Feel free to use your laptop in my talk!

# Databases for simulation of plasmas (elementary collisional data)

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19th International Summer School on "Low Temperature Plasma Physics: Basics and Applications" Master Class "Plasma Kinetics"

Physikzentrum Bad Honnef (Germany), October 4-11 2014





- Database Needs for Modeling and Simulation of Plasma Processing, Panel on Database Needs in Plasma Processing, 1996. National Research Council, ed., Washington, D.C.: National Academy Press.
- Low Temperature Plasma Science, Report of the Department of Energy Office of Fusion Energy Sciences Workshop on Low Temperature Plasmas March 25-27, 2008.

# priorities 2008

- Establish a clearinghouse for fundamental data for LTPS. A hierarchical evaluation, ranging from rough approximations to accurate and complete datasets, should be created. The data should be brought together, evaluated by experts, and made widely available by using up-to-date Web-based technologies.
- Create and support a standing body to identify needs, set priorities, and validate fundamental data in LTPS.
- Develop new approximate methods, scaling laws, and empirical formulas that can be used to quickly estimate unknown data.
- Via computation, provide fundamental data for large molecules, clusters, nanoparticles, and interactions with surfaces. This effort would link closely with developments in other fields, such as quantum chemistry, atomic, molecular, and optical physics, and surface physics, and utilize such powerful techniques as molecular dynamics simulation, quantum chemical codes, atomic structure techniques, and emerging high accuracy atomic and molecular scattering codes.
- A program of experimental measurements needs to be revitalized. New and existing laboratories and techniques should be used to measure key systems, providing key tests of theoretical and approximation method results, and to probe unique or complex situations not approachable with even the most powerful computational methods.



www.lxcat.net

# LXCAT (PRONOUNCED "ELECSCAT")

### Plasma Data Exchange Project

- The Plasma Data Exchange Project is a communitybased project which was initiated as a result of a public discussion held at the 2010 Gaseous Electronics Conference (GEC), a leading international meeting for the Low-Temperature Plasma community.
- This project aims to address, at least in part, the wellrecognized needs for the community to organize the means of collecting, evaluating and sharing data both for modeling and for interpretation of experiments.



# LXCAT: contributors (Sep. 2014)

- BSR (quantum-mechanical calculations by O Zatsarinny and K Bartschat)
- BIAGI (compilation of electron cross sections used by S F Biagi)
- BORDAGE (Compilation of electron cross sections used by M-C Bordage)
- BRAY
- DUTTON
- FLINDERS
- HAYASHI
- IST-LISBON
- ITIKAWA
- LAPLACE (Review of measurements

after 1975)

- MORGAN (Kinema Research & Software)
- NGFSRDW
- PHELPS
- PUECH
- QUANTEMOL
- SIGLO
- TRINITI
- URQUIJO (compilation of De Urquijo)

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- VIEHLAND
- UBC

New contributors are welcome!

### LXCAT: electrons

### Complete sets of cross sections for electron scattering from ground state neutral atoms and molecules.

The energy range of interest is from 0 to some 100's of eV and higher. A complete set of cross sections consists of elastic momentum transfer, and total cross sections for the processes of ionization, attachment and excitation. Complete sets of cross sections are needed as input to a Boltzmann equation solver to determine the electron or ion energy distribution function.

#### Partial sets of electron-neutral scattering cross sections.

Partial sets of electron neutral scattering cross sections are also included on this site. These include additional data concerning electron collisions with ground state molecules - such as total scattering, total elastic scattering - not used in the Boltzmann calculations. These also include cross sections for electron impact ionization of metastable or radicals, needed for the calculation of stepwise ionization, for example.

#### Differential scattering cross sections.

#### Measured electron swarm & transport data.

Swarm data consist of electron transport and rate coefficients as functions of reduced electric field strength, E/N, the ratio of the electric field to the neutral density. At present, we have excluded swarm data measured in the presence of magnetic fields, where a large body of data exist. This may be included in the future if users are interested.

### LXCAT: ions

#### Ion-neutral interaction potentials.

Ion neutral interaction potentials can be used to calculate differential cross sections for ion-neutral scattering.

