Uploading data to LXCat databases for electron scattering cross sections

> The LXCat team Version January 2019

These instructions use as an example the SIGLO database but can be applied in general by replacing "SIGLO" with any other database name.

The structure of the databases for other data types is somewhat different but can be easily inferred from the description here.

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Accessing the login page



Account information page

- 1) Change password, if desired.
- 2) Change language, if desired.
- 3) Access database(s) by clicking on the symbol "+ ".



Database structure & contents

Element name	Contents							
SIGLO								
SIGLOelec_cs	Cross section (CS) data tables with identifying information in header for each process. Tables are 2-columns (energy in eV, CS in m ² .							
SIGLOelec_cs_groups	Group names, if any, with identifying information							
SIGLO_DATABASE	Description of the database as a whole, with contact information for the contributors.							
SIGLO_LIST_OF_SPECIES	List of species for which data are available in this database							
SIGLO_PUBLICATIONS	Notes, publication, posters, etc, if any.							

Note that SIGLO__elec_cs and SIGLO__elec_cs_groups are subelements of SIGLO and accessible by clicking on the "+" symbol preceeding "SIGLO".

SIGLO_DATABASE: Database description & contact information

$\leftarrow \top \rightarrow \qquad \checkmark$	PUBLIC	VAMDC	FULL NAME	DESCRIPTION	CONTACT	HOW TO REFERENCE	KEY (AUTO)
□ <pre></pre>	ON	NOSET		The SIGLO database is the "in-house" data used by	LC Pitchford and JP Boeuf pitchford@@lapla		1

- 🗊 Serveur: localhost:3306 » 🍵 Base de données: lxcat_contributors » 🐻 Table: SIGLO_DATABASE												
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PUBLIC	enum			● ON ○ OFF								
VAMDC	enum			NOSET								
FULL NAME	varchar(1024)		~									
DESCRIPTION	text			The SIGLO database is the "in-hot data used by the group GREPHE at LAPLACE in Toulouse. The data are from different sources as indicat each gas. Please refer to origins sources in publications. An early version of this data file, "siglo.sec", was distribute BOLSIG. The main changes in the present version are : The format has been changed compatible with BOLSIG. 	ise" ; taken red for il ed with i to be longer							
CONTACT	text			LC Pitchford and JP Boeuf pitchford@@laplace.univ-tls and jpb@@laplace.univ-tlse.fr	se.fr /							

Definitions of parameters

Parameter	Definition
PUBLIC	If ON, then accessible to all visitors to LXCat. If OFF, then accessible only to owner (useful for debugging).
VAMDC	Contributors can choose whether or not they want their data accessible via VAMDC.
FULL NAME	Default is the short database name (eg SIGLO).
DESCRIPTION	This information is displayed on the LXCat website at <u>www.lxcat.net/SIGLO</u> .
CONTACT	How to contact the contributors of this database.

SIGLO_LIST_OF_SPECIES: list of target species

IMPORTANT: The target species name must be on this list before cross section data for this species can be added to the database.



Click here to edit the species name.

SIGLO__elec_cs_groups: List of "groups" with brief descriptions

It is possible to organize the data into "groups" with common properties and to comment on those properties in SIGLO__elec_cs-groups.

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✓ Affichage des lignes	✓ Affichage des lignes 0 - 15 (total de 16, Traitement en 0.0001 secondes.)												
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🔄 🥜 Modifier 👫 Cop	ier 🤤 Effacer Ne	J. Meunier, Ph. Belenguer and J.P. Boeuf, J. Appl											

Click here to edit the group name.

The SIGLO database uses "groups" to give references for the compilation of data for each species. Other more creative uses of "groups" could be imagined.

Information for each scattering process

FIELD	DESCRIPTION
TARGET SPECIES	Selected from predefined list of species (SIGLO_LIST_OF_SPECIES)
FINAL STATE	User defined
COMPLETE SET	"YES" if and only if these data are to be used with others for the same target species, from the same database, in a Boltzmann solver
TYPE OF DATA	The following are allowed data types : 'ELASTIC: eV m2','EXCITATION: eV m2','IONIZATION: eV m2','ATTACHMENT: eV m2'. 'RECOMBINATION : eV m2' will be added to this list. Other data types (eg ROTATION, VIBRATIONAL, EFFECTIVE)exist but are useful only in Boltzmann solvers and for complete sets of data.
MASS RATIO (m/M)	Required for ELASTIC scattering. NULL or blank for all others.
THRESHOLD ENERGY (E) in eV	Required for all except ELASTIC scattering. NULL or blank for ELASTIC.
STAT WEIGHT RATIO (g1/g0)	Useful for some applications, but not required
GROUP LABEL	Selected from the list in SIGLO_elec_cs-groups , or NULL
THIS DATA COMMENT	Additional information as needed. Such could include references specific to this particular process
DATA	2-column data table : energy (in eV) and cross section (in m2)

SIGLO__elec_cs : data tables for each process

Below is a screen shot from SIGLO__elec_cs to illustrate how the actual data exist in the databases.

