified 08/06/11

The Landau-Lifshitz cross section for the angular integrated cross section using a polarization potential is

```
In[1017]:= totalQ =
            gammaLL * alphaau ^ (2 / 3) * (mr / me / 4 * ry / enrel) ^ (1 / 3) //. enrel -> enrelau * 2 * ry
```

$$\text{Out[1017]= } 5.68629 \text{alphaau}^{2/3} \left(\frac{\text{mr}}{\text{enrelau me}} \right)^{1/3}$$

From Massey and Burhop (1952), p. 370, Eq. (17), we can calculate the equivalent hard sphere radius as

```
In[1018]:= radius = a /. (Solve[2 * Pi * a ^ 2 == totalQ, a][[1]])
```

$$\text{Out[1018]= } -0.951316 \text{alphaau}^{1/3} \left(\frac{\text{mr}}{\text{enrelau me}} \right)^{1/6}$$

From Massey and Burhop (1952), p. 370, Eq. (20), we can calculate $I(\theta)$ as

```
In[1019]:= limitingIMB = kao^2 * radius^4 / 4
```

$$\text{Out[1019]= } 0.204757 \text{ alphaau}^{4/3} \text{ kao}^2 \left(\frac{\text{mr}}{\text{enrelau me}} \right)^{2/3}$$

Solve for the angle θ_D by setting the empirical cross section at $\theta_D = 0$ equal to the cross section from Landau and Lifshitz.

```
In[1020]:= sold = Solve[(limitingI /. cSmall -> 0) == limitingIMB, thetaD]
```

$$\text{Out[1020]= } \left\{ \left\{ \theta_D \rightarrow 1.11922 / \left(\text{alphaau}^{5/6} \sqrt{\text{enrelau}} \text{ kao}^2 \left(\frac{\text{mr}}{\text{enrelau me}} \right)^{2/3} \right)^{2/5} \right\} \right\}$$

```
In[1021]:= thetaD0 = thetaD /. sold[[1]]
```

$$\text{Out[1021]= } 1.11922 / \left(\text{alphaau}^{5/6} \sqrt{\text{enrelau}} \text{ kao}^2 \left(\frac{\text{mr}}{\text{enrelau me}} \right)^{2/3} \right)^{2/5}$$

Empirically, try an increase variable increase at low energies and a decrease at high energies

```
In[1022]:= thetaDFit0 =  
(thetaD0 /. {kao -> Sqrt[mr / me * enrelau], alphaau -> 0.808 / (0.529)^3, enrelau ->  
enrel / 27.3}) /. {me -> 9.11 * 10^-31, mr -> 2 / 3 * 1.673 * 10^-27} // PowerExpand
```

$$\text{Out[1022]= } \frac{0.016725}{\text{enrel}^{1/3}}$$

```
In[1023]:= thetaDFit :=  
0.85 * (thetaD0 / (1 + (enrelau * 27.3 / 0.25)^1)^0.05 /. {kao -> Sqrt[mr / me * enrelau],  
alphaau -> 0.808 / (0.529)^3, enrelau -> enrel / 27.3}) /. {  
me -> 9.11 * 10^-31, mr -> 2 / 3 * 1.673 * 10^-27} // PowerExpand  
thetaDFit = (thetaD0 / 1.5 /. {kao -> Sqrt[mr / me * enrelau],  
alphaau -> 0.808 / (0.529)^3, enrelau -> enrel / 27.3}) /. {  
me -> 9.11 * 10^-31, mr -> 2 / 3 * 1.673 * 10^-27} // PowerExpand
```

```
In[1024]:= thetaDFit /. enrel -> 0.1
```

$$\text{Out[1024]= } 0.030117$$

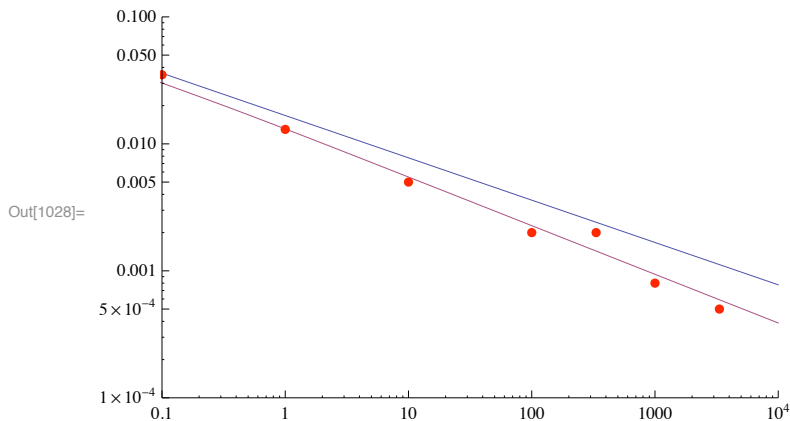
```
In[1025]:= thetaDFitPlot = LogLogPlot[{thetaDFit0, thetaDFit},  
{enrel, 0.01, 10000}, PlotRange -> {{0.1, 10000}, {0.0001, 0.1}}];
```

```
In[1026]:= eyeballTable = {{0.1, 0.035}, {1, 0.013}, {10, 0.005},  
{100, 0.002}, {333, 0.002}, {1000, 0.0008}, {3333, 0.0005}}
```

$$\text{Out[1026]= } \left\{ \left\{ 0.1, 0.035 \right\}, \left\{ 1, 0.013 \right\}, \left\{ 10, 0.005 \right\}, \left\{ 100, 0.002 \right\}, \left\{ 333, 0.002 \right\}, \left\{ 1000, 0.0008 \right\}, \left\{ 3333, 0.0005 \right\} \right\}$$

```
In[1027]:= trialDPlot = ListLogLogPlot[%,  
PlotRange -> {{0.01, 10000}, {10^-4, 0.1}}, PlotStyle -> plotColorsPoints];
```

```
In[1028]:= Show[thetaDFitPlot, trialDPlot]
```



■ Scattering below rainbow angle only

The preceding applies when there is no cutoff beyond the rainbow angle discussed below. When there is a cutoff, we approximate the distribution by chopping the distribution at θ_{Ra} . From below, an empirical relation for θ_{Ra} is $3.56/\text{enrel}$ for $\text{enrel} > 1.134$ eV and π for $\text{enrel} < 1.134$ eV. Of course, we would rather have a more gradual cutoff.

```
In[1029]:= qTotalIsmallRa:=2*Pi*Integrate[(ismall*Sin[theta0]/.thetaD->0),{theta0,theta1,thetaRa},
Assumptions->{ry>0,alphaau>0,ao>0,enrelau>0,theta0>0,Pi>=thetaRa>theta1>0}]
```

```
In[1030]:= qTotalIsmallRa
```

$$\text{Out[1030]} = \frac{1}{4} \sqrt{\frac{3}{2}} \sqrt{\frac{\text{alphaau}}{\text{enrelau}}} \pi^{3/2} \left(\frac{2}{\sqrt{\theta_{1}}} - \frac{2}{\sqrt{\theta_{Ra}}} \right)$$

In the following, $\text{Pi} \geq \theta_{Ra} \geq \theta_{\text{Cum}} > \theta_{1} > 0$

```
In[1031]:= cumulativeIsmallRa:=2*Pi*Integrate[ismall*Sin[theta0],{theta0,theta1,thetaCum},
Assumptions->{ry>0,alphaau>0,ao>0,enrelau>0,theta0>0,Pi>=thetaRa>=thetaCum>theta1>0,
0<theta1<Pi,Pi>thetaCum>0,Pi>thetaD>0}]/qTotalIsmallRa
```

```
In[1032]:= If[calcAll==1,cumulativeIsmallRa//PowerExpand//FullSimplify]
```

■ Exact classical scattering

From `c://mathbook/helium/HeHepcollisions/ClassicalFit2.nb` an exact solution for the classical scattering is

```
In[1033]:= ithetaClassicalExact :=
-(((1 + Sqrt[1 - (4 * a) / p^4])^(3 / 2) * Sqrt[1 / 2 - (2 * a) / p^4] * p^6 *
(2 * a + (-1 + Sqrt[1 - (4 * a) / p^4]) * p^4) *
(4 * a + (-1 + Sqrt[1 - (4 * a) / p^4]) * p^4) *
Csc[(2 * Sqrt[2] * EllipticK[-((2 * a + (-1 + Sqrt[1 - (4 * a) / p^4]) * p^4) /
(2 * a))]) / Sqrt[1 + Sqrt[1 - (4 * a) / p^4]]]) /
(16 * a^2 * ((-1 + Sqrt[1 - (4 * a) / p^4]) * p^4 *
EllipticE[-((2 * a + (-1 + Sqrt[1 - (4 * a) / p^4]) * p^4) / (2 * a))] +
(4 * a + (-1 + Sqrt[1 - (4 * a) / p^4]) * p^4) *
EllipticK[-((2 * a + (-1 + Sqrt[1 - (4 * a) / p^4]) * p^4) / (2 * a))]))))
```

Here p is the impact parameter, θ is the scattering angle, and $a = C4/\text{enrelau}$, where $C4$ is the polarizability in Hartree* ao^4 .

```
In[1034]:= thetaClaEx:= Pi - (2*Sqrt[2]*EllipticK[-((2*a + (-1 + Sqrt[1 - (4*a)/p^4])*p^4)/(2*a))]/
Sqrt[1 + Sqrt[1 - (4*a)/p^4]])
```


In[1035]:= **thetaClaEx**

$$\text{Out[1035]= } \pi - \frac{2\sqrt{2} \text{EllipticK}\left[-\frac{2a + \left(-1 + \sqrt{1 - \frac{4a}{p^4}}\right)p^4}{2a}\right]}{\sqrt{1 + \sqrt{1 - \frac{4a}{p^4}}}}$$

Solve[{theta1==thetaClaEx,ithetaExact==ithetaClassicalExact},ithetaExact,p]//PowerExpand

Mathematica apparently does not know how to solve these equations for `ithetaExact` as a function of `theta1`, so we make the `Solve[]` not evaluatable. I should try replacing $4a/p^4$ with x and eliminating x .

In[1036]:= **thetaDFit**

$$\text{Out[1036]= } \frac{0.0142162}{\text{enrel}^{1/3} (1 + 4. \text{enrel})^{0.05}}$$

■ Screened Coulomb scattering

■ Modified screened Coulomb scattering

From our earlier work, the modified differential scattering cross section $i(\text{thetaC}, \text{betaC}, \text{enrel})$ in center-of-mass coordinates is assumed to be

In[1037]:= **iModSC = aC*(1 + 2*betaC - Cos[thetaC])^-2 +bC //PowerExpand**

$$\text{Out[1037]= } bC + \frac{aC}{(1 + 2 \text{betaC} - \text{Cos}[\text{thetaC}])^2}$$

where `thetaC` is the scattering angle and `betaC` is the "modified screening parameter". Here both `betaC` and `aC` are functions of energy. For `betaC = 0` we have Coulomb or Rutherford scattering. For `betaC = 0.5` the scattering is isotropic. Note that this function is asymmetric about $\pi/2$ as expected for non-identical particles.

In[1038]:= **totalModSC=Integrate[iModSC,{thetaC,0,Pi},Assumptions->{aC>0,betaC>0,bC>0}]**

$$\text{Out[1038]= } bC \pi + \frac{aC (\pi + 2 \text{betaC} \pi)}{8 (\text{betaC} (1 + \text{betaC}))^{3/2}}$$

■ Screened Coulomb potential only from screenedCoulomb.nb

In[1039]:= **Clear[ry, mr, me, hbar, k, ao]**

It is customary to treat each atom of the H_2 separately, so the one doubles the cross section for $H^+ + H$.

We write the screened Coulomb potential in eV versus radius r in a.u. Here `ascr` is the screening length, `ry` is the Rydberg, and `z1` and `z2` are the nuclear charges.

In[1040]:= **screenpoten[r_] = 2 * z1 * z2 * ry / r * Exp[-r / ascr]**

$$\text{Out[1040]= } \frac{2 e^{-\frac{r}{\text{ascr}}} \text{ry} z1 z2}{r}$$

From McDaniel, Mitchell, and Rudd (1993) p. 342 and Schiff (1949) p. 168 the differential cross section for this potential is

```
In[1041]:= iscrHHp := (2 * mr * z1 * z2 * 2 * ry * ao / (hbar^2 * (K^2 + ascr^-2)))^2 / ao^2 // .  
{K -> 2 * k * Sqrt[(1 - Cos[thetaSC]) / 2], k -> Sqrt[2 * mr * enrelCoulomb] / hbar} //  
PowerExpand // FullSimplify
```

```
In[1042]:= iscrHHp
```

```
Out[1042]= (16 ascr^4 mr^2 ry^2 z1^2 z2^2) /  
(hbar^2 + 4 ascr^2 enrelCoulomb mr - 4 ascr^2 enrelCoulomb mr Cos[thetaSC])^2
```

where enrelCoulomb is the kinetic energy in COM and ry is the Rydberg, both in eV. This can be written as

```
In[1043]:= iscrMcD = iscrHHp /. {enrelCoulomb -> khbar^2 / (2 * mr), ry -> hbar^2 / (2 * me * ao^2)}
```

```
Out[1043]= (4 ascr^4 hbar^4 mr^2 z1^2 z2^2) / (ao^4 me^2 (hbar^2 + 2 ascr^2 khbar^2 - 2 ascr^2 khbar^2 Cos[thetaSC])^2)
```

where we sometimes use

```
kao = Sqrt[mrome * enrelCoulomb / ry];
```

```
khbar = Sqrt[2 * mr * enrelCoulomb];
```

Here enrel is in eV and so cancels the eV in ry. mrome is the ratio of the reduced mass to the electron mass.

To make contact with the modified Screened Coulomb formulas used in the upper part of this note book we note that

```
In[1044]:= bC = 0;
```

```
In[1045]:= aC = (mr * z1 * z2 * 2 * ry * ao / khbar^2)^2;
```

and

```
In[1046]:= betaC = 1 / 2 * 1 / 2 * (kao * ascr)^-2;
```

■ For H+ -H2 collisions

ascr from McDaniel 1993 Eq. 4-3-6 in a.u.

```
In[1047]:= Clear[qe, mr]
```

From McDaniel (1964). We need to get enrelCoulomb for use in converting H+ + H screened Coulomb collision formula to function of enrel in H+ + H2 collision. Do not forget to double collision cross section for two H+'s in H2.

```
In[1048]:= Solve[{enrel == mH * 2 * mH / (mH + 2 mH) * vo^2 / 2,
  enrelCoulomb == mH * mH / (mH + mH) * vrel^2 / 2,
  mH * 2 * mH / (mH + 2 * mH) * vo == mH * vrel}, enrelCoulomb, {vo, vrel}]
```

```
Out[1048]:= {{enrelCoulomb ->  $\frac{\text{enrel}}{3}$ }}
```

```
In[1049]:= enrelCoulomb = enrelCoulomb /. %[[1]]
```

```
Out[1049]:=  $\frac{\text{enrel}}{3}$ 
```

Note that this solution is for the relative energy of the incident H+ and differs from the solution for the laboratory energy of the incident H+ (or D+) needed for the D + D reaction in the notebooks Boris09Notes070611_7.nb and BOR09AsymmSpatialFusion070611_7.nb.

```
In[1050]:= values = Dispatch[{ry -> 13.6,
  ascr -> 1 / Sqrt[2], (*for H*)
  z1 -> 1, z2 -> 1,
  mr -> 1.008 * 1.008 / (1.008 + 1.008) * 1.672 * 10^-27, (*only correct for H+ + H*)
  mrome -> 1.008 * 1.008 / (1.008 + 1.008) * 1836, (*only correct for H+ + H*)
  qe -> 1.602 * 10^-19,
  ao -> 0.529 * 10^-10,
  hbar -> 1.054 * 10^-34,
  alphaau -> 4.5}]
```

```
Out[1050]:= Dispatch[{{ry -> 13.6, ascr ->  $\frac{1}{\sqrt{2}}$ , z1 -> 1,
  z2 -> 1, mr ->  $8.42688 \times 10^{-28}$ , mrome -> 925.344, qe ->  $1.602 \times 10^{-19}$ ,
  ao ->  $5.29 \times 10^{-11}$ , hbar ->  $1.054 \times 10^{-34}$ , alphaau -> 4.5}}, -DispatchTables -]
```

From above in atomic units and doubling the cross section to account for two H atoms in H2.

```
In[1051]:= aC1=2*a/ao^2
```

```
Out[1051]:=  $\frac{2 a}{a_0^2}$ 
```

```
In[1052]:= iscr := 2 * iscrHHp
```

```
In[1053]:= iscr
```

```
Out[1053]:=  $(32 m r^2 r y^2 z_1^2 z_2^2) / \left( \hbar^4 \left( \frac{1}{a_{scr}^2} - (4 \text{enrel} m r (-1 + \text{Cos}[\text{thetaSC}])) / (3 \hbar^2) \right)^2 \right)$ 
```

Consider these examples

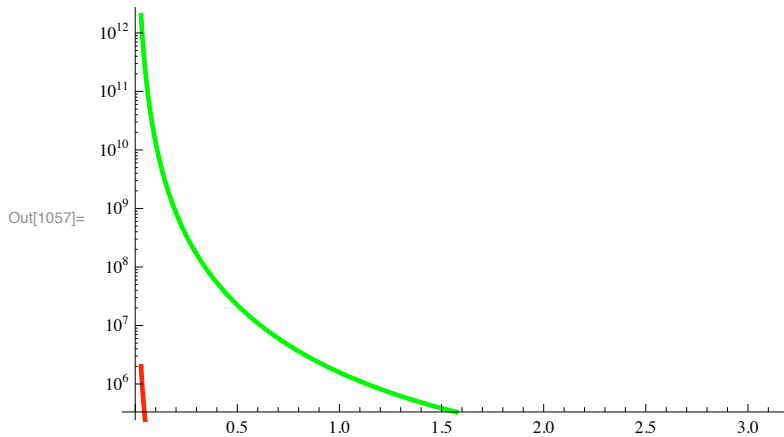
```
In[1054]:= (iscr/.enrel->100/.values)*UnitStep[Pi/2-thetaSC]
```

```
Out[1054]:=  $\left( 3.40564 \times 10^{85} \text{UnitStep}\left[\frac{\pi}{2} - \text{thetaSC}\right] \right) / \left( 2 - 1.0114 \times 10^{43} (-1 + \text{Cos}[\text{thetaSC}]) \right)^2$ 
```

```
In[1055]:= LogPlot[(iscr/.enrel->100/.values)*UnitStep[Pi/2-thetaSC], {thetaSC,0,Pi}, (*PlotRange
PlotStyle->plotColorsLines[[1]]];
```

```
In[1056]:= LogPlot[(iscr/.enrel->0.1/.values)*UnitStep[Pi/2-thetaSC], {thetaSC,0,Pi}, (*PlotRange
PlotStyle->plotColorsLines[[3]]];
```

```
In[1057]:= Show[% , %%]
```



```
In[1058]:= iscr1 = iscr /. values
```

```
Out[1058]=  $3.40564 \times 10^{85} / (2 - 1.0114 \times 10^{41} \text{enrel} (-1 + \text{Cos}[\text{thetaSC}]))^2$ 
```

```
In[1059]:= totaliscr=Integrate[iscr1,{thetaSC,0,Pi},Assumptions->{Pi>=enrel>0}]
```

```
Out[1059]= ConditionalExpression[
$$\frac{1}{(2. + 2.02281 \times 10^{41} \text{enrel})^{7/2}} 3.40564 \times 10^{85}$$


$$\left( \left( (-3.21365 \times 10^{73} + 0. i) - (3.2503 \times 10^{114} + 0. i) \text{enrel} \right) \text{enrel}^2 \sqrt{2. + 2.02281 \times 10^{41} \text{enrel}} + \right.$$


$$\left. (-5.65685 - 1.43034 \times 10^{42} \text{enrel} - 1.15732 \times 10^{83} \text{enrel}^2 - 2.92629 \times 10^{123} \text{enrel}^3) \right.$$


$$\text{ArcTan} \left[ 1.11072 \times 10^{-9} \sqrt{2. + 2.02281 \times 10^{41} \text{enrel}} \right] +$$


$$\left. (5.65685 + 1.43034 \times 10^{42} \text{enrel} + 1.15732 \times 10^{83} \text{enrel}^2 + 2.92629 \times 10^{123} \text{enrel}^3) \right.$$


$$\left. \text{ArcTan} \left[ 4.50158 \times 10^8 \sqrt{2. + 2.02281 \times 10^{41} \text{enrel}} \right] \right], \text{enrel} < 1.03398 \times 10^{-25}]$$

```

```
In[1060]:= Clear[a,b,beta]
```

■ Differential cross section near "rainbow angle".

This problem is discussed by Bransden, "Atomic Collision Theory" (Benjiman, New York, 1970), p.93 under semiclassical scattering theory (WKB?). The rainbow angle occurs when the classical deflection function passes through a maximum. The differential cross section for theta0 near thetaR is then given by Bransden's Eq. (2-155) as

Keep in mind that this solution is intended to apply only near the rainbow angle and does

not contain information as to the scattering potential over a significant range of energies or distance.

```
In[1061]:= iRainbow=2*Pi/k^2*(1r+1/2)/Sin[theta0]*qA^(-2/3)*Abs[AiryAi[(thetaR-theta0)/qA^(1/3)]]
```

$$\text{Out[1061]} = \frac{1}{k^2 qA^{2/3}} 2 \left(\frac{1}{2} + 1r \right) \pi \text{Abs} \left[\text{AiryAi} \left[\frac{-\text{theta0} + \text{thetaR}}{qA^{1/3}} \right] \right]^2 \text{Csc}[\text{theta0}]$$

where

$$qA = 1/2 * D[\text{theta0}, \{1r, 2\}]$$

It would appear that the above is $2\pi d\sigma/d\Omega = d\sigma/d\theta / \sin\theta$. Presumably, this is in atomic units.

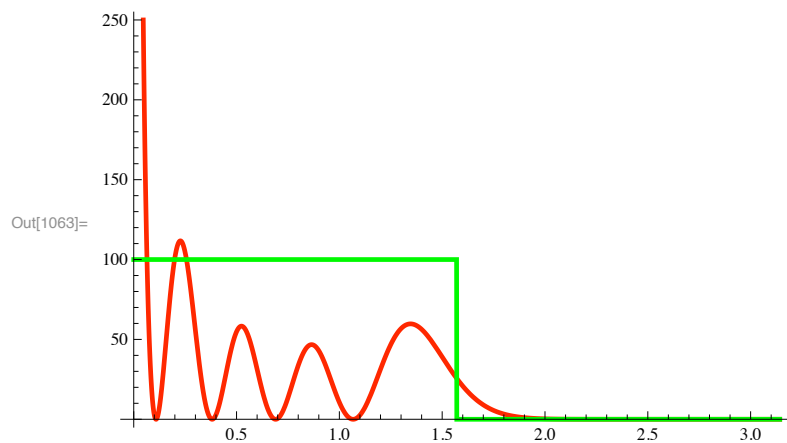
The constants used in the following example are arbitrary, i.e., $qA = 0.01$ a.u. and the angle of the rainbow peak thetaR .

We effectively change the sign of the argument of the Airy function when we plot for $\text{theta0} < \text{thetaR}$ and for $\text{theta0} > \text{thetaR}$.

```
In[1062]:= iRainbow=2*Pi/k^2*(1r+1/2)/Sin[theta0]*qA^(-2/3)*AiryAi[-(thetaR-theta0)/qA^(1/3)]^2
```

$$\text{Out[1062]} = \frac{1}{k^2 qA^{2/3}} 2 \left(\frac{1}{2} + 1r \right) \pi \text{AiryAi} \left[-\frac{\text{theta0} + \text{thetaR}}{qA^{1/3}} \right]^2 \text{Csc}[\text{theta0}]$$

```
In[1063]:= iRainbowPlot=Plot[{(iRainbow//.{1r->1,qA->.010,k->1,thetaR->Pi/2}), (UnitStep[thetaR-the-
{theta0,0,Pi}, (*PlotRange->{{0,Pi},{0,100}},*) PlotStyle->plotColorsLines[{{1,3}}]]
```



I do not understand this plot and do not see anyway to make use of it. It looks to me like the horizontal axis is reversed.