The previous slide defines the contents of each of the columns here, and the next slides shows how to upload such data.

Image: Browse Image: SQL Search Image: Insert Image: Export Image: Insert Image: Export Image: Operations Image: Square search Image:													
Showing rows 0 - 2 (3 total, Query took 0.0007 seconds.)													
SELECT * FROM `SIGLO_el	SELECT * FROM `SIGLO_elec_cs` WHERE `TARGET SPECIES` LIKE 'Ar'												
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+ Options													
←⊤→ ▼	TARGET SPECIES	FINAL STATE	COMPLETE SET	TYPE OF DATA	MASS RATIO (m/M)	THRESHOLD ENERGY (E) in eV	STAT WEIGHT RATIO (g1/g0)	GROUP	THIS DATA COMMENT	DATA	LAST UPDATE	ID (AUTO)	
🗌 🥜 Edit 👫 Copy 🥥 Delete	Ar	Ar	YES	EFFECTIVE: eV m2	0.0000136	NULL	NULL	Ar	EFFECTIVE MOMENTUM- TRANSFER CROSS SECTION	0 7.5E- 1E-3 7.9 20 0.002 7.1E-20 0.003 6.7E	0 2011-06-06 18:21:14 E-	2	
Copy 🥥 Delete	Ar	Ar*(11.5eV)	YES	EXCITATION: eV m2	NULL	11.5	NULL	Ar	All excitation is grouped into this one level.	11.5 0 12.7 7E 22 13.7 1.41E-2 14.7 2.28E-2	2010-06-23 11:41:34 1	3	

This information is inserted automatically. Users shouldn't touch these columns!!

INSERT data: Click on button in upper horizontal bar. Data for each field (defined on p 9) are inserted by hand. The 2-column table of (energy CS) can be copied and pasted from another application. It is recommended that new users begin by inserting data in this way to become familiar with the options.

or **IMPORT** data: Click on "import" to upload a data file in following format:

INSERT INTO `SIGLO elec cs` (`TARGET SPECIES`, `FINAL STATE`, `COMPLETE SET`, `TYPE OF DATA`, `MASS RATIO (m/M)`, `THRESHOLD ENERGY (E) in eV', 'STAT WEIGHT RATIO (g1/g0)', 'GROUP LABEL', 'THIS DATA COMMENT', 'DATA') VALUES ('Ar', 'Ar', 'YES', 'ELASTIC: eV | m2', 1.36e-05, NULL, NULL, 'Magboltz v11.2', 'From Biagi elastic MOMENTUM-TRANSFER CROSS SECTION', 7.1E-20 '0. 1E-3 6.2984E-20 730. 2.247E-21 964. 1.8582E-21'), ('Ar', 'Ar(*)', 'YES', 'EXCITATION: eV | m2', NULL, 6., NULL, 'Magboltz v11.2', 'excitation any comment allowed here', 3.44754E-19 '0 3.44754E-19 1E-4 100. 4.2866E-21 ');

Between the parenthesis in the first line of the file to be IMPORTed are the names of the columns in SIGLO__elec_cs. (There is no carriage return/line feed; this is one long line.)

Attention: Be careful with the symbol "`" in the first line - this is not the same as the symbol "'" which appears in the following lines. Note that there are two underline symbols in SIGLO__elec_cs.

In the IMPORT example on the previous page, there are data for two different processes, ELASTIC and EXCITATION. Data are supplied for each of the column named in the first line.

The data for the two different processes are separated by a comma, and the end of the input is indicated by a semicolon.

Contact the LXCat team if you have any problems.

SIGLO_PUBLICATIONS: Articles, presentations, posters, notes, etc.

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14-Oct-19

See <u>https://www.lxcat.net/notes/</u> for a full list of such publications on LXCat.¹³