Bransden (1970) gives the asymptotic forms for $x \rightarrow -\infty$ as

```
In[1064]:= limitAiryAiNeg := 3^(-1/3)/Sqrt[Pi]/(-x)^(1/4)*Cos[2/3*(-x)^(3/2)-Pi/4]/.x->(thetaR-th
```

The average of the oscillatory limit is

```
In[1065]:= asymAvgNeg:=2*Pi/k^2*(1r+1/2)/Sin[theta0]*qA^(-2/3)*(Abs[3^(-1/3)/Sqrt[Pi]/(-x)^(1/4)/  
x->(thetaR-theta0)/qA^(1/3)])^2// PowerExpand
```

```
In[1066]:= asymAvgNeg/.{1r->1,qA->.010,thetaR->Pi/2,k->1}
```

```
Out[1066]= 14.4225 Csc[theta0]
```

$$\frac{14.4225 \operatorname{Csc}[\theta_0]}{\sqrt{\operatorname{Abs}\left[\frac{\pi}{2} - \theta_0\right]}}$$

We change the sign of x in the Airy function

```
In[1067]:= asymAvgNeg2:=2*Pi/k^2*(1r+1/2)/Sin[theta0]*qA^(-2/3)*(Abs[3^(-1/3)/Sqrt[Pi]/(-x)^(1/4)  
x->(thetaR-theta0)/qA^(1/3)])^2// PowerExpand
```

Bransden (1970) gives the asymptotic forms for $x \rightarrow +\infty$ as

```
In[1068]:= limitAiryAiPos = 3^(-1/3)/Sqrt[Pi]/(x)^(1/4)*Exp[-2/3*(x)^(3/2)]/.x->(theta0-thetaR)/q
```

```
Out[1068]=
```

$$\frac{e^{-\frac{2}{3} \left(\frac{\theta_0 - \theta_{\text{R}}}{qA^{1/3}} \right)^{3/2}}}{3^{1/3} \sqrt{\pi} \left(\frac{\theta_0 - \theta_{\text{R}}}{qA^{1/3}} \right)^{1/4}}$$

We do not change the sign of x in the Airy function

```
In[1069]:= limitRainbowPos=2*Pi/k^2*(1r+1/2)/Sin[theta0]*qA^(-2/3)*(Abs[limitAiryAiPos])^2
```

```
Out[1069]=
```

$$\left(2 e^{-\frac{4}{3} \operatorname{Re}\left[\left(\frac{\theta_0 - \theta_{\text{R}}}{qA^{1/3}}\right)^{3/2}\right]} \left(\frac{1}{2} + 1r\right) \operatorname{Csc}[\theta_0] \right) / \left(3^{2/3} k^2 qA^{2/3} \sqrt{\operatorname{Abs}\left[\frac{\theta_0 - \theta_{\text{R}}}{qA^{1/3}}\right]} \right)$$

Assume a value for thetaR

```
In[1070]:= thetaR = pi / 2 (*3pi/4*)
```

```
Out[1070]=
```

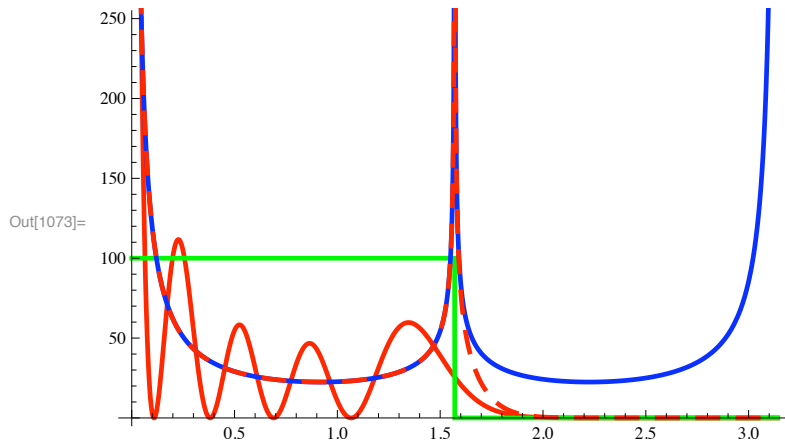
$$\frac{\pi}{2}$$

```
In[1071]:= asymAvgNegPlot=Plot[(asymAvgNeg2//.{1r->1,qA->.010,k->1}), {theta0,0,Pi}, PlotRange->{  
PlotStyle->plotColorsLines[[5]]];
```

```
In[1072]:= limitRainbowPosPlot=Plot[(limitRainbowPos/.{1r->1,qA->.010,k->1}), {theta0,0,Pi},  
PlotRange->{{0,Pi},{-0,1000}}, PlotStyle->plotColorsLines[[10]]];
```

In[1073]:=

```
Show[iRainbowPlot, asymAvgNegPlot, limitRainbowPosPlot]
```



In[1074]:=

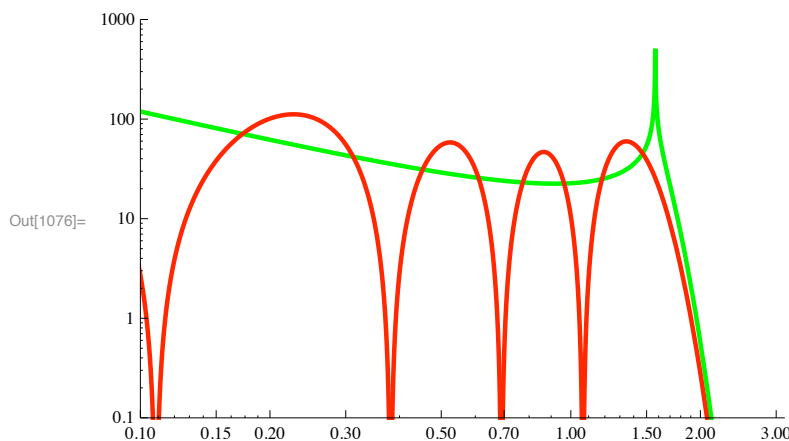
```
iRainbowLogLogPlot=LogLogPlot[{(iRainbow/.{lr->1,qA->.010,k->1})}, {theta0,0.01,Pi},
PlotRange->{{0.1,Pi},{10^-1,1000}}, PlotStyle->plotColorsLines[[1]]];
```

In[1075]:=

```
limitRainbowPosLogLogPlot=LogLogPlot[(limitRainbowPos/.{lr->1,qA->.010,k->1}), {theta0
PlotRange->{{0.1,Pi},{10^-1,1000}}, PlotStyle->plotColorsLines[[3]]];
```

In[1076]:=

```
Show[limitRainbowPosLogLogPlot, iRainbowLogLogPlot]
```



I have reversed the sign of the argument of the Airy function and its limiting approximations from those of Bransden in order to get a reasonable plot. Note that this is different than changing from $\theta_R - \theta_0$ to $\theta_0 - \theta_R$ everywhere. Obviously, I am confused.

```
Series[iRainbow, {theta0,0,4}]
```

In[1077]:=

iRainbow*Sin[theta0]

$$\text{Out[1077]= } \frac{2 \left(\frac{1}{2} + \text{lr} \right) \pi \text{AiryAi} \left[-\frac{\pi - \text{theta0}}{qA^{1/3}} \right]^2}{k^2 qA^{2/3}}$$

■ **Some rainbow angles from the literature are:**

Some of these are from vibrational excitation data. It appears that these are values at the local maximum versus theta. See Krstic and Schultz (1999) Fig. 3 and my old graphs. I believe that the energies are COM energies, as is enrel.

In[1078]:=

thetaRGiese74={ {6,35}, {10,22}, {16,13.5}, {25,8} }; (*eV,deg*)

In[1079]:=

thetaRSchinke={ {4.67,44}, {6,33} }; (*eV,deg*)

In[1080]:=

thetaRMcGuire76={ {3.7,56} }; (*eV,deg*)

In[1081]:=

thetaRMcGuire80={ {10,22} }; (*eV,deg*)

In[1082]:=

thetaRGianturco95={ {20,10.5} }; (*eV,deg*)

From Fig. 2 of Gao et al, Phys. Rev. A 44, 5599 (1991) for "direct scattering". Figure 3 for single charge transfer gave different angles in the same general range.

In[1083]:=

thetaRRice={ {333,0.4}, {1000,0.27}, {3333,0.12} };

In[1084]:=

**ListPlot[{thetaRGiese74, thetaRSchinke, thetaRMcGuire76, thetaRMcGuire80, thetaRGiantu
PlotRange->{{0,100},{0,180}}];**

This plot shows that the various calculations of the rainbow angle agree rather well.

In[1085]:=

Join[thetaRGiese74, thetaRSchinke, thetaRMcGuire76, thetaRMcGuire80, thetaRGianturco95

In[1086]:=

rainbowLogLogPlot=ListLogLogPlot[%,PlotRange->{{0.1,10000},{0.1,1000}},PlotStyle->plot

Empirically, I get the following fit to the Rainbow angle data.

In[1087]:=

rainbowAngleFit := 2 * π / (1 + (enrel / 0.57) ^ 4) ^ 0.25

In[1088]:=

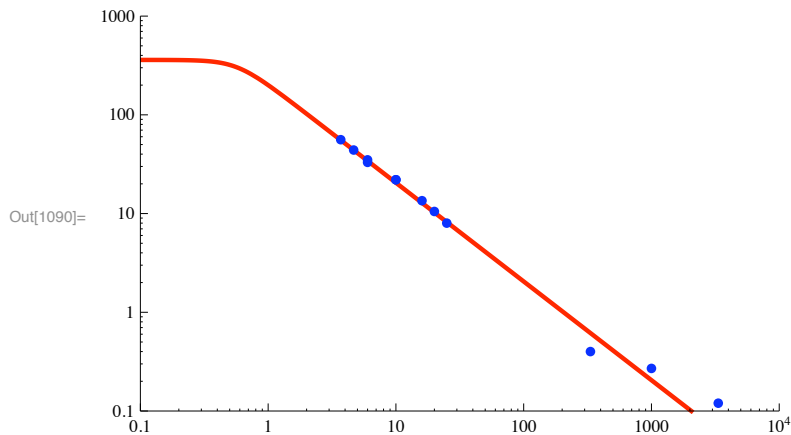
rainbowAngleFit

$$\text{Out[1088]= } \frac{2 \pi}{(1 + 9.47328 \text{enrel}^4)^{0.25}}$$

The $1/\text{enrel}$ dependence corresponds with a constant value of the normalized angle variable "theta*tau" behavior in theory. Note that the following plot is of the rainbow angle in degrees versus energy in eV to agree with experiment.

```
In[1089]:= rainbowFitPlot=LogLogPlot[180/π*rainbowAngleFit, {enrel,0.1,10000},PlotRange->{{0.1,10},
PlotStyle->plotColorsLines];
```

```
In[1090]:= Show[rainbowFitPlot, rainbowLogLogPlot]
```



Note that this plot is of the angle in degrees, while the fit is in radians. Also, note that the fit at angles greater than 180 deg is presumably unrealistic, but is important so as to make the rainbow structure in our empirical formula disappear at low collision energies.

The question now is how to use this scaling of the rainbow angle to modify the empirical differential cross section.

```
In[1091]:= thetaDFit
```

$$\text{Out[1091]} = \frac{0.0142162}{\text{enrel}^{1/3} (1 + 4. \text{enrel})^{0.05}}$$

■ Empirical differential cross section

```
In[1092]:= Clear[thetaR]
```

The presence of a first order singularity as $\theta_0 \rightarrow 0$ makes it important that I find some way to approximate the diffraction region at very small angles.

This formula is based on our observation that one can get a much better fit to the Krstic & Schultz theory at 10 eV by combining the small angle polarization formula with the Airy function description of the angles near the Rainbow angle at angles $\theta_E < \theta_{Ra}$. Note that we have arranged for the constant c_{Rain} to be set to zero at when $\theta_{Ra} > \pi$.

In principle, something like the following would be a way of applying a cutoff near the rainbow angle.

```
iEmpiricalR1:=(iRainbow2/.thetaE->theta0)*UnitStep[Pi-thetaRa]+ismall*UnitStep[thetaRa
```

In use, thetaRa = rainbowAngleFit or some "to be determined" factor times it. The magnitude of cRain is still to be determined so as to give a smooth transition at and near theta0 = thetaR between the green curve representing iRainbow2 and ismall. However, iRainbow2 has a singularity at thetaR. We therefore fall back on our old procedure of multiplying by a function that falls off at theta0 values larger than thetaR. Because the usual power-law roll-off is nowhere near fast enough, we try an exponential. The problem is to find the energy dependence of the two coefficients. The choices in the next cell work reasonably well for thetaR of pi/4 and pi/2.

```
iEmpiricalR := ismall / (1 + 0.1 * Exp[13 * (theta0 - thetaR) / thetaR]) / Sqrt[thetaR]]
```

In[1093]= **ismall**

$$\text{Out[1093]= } \frac{\sqrt{\text{alphaau}} \sqrt{\frac{3\pi}{2}} \text{theta0 Csc[theta0]}}{8 \sqrt{\text{enrelau}} (\text{theta0}^{5/2} + \text{thetaD}^{5/2})}$$

We add an increase near the rainbow angle at smaller angles than the sharp drop off.

```
iEmpiricalR := Piecewise[{{ismall + cSmall, thetaR > Pi},
  {ismall (1 + 0.1 * Exp[5 * (theta0 - 0.6 * thetaR) / Sqrt[thetaR]]) /
    (1 + 0.1 * Exp[16 * (theta0 - 0.9 * thetaR) / Sqrt[thetaR]]) + cSmall,
  theta0 < 3 Sqrt[thetaR] && thetaR < Pi}, {cSmall,
  theta0 > 3 Sqrt[thetaR] && thetaR < Pi}}]
```

09/05/11 The following is our principal result: For an empirical fit to various sources of $d\sigma/d\Omega = d\sigma/d\theta (2\pi \sin[\theta])^{-1}$, we propose

```
In[1094]= iEmpiricalR := Piecewise[{{ismall + cSmall, thetaR > Pi},
  {ismall / (1 + ((theta0 - 0.9 * thetaR) / thetaR) ^ 4) ^ 0.5 + cSmall,
  theta0 < 3 Sqrt[thetaR] && thetaR < Pi},
  {cSmall, theta0 > 3 Sqrt[thetaR] && thetaR < Pi}}]
```

where ismall, cSmall, thetaD, and thetaR are defined elsewhere in this notebook.

In[1095]= **iEmpiricalR**

$$\text{Out[1095]= } \left\{ \begin{array}{ll} \frac{c\text{Small} + \left(\sqrt{\text{alphaau}} \sqrt{\frac{3\pi}{2}} \text{theta0 Csc[theta0]} \right)}{\left(8 \sqrt{\text{enrelau}} (\text{theta0}^{5/2} + \text{thetaD}^{5/2}) \right)} & \text{thetaR} > \pi \\ \frac{c\text{Small} + \left(\sqrt{\text{alphaau}} \sqrt{\frac{3\pi}{2}} \text{theta0 Csc[theta0]} \right)}{\left(8 \sqrt{\text{enrelau}} (\text{theta0}^{5/2} + \text{thetaD}^{5/2}) \right) \left(1 + (\text{theta0} - 0.9 \text{thetaR})^4 / \text{thetaR}^4 \right)^{0.5}} & \text{theta0} < 3 \sqrt{\text{thetaR}} \ \&\& \ \text{thetaR} < \pi \\ c\text{Small} & \text{theta0} > 3 \sqrt{\text{thetaR}} \ \&\& \ \text{thetaR} < \pi \\ 0 & \text{True} \end{array} \right.$$

```
In[1096]:= thetaDFit
```

```
Out[1096]= 
$$\frac{0.0142162}{\text{enrel}^{1/3} (1 + 4. \text{enrel})^{0.05}}$$

```

```
In[1097]:= iEmpiricalTest =
```

```
  iEmpiricalR //. {thetaD -> thetaDFit, alphaau -> 0.808 / (0.529)^3, enrelau -> 10 / 27.2,
  cSmall -> 0.1, thetaR -> rainbowAngleFit, enrel -> 10}
```

```
Out[1097]= 
$$\begin{cases} 0.1 + (1.04553 \text{theta0} \text{Csc}[\text{theta0}]) / & \text{theta0} < 1.79535 \\ \left( (1 + 60.7835 (-0.322327 + \text{theta0})^4)^{0.5} (2.22346 \times 10^{-6} + \text{theta0}^{5/2}) \right) & \\ 0.1 & \text{theta0} > 1.79535 \\ 0 & \text{True} \end{cases}$$

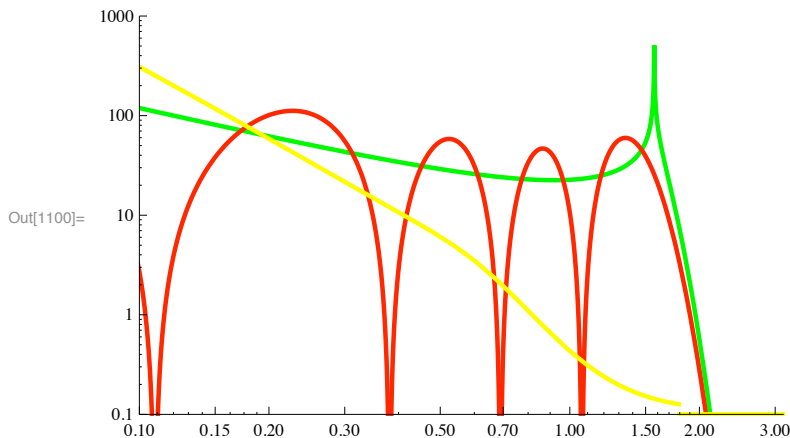
```

```
In[1098]:= iEmpiricalRPlot = Plot[Evaluate[%, {theta0, 0.01, Pi},
  PlotRange -> {{0., Pi}, {0, 1000}}, PlotStyle -> plotColorsLines[[7]]];
```

```
In[1099]:=
```

```
iEmpiricalRLogLogPlot=LogLogPlot[Evaluate[iEmpiricalR//.{thetaD->thetaDFit,alphaau->0.
cSmall->0.1,thetaR->rainbowAngleFit,enrel->10}], {theta0,0.01,Pi},PlotRange->{{0.1,Pi}
PlotStyle->plotColorsLines[[7]]];
```

```
In[1100]:= Show[limitRainbowPosLogLogPlot, iRainbowLogLogPlot, iEmpiricalRLogLogPlot]
```



The iEmpirical plot is not supposed to agree with the rainbow solution, which is extended well beyond its range of applicability near $\text{Pi}/2$.

■ Additive constant

```
In[1101]:= Clear[enrel]
```

I need to come up with a contribution to the Empirical profile that applies at large angles. Consider a term c_{Small} that is independent of angle and decreases with increasing enrel , e.g.,

The values used thus far are

```
In[1102]:= cSmallTable =
```

```
{ {0.1, 7.}, {1, 3.}, {10, 0.003}, {100, 0.00005}, {333, 0}, {1000, 0}, {3333, 0}
```

```
Out[1102]= {{0.1, 7.}, {1, 3.}, {10, 0.003}, {100, 0.00005}, {333, 0}, {1000, 0}, {3333, 0}}
```

```
In[1103]:= cSmallTablePlot = ListLogLogPlot[cSmallTable,
```

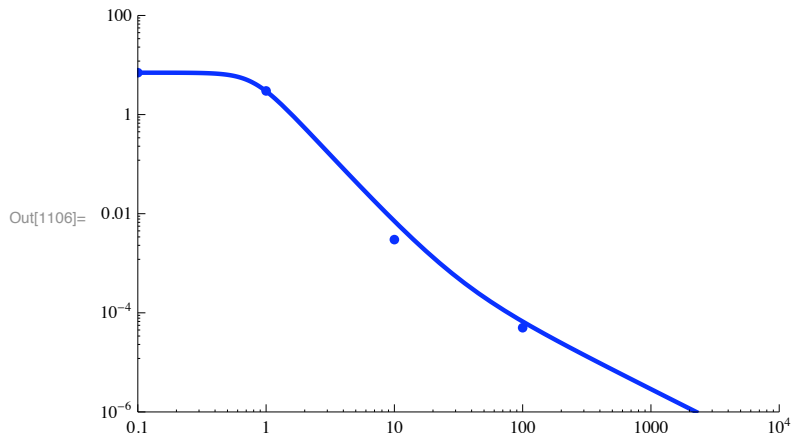
```
PlotRange -> {{0.1, 10000}, {10^-6, 10^2}}, PlotStyle -> plotColorsPoints[[5]]];
```

Try the following. It is strictly an empirical parameter, chosen to approximate large angle behavior.

```
In[1104]:= cSmallFit := 7 / (1 + (enrel / 0.8) ^ 4) ^ 0.7 * (1 + (enrel / 30) ^ 1.5)
```

```
In[1105]:= cSmallFitPlot = LogLogPlot[cSmallFit, {enrel, 0.1, 10000},
  PlotRange -> {{0.1, 10000}, {10^-6, 10^2}}, PlotStyle -> plotColorsLines[[5]]];
```

```
In[1106]:= Show[cSmallFitPlot, cSmallTablePlot]
```



The points are from my eyeball fits to Krstic and Schultz (1999).

■ Cumulative probability

The cumulative probability is used in Monte Carlo calculations

```
In[1107]:= cumulativeIsSmallPol /. {theta1 -> 0.001, cSmall -> 0, thetaD -> thetaDFit} //
  PowerExpand // Cancel
```

```
Out[1107]= 
$$\frac{-0.0321972 + 1.01817 \sqrt{\text{thetaCum}}}{\sqrt{\text{thetaCum}}}$$

```

```
In[1108]:= Plot[%, {thetaCum, 0.001, Pi}, PlotRange -> {{0, Pi}, {0, 1}}];
```

```
In[1109]:= iRainbowExample = (iRainbow /. {lr -> 1, qA -> .010, thetaR -> Pi/2, k -> 1})
```

```
Out[1109]= 203.051 AiryAi[-4.64159 (Pi/2 - theta0)]^2 Csc[theta0]
```

```
In[1110]:= 203.05068584529502` Abs[AiryAi[-4.641588833612778` (Pi/2 - theta0)]]^2 Csc[theta0]
```

```
Out[1110]= 203.051 Abs[AiryAi[-4.64159 (Pi/2 - theta0)]]^2 Csc[theta0]
```

```
In[1111]:= NIntegrate[iRainbowExample*Sin[theta0], {theta0, 0.01, 0.1*Pi}]/(NIntegrate[iRainbowExam
```

```
Out[1111]= 0.0473777
```

```
In[1112]:= NIntegrate[ (asymAvgNeg2*Sin[theta0] /. {lr->1, qA->.010, thetaR->Pi/2, k->1}), {theta0, 0.00
```

```
Out[1112]= 3.80514
```

```
In[1113]:= Clear[thetaSC]
```

```
In[1114]:= NIntegrate[ (iscr/.enrel->100/.values)*Sin[thetaSC]*UnitStep[Pi/2-thetaSC], {thetaSC, 0.0
```

```
Out[1114]= 6651.81
```

```
In[1115]:= NIntegrate[ (iscr/.enrel->100/.values)*Sin[thetaSC]*UnitStep[Pi/2-thetaSC], {thetaSC, 0.0
```

```
Out[1115]= 6658.28
```

```
In[1116]:= ismall
```

$$\frac{\sqrt{\text{alphaau}} \sqrt{\frac{3\pi}{2}} \text{theta0} \text{Csc}[\text{theta0}]}{8 \sqrt{\text{enrelau}} (\text{theta0}^{5/2} + \text{thetaD}^{5/2})}$$

```
In[1117]:= thetaDFit
```

$$\frac{0.0142162}{\text{enrel}^{1/3} (1 + 4. \text{enrel})^{0.05}}$$

```
In[1118]:= NIntegrate[ (ismall*Sin[theta0] //. {enrelau->1, alphaau->4.5, thetaD->thetaDFit, cSmall->0}
{theta0, 0.01, Pi/10}]
```

NIntegrate::inumr :

The integrand $\left(0.575621 \text{theta0} \text{UnitStep}\left[\frac{\pi}{2} - \text{theta0}\right]\right) / \left(0.0000240969 \left(\frac{1}{\text{enrel}^{1/3} \ll 1 \gg^{0.05}} + \text{theta0}^{5/2}\right)\right)$ has evaluated to non-numerical values for all sampling points in the region with boundaries $\{(0.01, 0.314159)\}$. \gg

```
Out[1118]= NIntegrate[
(ismall Sin[theta0] //. {enrelau -> 1, alphaau -> 4.5, thetaD -> thetaDFit, cSmall -> 0})
UnitStep[Pi/2 - theta0], {theta0, 0.01, Pi/10}]
```

```
In[1119]:= case1Norm = NIntegrate[iRainbowExample * Sin[theta0], {theta0, 0.001, Pi}];
```

The following case1 is multiplied by 0.95 so as to differentiate between the plots for cases 1 and 2.

```
In[1120]:= case1 := If[calcAll == 1,
0.95 * NIntegrate[iRainbowExample * Sin[theta0], {theta0, 0.001, thetaCum}] /
NIntegrate[iRainbowExample * Sin[theta0],
{theta0, 0.001, Pi}];
```

In[1121]:=

```

case1Plot = Plot[case1, {thetaCum, 0, Pi}, PlotRange -> {{0, Pi}, {0, 1}},
  PlotStyle -> plotColorsLines[[1]], PlotPoints -> 100];

case2Norm = NIntegrate[iRainbowExample * Sin[theta0], {theta0, 0.0001, Pi}];

case2 := If[calcAll == 1,
  NIntegrate[iRainbowExample * Sin[theta0], {theta0, 0.0001, thetaCum}] / case2Norm];

case2Plot = Plot[case2, {thetaCum, 0, Pi}, PlotRange -> {{0, Pi}, {0, 1}},
  PlotStyle -> plotColorsLines[[2]], PlotPoints -> 100];

case3Norm = NIntegrate[
  (asymAvgNeg2 * Sin[theta0] /. {lr -> 1, qA -> .010, thetaR -> Pi / 2, k -> 1}),
  {theta0, 0.0001, Pi / 2}]

case3 := If[calcAll == 1, (NIntegrate[
  (asymAvgNeg2 * Sin[theta0] /. {lr -> 1, qA -> .010, thetaR -> Pi / 2, k -> 1}) *
  UnitStep[Pi / 2 - theta0], {theta0, 0.0001, thetaCum}]) / case3Norm]

case3Plot = Plot[case3, {thetaCum, 0, Pi}, PlotRange -> {{0, Pi}, {0, 1}},
  PlotStyle -> plotColorsLines[[3]], PlotPoints -> 100];

case4Norm = NIntegrate[(iscr /. enrel -> 0.1 /. values) *
  Sin[thetaSC] * UnitStep[Pi / 2 - thetaSC], {thetaSC, 0.01, Pi / 2}]

case4 := If[calcAll == 1,
  NIntegrate[(iscr /. enrel -> 0.1 /. values) * Sin[thetaSC] * UnitStep[Pi / 2 - thetaSC],
  {thetaSC, 0.01, thetaCum}] / case4Norm]

case4Plot = Plot[case4, {thetaCum, 0, Pi}, PlotRange -> {{0, Pi}, {0, 1}},
  PlotStyle -> plotColorsLines[[4]], PlotPoints -> 100];

case5Norm = NIntegrate[
  (ismall * Sin[theta0] /. {enrelau -> 0.1 / 27.211, alphaau -> 4.5, thetaD -> thetaDFit,
  cSmall -> 0}) * UnitStep[Pi / 2 - theta0], {theta0, 0.01, Pi}]

case5 := If[calcAll == 1, NIntegrate[(ismall * Sin[theta0] /.
  {enrelau -> 0.1 / 27.211, alphaau -> 4.5, thetaD -> thetaDFit}) *
  UnitStep[Pi / 2 - theta0], {theta0, 0.01, thetaCum}] / case5Norm]

case5Plot = Plot[case5, {thetaCum, 0, Pi}, PlotRange -> {{0, Pi}, {0, 1}},
  PlotStyle -> plotColorsLines[[5]], PlotPoints -> 100];

```

```

cumulativeIsmallPlot = Plot[Evaluate[cumulativeIsmallPol /.
  {theta1 -> 0.001, enrelau -> 0.1 / 27.211, alphaau -> 4.5, thetaD -> thetaDFit}],
  {thetaCum, 0.001, Pi}, PlotRange -> {{0.001, Pi}, {0, 1}},
  PlotStyle -> plotColorsLines[[6]], PlotPoints -> 100];

```

```
Show[{case1Plot, case2Plot, case3Plot, case4Plot, case5Plot, cumulativeIsmallPlot}]
```

The agreement between the red (thetaMin=0.001)(multiplied by 0.95 to separate curves), orange (thetaMin=0.0001), and green (avg of iRainbow) curves for various lower limits to theta is good. The agreement for the other approximations is bad.

Note that the contribution from angles beyond the rainbow angle to the cumulative scattering probability for large angles is negligible, i.e., in this approximation the differential cross section may be reasonably be assumed to be zero.

Differential cross sections from Simko et al (1997) and Simko (thesis 1997)

The form of the differential cross section assumed by Simko et al for all inelastic collisions is proportional to

In[1122]:=

```
iSimko=1/(1+alphaS*epsilon/epsilonk*Sin[thetaS/2])^betaS/.{alphaS->0.5,betaS->2.1}
```

Out[1122]=

$$\frac{1}{\left(1 + \frac{0.5 \epsilon \sin\left[\frac{\theta_{\text{S}}}{2}\right]}{\epsilon_{\text{k}}}\right)^{2.1}}$$

where alphaS = 0.5 and betaS = 2.1 are numbers that are chosen to fit H+ in H2 mobility data for E/N < 100 Td.

In[1123]:=

```
iSimko1=iSimko/.epsilon->x*epsilonk
```

Out[1123]=

$$\frac{1}{\left(1 + 0.5 x \sin\left[\frac{\theta_{\text{S}}}{2}\right]\right)^{2.1}}$$

The contribution of the inelastic processes to the momentum transfer cross section relative to the total cross section is

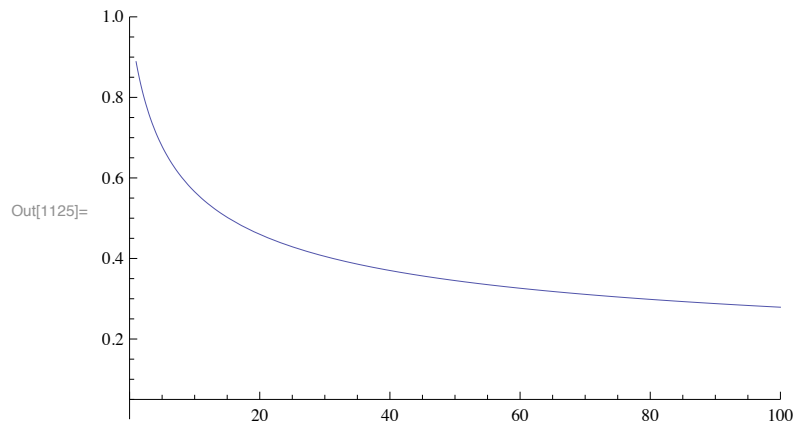
In[1124]:=

```
relqmksimko=2*Pi*Integrate[iSimko1*(1-Cos[thetaS])*Sin[thetaS],{thetaS,0,Pi},Assumptio
(2*Pi*Integrate[iSimko1*Sin[thetaS],{thetaS,0,Pi},Assumptions->x>=1)]//Simplify
```

```
Out[1124]= ((1. + (0.500022 + 0.0000111803 x) x)11/10
  ((x2 (-145.455 (1. + 0.0000223607 x)1/10 + 145.455 (1. + 0.5 x)1/10 +
    (-80.0033 (1. + 0.0000223607 x)1/10 + 72.7309 (1. + 0.5 x)1/10) x +
    (-0.00178885 (1. + 0.0000223607 x)1/10 + 0.00178885 (1. + 0.5 x)1/10) x2)) /
  (1. + 0.500022 x + 0.0000111803 x2)11/10 +
  (x2 (-145.455 (1. + 0.0000223607 x)1/10 + 145.455 (1. + 0.5 x)1/10 +
    x (-80.0033 (1. + 0.0000223607 x)1/10 + 72.7309 (1. + 0.5 x)1/10 -
    0.00178885 (1. + 0.0000223607 x)1/10 x + 0.00178885 (1. + 0.5 x)1/10 x)) /
  (1. + (0.500022 + 0.0000111803 x) x)11/10 + (-17503.9 (2. + 0.0000447214 x)1/10 +
    17503.9 (2. + 1. x)1/10 +
    x2 (1006.26 (2. + 0.0000447214 x)1/10 - 1246.94 (2. + 1. x)1/10) +
    x3 (722.059 (2. + 0.0000447214 x)1/10 - 623.608 (2. + 1. x)1/10) +
    x4 (0.0161452 (2. + 0.0000447214 x)1/10 - 0.015338 (2. + 1. x)1/10) +
    x (-9627.55 (2. + 0.0000447214 x)1/10 + 8752.39 (2. + 1. x)1/10)) /
  (4. + 2.00009 x + 0.0000447214 x2)11/10)) /
  (x2 (-145.455 (1. + 0.0000223607 x)1/10 + 145.455 (1. + 0.5 x)1/10 +
    x (-80.0033 (1. + 0.0000223607 x)1/10 + 72.7309 (1. + 0.5 x)1/10 -
    0.00178885 (1. + 0.0000223607 x)1/10 x + 0.00178885 (1. + 0.5 x)1/10 x))
```

In[1125]:=

```
Plot[relqmksimko,{x,1,100},PlotRange->{{0,100},{0.001,1}}]
```



For later comparison with Krstic and Schultz, we plot the differential cross section for H+ + H2 scattering. First we need to normalize the Simko et al formula

In[1126]:=

```
normiSimko=(1/(1+alphaS*epsilon/epsilonk*Sin[thetaS/2])^betaS/.
{alphaS->0.5,betaS->2.1})/Integrate[Sin[thetaS]/(1+alphaS*epsilon/epsilonk*Sin[thetaS/
{alphaS->0.5,betaS->2.1},{thetaS,0,Pi}, Assumptions->{epsilon>0,epsilonk>0}]]//Simplify
```

$$\text{Out[1126]= } \frac{\epsilon^2 (0.0000223607 \epsilon + 1. \epsilon_k)^2 (0.5 \epsilon + 1. \epsilon_k)^2}{\left(\epsilon_k^3 \left(\epsilon^3 \left(0.000894427 (1. + (0.0000223607 \epsilon) / \epsilon_k)^{9/10} - 4. \times 10^{-8} \left(1. + \frac{0.5 \epsilon}{\epsilon_k} \right)^{9/10} \right) + \epsilon^2 \left(36.3672 (1. + (0.0000223607 \epsilon) / \epsilon_k)^{9/10} - 0.00357778 \left(1. + \frac{0.5 \epsilon}{\epsilon_k} \right)^{9/10} \right) \epsilon_k + \epsilon \left(145.458 (1. + (0.0000223607 \epsilon) / \epsilon_k)^{9/10} - 80.0065 \left(1. + \frac{0.5 \epsilon}{\epsilon_k} \right)^{9/10} \right) \epsilon_k^2 + \left(145.455 (1. + (0.0000223607 \epsilon) / \epsilon_k)^{9/10} - 145.455 \left(1. + \frac{0.5 \epsilon}{\epsilon_k} \right)^{9/10} \right) \epsilon_k^3 \right) \left(1 + \frac{0.5 \epsilon \sin\left[\frac{\theta_S}{2}\right]}{\epsilon_k} \right)^{2.1}}$$

In[1127]:=

```
normiSimko1=normiSimko/.epsilon->x*epsilonk//Simplify
```

$$\text{Out[1127]= } \frac{(1. + 0.0000223607 x)^2 (1. + 0.5 x)^2 x^2}{\left((145.455 (1. + 0.0000223607 x)^{9/10} - 145.455 (1. + 0.5 x)^{9/10} + (145.458 (1. + 0.0000223607 x)^{9/10} - 80.0065 (1. + 0.5 x)^{9/10}) x + (36.3672 (1. + 0.0000223607 x)^{9/10} - 0.00357778 (1. + 0.5 x)^{9/10}) x^2 + (0.000894427 (1. + 0.0000223607 x)^{9/10} - 4. \times 10^{-8} (1. + 0.5 x)^{9/10}) x^3 \right) \left(1 + 0.5 x \sin\left[\frac{\theta_S}{2}\right] \right)^{2.1}}$$

For J = 0-2 rotational excitation at 10 eV, qrSimko=4E-20 m²/(0.529E-10)² = 14 compared to qm = 1.6E-20/(.529E-10)² = 5.72.

In[1128]:=

```
qrSimkoIPlot=LogPlot[(qrSimko*normiSimko)/.{epsilon->10,epsilonk->0.045,qrSimko->14.},
PlotRange->{{0,Pi},{0.01,10^5}}, PlotStyle->plotColorsLines[[5]]];
```

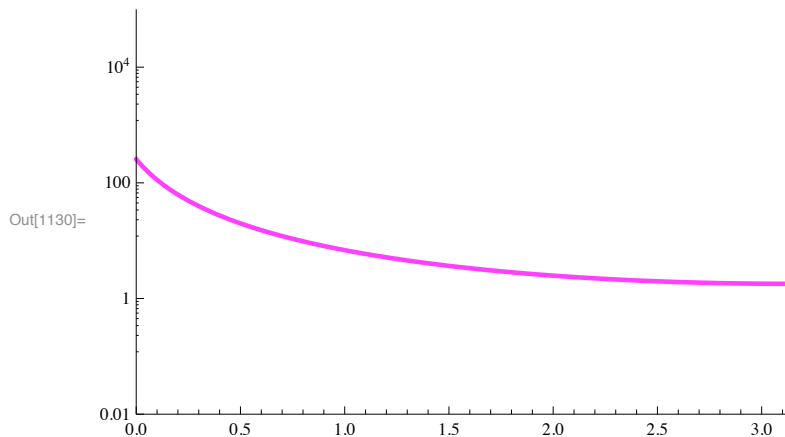
In[1129]:=

```
qrSimkoI2Plot=LogLogPlot[((qrSimko*normiSimko*2*Pi*Sin[thetaS])/.{epsilon->10,epsilonk
PlotRange->{{0.001,4},{10^-4,101000.}}, PlotStyle->plotColorsLines[[5]]];
```

For $v = 0-1$ vibrational excitation at 10 eV, $qv_{\text{Simko}}=4E-20 \text{ m}^2/(0.529E-10)^2 = 14$ compared to $q_m = 1.6E-20/(.529E-10)^2 = 5.72$.

Plot $d\sigma/d\Omega$

```
In[1130]:= qvSimkoIPlot=LogPlot[(qvSimko*normiSimko)/.{epsilon->10,epsilonk->0.52,qvSimko->14.},{PlotRange->{{0,Pi},{0.01,10^5}},PlotStyle->plotColorsLines[[6]]]
```



Plot $d\sigma/d\theta$

```
In[1131]:= qvSimkoI2Plot=LogLogPlot[(qvSimko*normiSimko*2*Pi*Sin[thetaS])/.{epsilon->10,epsilonk->0.52,qvSimko->14.},{PlotRange->{{0.001,4},{10^-4,101000.}},PlotStyle->plotColorsLines[[6]]];
```

Momentum transfer weighting

```
In[1132]:= qmSimkoImPlot=Plot[(qvSimko*normiSimko*Sin[thetaS](1-Cos[thetaS])/.{epsilon->10,epsilonk->0.52,qvSimko->14.},{thetaS,0,Pi},{PlotRange->{{0.0,Pi},{0,12.}},PlotStyle->plotColorsLines[[6]]];
```

```
In[1133]:= Clear[thetaR, thetaD, cSmall]
```

Krstic and Schultz differential cross sections

Krstic and Schultz (1999) provide their differential cross sections in the form of tables of $2\pi\sin\theta d\sigma/d\omega = d\sigma/d\theta$

- For 0.1 eV in CM, Krstic and Schultz give tabulated results:

```
In[1134]:= Flatten[Take[Import["h2hpeldiff-0.txt","CSV"],6]]
```

```
Out[1134]= {Differential Elastic (EL) Cross Section vs. CM scattering angle (theta),
for H++H2 at ~ .1000 eV CM Energy,
The Cross sections are multiplied by 2*pi*sin(theta)!,
Ref.: P.S. Krstic and D.R. Schultz, Atomic and Plasma-Material Interaction,
Data for Fusion, Vol.8, IAEA, Vienna, (1998)., }
```

```
In[1135]:= krstic01Data=Join[{{0, 0}},Drop[Drop[Import["h2hpeldiff-0.txt","Table"],13],-2]];
```

Because Krstic & Schultz did not use a constant step size in their table, we have to interpolate in order to integrate.

Skip next cell.

```
Table[krstic01Data[[j + 1, 1]] - krstic01Data[[j, 1]], {j, Length[krstic01Data] - 1}]
```

```
In[1136]:= krstic01LogLogPlot=ListLogLogPlot[krstic01Data,PlotRange->{{0.001,Pi},{1,10100}}];
```

```
In[1137]:= krstic01LogPlot=ListLogPlot[krstic01Data,PlotRange->{{0.001,Pi},{1,10100}}];
```

```
In[1138]:= diffQ01=Table[{{#[[j,1]],#[[j,2]]/(2*Pi*Sin[#[[j,1]])}},{j,2,Length[#]}]&[krstic01Data]
```

```
In[1139]:= diffQ01LogPlot=ListLogPlot[diffQ01,PlotRange->{{0,Pi},{0.0999,100000}}];
```

```
In[1140]:= diffQ01LogLogPlot=ListLogLogPlot[diffQ01,PlotRange->{{0.01,Pi},{0.0999,100000}}];
```

Assume cSmall

```
cSmall = 7;
```

```
In[1141]:= cSmall = cSmallFit /. enrel -> 0.1
```

```
Out[1141]= 7.00015
```

```
In[1142]:= thetaD = thetaDFit /. {enrel -> 0.1, alphaau -> 0.808 / (0.529)^3}
```

```
Out[1142]= 0.030117
```

```
thetaD = 0.035
```

```
In[1143]:= thetaR = rainbowAngleFit /. enrel -> 0.01 / 27.211
```

```
Out[1143]= 6.28319
```

```
In[1144]:= me = 9.11 * 10^-31; mr = 2 / 3 * 1.673 * 10^-27;
```

```
In[1145]:= ismall01=(ismall//. {ry->13.6,alphaau->0.808/(0.529)^3,enrelau->0.1/27.211,thetaD->the
```

```
Out[1145]= 7.00015 +  $\frac{10.4574 \theta_0 \text{Csc}[\theta_0]}{0.000157408 + \theta_0^{5/2}}$ 
```

```
In[1146]:= smallAngleClassical01LogPlot =  
LogPlot[2 * Pi * ismall01 * Sin[theta0] /. {ry -> 13.6, alphaau -> 0.808 / (0.529)^3,  
enrelau -> 0.1 / 27.211, thetaD -> thetaDFit}, {theta0, 0, Pi},  
PlotRange -> {{0, Pi}, {1, 100 000.}}, PlotStyle -> {Hue[0.5], Thickness[0.007]}];
```

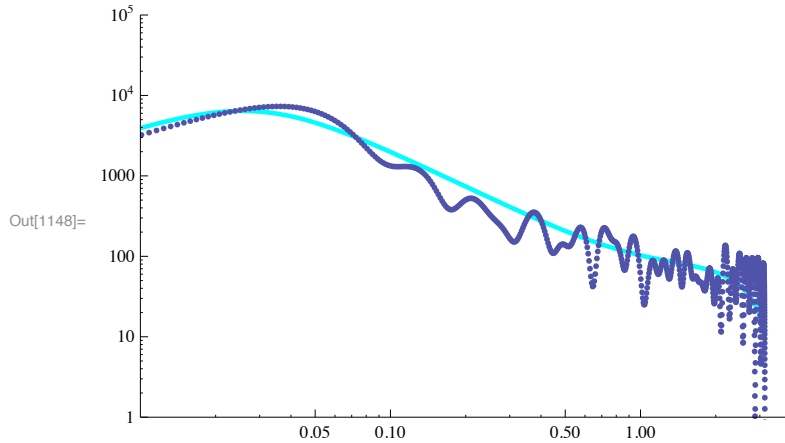
This has a singularity at small angles and must be replaced by the quantum formulation of Massey et al.

In[1147]:=

```
smallAngleClassical01LogLogPlot2 =
  LogLogPlot[(2 * Pi * ismall01 * Sin[theta0]) /. {ry -> 13.6,
    alphaau -> 0.808 / (0.529) ^ 3, enrelau -> 0.1 / 27.211, thetaD -> thetaDFit},
    {theta0, 0.001, Pi}, PlotRange -> {{0.01, 4}, {1, 100 000.}},
    PlotStyle -> {Hue[0.5], Thickness[0.007]}];
```

In[1148]:=

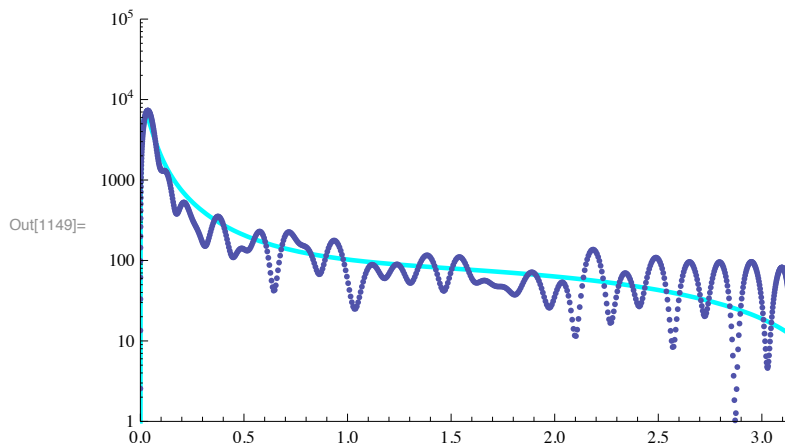
```
Show[smallAngleClassical01LogLogPlot2, krstic01LogLogPlot, DisplayFunction->$DisplayFunc
```



This plot shows that the modification of the small angle model works reasonably well at θ_0 below about 0.1 radian.

In[1149]:=

```
Show[smallAngleClassical01LogPlot, krstic01LogPlot, DisplayFunction->$DisplayFunction]
```



■ Modified classically exact formula

Here we have added a constant, c_{Small}

p_c is the impact parameter which leads to spiraling trajectory. The `thetaClassicalExact`

function shows a singularity at scattering angles near π .

```
In[1150]:= pc=(4*a)^(1/4)/.a->4.50/2/(0.1/27.2)
```

```
Out[1150]= 7.03401
```

Note that we will add an arbitrary constant cSmall to this differential cross section.

```
In[1151]:= ithetaClassicalExact01=(ithetaClassicalExact+cSmall)/. {a->4.50/2/(0.1/27.2)}
```

```
Out[1151]= 7.00015 -  $\left( 1.6687 \times 10^{-7} \left( 1 + \sqrt{1 - \frac{2448.}{p^4}} \right)^{3/2} \sqrt{\frac{1}{2} - \frac{1224.}{p^4}} \right.$   

 $p^6 \left( 1224. + \left( -1 + \sqrt{1 - \frac{2448.}{p^4}} \right) p^4 \right) \left( 2448. + \left( -1 + \sqrt{1 - \frac{2448.}{p^4}} \right) p^4 \right)$   

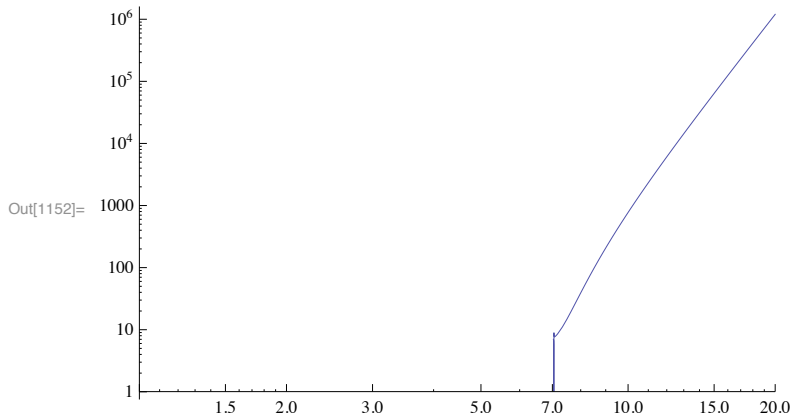
 $\text{Csc} \left[ \left( 2 \sqrt{2} \text{EllipticK} \left[ -0.000816993 \left( 1224. + \left( -1 + \sqrt{1 - \frac{2448.}{p^4}} \right) p^4 \right) \right] \right) / \right.$   

 $\left. \left( \sqrt{1 + \sqrt{1 - \frac{2448.}{p^4}}} \right) \right] /$   

 $\left( \left( -1 + \sqrt{1 - \frac{2448.}{p^4}} \right) p^4 \text{EllipticE} \left[ -0.000816993 \left( 1224. + \left( -1 + \sqrt{1 - \frac{2448.}{p^4}} \right) p^4 \right) \right] + \right.$   

 $\left. \left( 2448. + \left( -1 + \sqrt{1 - \frac{2448.}{p^4}} \right) p^4 \right) \text{EllipticK} \left[ -0.000816993 \left( 1224. + \left( -1 + \sqrt{1 - \frac{2448.}{p^4}} \right) p^4 \right) \right] \right)$ 
```

```
In[1152]:= LogLogPlot[{ithetaClassicalExact01}, {p, pc, 20}, PlotRange->{{1, 20}, All}]
```



```
In[1153]:= FindRoot[ithetaClassicalExact01, {p, pc}]
```

```
Out[1153]= {p -> 6.93319 - 0.752301 i}
```

I have no idea what this complex root means.

We need to evaluate ithetaClassicalExact01 and thetaExact01 for $p \geq pc$, the spiraling impact parameter.

```
In[1154]:= thetaExact01=thetaClaEx/.a->4.50/2/(0.1/27.2)
```

$$\text{Out[1154]= } \pi - \left(2 \sqrt{2} \text{EllipticK} \left[-0.000816993 \left(1224. + \left(-1 + \sqrt{1 - \frac{2448.}{p^4}} \right) p^4 \right) \right] \right) / \left(\sqrt{1 + \sqrt{1 - \frac{2448.}{p^4}}} \right)$$

```
In[1155]:= FindRoot[1 / thetaExact01, {p, pc}]
```

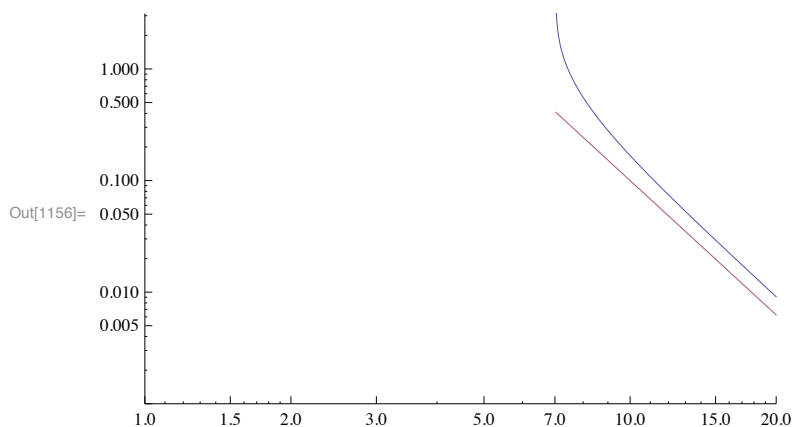
FindRoot::lstol :

The line search decreased the step size to within tolerance specified by AccuracyGoal and PrecisionGoal but was unable to find a sufficient decrease in the merit function. You may need more than MachinePrecision digits of working precision to meet these tolerances. >>

```
Out[1155]= {p -> 7.03401}
```

Note the following change of sign. The singularities in thetaExact and ithetaClassicalExact occur at $p = pc$.

```
In[1156]:= LogLogPlot[{-thetaExact01, 1000 * p^-4},
  {p, pc, 20}, PlotRange -> {{1, 20}, {0.001, Pi}}]
```



Since I cannot make ParametricPlot[] work, I will try making tables of thetaExact01 and ithetaClassicalExact01 versus p.

```
ParametricPlot[{-thetaExact01 /. p -> 1/x},
  {ithetaClassicalExact01 /. p -> 1/x}, {x, -1/pc, 1/pc}]
```

We use a nonuniform angle scale to see the behavior near a scattering angle of π .

```
In[1157]:= delpList = {0.001, 0.002, 0.003, 0.008, 0.01, 0.012, 0.014, 0.015,
0.0152, 0.0155, 0.0157, 0.0158, 0.01585, 0.0159, 0.01595, 0.016,
0.0165, 0.017, 0.02, 0.03, 0.1, 0.3, 0.5, 1., 2., 3., 4., 7., 10.};
```

```
In[1158]:= classicalExact01Table1=Table[{delpList[[j]],#[[j]],-thetaExact01/.p->#[[j]], ithetaCla
{j,1,Length[delpList]}}&[pc+delpList];
```

```
In[1159]:= classicalExact01Table=Table[#[[j,3]],#[[j,4]],{j,Length[#]}]&[classicalExact01Table1
```

```
In[1160]:= classicalExact01Plot=ListLogPlot[classicalExact01Table, PlotRange->{{0,2*Pi},{0.1,10^5}
PlotStyle->plotColorsLines[[3]]];
```

```
In[1161]:= ismall01LogPlot = LogPlot[ismall01 /. {ry -> 13.6, alphaau -> 0.808 / (0.529)^3,
enrelau -> 0.1 / 27.211, thetaD -> thetaDFit}, {theta0, 0, Pi},
PlotRange -> {{0, Pi}, {1, 100 000.}}, PlotStyle -> plotColorsLines[[13]]];
```

```
In[1162]:= thetaR = rainbowAngleFit /. enrel -> 0.1;
```

```
In[1163]:= iEmpirical01LogPlot = LogPlot[iEmpiricalR /. {ry -> 13.6, alphaau -> 0.808 / (0.529)^3,
enrelau -> 0.1 / 27.211, thetaD -> thetaDFit}, {theta0, 0, Pi},
PlotRange -> {{0, Pi}, {1, 100 000.}}, PlotStyle -> plotColorsLines[[7]]];
```

```
In[1164]:= asymAvg01Neg2LogPlot =
LogPlot[(asymAvgNeg2 /. {lr -> 0.05, qA -> .002, k -> 0.5}), {theta0, 0, Pi},
PlotRange -> {{0, Pi}, {1, 100 000}}, PlotStyle -> plotColorsLines[[6]]];
```

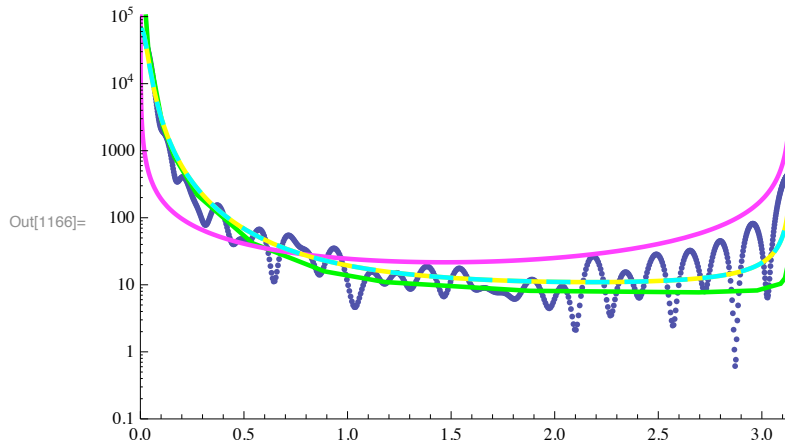
decreasing qA seems to lower the wavelength of the oscillations; decreasing k increases the magnitude of the cross section and the oscillations; decreasing lr slowly decreases the amplitude of the oscillations; thetaR changes the position of the right hand singularity for thetaR< π .

```
In[1165]:= iEmpiricalR /.
{alphaau -> 0.808 / (0.529)^3, enrelau -> 0.1 / 27.211, thetaD -> thetaDFit}
```

```
Out[1165]= 7.00015 +  $\frac{10.4574 \text{ theta0 Csc}[\text{theta0}]}{0.000157408 + \text{theta0}^{5/2}}$ 
```

In[1166]:=

```
Show[diffQ01LogPlot, classicalExact01Plot, asymAvg01Neg2LogPlot, iEmpirical01LogPlot, is
```



Out[1166]=

black points - Krstic and Scultz, yellow - Empirical, cyan - ismall (angle), green - Classical Exact, magenta - based on rainbow,

We see that empirically the small angle approximation (cyan) works better than the classical "exact" (green) solution at scattering angles near π . Both analytical solutions fail at very low angles, where diffraction effects become important. See Massey and Mohr. The fit of the Rainbow solution would be better if the direction of angles were reversed, but we need to remember that this solution has no information on the form of the potential well.

In[1167]:=

```
runTime = TimeUsed[] - startTime
```

Out[1167]= 42.368

In[1168]:= `krstic01Fcn = Interpolation[krstic01Data][x]`Out[1168]= `InterpolatingFunction[{{0., 3.14158}}, <>][x]`

In[1169]:=

```
total01=NIntegrate[krstic01Fcn, {x,0,krstic01Data[[-1,1]]}]
```

Out[1169]= 778.452

```
cumProbKrstic01[theta_] :=  
  Integrate[krstic01Fcn, {x, 0, theta}] / total01 (* Cumulative Distr. Func. *)
```

In[1171]:=

```
runTime = TimeUsed[] - startTime
```

Out[1171]= 42.383

In[1172]:=

```
bins = 3000;
```

In[1173]:=

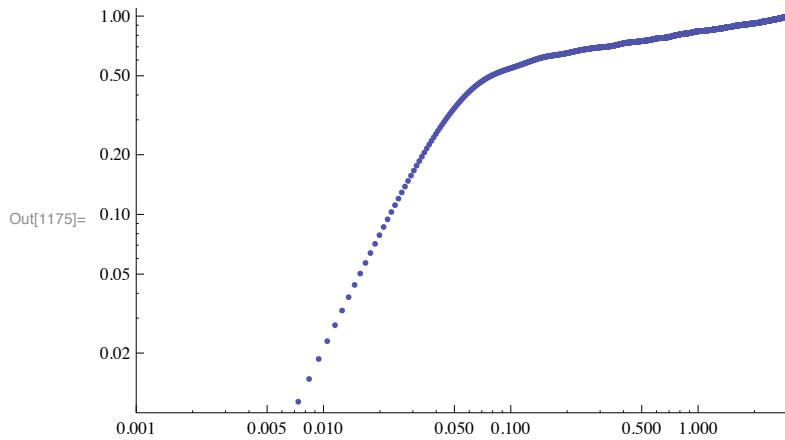
```
cumProbKrstic01Table =  
  Table[{(j - 1) * Pi / bins * 1., cumProbKrstic01[(j - 1) * Pi / bins]}, {j, 1, bins}];
```



```
In[1174]:= runTime = TimeUsed[] - startTime
```

```
Out[1174]= 51.369
```

```
In[1175]:= cumProbKrstic01Plot=ListLogLogPlot[cumProbKrstic01Table,PlotRange->{{0.001,Pi},{0.01,1
```



```
In[1176]:= totalEmp01 =  
  NIntegrate[(iEmpiricalR * 2 * Pi * Sin[theta0] /. {alphaau -> 0.808 / (0.529)^3,  
    enrelau -> 0.1 / 27.211, thetaD -> thetaDFit, enrel -> 0.1}), {theta0, 0, Pi}]
```

```
Out[1176]= 823.276
```

```
In[1177]:= cumProbEmp01[theta_] := NIntegrate[  
  (iEmpiricalR * 2 * Pi * Sin[theta0] / totalEmp01 /. {alphaau -> 0.808 / (0.529)^3,  
    enrelau -> 0.1 / 27.211, thetaD -> thetaDFit, enrel -> 0.1}), {theta0, 0, theta}]
```

In[1178]:=

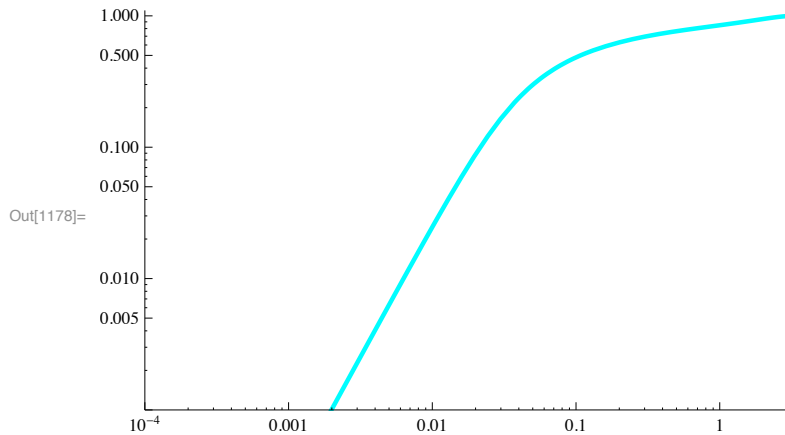
```
cumProbEmp01Plot = LogLogPlot[cumProbEmp01[theta], {theta, 0.0001, Pi},
  PlotRange -> {{0.0001, Pi}, {0.001, 1.1}}, PlotStyle -> plotColorsLines[[4]]]
```

NIntegrate::nlm : theta0 = theta is not a valid limit of integration. >>

NIntegrate::nlm : theta0 = theta is not a valid limit of integration. >>

NIntegrate::nlm : theta0 = theta is not a valid limit of integration. >>

General::stop : Further output of NIntegrate::nlm will be suppressed during this calculation. >>



In[1179]:=

```
cumProbSmall01Plot=LogLogPlot[Evaluate[cumulativeISmallPol//.
  {alphaau->5.4, enrelau->0.1/27.211, theta1->0.03,thetaD->thetaDFit}], {thetaCum,0.001,
  PlotRange->{{0.001,Pi},{0.01,1.1}}, PlotStyle->plotColorsLines[[5]]];
```

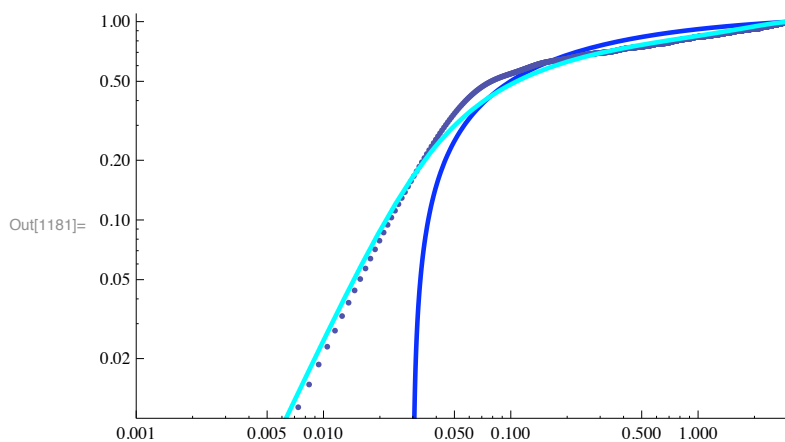
In[1180]:=

```
runTime = TimeUsed[] - startTime
```

Out[1180]= 63.646

In[1181]:=

```
Show[cumProbSmall01Plot,cumProbKrstic01Plot,cumProbEmp01Plot]
```



This shows our fit is much too small at low angles

In[1182]:= **Clear[thetaR, thetaD, cSmall]**

■ For 1 eV in CM, Krstic and Schultz give

```
In[1183]:= Flatten[Take[Import["h2hpeldiff-1.txt", "CSV"], 6]]
```

```
Out[1183]= {Differential Elastic (EL) ) Cross Setion vs. CM scattering angle (theta),
  for H++H2 at ~ 1.0000 eV CM Energy,
  The Cross sections are multiplied by 2*pi*sin(theta)!,
  Ref.: P.S. Krstic and D.R. Schultz, Atomic and Plasma-Material Interaction,
  Data for Fusion, Vol.8, IAEA, Vienna, (1998)., }
```

```
In[1184]:= krstic1Data = Join[{{0, 0}}, Drop[Drop[Import["h2hpeldiff-1.txt", "Table"], 13], -2]];
```

```
In[1185]:= Export["krstic1Data.txt", %, "Table"]
```

```
Out[1185]= krstic1Data.txt
```

These data are $d\sigma/d\theta$. To get $d\sigma/d\Omega$, divide by $2\pi\sin[\theta]$

```
In[1186]:= diffQ1=Table[#[[j,1]],#[[j,2]]/(2*Pi*Sin#[[j,1]])],{j,2,Length[#]}&[krstic1Data];
```

```
In[1187]:= diffQ1LogPlot=ListLogPlot[diffQ1,PlotRange->{{-0.001,Pi},{0.999,10^6}}];
```

```
In[1188]:= diffQ1LogLogPlot=ListLogLogPlot[diffQ1,PlotRange->{{0.0001,10},{0.999,10^6}}];
```

Assume cSmall.

```
In[1189]:= cSmall = 3;
```

```
In[1190]:= cSmall = cSmallFit /. enrel -> 1
```

```
Out[1190]= 2.96495
```

```
In[1191]:= thetaD = thetaDFit /. {enrel -> 1, alphaau -> 0.808 / (0.529)^3}
```

```
Out[1191]= 0.013117
```

```
thetaD = 0.013;
```

```
In[1192]:= thetaR = rainbowAngleFit /. enrel -> 1
```

```
Out[1192]= 3.49268
```

```
In[1193]:= iEmpiricalR //. {alphaau -> 0.808 / (0.529)^3, enrelau -> 1 / 27.211, thetaD -> thetaDFit}
```

```
Out[1193]= 2.96495 +  $\frac{3.30693 \text{ theta0 Csc}[\text{theta0}]}{0.0000197056 + \text{theta0}^{5/2}}$ 
```

```
In[1194]:= iEmpiricalLogPlot = LogPlot[Evaluate[{iEmpiricalR /.
  {alphaau -> 0.808 / (0.529)^3, enrelau -> 1 / 27.211, thetaD -> thetaDFit}],
  {theta0, 0, Pi}, PlotRange -> {{0, Pi}, {1, 100000.}},
  PlotStyle -> plotColorsLines[[7]]];
```

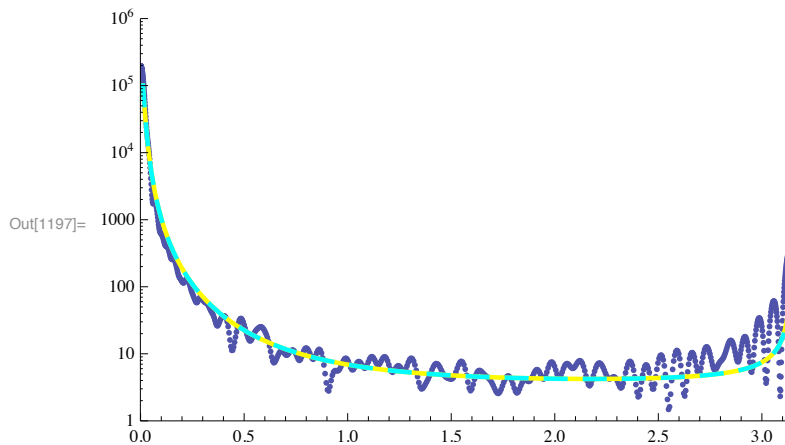
```
In[1195]:= ismall1=(ismall1 /. {ry->13.6,alphaau->0.808/(0.529)^3,enrelau->1/27.211,thetaD->thetaD
```

$$\text{Out[1195]= } 2.96495 + \frac{3.30693 \theta_0 \text{Csc}[\theta_0]}{0.0000197056 + \theta_0^{5/2}}$$

This has a singularity at small angles and should be replaced by the quantum formulation of Massey et al.

```
In[1196]:= smallAngleClassicalPlot =
  LogPlot[ismall1 /. {ry -> 13.6, alphaau -> 0.808 / (0.529)^3,
    enrelau -> 1 / 27.211, thetaD -> thetaDFit}, {theta0, 0, Pi},
  PlotRange -> {{0, Pi}, {1, 100000.}}, PlotStyle -> plotColorsLines[[13]]];
```

```
In[1197]:= Show[diffQ1LogPlot, iEmpiricalLogPlot, smallAngleClassicalPlot]
```



```
In[1198]:= krstic1Plot=ListLogLogPlot[krstic1Data,PlotRange->{{0.001,4},{1,101000}}];
```

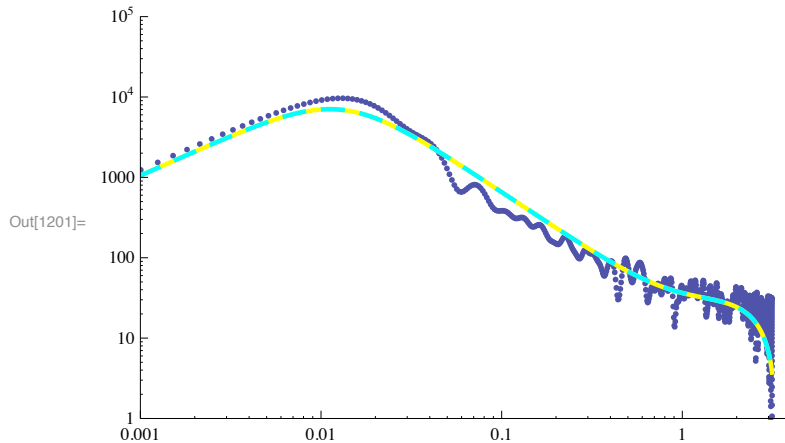
These data are $d\sigma/d\theta$.

```
In[1199]:= smallAngleClassicalKSLogLogPlot = LogLogPlot[
  (2 * Pi * ismall1 * Sin[theta0]) /. {ry -> 13.6, alphaau -> 0.808 / (0.529)^3,
    enrelau -> 1. / 27.211, thetaD -> thetaDFit}, {theta0, 0.001, Pi},
  PlotRange -> {{0.001, 4}, {1, 10^5}}, PlotStyle -> plotColorsLines[[13]]];
```

```
In[1200]:= iEmpiricalKSLogLogPlot =
  LogLogPlot[(2 * Pi * Sin[theta0] * iEmpiricalR /. {alphaau -> 0.808 / (0.529)^3,
    enrelau -> 1 / 27.211, thetaD -> thetaDFit}), {theta0, 0.001, Pi},
  PlotRange -> {{0.001, Pi}, {1, 10^5}}, PlotStyle -> plotColorsLines[[7]]];
```

In[1201]:=

```
Show[krstic1Plot, iEmpirical1KSLogLogPlot, smallAngleClassical1KSLogLogPlot]
```



In[1202]:=

```
krstic1Plot3=ListLogPlot[krstic1Data,PlotRange->{{0,Pi},{1,101000}}];
```

In[1203]:=

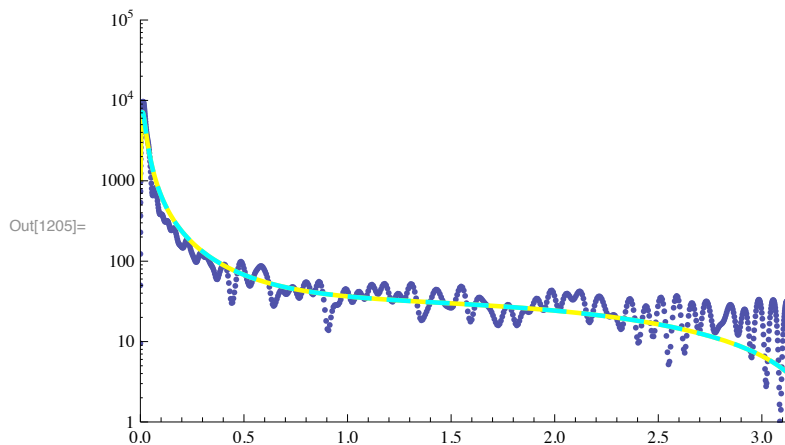
```
smallAngleClassical1KSLogPlot =
  LogPlot[(2 * Pi * ismall1 * Sin[theta0]) /. {ry -> 13.6, alphaau -> 0.808 / (0.529)^3,
    enrelau -> 1 / 27.211, thetaD -> thetaDFit}, {theta0, 0.01, Pi},
  PlotRange -> {{0, Pi}, {1, 101000.}}, PlotStyle -> plotColorsLines[[13]]];
```

In[1204]:=

```
iEmpirical1KSLogPlot =
  LogPlot[2 * Pi * Sin[theta0] * (iEmpiricalR /. {alphaau -> 0.808 / (0.529)^3,
    enrelau -> 1 / 27.211, thetaD -> thetaDFit}), {theta0, 0.001, Pi},
  PlotRange -> {{0, Pi}, {1, 100000.}}, PlotStyle -> plotColorsLines[[7]]];
```

In[1205]:=

```
Show[krstic1Plot3, iEmpirical1KSLogPlot, smallAngleClassical1KSLogPlot]
```



In[1206]:=

```
cumProbSmallQ1Plot=LogLogPlot[Evaluate[cumulativeIsmallPol /. {alphaau->5.4, enrelau->1
  theta1->0.01, thetaD->thetaDFit}], {thetaCum, 0.001, Pi}, PlotRange->{{0.001, Pi}, {0.01, 1.}
```

Here I have taken the lower limit to the integrals over ismall1 to be 0.01 rad, i.e., near the maximum of the experimental $\text{diffQ1}[\theta] * 2 * \pi * \text{Sin}[\theta]$ plot.

```
In[1207]:= runTime = TimeUsed[] - startTime
```

```
Out[1207]= 68.887
```

```
In[1208]:= krstic1Fcn = Interpolation[krstic1Data][x]
```

```
Out[1208]= InterpolatingFunction[{{0., 3.14158}}, <>][x]
```

```
In[1209]:= total1=NIntegrate[krstic1Fcn, {x,0,krstic1Data[[-1,1]]}]
```

```
Out[1209]= 420.996
```

```
In[1210]:= cumProbKrstic1[theta_] :=  
Integrate[krstic1Fcn, {x, 0, theta}] / total1 (* Cumulative Distr. Func. *)
```

```
In[1211]:= runTime = TimeUsed[] - startTime
```

```
Out[1211]= 68.918
```

```
In[1212]:= bins = 3000;
```

```
In[1213]:= cumProbKrstic1Table =  
Table[{(j - 1) * Pi / bins * 1., cumProbKrstic1[(j - 1) * Pi / bins]}, {j, 1, bins}];
```

```
In[1214]:= runTime = TimeUsed[] - startTime
```

```
Out[1214]= 77.872
```

```
In[1215]:= cumProbKrstic1Plot=ListLogLogPlot[cumProbKrstic1Table,PlotRange->{{0.001,Pi},{0.01,1.1}}
```

```
In[1216]:= totalEmp1 =  
NIntegrate[(iEmpiricalR * 2 * Pi * Sin[theta0] /. {alphaau -> 0.808 / (0.529)^3,  
enrelau -> 1 / 27.211, thetaD -> thetaDFit, enrel -> 1}), {theta0, 0, Pi}]
```

```
Out[1216]= 401.676
```

```
In[1217]:= cumProbEmp1[theta_] := NIntegrate[  
(iEmpiricalR * 2 * Pi * Sin[theta0] / totalEmp1 /. {alphaau -> 0.808 / (0.529)^3,  
enrelau -> 1 / 27.211, thetaD -> thetaDFit, enrel -> 1}), {theta0, 0, theta}]
```

```
In[1218]:= cumProbEmp1Plot = LogLogPlot[cumProbEmp1[theta], {theta, 0.0001, Pi},  
PlotRange -> {{0.0001, Pi}, {0.001, 1.1}}, PlotStyle -> plotColorsLines[[4]]];
```

NIntegrate::nlim : theta0 = theta is not a valid limit of integration. >>

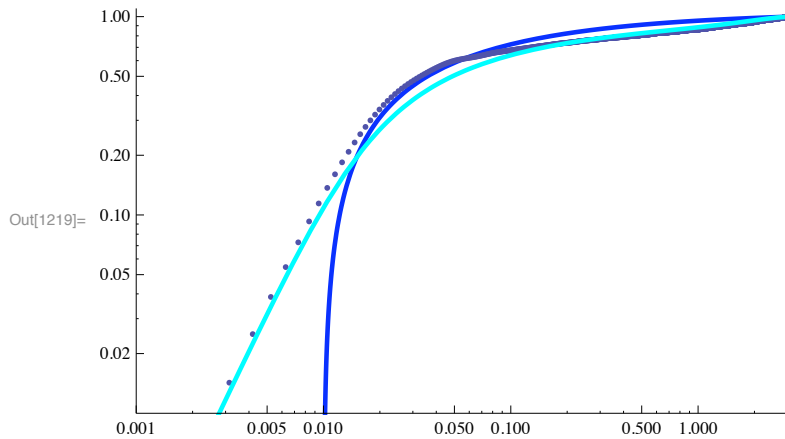
NIntegrate::nlim : theta0 = theta is not a valid limit of integration. >>

NIntegrate::nlim : theta0 = theta is not a valid limit of integration. >>

General::stop : Further output of NIntegrate::nlim will be suppressed during this calculation. >>

In[1219]:=

```
Show[cumProbSmallQ1Plot, cumProbKrstic1Plot, cumProbEmp1Plot]
```



In[1220]:=

```
Clear[a, ka]
```

In[1221]:=

```
ka0 := Sqrt[massAtom / massElectron * relenergy / 13.61 / .
  {massAtom -> 1.008 * 1836 * massElectron }]
```

In[1222]:=

```
ka0=ka0/.relenergy->1.
```

Out[1222]= 11.661

From Massey and Burhop (1952), the peak cross section at zero energy is $k^2 a^4 / 4 = (ka)^2 * a^2 / 4$. From Krstic and Schultz, $i_{zero} = 1.97 * 10^5 \text{ ao}^2$

```
izero=(ka)^2*a^2/4
```

or

In[1223]:=

```
a=(4*izero/k^2)^(1/4)/.{izero->1.97*10^5*ao^2,k->ka0/ao} //PowerExpand
```

Out[1223]= 8.72495 ao

In[1224]:=

```
Clear[thetaR, thetaD, cSmall]
```

■ For 10 eV in CM, Krstic and Schultz give

In[1225]:=

```
Flatten[Take[Import["h2hpeldiff10.txt", "CSV"], 6]]
```

```
Out[1225]= {Differential Elastic (EL) ) Cross Setion vs. CM scattering angle (theta),
  for H++H2 at ~ 10.0000 eV CM Energy,
  The Cross sections are multiplied by 2*pi*sin(theta)!,
  Ref.: P.S. Krstic and D.R. Schultz, Atomic and Plasma-Material Interaction,
  Data for Fusion, Vol.8, IAEA, Vienna, (1998)., }
```

```
In[1226]:= krstic10Data = Join[{0, 0}, Drop[Drop[Import[
  "c:\\users\\avp\\documents\\mathbook\\hydrogen\\h2hpcollisions\\h2hpeldiff10.
  txt", "Table"], 13], -2]]];
```

These data are $d\sigma/d\theta$ versus θ values. See Fig. 3 of Krstic and Schultz (1999). To get $d\sigma/d\Omega$, divide by $2\pi\sin[\theta]$, as is done next.

```
In[1227]:= diffQ10=Table[{#[[j,1]],#[[j,2]]/(2*Pi*Sin[#[[j,1]])}],{j,2,Length[#]-1}&[krstic10Dat
```

```
In[1228]:= diffQ10LogPlot=ListLogPlot[diffQ10,PlotRange->{{-0.001,Pi},{0.999,10^6}}];
```

```
In[1229]:= diffQ10LogLogPlot=ListLogLogPlot[diffQ10,PlotRange->{{0.0001,10},{0.999,10^6}}];
```

Back to $d\sigma/d\theta$ from Krstic & Schultz (1999).

```
In[1230]:= diffQm10=Table[{#[[j,1]],#[[j,2]]*(1-Cos[#[[j,1]])}],{j,Length[#]}&[krstic10Data];
```

```
In[1231]:= diffQm10Plot=ListPlot[diffQm10,PlotRange->{{0.0,Pi},{0.0,10}}];
```

From McDaniel, Mitchell, and Rudd, Atomic Collisions: Heavy Particle Collisions (Wiley, New York, 1993), p. 91, the classical differential scattering cross section in a. u. for a polarization potential of $V(r) = -c r^{-4} = -r\alpha\alpha\alpha\alpha^4/r^4$ at small angles is given by:

Assume a value for cSmall

```
In[1232]:= cSmall = cSmallFit /. enrel -> 10
```

```
Out[1232]= 0.00708236
```

```
In[1233]:= thetaD = thetaDFit /. {enrel -> 10, alphaau -> 0.808 / (0.529)^3}
```

```
Out[1233]= 0.00548039
```

```
thetaD = 0.005;
```

```
In[1234]:= thetaR = rainbowAngleFit /. enrel -> 10
```

```
Out[1234]= 0.358141
```

```
In[1235]:= iEmpirical10LogPlot = LogPlot[iEmpiricalR //. {ry -> 13.6, alphaau -> 0.808 / (0.529)^3,
  enrelau -> 10 / 27.211, thetaD -> thetaDFit}, {theta0, 0, Pi},
  PlotRange -> {{0, Pi}, {1, 100 000.}}, PlotStyle -> plotColorsLines[[4]]];
```

```
In[1236]:= ismall10=(ismall//. {ry->13.6,alphaau->0.808/(0.529)^3,enrelau->10/27.211,thetaD->thet
```

```
Out[1236]= 0.00708236 +  $\frac{1.04574 \text{ theta0 Csc}[\text{theta0}]}{2.22346 \times 10^{-6} + \text{theta0}^{5/2}}$ 
```

This has a singularity at small angles and should be replaced by the quantum formulation of Massey and Mohr for small angles.

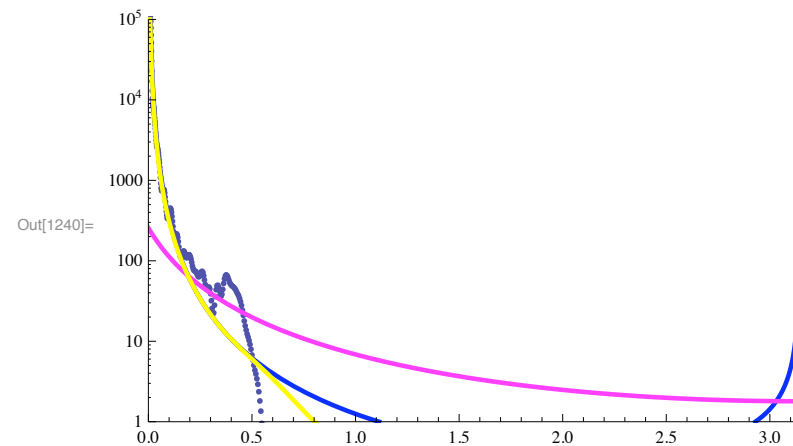

```
In[1237]:= smallAngleClassical10Plot =
  LogPlot[ismall10 /. {ry -> 13.6, alphaau -> 0.808 / (0.529)^3,
    enrelau -> 10 / 27.211, thetaD -> thetaDFit}, {theta0, 0, Pi},
  PlotRange -> {{0, Pi}, {1, 100 000.}}, PlotStyle -> plotColorsLines[[5]]];
```

```
In[1238]:= iEmpiricalR //.
  {alphaau -> 0.808 / (0.529)^3, enrelau -> 10 / 27.211, thetaD -> thetaDFit}
```

```
Out[1238]= { 0.00708236 + (1.04574 theta0 Csc[theta0]) /          theta0 < 1.79535
  ((1 + 60.7835 (-0.322327 + theta0)^4)^0.5 (2.22346 x 10^-6 + theta0^5/2))
  0.00708236          theta0 > 1.79535
  0                  True
```

```
In[1239]:= iEmpirical10LogPlot = LogPlot[iEmpiricalR //.
  {alphaau -> 0.808 / (0.529)^3, enrelau -> 10 / 27.211, thetaD -> thetaDFit},
  {theta0, 0, Pi}, PlotRange -> {{0, Pi}, {0.1, 100 000.}},
  PlotStyle -> plotColorsLines[[7]]];
```

```
In[1240]:= Show[smallAngleClassical10Plot, diffQ10LogPlot, qvSimkoIPlot, iEmpirical10LogPlot]
```



The Empirical (yellow) fit is good for angles below the rainbow peak, but is too small near the rainbow peak. The Simko fit (magenta) is good only over a very limited angular range.

The differential cross section for rotational excitation does not belong in the above plot since Krstic and Schultz did not consider it.

■ Now look at plots of scattering probability as used by Krstic and Schultz (1999)

These data are $d\sigma/d\theta$. To get $d\sigma/d\Omega$, divide by $2\pi\sin[\theta]$

```
In[1241]:= krstic10LogLogPlot=ListLogLogPlot[krstic10Data, PlotRange->{{0.001, 3.14}, {10^-3, 101000}}
```

```
In[1242]:= smallAngleClassical10Plot2 = LogLogPlot[(2 * Pi * ismall110 * Sin[theta0]) /. {ry -> 13.6,
  alphaau -> 0.808 / (0.529)^3, enrelau -> 10 / 27.211, thetaD -> thetaDFit},
  {theta0, 0.001, Pi}, PlotRange -> {{0.001, 3.14}, {10^-3, 10^6}},
  PlotStyle -> {Hue[0.5], Thickness[0.007]}];
```

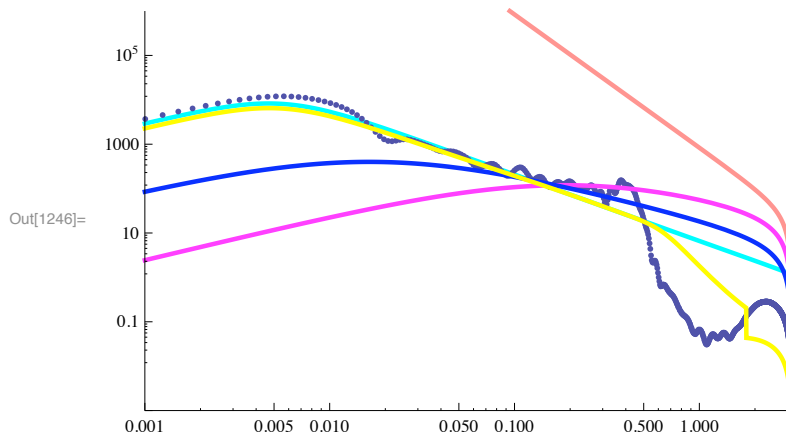
```
In[1243]:= iEmpirical10LogLogPlot = LogLogPlot[2 * Pi * iEmpiricalR * Sin[theta0] //.
  {alphaau -> 0.808 / (0.529)^3, enrelau -> 10 / 27.211, thetaD -> thetaDFit},
  {theta0, 0.001, Pi}, PlotRange -> {{0.001, Pi}, {0.001, 100 000.}},
  PlotStyle -> plotColorsLines[[7]]];
```

```
In[1244]:= iscr//.values/.{enrel->10}
```

```
Out[1244]= 1.84068 × 10-51 / (7.43556 × 10-27 - 7.43556 × 10-27 Cos[thetaSC])2
```

```
In[1245]:= scrCoul10LogLogPlot=LogLogPlot[(2*Pi*iscr*Sin[thetaSC]//.values/.enrel->10), {thetaSC,
  PlotRange->{{0.0001,3.14},{10^-3,10^6}},PlotStyle->plotColorsLines[[8]]];
```

```
In[1246]:= Show[smallAngleClassical10Plot2,krstic10LogLogPlot, qvSimkoI2Plot, qrSimkoI2Plot,
  scrCoul10LogLogPlot, iEmpirical10LogLogPlot]
```



■ Plot with momentum transfer weighting

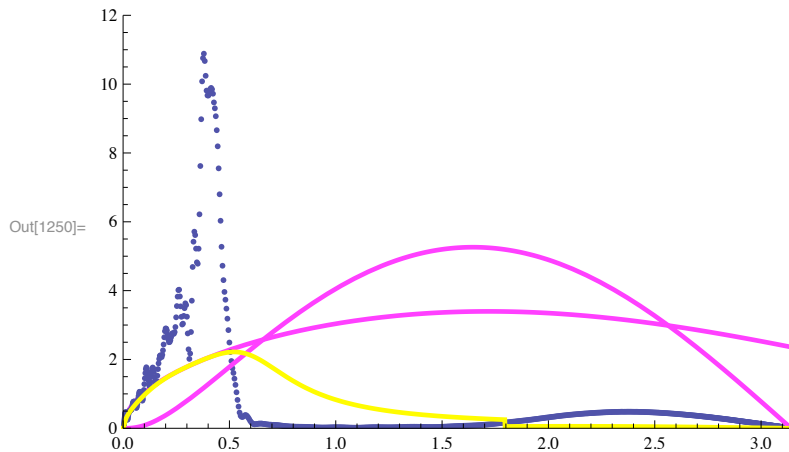
```
In[1247]:= smallAngleClassicalQm10Plot =
  Plot[(ismall110 * (1 - Cos[theta0]) * 2 * Pi * Sin[theta0]) /. {ry -> 13.6, alphaau ->
    0.808 / (0.529)^3, enrelau -> 10 / 27.211, thetaD -> thetaDFit}}, {theta0, 0, Pi},
  PlotRange -> {{0, Pi}, {0, 12.}}, PlotStyle -> plotColorsLines[[6]]];
```

This approaches $\theta_0 = 0$ as $\text{Sqrt}[\theta_0]$

```
In[1248]:= iRainbow10QmPlot=Plot[{(iRainbow2*(1-Cos[theta0])*2*Pi*Sin[theta0]/.
  {lr->100,qA->.00045,thetaR->0.145*Pi,k->Sqrt[2/2*1836*10./13.6])}], {theta0,0,Pi},
  PlotRange->{{0,Pi},{0.0,12}}, PlotStyle->plotColorsLines[[1]]];
```

```
In[1249]:= iEmpirical10QmPlot=Plot[{(iEmpiricalR*(1-Cos[theta0])*2*Pi*Sin[theta0] //
{alphaau -> 0.808/(0.529)^3, enrelau -> 10/27.211, thetaD -> thetaDFit}}, {theta0,0,Pi
PlotRange->{{0,Pi},{0.0,12}}, PlotStyle->plotColorsLines[[7]]];
```

```
In[1250]:= Show[smallAngleClassicalQm10Plot, diffQm10Plot, qmSimkoImPlot, iRainbow10QmPlot,iEmpir
```



Not a good fit, but comparable areas under the points and the yellow curve.

```
In[1251]:= NIntegrate[(iEmpiricalR * (1 - Cos[theta0]) * 2 * Pi * Sin[theta0] //
{alphaau -> 0.808 / (0.529)^3, enrelau -> 10 / 27.211, thetaD -> thetaDFit}),
{theta0, 0, Pi}]
```

Out[1251]= 1.94645

■ Cumulative scattering probability

```
In[1252]:= cumProbSmallQ10Plot=LogLogPlot[Evaluate[cumulativeIsmallPol/. {alphaau->0.808/(0.529)^
thetaD->thetaDFit}], {thetaCum,0.001,Pi}, PlotRange->{{0.001,Pi},{0.001,1}}, PlotStyle
```

```
In[1253]:= runTime = TimeUsed[] - startTime
```

Out[1253]= 96.764

```
In[1254]:= krstic10Fcn = Interpolation[krstic10Data][x]
```

Out[1254]= InterpolatingFunction[{{0., 3.14158}}, <>][x]

```
In[1255]:= total10=NIntegrate[krstic10Fcn, {x,0,krstic10Data[[-1,1]]}]
```

Out[1255]= 221.531

```
In[1256]:= cumProbKrstic10[theta_] :=
Integrate[krstic10Fcn, {x, 0, theta}] / total10 (* Cumulative Distr. Func. *)
```

```
In[1257]:= runTime = TimeUsed[] - startTime
```

```
Out[1257]= 96.796
```

```
In[1258]:= bins = 3000;
```

```
In[1259]:= cumProbKrstic10Table =  
  Table[{(j - 1) * Pi / bins * 1., cumProbKrstic10[(j - 1) * Pi / bins]}, {j, 1, bins}];
```

```
In[1260]:= runTime = TimeUsed[] - startTime
```

```
Out[1260]= 105.828
```

```
In[1261]:= cumProbKrstic10Plot=ListLogLogPlot[cumProbKrstic10Table,PlotRange->{{0.001,Pi},{0.01,1
```

```
In[1262]:= totalEmp10 =  
  NIntegrate[(iEmpiricalR * 2 * Pi * Sin[theta0] /. {alphaau -> 0.808 / (0.529)^3,  
    enrelau -> 10 / 27.211, thetaD -> thetaDFit, enrel -> 10}), {theta0, 0, Pi}]
```

```
Out[1262]= 147.424
```

```
In[1263]:= cumProbEmp10[theta_] := NIntegrate[  
  (iEmpiricalR * 2 * Pi * Sin[theta0] / totalEmp10 /. {alphaau -> 0.808 / (0.529)^3,  
    enrelau -> 10 / 27.211, thetaD -> thetaDFit, enrel -> 10}), {theta0, 0, theta}]
```

```
In[1264]:= cumProbEmp10Plot = LogLogPlot[cumProbEmp10[theta], {theta, 0.0001, Pi},  
  PlotRange -> {{0.0001, Pi}, {0.001, 1.1}}, PlotStyle -> plotColorsLines[[4]]];
```

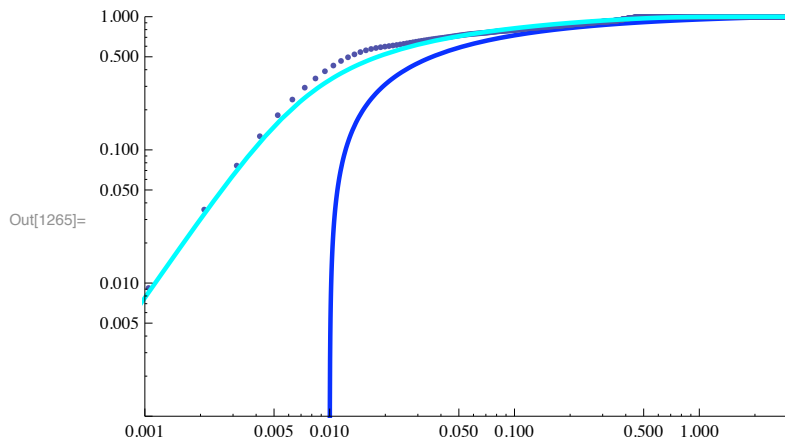
NIntegrate::nlm : theta0 = theta is not a valid limit of integration. >>

NIntegrate::nlm : theta0 = theta is not a valid limit of integration. >>

NIntegrate::nlm : theta0 = theta is not a valid limit of integration. >>

General::stop : Further output of NIntegrate::nlm will be suppressed during this calculation. >>

```
In[1265]:= Show[cumProbSmallQ10Plot, cumProbKrstic10Plot, cumProbEmp10Plot]
```



```
In[1266]:= Clear[thetaR, thetaD, cSmall]
```

■ For 100 eV in CM, Krstic and Schultz give

```
In[1267]:= Flatten[Take[Import["h2hpeldiff100.txt", "CSV"], 6]]
```

```
Out[1267]= {Differential Elastic (EL ) Cross Section vs. CM scattering angle (theta),
  for H++H2 at ~100.0000 eV CM Energy,
  The Cross sections are multiplied by 2*pi*sin(theta)!,
  Ref.: P.S. Krstic and D.R. Schultz, Atomic and Plasma-Material Interaction,
  Data for Fusion, Vol.8, IAEA, Vienna, (1998)., }
```

```
In[1268]:= krstic100Data =
  Join[{{0, 0}}, Drop[Drop[Import["h2hpeldiff100.txt", "Table"], 13], -2]];
```

```
In[1269]:= diffQ100=Table[{{%[[j,1]],%[[j,2]]/(2*Pi*Sin[%[[j,1]])}}, {j,2,Length[%]}];
```

```
In[1270]:= diffQ100Plot=ListLogPlot[%, PlotRange->{{-0.001, Pi}, {0.999*10^-5., 10100}}, DisplayFunci
```

```
In[1271]:= diffQ100LogPlot=ListLogLogPlot[%%, PlotRange->{{0.0001, 10}, {0.999*10^-5., 10100}}, Displa
```

here a = $\alpha_{\text{aa}}/2 \cdot \text{enrel}/27.12$

```
In[1272]:= a=4.50/2/(100/27.2)
```

```
Out[1272]= 0.612
```

here a = $\alpha_{\text{aa}}/2 \cdot \text{enrel}/27.12$

```
In[1273]:= pc=(4*a)^(1/4)
```

```
Out[1273]= 1.25084
```

Assume cSmall

```
In[1274]:= cSmall = 5. * 10^-5;
```

```
In[1275]:= cSmall = cSmallFit /. enrel -> 100
```

```
Out[1275]= 0.0000667021
```

```
In[1276]:= thetaD = thetaDFit /. {enrel -> 100, alphaau -> 0.808 / (0.529)^3}
```

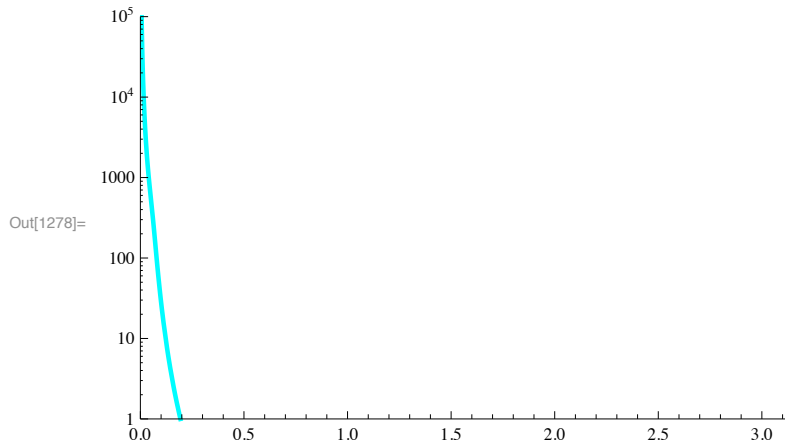
```
Out[1276]= 0.00226966
```

```
thetaD = 0.002;
```

```
In[1277]:= thetaR = rainbowAngleFit /. enrel -> 100
```

```
Out[1277]= 0.0358142
```

```
In[1278]:= iEmpirical100LogPlot = LogPlot[iEmpiricalR /. {ry -> 13.6, alphaau -> 0.808 / (0.529)^3, enrelau -> 100 / 27.211, thetaD -> thetaDFit}, {theta0, 0, Pi}, PlotRange -> {{0, Pi}, {1, 100 000.}}, PlotStyle -> plotColorsLines[[4]]]
```



From McDaniel, Mitchell, and Rudd, Atomic Collisions: Heavy Particle Collisions (Wiley, New York, 1993), p. 91, the classical differential scattering cross section in a. u. for a polarization potential of $V(r) = -c r^{-n} = -ry \cdot \alpha_{\text{au}} \cdot a_0^4 / r^n$ at small angles is given by:

```
In[1279]:= ismall100=ismall//. {ry->13.6,alphaau->0.808/(0.529)^3,enrelau->100/27.211,thetaD->the
```

```
Out[1279]= 
$$\frac{0.330693 \theta_0 \csc[\theta_0]}{2.45415 \times 10^{-7} + \theta_0^{5/2}}$$

```

This has a singularity at small angles and must be replaced by the quantum formulation of Massey et al.

If diffraction limits the polarization to $\theta > \theta_1 = 0.014$ rad as estimated below

```
In[1280]:= qTotalIsmallPol/.{ry->13.6,alphaau->0.808/(0.529)^3,enrelau->0.1/27.211}/.theta1->0.01
```

```
Out[1280]= 1036.49
```

This is to be compared to 122 calculated below for the total cross section using Massey-Mohr-Landau-Lifshitz. It shows that we have underestimated the diffraction angle.

```
In[1281]:= schrCoul100LogPlot=LogLogPlot[(2*Pi*iscr*Sin[thetaSC]//.values/.enrel->100), {thetaSC,0, Pi}, PlotRange->{{0.0001, Pi}, {10^-3, 10^6}}, PlotStyle->plotColorsLines[[8]]];
```

```
In[1282]:= smallAngleClassical100Plot = LogPlot[ismall100 /. {ry -> 13.6, alphaau -> 0.808 / (.529)^3, enrelau -> 100 / 27.211, thetaD -> thetaDFit}, {theta0, 0, Pi}, PlotRange -> {{0, Pi}, {10^-5, 100 000.}}, PlotStyle -> plotColorsLines[[5]]];
```

```
In[1283]:= ithetaClassicalExact100=ithetaClassicalExact;
```

The singularity does not occur very close to $p = p_c$. Lets assume it occurs near p_e , where by trial and error $\theta = \Pi$ at p_e of

```
In[1284]:= pe=1.25367;
```

```
In[1285]:= classicalExactTable1=Table[{pe*(1+.0001*j^3),theta100/.p->pe*(1+.0001*j^3), ithetaClas  
{j,0,50}}];
```

```
In[1286]:= classicalExactTable1=Table[{-%[[j,2]],%[[j,3]]},{j,Length[%]}];
```

```
In[1287]:= classicalExact1Plot=ListLogPlot[classicalExactTable1, PlotRange->{{0,Pi},{10^-5,10^7}}  
PlotStyle->plotColorsLines[[1]]];
```

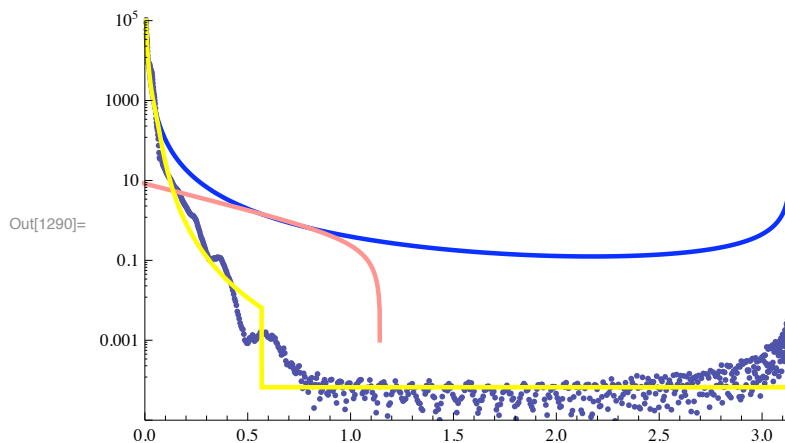
```
In[1288]:= iEmpiricalR //. {alphaau -> 0.808 / (0.529)^3, enrelau -> 100 / 27.211, thetaD -> thetaDFit}
```

```
Out[1288]= 
$$\begin{cases} 0.0000667021 + (0.330693 \theta_0 \operatorname{Csc}[\theta_0]) / & \theta_0 < 0.567739 \\ \left( (1 + 607829 \cdot (-0.0322327 + \theta_0)^4)^{0.5} (2.45415 \times 10^{-7} + \theta_0^{5/2}) \right) & \\ 0.0000667021 & \theta_0 > 0.567739 \\ 0 & \text{True} \end{cases}$$

```

```
In[1289]:= iEmpirical100LogPlot = LogPlot[iEmpiricalR //.  
{alphaau -> 0.808 / (0.529)^3, enrelau -> 100 / 27.211, thetaD -> thetaDFit},  
{theta0, 0, Pi}, PlotRange -> {{0, Pi}, {10^-5, 10^5}},  
PlotStyle -> plotColorsLines[[7]]];
```

```
In[1290]:= Show[smallAngleClassical100Plot,diffQ100Plot,classicalExact1Plot, scrCoul100LogPlot,iE
```



I am not sure what one learns from the comparison of the screened Coulomb cross section with the quantum calculation. The screened Coulomb result is a couple of orders of magnitude larger at most angles.

```
In[1291]:= krstic100Plot=ListLogLogPlot[krstic100Data, PlotRange->{{0.001,4},{10^-4,10^5}}, Displa
```

In[1292]:=

```
smallAngleClassical100Plot2 =
  LogLogPlot[(2 * Pi * ismall100 * Sin[theta0]) /. {ry -> 13.6,
    alphaau -> 0.808 / (0.529)^3, enrelau -> 100. / 27.211, thetaD -> thetaDFit},
    {theta0, 0.001, Pi}, PlotRange -> {{0.001, Pi}, {10^-4, 10^5}},
    PlotStyle -> {Hue[0.5], Thickness[0.007]}];
```

In[1293]:=

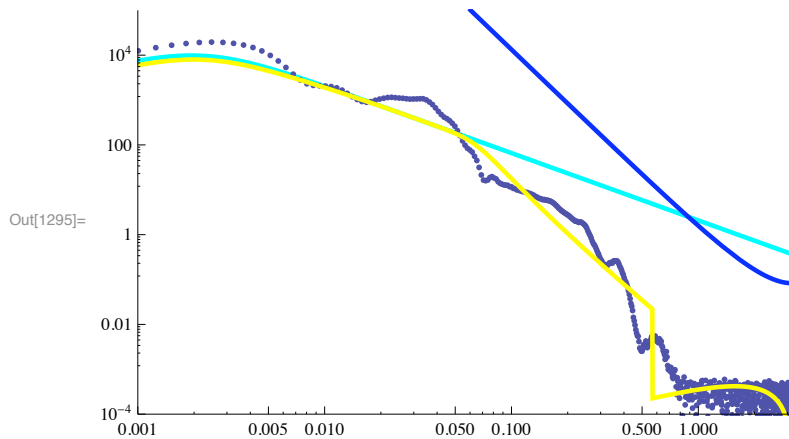
```
scrCoul100LogLogPlot=LogLogPlot[{Evaluate[{iscr/.values/.enrel->100}], {thetaSC,0.001,
  PlotRange->{{0.0001,Pi},{10^-4,10^5}}, PlotStyle->plotColorsLines[[5]]];
```

In[1294]:=

```
iEmpirical100LogLogPlot = LogLogPlot[2 * Pi * iEmpiricalR * Sin[theta0] /.
  {alphaau -> 0.808 / (0.529)^3, enrelau -> 100 / 27.211, thetaD -> thetaDFit},
  {theta0, 0.001, Pi}, PlotRange -> {{0.001, Pi}, {0.0001, 10^5}},
  PlotStyle -> plotColorsLines[[7]]];
```

In[1295]:=

```
Show[smallAngleClassical100Plot2,krstic100Plot, scrCoul100LogLogPlot,iEmpirical100LogL
```



In[1296]:=

```
cumProbSmall100Plot=LogLogPlot[Evaluate[cumulativeIsmallPol/. {alphaau->5.4, enrelau->
  theta1->0.01,thetaD->thetaDFit}], {thetaCum,0.001,Pi}, PlotRange->{{0.001,Pi},{0.001,1}
  PlotStyle->plotColorsLines[[5]]];
```

In[1297]:=

```
runTime = TimeUsed[] - startTime
```

Out[1297]= 141.785

In[1298]:=

```
krstic100Fcn = Interpolation[krstic100Data][x]
```

Out[1298]= InterpolatingFunction[{{0., 3.14158}}, <>][x]

In[1299]:=

```
total100=NIntegrate[krstic100Fcn, {x,0,krstic100Data[[-1,1]]}]
```

Out[1299]= 132.203

In[1300]:=

```
cumProbKrstic100[theta_] :=
  Integrate[krstic100Fcn, {x, 0, theta}] / total100 (* Cumulative Distr. Func. *)
```



```
In[1301]:= runTime = TimeUsed[] - startTime
```

```
Out[1301]= 141.801
```

```
In[1302]:= bins = 3000;
```

```
In[1303]:= cumProbKrstic100Table =  
  Table[{(j - 1) * Pi / bins * 1., cumProbKrstic100[(j - 1) * Pi / bins]}, {j, 1, bins}];
```

```
In[1304]:= runTime = TimeUsed[] - startTime
```

```
Out[1304]= 150.833
```

```
In[1305]:= cumProbKrstic100Plot=ListLogLogPlot[cumProbKrstic100Table,PlotRange->{{0.001,Pi},{0.01
```

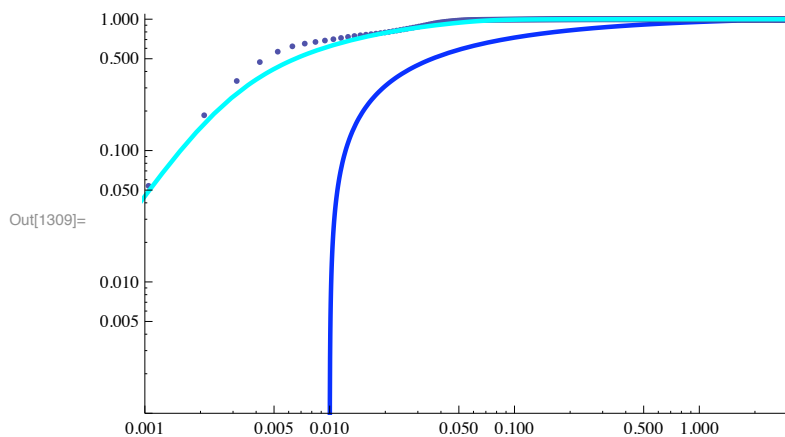
```
In[1306]:= totalEmp100 =  
  NIntegrate[(iEmpiricalR * 2 * Pi * Sin[theta0] /. {alphaau -> 0.808 / (0.529) ^ 3,  
    enrelau -> 100 / 27.211, thetaD -> thetaDFit, enrel -> 100}), {theta0, 0, Pi}]
```

```
Out[1306]= 70.4525
```

```
In[1307]:= cumProbEmp100[theta_] := NIntegrate[  
  (iEmpiricalR * 2 * Pi * Sin[theta0] / totalEmp100 /. {alphaau -> 0.808 / (0.529) ^ 3,  
    enrelau -> 100 / 27.211, thetaD -> thetaDFit, enrel -> 100}), {theta0, 0, theta}]
```

```
In[1308]:= cumProbEmp100Plot = Quiet[LogLogPlot[cumProbEmp100[theta], {theta, 0.0001, Pi},  
  PlotRange -> {{0.0001, Pi}, {0.01, 1.1}}, PlotStyle -> plotColorsLines[[4]]];
```

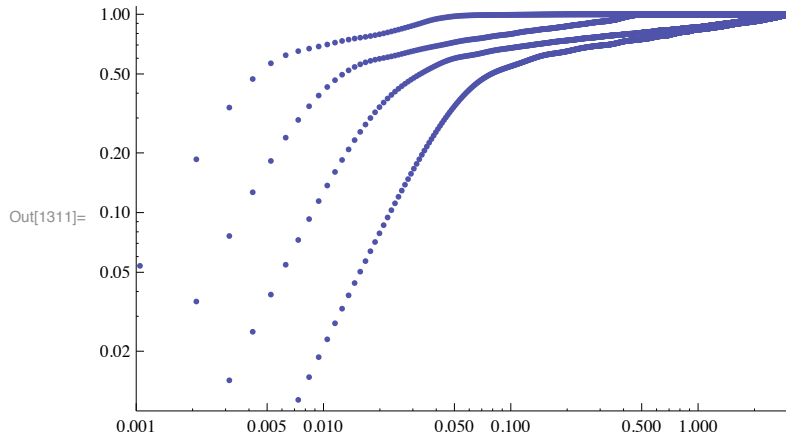
```
In[1309]:= Show[cumProbSmall100Plot, cumProbKrstic100Plot,cumProbEmp100Plot]
```



```
In[1310]:= Clear[a, ka]
```

■ Summary of Krstic & Schultz cumulative scattering data

```
In[1311]:= Show[cumProbKrstic01Plot, cumProbKrstic1Plot, cumProbKrstic10Plot, cumProbKrstic100Plot
```



```
In[1312]:= Clear[thetaR, thetaD, cSmall]
```

■ For 500 eV in Lab and 333 in COM, Stebbings et al (1988) give tabulated experimental results:

```
In[1313]:= Take[Import["hph2ri05.txt", "CSV"], -6]
```

```
Out[1313]= {{H+ + H2 from Smith et al
              (unpublished) (1988) Part of former file HPH2AN05.WK1 88/12/20},
             {EL = 5.00E+02 eV m = 1.00E+00 M = 2.00E+00},
             { 2mM/(m+M)^2 = 4.44E-01
               a=M^2 = 4.00E+00 THL*I(THL) del},
             {THL THL -c b cos(THg) THg I(THL)
               *sin(THL) DELCS tau ELCS},
             {rd deg cm2/str cm2/rd eVcm2/str keVdeg eVcm2},
             {Note: I(THL) extrapolated from .013 rd to 0.0175 rd}}
```

```
In[1314]:= dataRice333A=Drop[Import["hph2ri05.txt", "Table"], -6];
```

We add points at low angle based on L. Johnson (private communication 1989)

In[1315]=

```
dataRice333 = Join[{{0, 4. * 10^-10}},
  {{5. * 10^-2 / 57.3, 2. * 10^-10}}, {{8. * 10^-2 / 57.3, 1.02 * 10^-10}},
  Table[#[[j, 1]], #[[j, 7]], {j, Length[#]}] &[dataRice333A]
```

```
Out[1315]= {{0, 4. * 10^-10}, {0.0008726, 2. * 10^-10}, {0.00139616, 1.02 * 10^-10}, {0.0018, 5.51 * 10^-11},
  {0.0022, 3.28 * 10^-11}, {0.0026, 2.18 * 10^-11}, {0.003, 1.73 * 10^-11},
  {0.0034, 1.45 * 10^-11}, {0.0038, 1.23 * 10^-11}, {0.0042, 1. * 10^-11}, {0.0046, 8.29 * 10^-12},
  {0.005, 6.61 * 10^-12}, {0.0054, 5.61 * 10^-12}, {0.0058, 4.9 * 10^-12}, {0.0062, 4.4 * 10^-12},
  {0.0066, 4. * 10^-12}, {0.007, 3.73 * 10^-12}, {0.0074, 3.34 * 10^-12}, {0.0078, 2.85 * 10^-12},
  {0.0082, 2.46 * 10^-12}, {0.0086, 2.04 * 10^-12}, {0.009, 1.74 * 10^-12}, {0.0094, 1.45 * 10^-12},
  {0.0098, 1.14 * 10^-12}, {0.0102, 9.09 * 10^-13}, {0.0106, 7.21 * 10^-13}, {0.011, 6.07 * 10^-13},
  {0.0114, 5.11 * 10^-13}, {0.0118, 4.45 * 10^-13}, {0.0122, 3.87 * 10^-13},
  {0.0126, 3.3 * 10^-13}, {0.013, 3.12 * 10^-13}, {0.014, 2.05 * 10^-13}, {0.0148, 1.59 * 10^-13},
  {0.0157, 1.28 * 10^-13}, {0.0166, 1.07 * 10^-13}, {0.0175, 8.54 * 10^-14}}
```

```
ListLogLogPlot[dataRice333, PlotRange -> {{0.0001, 0.1}, {10^-14, 10^-9}}]
```

```
cSmall = 0
```

In[1316]=

```
cSmall = cSmallFit /. enrel -> 333
```

```
Out[1316]= 0.0000123162
```

In[1317]=

```
thetaD = thetaDFit /. {enrel -> 333, alphaau -> 0.808 / (0.529)^3}
```

```
Out[1317]= 0.00143129
```

```
thetaD = 0.002;
```

In[1318]=

```
thetaR = rainbowAngleFit /. enrel -> 330
```

```
Out[1318]= 0.0108528
```

In[1319]=

```
diffQRice333=Table[{dataRice333[[j,1]],dataRice333[[j,2]]/(0.528*10^-8)^2},{j,Length[d
```

We next convert the experimental data from the Lab frame to Center-of-Mass frame

From p. 9 of McDaniel (1964), we need to find the center-of-mass angles.

In[1320]=

```
Solve[Tan[thetaLab]==Sin[thetaCM]/(1/2+Cos[thetaCM]),thetaCM];
```

Solve::ifun : Inverse functions are being used by Solve, so
some solutions may not be found; use Reduce for complete solution information. >>

In[1321]=

```
thetaCM1[thetaLab_]=thetaCM/.%[[4]]
```

```
Out[1321]= ArcCos[1/4 (-1 + Cos[2 thetaLab] + sqrt(7 Cos[thetaLab]^2 + Cos[thetaLab]^2 Cos[2 thetaLab]))]
```

From p. 14 of McDaniel (1964) we need the COM differential cross section

$$\text{diffLab} = (1/4 + \cos[\text{thetaCM}] + 1)^{3/2} / (1 + 1/2 \cos[\text{thetaCM}]) * \text{diffCM}$$

so that

```
In[1322]:= diffCM[thetaCM_, diffLab_] := diffLab / (1/4 + Cos[thetaCM] + 1)^(3/2) / (1 + 1/2 * Cos[thetaCM])
```

```
In[1323]:= diffCM[thetaCM_, diffLab_]
```

$$\text{Out[1323]} = \text{diffLab}__ / \left(\left(1 + \frac{\cos[\text{thetaCM}__] }{2} \right) \left(\frac{5}{4} + \cos[\text{thetaCM}__] \right)^{3/2} \right)$$

```
In[1324]:= diffQCMRice333 = Table[{thetaCM1[diffQRice333[[j, 1]]], (diffCM[diffQRice333[[j, 1]]], diffQRice333[[j, Length[diffQRice333]]]}];
```

```
In[1325]:= diffQCMRice333Plot = ListLogLogPlot[diffQCMRice333, PlotRange -> {{0.0001, 10}, {1, 10^7}}, PlotStyle -> {Hue[0.5], Thickness[0.007]}];
```

```
In[1326]:= ismall333 = (ismall /. {ry -> 13.6, alphaau -> 0.808 / (0.529)^3, enrelau -> 333 / 27.211, thetaD -> theta0})
```

$$\text{Out[1326]} = \frac{0.181219 \text{ theta0} \text{ Csc}[\text{theta0}]}{7.75033 \times 10^{-8} + \text{theta0}^{5/2}}$$

```
In[1327]:= smallAngleClassical333Plot = LogLogPlot[ismall333, {theta0, 0.0001, Pi}, PlotRange -> {{0.0001, 10}, {1, 10^7}}, PlotStyle -> {Hue[0.5], Thickness[0.007]}];
```

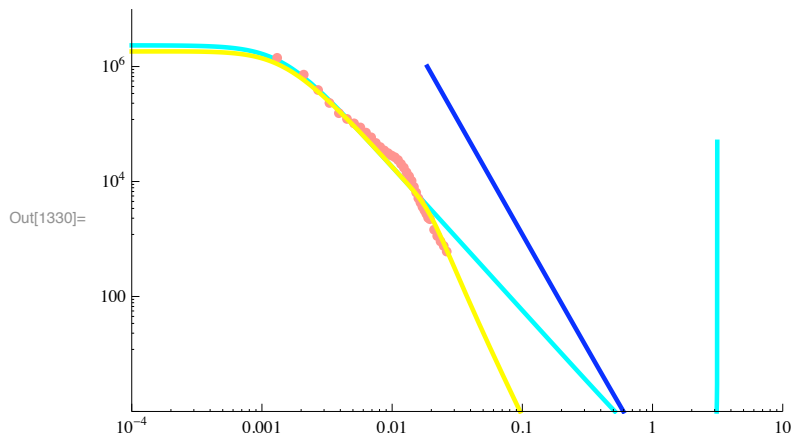
This has a singularity at small angles and must be replaced by the quantum formulation of Massey et al. and others.

```
In[1328]:= scrCoul333Plot = LogLogPlot[{Evaluate[isr /. values /. enrel -> 333]}, {thetaSC, 0.0001, Pi}, PlotRange -> {{0.0001, Pi}, {1, 10^6}}, PlotStyle -> plotColorsLines[[5]]];
```

```
In[1329]:= iEmpirical333LogPlot = LogLogPlot[Evaluate[iEmpiricalR /. {alphaau -> 0.808 / (0.529)^3, enrelau -> 333 / 27.211, thetaD -> thetaDFit, thetaR -> 0.01085}], {theta0, 0.0001, Pi}, PlotRange -> {{0.0001, Pi}, {1, 2. * 10^6}}, PlotStyle -> plotColorsLines[[7]]];
```

In[1330]=

```
Show[smallAngleClassical333Plot,diffQCMRice333Plot, scrCoul333Plot,iEmpirical333LogPlo
```



Out[1330]=

using the Krstic and Schultz type of plot gives

In[1331]=

```
rice333=Join[Table[{diffQCMRice333[[j,1]],diffQCMRice333[[j,2]]*2*Pi*Sin[diffQCMRice333[[j,Length[diffQCMRice333]]]}]]
```

Out[1331]=

```
{{0, 0.}, {0.0013089, 11654.2}, {0.00209424, 9509.85}, {0.0027, 6623.12},
{0.0033, 4818.76}, {0.0039, 3785.02}, {0.0045, 3465.82}, {0.0051, 3292.2},
{0.0057, 3121.24}, {0.0063, 2804.71}, {0.00689999, 2546.55}, {0.00749999, 2207.04},
{0.00809999, 2023.}, {0.00869999, 1897.86}, {0.00929999, 1821.73},
{0.00989998, 1762.97}, {0.0105, 1743.6}, {0.0111, 1650.51}, {0.0117, 1484.5},
{0.0123, 1347.07}, {0.0129, 1171.57}, {0.0135, 1045.76}, {0.0140999, 910.201},
{0.0146999, 746.058}, {0.0152999, 619.165}, {0.0158999, 510.368}, {0.0164999, 445.886},
{0.0170999, 389.017}, {0.0176999, 350.659}, {0.0182999, 315.293}, {0.0188999, 277.67},
{0.0194999, 270.858}, {0.0209998, 191.658}, {0.0221998, 157.147},
{0.0235498, 134.201}, {0.0248997, 118.615}, {0.0262497, 99.8034}}
```

In[1332]=

```
rice333Plot=ListLogLogPlot[%,PlotRange->{{0.0001,10},{1,100000.}}, DisplayFunction->Id
```

In[1333]=

```
smallAngleClassical333Plot2 = LogLogPlot[(2 * Pi * ismall1333 * Sin[theta0]) /.
{ry -> 13.6, alphaau -> 0.808 / (0.529)^3, enrelau -> 333 / 27.211},
{theta0, 0.0001, Pi}, PlotRange -> {{0.0001, 10}, {1, 100000.}},
PlotStyle -> {Hue[0.5], Thickness[0.007]}, DisplayFunction -> Identity];
```

The following screened Coulomb parameters are chosen to fit the Rice experiments

In[1334]=

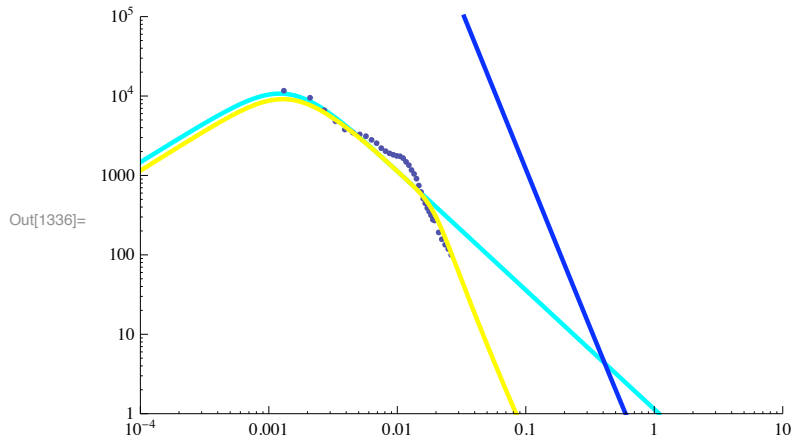
```
scrCoul333LogLogPlot=LogLogPlot[{Evaluate[(iscr//.values/.enrel->333)}], {thetaSC,0.00
PlotRange->{{0.0001,Pi},{1,10^5}}, PlotStyle->plotColorsLines[[5]]];
```

In[1335]=

```
iEmpirical333LogLogPlot =
LogLogPlot[2 * pi * iEmpiricalR * Sin[theta0] //. {alphaau -> 0.808 / (0.529)^3,
enrelau -> 333 / 27.211, thetaD -> thetaDFit}, {theta0, 0.0001, Pi},
PlotRange -> {{0.0001, Pi}, {1, 100000.}}, PlotStyle -> plotColorsLines[[7]]];
```

In[1336]:=

```
Show[smallAngleClassical333Plot2, rice333Plot, iEmpirical333LogLogPlot, scrCoul333LogLogP
```



Out[1336]=

The experimental data fails to show show a maximum at small angles, such as found at lower energies.

In[1337]:= `maxAngle = rice333[[-1, 1]]`

Out[1337]= 0.0262497

In the following, note that `rice333` is $d\sigma/d\theta$. We add contributions from large and small angles that are beyond the tabulated values.

In[1338]:=

```
rice333Fcn = Interpolation[rice333, InterpolationOrder -> 2][x]
```

Out[1338]= InterpolatingFunction[{{0., 0.0262497}}, <>][x]

In[1339]:=

```
qatt333rice = NIntegrate[rice333Fcn, {x, rice333[[1, 1]], rice333[[-1, 1]]}] +
  NIntegrate[100 / (x / 0.026)^4, {x, rice333[[-1, 1]], Pi}] +
  NIntegrate[rice333[[1, 2]], {x, 0, rice333[[1, 1]]}]
```

Out[1339]= 54.7951

Add on

In[1340]:=

```
Integrate[rice333[[2, 2]], {x, 0, rice333[[1, 1]]}]
```

Out[1340]= 0.

In[1341]:=

```
integrate333qmrice = NIntegrate[rice333Fcn * (1 - Cos[x]), {x, 0, maxAngle}] +
  NIntegrate[100 / (x / maxAngle)^4 * (1 - Cos[x]), {x, maxAngle, Pi}]
```

Out[1341]= 0.00231992

Note that the Sin^3 becomes Sin^2

```
In[1342]:= integrate333qvrice =
  NIntegrate[Interpolation[rice333][x] * (Sin[x]) ^ 2, {x, 0.0007, 0.02}] +
  NIntegrate[100 / (x / 0.026) ^ 4 * (Sin[x]) ^ 3, {x, 0.026, Pi}]
```

```
Out[1342]= 0.00253387
```

```
In[1343]:= cumProbSmall333Plot=LogLogPlot[Evaluate[cumulativeIsmallPol/. {alphaau->5.4, enrelau->
  theta1->0.01,thetaD->thetaDFit}], {thetaCum,0.001,Pi}, {PlotRange->{{0.001,Pi},{0.001,1}
  PlotStyle->plotColorsLines[[5]]];
```

```
In[1344]:= runTime = TimeUsed[] - startTime
```

```
Out[1344]= 200.598
```

```
In[1345]:= total333=NIntegrate[rice333Fcn, {x,0,maxAngle}]
```

```
Out[1345]= 53.953
```

```
In[1346]:= cumProbRice333[theta_] :=
  Integrate[rice333Fcn, {x, 0, theta}] / total333 (* Cumulative Distr. Func. *)
```

```
In[1347]:= runTime = TimeUsed[] - startTime
```

```
Out[1347]= 200.598
```

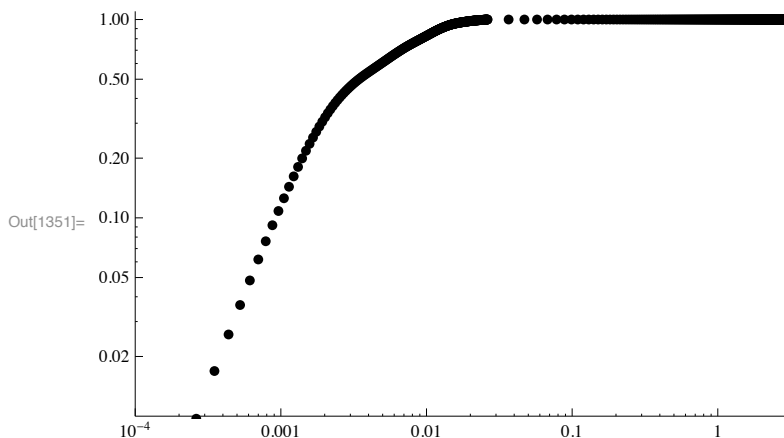
```
In[1348]:= bins = 300;
```

```
In[1349]:= cumProbRice333Table = Table[{(j - 1) * maxAngle / bins * 1.,
  cumProbRice333[(j - 1) * maxAngle / bins]}, {j, 1, bins}];
```

```
In[1350]:= runTime = TimeUsed[] - startTime
```

```
Out[1350]= 200.661
```

```
In[1351]:= cumProbRice333Plot=ListLogLogPlot[{cumProbRice333Table,Table[{maxAngle+(j-1)*(Pi-maxAn
  PlotRange->{{0.0001,Pi},{0.01,1.1}},PlotStyle->plotColorsPoints[{{9,9}}]]]
```



```
In[1352]:= runTime = TimeUsed[] - startTime
```

```
Out[1352]= 200.801
```

```
In[1353]:= totalEmp333 =  
NIntegrate[(iEmpiricalR * 2 * Pi * Sin[theta0] /. {alphaau -> 0.808 / (0.529)^3,  
enrelau -> 333 / 27.211, thetaD -> thetaDFit, enrel -> 333}), {theta0, 0, Pi}]
```

```
Out[1353]= 46.4093
```

```
In[1354]:= thetaR
```

```
Out[1354]= 0.0108528
```

```
In[1355]:= iEmpiricalR
```

```
Out[1355]= 
$$\begin{cases} 0.0000123162 + \left(0.27135 \sqrt{\text{alphaau } \theta_0 \text{ Csc}[\theta_0]}\right) / & \theta_0 < 0.31253 \\ \left(\sqrt{\text{enrelau}} \left(1 + 7.20837 \times 10^7 (-0.0097675 + \theta_0)^4\right)^{0.5} \right. \\ \left. \left(7.75033 \times 10^{-8} + \theta_0^{5/2}\right)\right) & \\ 0.0000123162 & \theta_0 > 0.31253 \\ 0 & \text{True} \end{cases}$$

```

```
In[1356]:= cumProbEmp333[theta_] = NIntegrate[  
(iEmpiricalR * 2 * Pi * Sin[theta0] / totalEmp333 /. {alphaau -> 0.808 / (0.529)^3,  
enrelau -> 333 / 27.211, thetaD -> thetaDFit, enrel -> 333}), {theta0, 0, theta}]
```

```
NIntegrate::nlm : theta0 = theta is not a valid limit of integration. >>
```

```
NIntegrate::nlm : theta0 = theta is not a valid limit of integration. >>
```

```
Out[1356]= 
$$\text{NIntegrate}\left[\frac{\text{iEmpiricalR } 2 \pi \text{ Sin}[\theta_0]}{\text{totalEmp333}} \text{ /. } \left\{\text{alphaau} \rightarrow \frac{0.808}{0.529^3},\right.\right.$$
  

$$\left.\left.\text{enrelau} \rightarrow \frac{333}{27.211}, \text{ thetaD} \rightarrow \text{thetaDFit}, \text{ enrel} \rightarrow 333\right\}, \{\theta_0, 0, \theta\}\right]$$

```


In[1357]:=

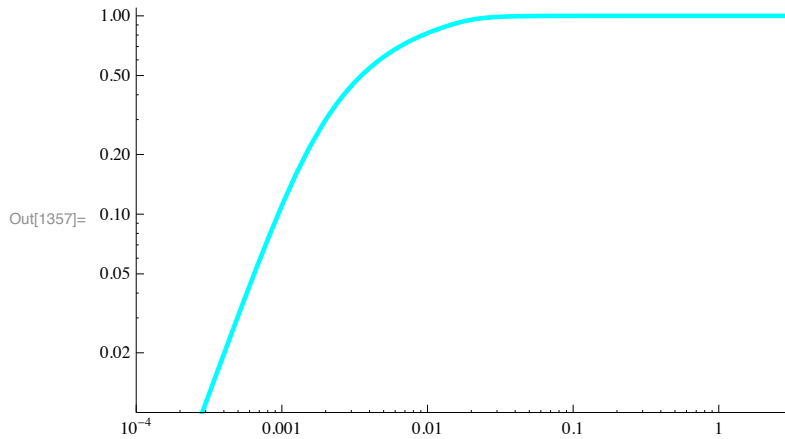
```
cumProbEmp333Plot = LogLogPlot[cumProbEmp333[theta], {theta, 0.0001, Pi},
  PlotRange -> {{0.0001, Pi}, {0.01, 1.1}}, PlotStyle -> plotColorsLines[[4]]]
```

NIntegrate::nlm : theta0 = theta is not a valid limit of integration. >>

NIntegrate::nlm : theta0 = theta is not a valid limit of integration. >>

NIntegrate::nlm : theta0 = theta is not a valid limit of integration. >>

General::stop : Further output of NIntegrate::nlm will be suppressed during this calculation. >>



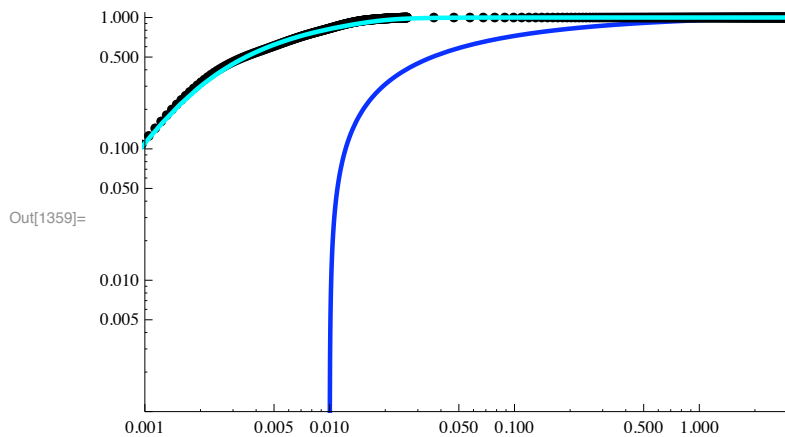
In[1358]:=

```
runTime = TimeUsed[] - startTime
```

Out[1358]= 258.646

In[1359]:=

```
Show[cumProbSmall1333Plot, cumProbRice333Plot, cumProbEmp333Plot]
```



```
In[1360]:= Clear[thetaR, thetaD, cSmall]
```

- For 1500 eV in Lab and 1000 in COM, Stebbings et al (1988) give tabulated experimental results:

In[1361]:=

```
Take[Import["hph2ri05.txt", "CSV"], -6]
```

```
Out[1361]= {{H+ + H2 from Smith et al
  (unpublished) (1988) Part of former file HPH2AN05.WK1 88/12/20},
 {EL = 5.00E+02 eV m = 1.00E+00 M = 2.00E+00},
 { 2mM/(m+M)^2 = 4.44E-01
  a=M^2 = 4.00E+00 THL*I(THL) del},
 {THL THL -c b cos(THg) THg I(THL)
  *sin(THL) DELCS tau ELCS},
 {rd deg cm2/str cm2/rd eVcm2/str keVdeg eVcm2},
 {Note: I(THL) extrapolated from .013 rd to 0.0175 rd}}
```

In[1362]:=

```
dataRice1000A=Drop[Import["hph2ri15.txt", "Table"], -6];
```

We add points at low angle based on L. Johnson (private communication 1989)

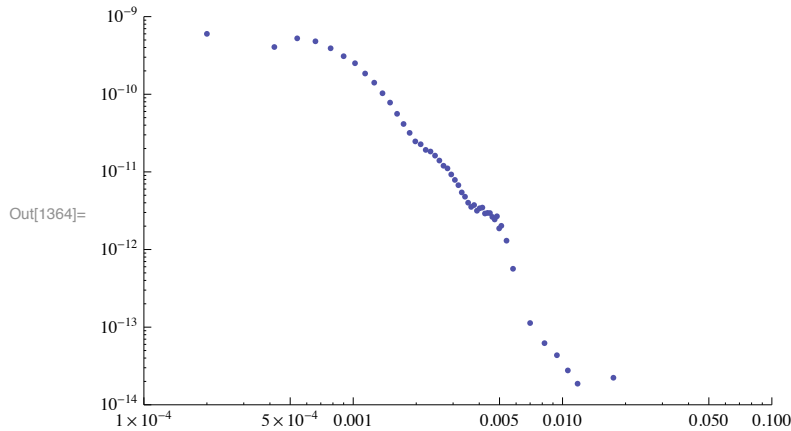
In[1363]:=

```
dataRice1000 = Join[{{0, 8. * 10^-10}}, {{0.0002, 6 * 10^-10}},
  Table[#[[j, 1]], #[[j, 7]]], {j, Length[#]}] &[dataRice1000A]
```

```
Out[1363]= {{0, 8. * 10^-10}, {0.0002,  $\frac{3}{5000000000}$ }, {0.00042, 4.06 * 10^-10}, {0.00054, 5.25 * 10^-10},
 {0.00066, 4.81 * 10^-10}, {0.00078, 3.91 * 10^-10}, {0.0009, 3.09 * 10^-10},
 {0.00102, 2.51 * 10^-10}, {0.00114, 1.85 * 10^-10}, {0.00126, 1.41 * 10^-10},
 {0.00138, 1.03 * 10^-10}, {0.0015, 7.81 * 10^-11}, {0.00162, 5.6 * 10^-11},
 {0.00174, 4.14 * 10^-11}, {0.00186, 3.18 * 10^-11}, {0.00198, 2.47 * 10^-11},
 {0.0021, 2.27 * 10^-11}, {0.00222, 1.92 * 10^-11}, {0.00234, 1.83 * 10^-11},
 {0.00246, 1.62 * 10^-11}, {0.00258, 1.4 * 10^-11}, {0.0027, 1.2 * 10^-11},
 {0.00282, 1.11 * 10^-11}, {0.00294, 9.27 * 10^-12}, {0.00306, 7.88 * 10^-12},
 {0.00318, 6.74 * 10^-12}, {0.0033, 5.44 * 10^-12}, {0.00342, 4.79 * 10^-12},
 {0.00354, 4.01 * 10^-12}, {0.00366, 3.54 * 10^-12}, {0.00378, 3.74 * 10^-12},
 {0.0039, 3.16 * 10^-12}, {0.00402, 3.4 * 10^-12}, {0.00414, 3.47 * 10^-12},
 {0.00426, 2.91 * 10^-12}, {0.00438, 2.96 * 10^-12}, {0.0045, 2.95 * 10^-12},
 {0.00462, 2.63 * 10^-12}, {0.00474, 2.44 * 10^-12}, {0.00486, 2.68 * 10^-12},
 {0.00498, 1.87 * 10^-12}, {0.0051, 2.02 * 10^-12}, {0.0054, 1.3 * 10^-12},
 {0.0058, 5.65 * 10^-13}, {0.007, 1.13 * 10^-13}, {0.0082, 6.22 * 10^-14}, {0.0094, 4.35 * 10^-14},
 {0.0106, 2.77 * 10^-14}, {0.0118, 1.87 * 10^-14}, {0.013, 8.35 * 10^-15}, {0.0142, 8.24 * 10^-15},
 {0.0154, 6.66 * 10^-15}, {0.0166, 7.05 * 10^-15}, {0.0175, 2.23 * 10^-14}}
```

In[1364]:=

```
ListLogLogPlot[dataRice1000, PlotRange -> {{0.0001, 0.1}, {10^-14, 10^-9}}]
```



Out[1364]=

```
cSmall = 0
```

In[1365]:=

```
cSmall = cSmallFit /. enrel -> 1000
```

Out[1365]= 2.88615×10^{-6}

In[1366]:=

```
thetaD = thetaDFit /. {enrel -> 1000, alphaau -> 0.808 / (0.529)^3}
```

Out[1366]= 0.000939022

```
thetaD = 0.0008;
```

In[1367]:=

```
thetaR = rainbowAngleFit /. enrel -> 1000
```

Out[1367]= 0.00358142

In[1368]:=

```
diffQRice1000=Table[{dataRice1000[[j,1]],dataRice1000[[j,2]]/(0.528*10^-8)^2},{j,Lengt
```

We next convert the experimental data from the Lab frame to Center-of-Mass frame

From p. 9 of McDaniel (1964), we need to find the center-of-mass angles.

In[1369]:=

```
Solve[Tan[thetaLab]==Sin[thetaCM]/(1/2+Cos[thetaCM]),thetaCM];
```

Solve::ifun : Inverse functions are being used by Solve, so some solutions may not be found; use Reduce for complete solution information. >>

In[1370]:=

```
thetaCM1[thetaLab_]=thetaCM/.%[[4]]
```

```
Out[1370]= ArcCos[1/4 (-1 + Cos[2 thetaLab] + Sqrt[2] Sqrt[7 Cos[thetaLab]^2 + Cos[thetaLab]^2 Cos[2 thetaLab]])]
```

From p. 14 of McDaniel (1964) we need the COM differential cross section

```
diffLab=(1/4+Cos[thetaCM]+1)^(3/2)/(1+1/2*Cos[thetaCM])*diffCM
```

so that

```
In[1371]:= diffCM[thetaCM_,diffLab_] := diffLab/(1/4+Cos[thetaCM]+1)^(3/2)/(1+1/2*Cos[thetaCM])
```

```
In[1372]:= diffCM[thetaCM_, diffLab_]
```

```
Out[1372]= diffLab_/((1 + Cos[thetaCM_]/2) (5/4 + Cos[thetaCM_] )^(3/2))
```

```
In[1373]:= diffQCMRice1000=Table[{thetaCM1[diffQRice1000[[j,1]]],(diffCM[diffQRice1000[[j,1]],diffQRice1000[[j,Length[diffQRice1000]]])};
```

```
In[1374]:= diffQCMRice1000Plot=ListLogLogPlot[diffQCMRice1000,PlotRange->{{0.0001,10},{1,10^7}},
```

```
In[1375]:= ismall1000=(ismall//. {ry->13.6,alphaau->0.808/(0.529)^3,enrelau->1000/27.211,thetaD->
```

```
Out[1375]= 0.104574 theta0 Csc[theta0]
           2.70203 x 10^-8 + theta0^5/2
```

```
In[1376]:= smallAngleClassical1000Plot = LogLogPlot[ismall1000, {theta0, 0.0001, Pi},
           PlotRange -> {{0.0001, 10}, {1, 10^7}}, PlotStyle -> {Hue[0.5], Thickness[0.007]}];
```

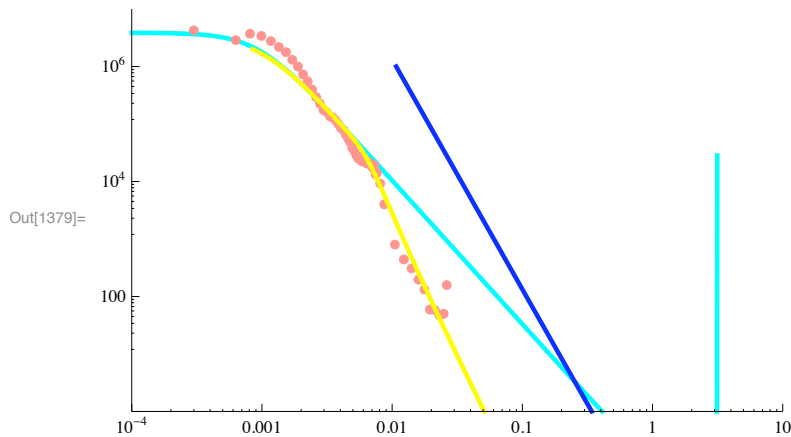
This has a singularity at small angles and must be replaced by the quantum formulation of Massey et al. and others.

```
In[1377]:= scrCoul1000Plot=LogLogPlot[{Evaluate[isrcr//.values/.enrel->1000]}, {thetaSC,0.0001,Pi},
           PlotRange->{{0.0001,Pi},{1,10^6}}, PlotStyle->plotColorsLines[[5]]];
```

```
In[1378]:= iEmpirical1000LogPlot =
           LogLogPlot[Evaluate[iEmpiricalR //. {alphaau -> 0.808 / (0.529)^3,
           enrelau -> 1000 / 27.211, thetaD -> thetaDFit, thetaR -> 0.01085}],
           {theta0, 0.0001, Pi}, PlotRange -> {{0.0001, Pi}, {1, 2. * 10^6}},
           PlotStyle -> plotColorsLines[[7]]];
```

In[1379]=

```
Show[smallAngleClassical1000Plot,diffQCMRice1000Plot, scrCoul1000Plot,iEmpirical1000Lo
```



Out[1379]=

using the Krstic and Schultz type of plot gives

In[1380]=

```
rice1000=Join[Table[{diffQCMRice1000[[j,1]],diffQCMRice1000[[j,2]]*Pi*Sin[diffQCMRice1000[[j,Length[diffQCMRice1000]]]}]]
```

```
Out[1380]= {{0, 0.}, {0.0003, 8013.45}, {0.00063, 11387.1}, {0.00081, 18931.8},
{0.00099, 21199.6}, {0.00117, 20366.2}, {0.00135, 18571.2}, {0.00153, 17096.7},
{0.00171, 14083.6}, {0.00189, 11863.9}, {0.00207, 9491.93}, {0.00225, 7823.13},
{0.00243, 6058.17}, {0.00261, 4810.47}, {0.00279, 3949.83}, {0.00297, 3265.88},
{0.00315, 3183.34}, {0.00333, 2846.38}, {0.00351, 2859.6}, {0.00369, 2661.27},
{0.00387, 2412.05}, {0.00405, 2163.63}, {0.00423, 2090.31}, {0.00441, 1819.98},
{0.00459, 1610.22}, {0.00477, 1431.28}, {0.00495, 1198.81}, {0.00513, 1093.96},
{0.00531, 947.952}, {0.00549, 865.213}, {0.00567, 944.066}, {0.00585, 822.982},
{0.00603, 912.733}, {0.00621, 959.331}, {0.00639, 827.831}, {0.00656999, 865.774},
{0.00674999, 886.489}, {0.00692999, 811.403}, {0.00710999, 772.338},
{0.00728999, 869.781}, {0.00746999, 621.885}, {0.00764999, 687.956},
{0.00809999, 468.788}, {0.00869999, 218.835}, {0.0105, 52.8222}, {0.0123, 34.06},
{0.0140999, 27.306}, {0.0158999, 19.6078}, {0.0176999, 14.7356}, {0.0194999, 7.24893},
{0.0212998, 7.81378}, {0.0230998, 6.84923}, {0.0248997, 7.8153}, {0.0262497, 26.0611}}
```

In[1381]=

```
rice1000Plot=ListLogLogPlot[%,PlotRange->{{0.0001,10},{1,100000.}}, DisplayFunction->I
```

In[1382]=

```
smallAngleClassical1000Plot2 = LogLogPlot[(2 * Pi * ismall1000 * Sin[theta0]) /.
{ry -> 13.6, alphaau -> 0.808 / (0.529)^3, enrelau -> 1000 / 27.211},
{theta0, 0.0001, Pi}, PlotRange -> {{0.0001, 10}, {1, 100000.}},
PlotStyle -> {Hue[0.5], Thickness[0.007]}, DisplayFunction -> Identity];
```

The following screened Coulomb parameters are chosen to fit the Rice experiments

In[1383]=

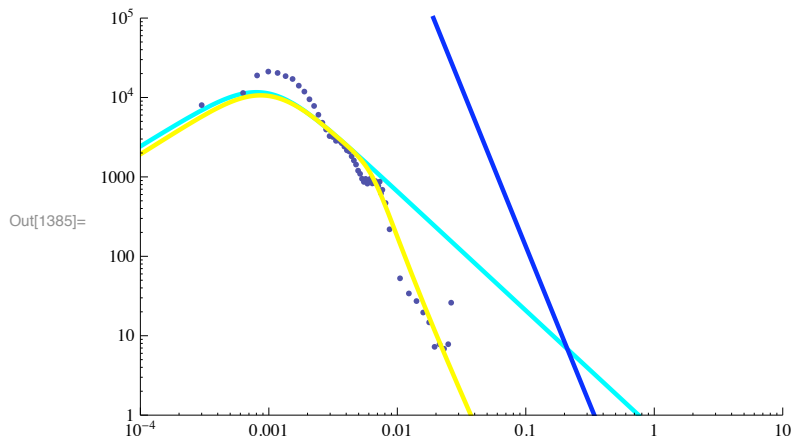
```
scrCoul1000LogLogPlot=LogLogPlot[{Evaluate[isacr//.values/.enrel->1000]}, {thetaSC,0.
PlotRange->{{0.0001,Pi},{1,10^5}}, PlotStyle->plotColorsLines[[5]]];
```

In[1384]:=

```
iEmpirical1000LogLogPlot =
LogLogPlot[2 *  $\pi$  * iEmpiricalR * Sin[theta0] /. {alphaau -> 0.808 / (0.529) ^ 3,
enrelau -> 1000 / 27.211, thetaD -> thetaDFit}, {theta0, 0.0001, Pi},
PlotRange -> {{0.0001, Pi}, {1, 100 000.}}, PlotStyle -> plotColorsLines[7]]];
```

In[1385]:=

```
Show[smallAngleClassical1000Plot2, rice1000Plot, iEmpirical1000LogLogPlot, scrCoul1000Log
```



Out[1385]=

The experimental data fails to show a maximum at small angles, such as found at lower energies.

In[1386]:=

```
maxAngle = rice1000[[-1, 1]]
```

Out[1386]= 0.0262497

In the following, note that rice1000 is $d\sigma/d\theta$. We add contributions from large and small angles that are beyond the tabulated values.

In[1387]:=

```
rice1000Fcn = Interpolation[rice1000, InterpolationOrder -> 2][x]
```

Out[1387]= InterpolatingFunction[{{0., 0.0262497}}, <>][x]

In[1388]:=

```
qatt1000rice = NIntegrate[rice1000Fcn, {x, rice1000[[1, 1]], rice1000[[-1, 1]]}] +
NIntegrate[100 / (x / 0.026) ^ 4, {x, rice1000[[-1, 1]], Pi}] +
NIntegrate[rice1000[[1, 2]], {x, 0, rice1000[[1, 1]]}]
```

Out[1388]= 41.9818

Add on

In[1389]:=

```
Integrate[rice1000[[2, 2]], {x, 0, rice1000[[1, 1]]}]
```

Out[1389]= 0.

In[1390]:=

```
qm1000rice = NIntegrate[rice1000Fcn * (1 - Cos[x]), {x, 0, maxAngle}] +
NIntegrate[100 / (x / maxAngle) ^ 4 * (1 - Cos[x]), {x, maxAngle, Pi}]
```

Out[1390]= 0.00106722

Note that the Sin³ becomes Sin²

```
In[1391]:= qv1000rice = NIntegrate[Interpolation[rice1000][x] * (Sin[x])^2, {x, 0.0007, 0.02}] +  
NIntegrate[100 / (x / 0.026)^4 * (Sin[x])^3, {x, 0.026, Pi}]
```

Out[1391]= 0.000484655

```
In[1392]:= cumProbSmall1000Plot=LogLogPlot[Evaluate[cumulativeIsmallPol/. {alphaau->5.4, enrelau-  
theta1->0.01,thetaD->thetaDFit}], {thetaCum,0.001,Pi}, PlotRange->{{0.0001,Pi},{0.001,  
PlotStyle->plotColorsLines[[5]]];
```

```
In[1393]:= total1000=NIntegrate[rice1000Fcn, {x,0,maxAngle}]
```

Out[1393]= 41.1396

```
In[1394]:= cumProbRice1000[theta_] :=  
Integrate[rice1000Fcn, {x, 0, theta}] / total1000 (* Cumulative Distr. Func. *)
```

```
In[1395]:= bins = 300;
```

```
In[1396]:= cumProbRice1000Table = Table[{(j - 1) * maxAngle / bins * 1.,  
cumProbRice1000[(j - 1) * maxAngle / bins]}, {j, 1, bins}];
```

```
In[1397]:= runTime = TimeUsed[] - startTime
```

Out[1397]= 264.729

```
In[1398]:= cumProbRice1000Plot=ListLogLogPlot[{cumProbRice1000Table,Table[{maxAngle+(j-1)*(Pi-max  
PlotRange->{{0.0001,Pi},{0.01,1.1}},PlotStyle->plotColorsPoints[{{9,9}}]}];
```

```
In[1399]:= thetaR
```

Out[1399]= 0.00358142

```
In[1400]:= iEmpiricalR
```

```
Out[1400]= 
$$\begin{cases} 2.88615 \times 10^{-6} + \left(0.27135 \sqrt{\text{alphaau}} \text{theta0} \text{Csc}[\text{theta0}]\right) / & \text{theta0} < 0.179535 \\ \left(\sqrt{\text{enrelau}} \left(1 + 6.07829 \times 10^9 (-0.00322327 + \text{theta0})^4\right)^{0.5} \right. \\ \quad \left. (2.70203 \times 10^{-8} + \text{theta0}^{5/2})\right) & \\ 2.88615 \times 10^{-6} & \text{theta0} > 0.179535 \\ 0 & \text{True} \end{cases}$$

```

```
In[1401]:= totalEmp1000 =  
NIntegrate[(iEmpiricalR * 2 * Pi * Sin[theta0] /. {alphaau -> 0.808 / (0.529)^3,  
enrelau -> 1000 / 27.211, thetaD -> thetaDFit, enrel -> 1000}), {theta0, 0, Pi}]
```

Out[1401]= 30.1539

```
In[1402]:= cumProbEmp1000[theta_] := NIntegrate[
  (iEmpiricalR * 2 * Pi * Sin[theta0] / totalEmp1000 /. {alphaau -> 0.808 / (0.529)^3,
    enrelau -> 1000 / 27.211, thetaD -> thetaDFit, enrel -> 1000}), {theta0, 0, theta}]
```

```
In[1403]:= cumProbEmp1000Plot = LogLogPlot[cumProbEmp1000[theta], {theta, 0.0001, Pi},
  PlotRange -> {{0.0001, Pi}, {0.01, 1.1}}, PlotStyle -> plotColorsLines[4]];
```

NIntegrate::nlim : theta0 = theta is not a valid limit of integration. >>

NIntegrate::nlim : theta0 = theta is not a valid limit of integration. >>

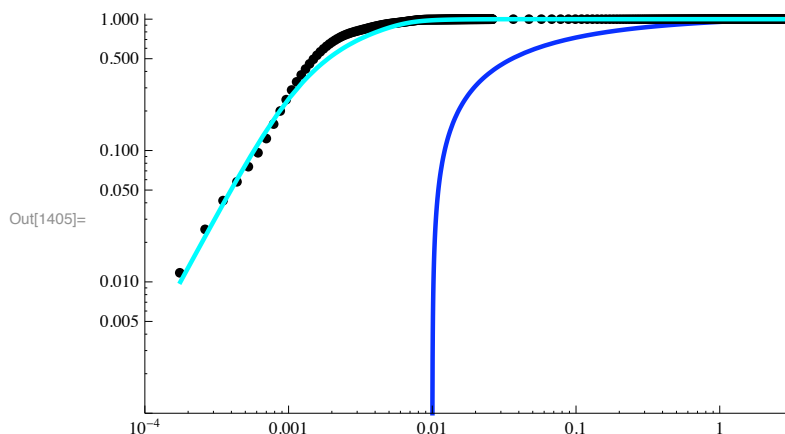
NIntegrate::nlim : theta0 = theta is not a valid limit of integration. >>

General::stop : Further output of NIntegrate::nlim will be suppressed during this calculation. >>

```
In[1404]:= runTime = TimeUsed[] - startTime
```

Out[1404]= 328.253

```
In[1405]:= Show[cumProbSmall1000Plot, cumProbRice1000Plot, cumProbEmp1000Plot]
```



```
In[1406]:= Clear[thetaR, thetaD, cSmall]
```

- For 5000 eV in Lab, 3333 eV in CM: Stebbings et al (1988) give tabulated experimental results:

- For 5000 eV in Lab, Stebbings et al (1988) give tabulated experimental results:

```
In[1407]:= Flatten[Take[Import["hph2ri50.txt", "Table"], -5]]
```

```
Out[1407]= {EL, =5.00E+03eV, m, =, 1., M, =, 2., 2mM/(m+M)^2, =4.44E-01,
  a=M^2, =4.00E+00, THL*I(THL), THL, THL, -c, b, cos(THg), THg,
  I(THL)*sin(THL), DELCS, tau, rd, deg, cm2/str, cm2/rd, eVcm2/str, keVdeg}
```

```
In[1408]:= Drop[Import["hph2ri50.txt", "Table"], -6];
```

The added point at $\{0.6 \cdot 10^{-9}\}$ is based on a very rough extrapolation of the preliminary plot from L. Johnson at Rice received 8/15/89


```
In[1409]:= diffQRice3333=Join[{0,6.*10^-9},Table[{{j,1}},%[[j,7]]/(0.528*10^-8)^2},{j,Length[
```

```
Out[1409]= {{0, 6. × 10-9}, {0.00042, 1.84731 × 107}, {0.00054, 1.15143 × 107},
{0.00066, 8.32185 × 106}, {0.00078, 4.98594 × 106}, {0.0009, 2.87678 × 106},
{0.00102, 1.77198 × 106}, {0.00114, 982 840.}, {0.00126, 369 462.},
{0.00138, 294 493.}, {0.0015, 147 785.}, {0.00162, 206 253.}, {0.00174, 341 842.},
{0.00186, 358 701.}, {0.00198, 390 984.}, {0.0021, 337 537.}, {0.00222, 226 699.},
{0.00234, 193 698.}, {0.00246, 151 372.}, {0.00258, 134 154.},
{0.0027, 69 229.2}, {0.00282, 66 718.3}, {0.00294, 42 685.4}, {0.00306, 53 087.7},
{0.00318, 27 153.6}, {0.0033, 23 566.6}, {0.00342, 22 024.2}, {0.0046, 10 832.8},
{0.0058, 7174.01}, {0.007, 4053.32}, {0.0082, 2231.12}, {0.0094, 1560.35},
{0.0106, 993.601}, {0.0118, 670.77}, {0.013, 299.515}, {0.0142, 295.569}}
```

The original data of column 7 is in cm²/str versus angle in rd. from column 1.

We next convert the experimental data to Center-of-Mass

From p. 9 of McDaniel (1964), we need to find the center-of-mass angles. We have done this above and do not repeat.

```
In[1410]:= diffQCMRice3333=Table[{thetaCM1[diffQRice3333[[j,1]]],diffCM[diffQRice3333[[j,1]],diff
{j,Length[diffQRice3333]}];
```

```
In[1411]:= diffQCMRice3333Plot=ListLogLogPlot[diffQCMRice3333,PlotRange->{{0.001,10},{1,1.01*10^7
```

■ Classical small angle formula

Assume cSmall

```
cSmall = 0;
```

```
In[1412]:= cSmall = cSmallFit /. enrel -> 3333
```

```
Out[1412]= 6.00832 × 10-7
```

```
In[1413]:= thetaD = thetaDFit /. {enrel -> 3333, alphaau -> 0.808 / (0.529) ^ 3}
```

```
Out[1413]= 0.000591915
```

```
thetaD = 0.0005;
```

```
In[1414]:= thetaR = rainbowAngleFit /. enrel -> 3330
```

```
Out[1414]= 0.0010755
```

```
In[1415]:= ismall3333=ismall //. {ry->13.6,alphaau->0.808/(0.529)^3,enrelau->3333/27.211,thetaD->t
```

```
Out[1415]= 
$$\frac{0.0572806 \text{ theta0 Csc}[\text{theta0}]}{8.5241 \times 10^{-9} + \text{theta0}^{5/2}}$$

```

```
In[1416]:= smallAngleClassical3333Plot =
LogLogPlot[ismall3333 /. {ry -> 13.6, alphaau -> 0.808 / (0.529)^3,
enrelau -> 3333 / 27.211, thetaD -> thetaDFit}, {theta0, 0.0001, Pi},
PlotRange -> {{0.0001, 10}, {10, 10^7}}, PlotStyle -> plotColorsLines[[4]]];

In[1417]:= totalClassicalSmall=NIntegrate[(ismall3333/.{enrelau->3333/27.211}),{theta0,0.0008,0.0

Out[1417]= 1416.27

In[1418]:= totalClassicalSmall=NIntegrate[(ismall3333/.enrelau->3333/27.211),{theta0,0.0008,Pi}]

Out[1418]= 1454.85
```

Very little of the integral cross section comes from large angles as seen by changing the limits.

The following screened Coulomb parameters are chosen to fit the Rice experiments

```
In[1419]:= scrCoul3333Plot=LogLogPlot[{Evaluate[isrcr//.values/.enrel->3333]}, {thetaSC,0.0001,P
PlotRange->{{0.0001,Pi},{10,10^7}}, PlotStyle->plotColorsLines[[5]]];
```

This shows that the screened Coulomb differential cross section varies approximately as θ^4 at large angles.

```
In[1420]:= iEmpiricalR

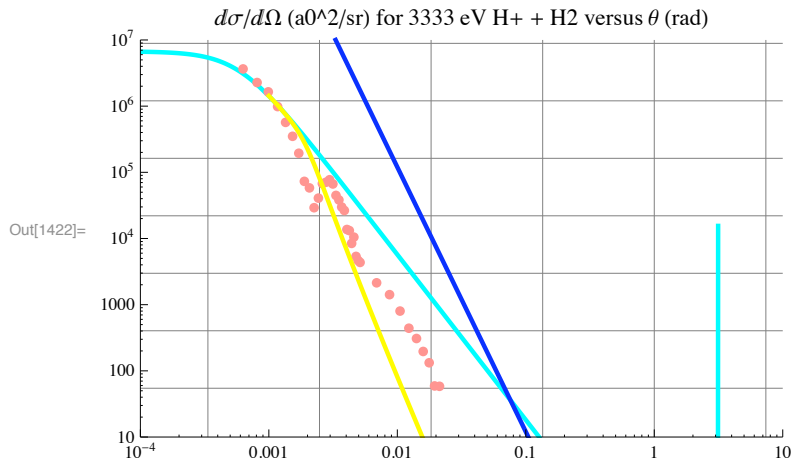
Out[1420]= 
$$\begin{cases} 6.00832 \times 10^{-7} + \left(0.27135 \sqrt{\text{alphaau}} \theta_0 \text{Csc}[\theta_0]\right) / & \theta_0 < 0.0983845 \\ \left(\sqrt{\text{enrelau}} \left(1 + 7.47409 \times 10^{11} (-0.00096795 + \theta_0)^4\right)^{0.5} \right. \\ \left. (8.5241 \times 10^{-9} + \theta_0^{5/2}) \right) & \\ 6.00832 \times 10^{-7} & \theta_0 > 0.0983845 \\ 0 & \text{True} \end{cases}$$

```

```
In[1421]:= iEmpirical3333LogLogPlot =
LogLogPlot[Evaluate[iEmpiricalR /. {alphaau -> 0.808 / (0.529)^3,
enrelau -> 3333 / 27.211, thetaD -> thetaDFit, thetaR -> 0.001085}],
{theta0, 0.001, Pi}, PlotRange -> {{0.001, Pi}, {10, 10^7}},
PlotStyle -> plotColorsLines[[7]]];
```

In[1422]:=

```
Show[smallAngleClassical3333Plot,diffQCMRice3333Plot,scrCoul3333Plot,iEmpirical3333Lo
GridLines->Automatic,PlotLabel->"dσ/dΩ (a0^2/sr) for 3333 eV H+ + H2 versus θ (rad)"]
```



This plot shows that the screened Coulomb model has the right shape but the wrong magnitude by over two orders of magnitude compared to experiment. Our Empirical fit is better, but drops too rapidly at large angles.

In[1423]:= **thetaR**

Out[1423]= 0.0010755

Most of the total cross section integral comes from outside $\theta_0 = 0.008$ rad, i.e., from the very forward scattering.

In[1424]:=

```
totalCrossSection=Integrate[ 10^6*(theta0/.001)^-4,{theta0,0.0008,Pi}]
```

Out[1424]= 651.034

■ $d\sigma/d\theta$ or KS type plot

In[1425]:=

```
rice3333=Table[{diffQCMRice3333[[j,1]],diffQCMRice3333[[j,2]]*2*Pi*Sin[diffQCMRice3333
```

In[1426]:=

```
riceKS3333Plot=ListLogLogPlot[%,PlotRange->{{0.0001,10},{1,10^5}},PlotStyle->plotColor
```

In[1427]:=

```
smallAngleClassicalKS3333Plot2 =
  LogLogPlot[(2 * Pi * ismall13333 * Sin[theta0]) /. {ry -> 13.6,
    alphaau -> 0.808 / (0.529)^3, enrelau -> 3333 / 27.211, thetaD -> thetaDFit},
  {theta0, 0.0001, Pi}, PlotRange -> {{0.0001, 10}, {1, 10^5}},
  PlotStyle -> {Hue[0.5], Thickness[0.007]}];
```

In[1428]:=

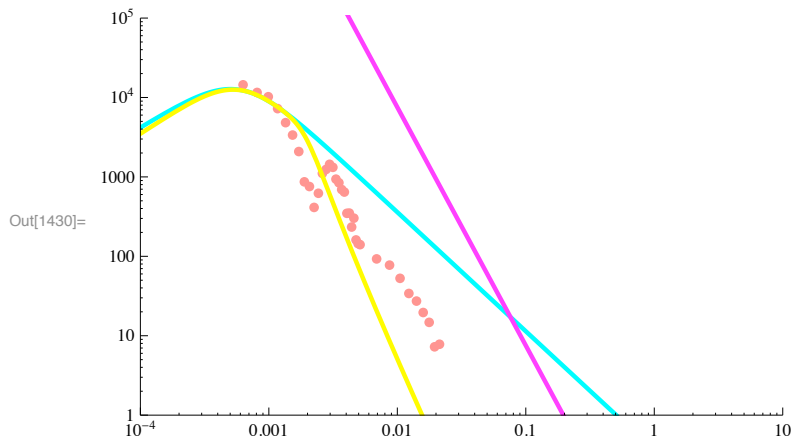
```
scrCoulKS3333Plot=LogLogPlot[2*Pi*Sin[thetaSC]*(iscr//.values/.enrel->3333), {thetaSC,
PlotRange->{{0.0001,4},{1,5.*10^5}},PlotStyle->plotColorsLines[[6]]];
```

In[1429]:=

```
iEmpirical3333KSLogLogPlot =
LogLogPlot[2 *  $\pi$  * iEmpiricalR * Sin[theta0] /. {alphaau -> 0.808 / (0.529) ^ 3,
enrelau -> 3333 / 27.211, thetaD -> thetaDFit}, {theta0, 0.0001, Pi},
PlotRange -> {{0.0001, Pi}, {1, 10^5}}, PlotStyle -> plotColorsLines[[7]]];
```

In[1430]:=

```
Show[smallAngleClassicalKS3333Plot2, riceKS3333Plot, scrCoulKS3333Plot, iEmpirical3333K
```



Out[1430]=

In the following, note that rice333 is $d\sigma/d\theta$, so that the $2*\pi*\sin[x]$ is not applied.

In[1431]:=

```
qatt3333rice = NIntegrate[Interpolation[rice3333][x], {x, 0.0007, 0.02}] +
NIntegrate[7.3 / (x / 0.02) ^ 4, {x, 0.02, Pi}] +
Integrate[rice3333[[1, 2]], {x, 0, rice3333[[1, 1]]}]
```

Out[1431]= 10.4263

In[1432]:=

```
rice3333[[1, 1]]
```

Out[1432]= 0

In[1433]:=

```
maxAngle = rice3333[[-1, 1]]
```

Out[1433]= 0.0212998

In[1434]:=

```
NIntegrate[Interpolation[rice3333][x], {x, rice3333[[1, 1]], rice3333[[-1, 1]]}]
```

Out[1434]= 19.3786

In[1435]:=

```
total3333rice =
NIntegrate[Interpolation[rice3333][x], {x, rice3333[[1, 1]], rice3333[[-1, 1]]}] +
NIntegrate[7.3 / (x / 0.02) ^ 4, {x, rice3333[[-1, 1]], Pi}] +
NIntegrate[rice3333[[1, 2]], {x, 0, rice3333[[1, 1]]}]
```

Out[1435]= 19.4189

In[1436]:=

```
Integrate[rice3333[[1, 2]], {x, 0, rice3333[[1, 1]]}]
```

Out[1436]= 0

```
In[1437]:= qm3333rice = NIntegrate[Interpolation[rice3333][x] * (1 - Cos[x]), {x, 0.0007, 0.02}] +  
NIntegrate[7.3 / (x / 0.02) ^ 4 * (1 - Cos[x]), {x, 0.026, Pi}]
```

```
Out[1437]= 0.000076049
```

Note that the Sin³ becomes Sin²

```
In[1438]:= qv3333rice = NIntegrate[Interpolation[rice3333][x] * (Sin[x]) ^ 2, {x, 0.0007, 0.02}] +  
NIntegrate[7.3 / (x / 0.02) ^ 4 * (Sin[x]) ^ 3, {x, 0.026, Pi}]
```

```
Out[1438]= 0.000112106
```

```
In[1439]:= runTime = TimeUsed[] - startTime
```

```
Out[1439]= 331.793
```

```
In[1440]:= cumProbSmall3333Plot=LogLogPlot[Evaluate[cumulativeIsmallPol/. {alphaau->5.4, enrelau-  
theta1->0.01,thetaD->thetaDFit}], {thetaCum,0.001,Pi}, PlotRange->{{0.0001,Pi},{0.001,  
PlotStyle->plotColorsLines[[5]]];
```

```
In[1441]:= rice3333Fcn = Interpolation[rice3333, InterpolationOrder -> 2][x]
```

```
Out[1441]= InterpolatingFunction[{{0., 0.0212998}}, <>][x]
```

```
In[1442]:= maxAngle
```

```
Out[1442]= 0.0212998
```

```
In[1443]:= total3333=NIntegrate[rice3333Fcn, {x,0,maxAngle}]
```

```
Out[1443]= 17.8392
```

```
In[1444]:= cumProbRice3333[theta_] :=  
Integrate[rice3333Fcn, {x, 0, theta}] / total3333 (* Cumulative Distr. Func. *)
```

```
In[1445]:= runTime = TimeUsed[] - startTime
```

```
Out[1445]= 333.837
```

```
In[1446]:= bins = 300;
```

```
In[1447]:= cumProbRice3333Table = Table[{(j - 1) * maxAngle / bins * 1.,  
cumProbRice3333[(j - 1) * maxAngle / bins]}, {j, 1, bins}];
```

```
In[1448]:= runTime = TimeUsed[] - startTime
```

```
Out[1448]= 333.899
```

```
In[1449]:= Table[{maxAngle + j * (Pi - maxAngle) / bins, 1}, {j, bins}];
```

```
In[1450]:= cumProbRice3333Plot=ListLogLogPlot[{cumProbRice3333Table,Table[{maxAngle+j*(Pi-maxAngle) / bins, 1}],PlotRange->{{0.0001,Pi},{0.01,1.1}},PlotStyle->plotColorsPoints[{{9,9}}];
```

```
In[1451]:= totalEmp3333 =  
NIntegrate[(iEmpiricalR * 2 * Pi * Sin[theta0] /. {alphaau -> 0.808 / (0.529)^3,  
enrelau -> 3333 / 27.211, thetaD -> thetaDFit, enrel -> 3333}), {theta0, 0, Pi}]
```

```
Out[1451]= 17.0119
```

```
In[1452]:= bins = 3000;
```

```
In[1453]:= cumProbEmp3333[theta_] := NIntegrate[  
(iEmpiricalR * 2 * Pi * Sin[theta0] / totalEmp3333 /. {alphaau -> 0.808 / (0.529)^3,  
enrelau -> 3333 / 27.211, thetaD -> thetaDFit, enrel -> 3333}), {theta0, 0, theta}]
```

```
In[1454]:= cumProbEmp3333Plot = LogLogPlot[cumProbEmp3333[theta], {theta, 0.0001, Pi},  
PlotRange -> {{0.0001, Pi}, {0.01, 1.1}}, PlotStyle -> plotColorsLines[4];
```

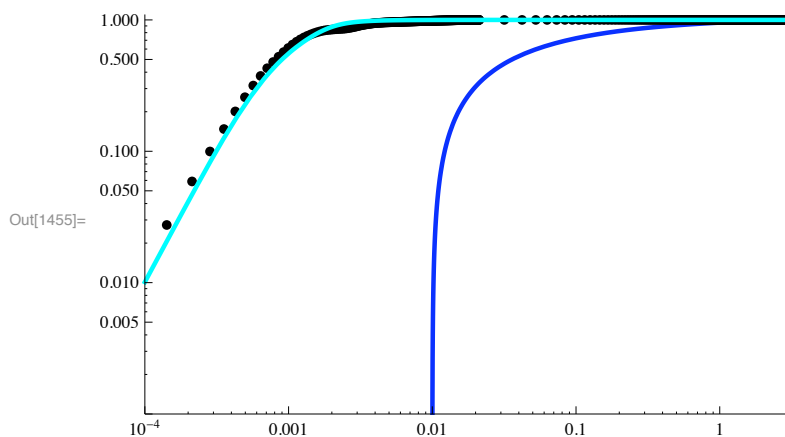
NIntegrate::nlm : theta0 = theta is not a valid limit of integration. >>

NIntegrate::nlm : theta0 = theta is not a valid limit of integration. >>

NIntegrate::nlm : theta0 = theta is not a valid limit of integration. >>

General::stop : Further output of NIntegrate::nlm will be suppressed during this calculation. >>

```
In[1455]:= Show[cumProbSmall13333Plot, cumProbRice3333Plot,cumProbEmp3333Plot]
```

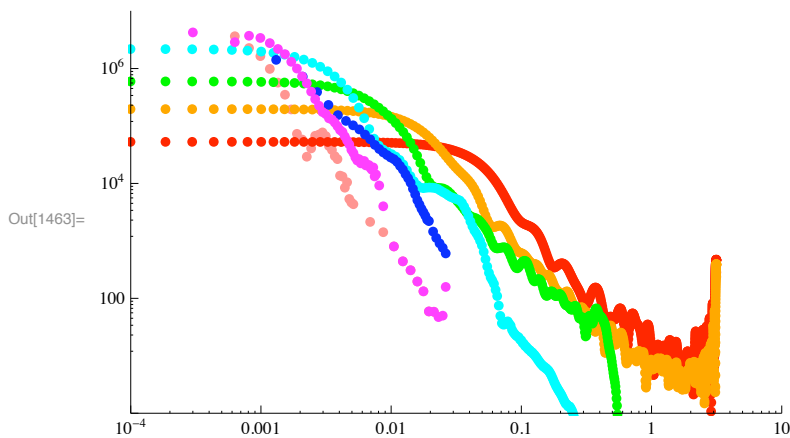


Compare experimental differential cross sections in COM

```

In[1456]:= diffQ01LogLogPlotA=ListLogLogPlot[diffQ01,PlotRange->{{0.0001,Pi},{0.0999,10^7}},PlotStyl
In[1457]:= diffQ1LogLogPlotA=ListLogLogPlot[diffQ1,PlotRange->{{0.0001,Pi},{0.0999,10^7}},PlotStyl
In[1458]:= diffQ10LogLogPlotA=ListLogLogPlot[diffQ10,PlotRange->{{0.0001,Pi},{0.0999,10^7}},PlotStyl
In[1459]:= diffQ100LogLogPlotA=ListLogLogPlot[diffQ100,PlotRange->{{0.0001,Pi},{0.0999,10^7}},PlotStyl
In[1460]:= diffQCMRice333PlotA=ListLogLogPlot[diffQCMRice333,PlotRange->{{0.0001,10},{1,10^7}},PlotStyl
In[1461]:= diffQCMRice1000PlotA=ListLogLogPlot[diffQCMRice1000,PlotRange->{{0.0001,10},{1,10^7}},PlotStyl
In[1462]:= diffQCMRice3333PlotA=ListLogLogPlot[diffQCMRice3333,PlotRange->{{0.0001,10},{1,1.01*10^7}},PlotStyl
In[1463]:= Show[diffQCMRice3333PlotA,diffQ01LogLogPlotA,diffQ1LogLogPlotA,diffQ10LogLogPlotA,diffQ100LogLogPlotA,
diffQCMRice333PlotA,diffQCMRice1000PlotA]

```

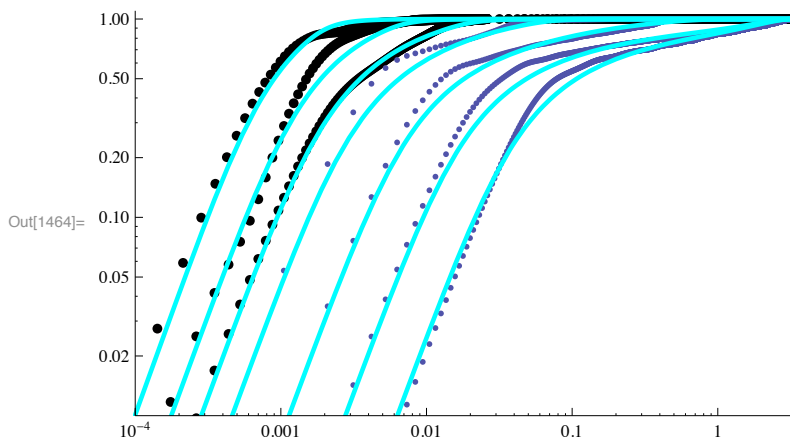


I see no obvious inconsistency between Krstic-Schultz and the Rice data, but this should be checked further.

```

In[1464]:= Show[cumProbRice3333Plot, cumProbRice1000Plot, cumProbRice333Plot,
cumProbKrstic01Plot, cumProbKrstic1Plot, cumProbKrstic10Plot,
cumProbKrstic100Plot, cumProbEmp3333Plot, cumProbEmp1000Plot, cumProbEmp333Plot,
cumProbEmp100Plot, cumProbEmp10Plot, cumProbEmp01Plot]

```



Except at the lowest energy, these fits are a start. I need to look more carefully at the behavior of the cumulative probability at low angles, e.g., the dependence on poorly known

experimental and extrapolated angular distributions at low angle for the high energy cases. Changes in the rainbow angle fit and the cSmallFit had little effect at the small angles. The more sensitive parameter is thetaD, where we raised the initial fit at low energies and lowered it at high energies.

Angular integrated cross sections

```
In[1465]:= Clear[thetaD, thetaR, cSmall]
```

```
In[1466]:= thetaDFit
```

```
Out[1466]= 
$$\frac{0.0142162}{\text{enrel}^{1/3} (1 + 4. \text{enrel})^{0.05}}$$

```

```
In[1467]:= rainbowAngleFit
```

```
Out[1467]= 
$$\frac{2 \pi}{(1 + 9.47328 \text{enrel}^4)^{0.25}}$$

```

■ Beam attenuation cross section

```
In[1468]:= ao = 0.529 * 10^-10
```

```
Out[1468]=  $5.29 \times 10^{-11}$ 
```

```
In[1469]:= qtotalLL //. polDispatch //. alphaau -> 0.808 / (0.529)^3
```

```
Out[1469]= 
$$\frac{567.199}{\text{enrel}^{1/3}}$$

```

```
In[1470]:= thetaDFit
```

```
Out[1470]= 
$$\frac{0.0142162}{\text{enrel}^{1/3} (1 + 4. \text{enrel})^{0.05}}$$

```

From above

```
In[1471]:= totaliscr
```

```
Out[1471]= ConditionalExpression[
$$\frac{1}{(2. + 2.02281 \times 10^{41} \text{enrel})^{7/2}} 3.40564 \times 10^{85}$$
  


$$\left( \left( (-3.21365 \times 10^{73} + 0. \text{i}) - (3.2503 \times 10^{114} + 0. \text{i}) \text{enrel} \right) \text{enrel}^2 \sqrt{2. + 2.02281 \times 10^{41} \text{enrel}} + \right.$$
  


$$\left. (-5.65685 - 1.43034 \times 10^{42} \text{enrel} - 1.15732 \times 10^{83} \text{enrel}^2 - 2.92629 \times 10^{123} \text{enrel}^3) \right.$$
  


$$\text{ArcTan} \left[ 1.11072 \times 10^{-9} \sqrt{2. + 2.02281 \times 10^{41} \text{enrel}} \right] +$$
  


$$\left. (5.65685 + 1.43034 \times 10^{42} \text{enrel} + 1.15732 \times 10^{83} \text{enrel}^2 + 2.92629 \times 10^{123} \text{enrel}^3) \right.$$
  


$$\left. \text{ArcTan} \left[ 4.50158 \times 10^8 \sqrt{2. + 2.02281 \times 10^{41} \text{enrel}} \right] \right], \text{enrel} < 1.03398 \times 10^{-25}]$$

```

```
In[1472]:= qattRicePlot =
```

```
ListLogLogPlot[{{333, qatt333rice}, {1000, qatt1000rice}, {3333, qatt3333rice}},  

PlotRange -> {{0.1, 10000}, {10, 10^4}}, PlotStyle -> plotColorsPoints[{{9}}];
```



```

In[1473]:= attPolISCRQPlot =
  LogLogPlot[{Evaluate[qtotalLL // . polDispatch // . alphaau -> 0.808 / (0.529)^3],
    Evaluate[totaliscr]}, {enrel, 0.1, 10000},
  PlotRange -> {{0.1, 10000}, {1, 10^4}}, GridLines -> Automatic,
  PlotLabel -> "Beam attenuation cross section (m^2) vs relative energy (eV)",
  PlotStyle -> plotColorsLines[{{7, 8}}]];

In[1474]:= Import["h2hpkrstic.txt", "CSV"] // TableForm;

In[1475]:= krsticHpH2Table = Drop[Drop[Import["h2hpkrstic.txt", "Table"], 4], -1];

In[1476]:= Table[{krsticHpH2Table[[j, 1]], krsticHpH2Table[[j, 2]]}, {j, Length[krsticHpH2Table]}]

Out[1476]:= {{0.1, 778.452}, {0.1995, 675.857}, {0.5012, 523.936}, {1., 420.996}, {1.995, 338.864},
  {5.012, 267.759}, {10., 221.53}, {19.95, 178.201}, {50.12, 144.591}, {100., 132.202}}

In[1477]:= H2HpAttenQKrsticPlot = ListLogLogPlot[Table[{krsticHpH2Table[[j,1]], krsticHpH2Table[[j,2]]}, {j, Length[krstic
  PlotRange -> {{0.1,10000.},{10,10000.}}, PlotStyle -> plotColorsPoints[[6]]];

  Note that the data is in atomic units versus relative energy

In[1478]:= iEmpiricalR

Out[1478]:= 
$$\begin{cases}
c_{\text{Small}} + \frac{0.27135 \sqrt{\alpha_{\text{aa}}} \theta_0 \csc[\theta_0]}{\sqrt{\text{enrelau}} (\theta_0^{5/2} + \theta_0^{D^{5/2}})} & \theta_0 > \pi \\
c_{\text{Small}} + \frac{0.27135 \sqrt{\alpha_{\text{aa}}} \theta_0 \csc[\theta_0]}{\sqrt{\text{enrelau}} (\theta_0^{5/2} + \theta_0^{D^{5/2}}) \left(1 + \frac{(\theta_0 - 0.9 \theta_0^{\text{rainbow}})^4}{\theta_0^4}\right)^{0.5}} & \theta_0 < 3 \sqrt{\theta_0^{\text{rainbow}}} \ \&\& \ \theta_0 < \pi \\
c_{\text{Small}} & \theta_0 > 3 \sqrt{\theta_0^{\text{rainbow}}} \ \&\& \ \theta_0 < \pi \\
0 & \text{True}
\end{cases}$$

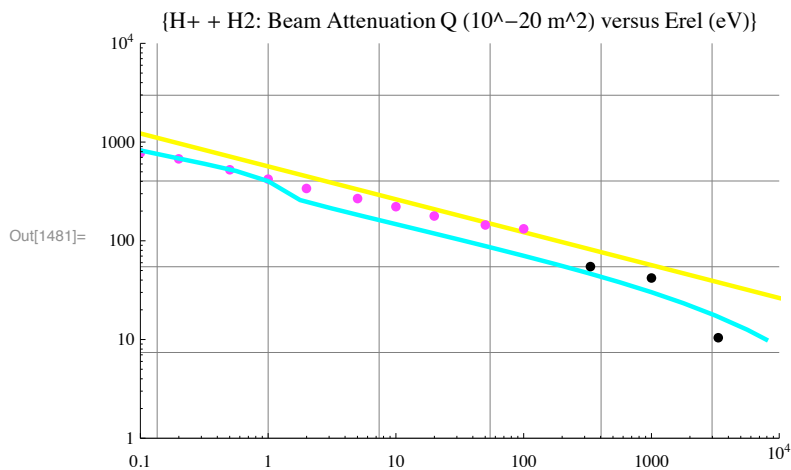

In[1479]:= qattEmpiricalTable = Table[
  {0.01 * 10^((j - 1) / 4), NIntegrate[Evaluate[(iEmpiricalR * 2 * Pi * Sin[theta0] //
  {alphaau -> 0.808 / (0.529)^3, enrelau -> 0.01 * 10^((j - 1) / 4) / 27.211,
  thetaD -> thetaDFit, thetaR -> rainbowAngleFit, enrel -> 0.01 * 10^((j - 1) / 4),
  cSmall -> cSmallFit}], {theta0, 0, Pi}]}, {j, 25}]

Out[1479]:= {{0.01, 1584.51}, {0.0177828, 1341.98}, {0.0316228, 1137.8},
  {0.0562341, 966.504}, {0.1, 823.276}, {0.177828, 703.743},
  {0.316228, 603.038}, {0.562341, 509.291}, {1., 401.676}, {1.77828, 258.636},
  {3.16228, 212.484}, {5.62341, 176.648}, {10., 147.424}, {17.7828, 123.02},
  {31.6228, 102.488}, {56.2341, 85.1483}, {100., 70.4525}, {177.828, 57.9459},
  {316.228, 47.2527}, {562.341, 38.0682}, {1000., 30.1539}, {1778.28, 23.3349},
  {3162.28, 17.4937}, {5623.41, 12.5632}, {10000., 8.52108}}

In[1480]:= qattEmpiricalLogLogPlot =
  ListLogLogPlot[qattEmpiricalTable, PlotRange -> {{0.1, 10000}, {10, 10^4}},
  Joined -> True, PlotStyle -> plotColorsLines[{{4}}]];

```

```
In[1481]:= Show[{attPolISCRQPlot, H2HpAttenQKrsticPlot, qattEmpiricalLogLogPlot, qattRicePlot},
  PlotLabel -> {"H+ + H2: Beam Attenuation Q (10^-20 m^2) versus Erel (eV)"},
  GridLines -> Automatic]
```



Magenta points - Krstic&Schultz, black points - Rice, cyan line - iEmpirical, yellow line - polarization

The Rice qatt data represented by the black points are somewhat uncertain, since data is not available at very small scattering angles.

■ Angular integrated cross sections - diffusion or momentum transfer cross section

```
In[1482]:= integrate333qmrice
```

```
Out[1482]:= 0.00231992
```

```
In[1483]:= qm3333rice
```

```
Out[1483]:= 0.000076049
```

```
In[1484]:= qmRicePlot =
```

```
ListLogLogPlot[{{333, integrate333qmrice}, {1000, qm1000rice}, {3333, qm3333rice}},
  PlotRange -> {{0.1, 10 000}, {10^-5, 10^3}}, PlotStyle -> plotColorsPoints[{{9}}];
```

```
In[1485]:= polQmPlot = LogLogPlot[ Evaluate[masonPolarQ],
```

```
{enrel, 0.1, 10 000}, PlotRange -> {{0.1, 1000}, {10^-5, 10^3}},
  PlotLabel -> "Diffusion cross section (m^2) vs relative energy (eV)",
  GridLines -> Automatic, PlotStyle -> plotColorsLines[{{15, 1}}];
```

```
In[1486]:= H2HpQmKrsticPlot = ListLogLogPlot[Table[{krsticHpH2Table[[j,1]], krsticHpH2Table[[j,4]],{j,Length[krsticHpH2Table]}],
  PlotRange -> {{0.1,10000.},{10^-5,10^3}}, PlotStyle -> plotColorsPoints[{{6}}];
```

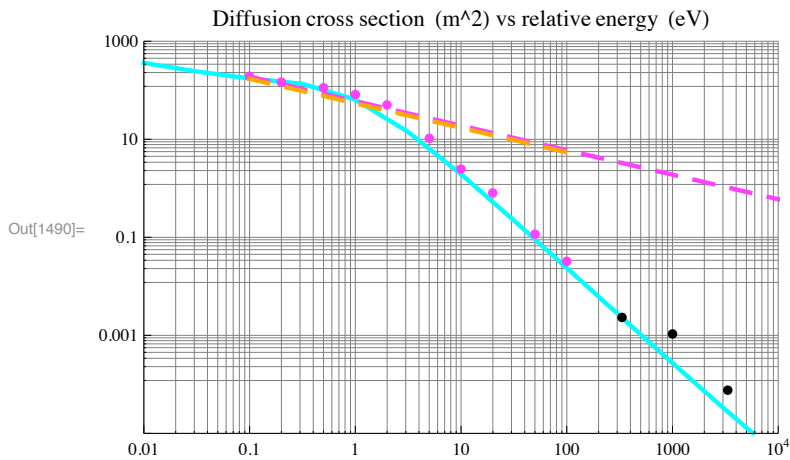
```
In[1487]:= H2HpKrsticLangevinPlot = ListLogLogPlot[Table[{krsticHpH2Table[[j,1]], krsticHpH2Table[[j,8]]/ao^2},{j,Length[krsticHpH2Table]}],
  PlotRange -> {{0.1,10000.},{10^-5,10^3}}, PlotStyle -> plotColorsLines[{{11}}];
```

```
In[1488]:= qmEmpiricalTable = Table[{0.01 * 10^((j - 1) / 2),
  NIntegrate[{iEmpiricalR * (1 - Cos[theta0]) * 2 * Pi * Sin[theta0] //
  {alphaau -> 0.808 / (0.529)^3, enrelau -> 0.01 * 10^((j - 1) / 2) / 27.211,
  thetaD -> thetaDFit, thetaR -> rainbowAngleFit, enrel -> 0.01 * 10^((j - 1) / 2),
  cSmall -> cSmallFit}}, {theta0, 0, Pi}], {j, 13}]
```

```
Out[1488]:= {{0.01, 360.512}, {0.0316228, 241.785}, {0.1, 174.643},
  {0.316228, 135.385}, {1., 64.7186}, {3.16228, 14.1017}, {10., 1.94645},
  {31.6228, 0.220295}, {100., 0.0237115}, {316.228, 0.00252889},
  {1000., 0.00027267}, {3162.28, 0.0000304249}, {10 000., 3.69012 * 10^-6}}
```

```
In[1489]:= qmEmpiricalLogLogPlot = ListLogLogPlot[qmEmpiricalTable,
  PlotRange -> {{0.01, 10 000}, {10^-5, 10^3}}, PlotStyle -> plotColorsLines[{{4}}],
  PlotLabel -> "Diffusion cross section (m^2) vs relative energy (eV)",
  GridLines -> Automatic, Joined -> True];
```

```
In[1490]:= Show[qmEmpiricalLogLogPlot, polQmPlot,
  H2HpQmKrsticPlot, H2HpKrsticLangevinPlot, qmRicePlot]
```



Magenta points - Krstic&Schultz, black points - Rice, cyan line - iEmpirical, dashed red line - Krstic's polarization, dashed magenta line - polarization (McDaniel)

These results are independent of thetaD, as shown by large changes in thetaDFit.

■ Angular integrated cross sections - viscosity cross section

```
In[1491]:= integrate333qvrice
```

```
Out[1491]= 0.00253387
```

```
In[1492]:= qv3333rice
```

```
Out[1492]= 0.000112106
```

```
In[1493]:= qvRicePlot =
```

```
ListLogLogPlot[{{333, integrate333qvrice}, {1000, qv1000rice}, {3333, qv3333rice}},
  PlotRange -> {{0.1, 10 000}, {10^-5, 10^3}}, PlotStyle -> plotColorsPoints[{{9}}];
```

From Phelps (1994) for isotropic scattering, $Q_v = 2/3Q_m$

```
In[1494]:= polQvPlot = LogLogPlot[{Evaluate[masonPolarQ]},
  {enrel, 0.1, 10 000}, PlotRange -> {{0.01, 10 000}, {10^-5, 10^3}},
  PlotLabel -> "Viscosity cross section (m^2) vs relative energy (eV)",
  GridLines -> Automatic, PlotStyle -> plotColorsLines[{{15, 1}}];
```

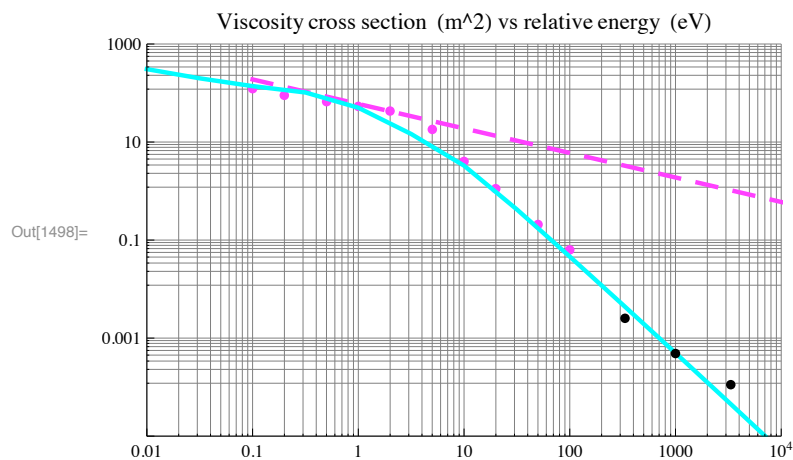
```
In[1495]:= H2HpQvKrsticPlot = ListLogLogPlot[Table[{krsticHpH2Table[[j,1]], krsticHpH2Table[[j,6]]}, {j, Length[krsticHpH:
  PlotRange -> {{0.1,10000.},{10^-5,10^3}}, PlotStyle -> plotColorsPoints[{{6}}];
```

```
In[1496]:= qvEmpiricalTable =
  Table[{0.01 * 10^((j - 1) / 2), NIntegrate[(iEmpiricalR * 2 * Pi * (Sin[theta0])^3 //.
{alphaau -> 0.808 / (0.529)^3, enrelau -> 0.01 * 10^((j - 1) / 2) / 27.211,
thetaD -> thetaDFit, thetaR -> rainbowAngleFit, enrel -> 0.01 * 10^((j - 1) / 2),
cSmall -> cSmallFit)}, {theta0, 0, Pi}]], {j, 13}]
```

```
Out[1496]:= {{0.01, 307.187}, {0.0316228, 199.48}, {0.1, 138.19},
  {0.316228, 102.568}, {1., 50.093}, {3.16228, 14.5937}, {10., 3.30079},
  {31.6228, 0.421055}, {100., 0.0460619}, {316.228, 0.00483133},
  {1000., 0.000496864}, {3162.28, 0.0000500672}, {10000., 4.96866 * 10^-6}}
```

```
In[1497]:= qvEmpiricalLogLogPlot =
  ListLogLogPlot[qvEmpiricalTable, PlotRange -> {{0.1, 10000}, {10^-5, 10^3}},
  Joined -> True, PlotStyle -> plotColorsLines[[{4}]]];
```

```
In[1498]:= Show[polQvPlot, H2HpQvKrsticPlot, qvEmpiricalLogLogPlot, qvRicePlot]
```



Magenta points - Krstic&Schultz, black points - Rice, cyan line - iEmpirical, dashed magenta line - polarization (McDaniel)

```
In[1499]:= runTime = TimeUsed[] - startTime
```

```
Out[1499]= 432.086
```

```
In[1500]:= EmitSound[Sound[{Play[Sin[440 * 2 * Pi * t] * Sin[2 Pi * t]^2, {t, 0, 0.5}}]]]
```

```
In[1501]:= Quit[]
```