#### Ion-neutral scattering cross sections.

The limited ion-neutral cross section data available on this site were derived assuming that the differential scattering can be reasonably well approximated as the sum of an isotropic part and a backscatter part. These two components are provided as functions of the center or mass energy.

#### Measured ion swarm & transport data.

Swarm data consist of ion transport and rate coefficients as functions of reduced electric field strength, E/N, the ratio of the electric field to the neutral density. At present, we have excluded swarm data measured in the presence of magnetic fields, where a large body of data exist. This may be included in the future if users are interested.

### LXCAT: photons

#### Databases containing oscillator strengths

Oscillator strength is a quantity that expresses the probability of absorption or emission of electromagnetic radiation in transitions between energy levels of an atom or molecule. These data, combined with a suitable model such as BEF scaling (Y-K Kim, Phys Rev A, 2001), can be used to infer the energy dependence and magnitude of electron-neutral scattering cross sections for specific processes for energies greater than several times the threshold energy.

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Retrieving scattering cross sections

See MC 01 Stephen Bruckman, Electron-scattering cross-sections: measurements & calculations









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### LXCAT step-by-step example

Online calculated electron swarm parameters











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### LXCAT step-by-step example

Comparison of measured and calculated swarm parameters

#### HOME HOW TO USE CONTRIBUTORS DATA CENTER ONLINE CALCULATIONS DOCS AND LINKS DISCUSSION BOARD 3 RESET UPDATE LIST OF SPECIES RUN CALCULATIONS » ⊙ non-Maxwellian EEDF I O Maxwellian EEDF E/N = DTd About the solver eV Te = Swarm parameters are calculated here using BOLSIG+ (ver. 1.2) solver for the numerical solution of the Boltzmann equation for K # points = Tgas = electrons in weakly ionized gases in uniform electric fields, conditions which typically appear in the bulk of collisional low-temperature plasmas. It has been developed by Gerjan Hagelaar (LAPLACE, France). SPECIES MOLE FRACTIONS Note that BOLSIG+ makes use of the classical "2-term approximation". Some of the data sets on this site were developed for use with Monte Carlo or "multiterm" Boltzmann solvers and errors may be introduced by the 2-term approximation used in BOLSIG+. We have 02 = tried to indicate when this could be of concern. Please consult BOLSIG+ for the details and to download the complete freeware application for Windows. Users of this site are kindly requested to reference to BOLSIG+ and the appropriate cross section databases in all publications making use of data from this site. Mobility x Gas density Diffusion coefficient x Gas density www.ixcat.net 29 Sep 2014 Reduced Townsend coeffici Electron energy N2 (0.8, Phelps) + O2 (0.2, Phelps) 10<sup>26</sup> Reaction rates Electron energy distribution functions Electron cross sections (new window) varm parameters in text file Mobility x Gas density, (m V s)<sup>-1</sup> All figures in zip archive 102 ss section input file Assign label Submit 10<sup>2</sup> 10<sup>23</sup> 10<sup>3</sup>

35



10 100 10 102 Reduced electric field, Td

	8 databases I 264 x 60 species I 129.8k records I updated: 23 September 2014	STEP 1: SELECT DATA TYPE & CLICK NEXT
Databases containing meas	sured electron and ion swarm data	« PREV NEXT »
Swarm data consist of electron and ion tra	ansport and rate coefficients as functions of reduced electric field strength,	SCATTERING CROSS SECTIONS
E/N, the ratio of the electric field to the ne presence of magnetic fields, where a large	utral density. At present, we have excluded swarm data measured in the e body of data exist. This may be included in the future if users are	DIFFERENTIAL SCATTERING CROSS SECTIONS
interested.		INTERACTION POTENTIALS
		OSCILLATOR STRENGTHS
		SWARM / TRANSPORT DATA
		GLOBAL SPECIES FILTERING
		ELECTRONS
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data type » databases » first species » second species » Ground states	data groups - processes - output     STEP 4: SELECT SECOND SPECIES & CLICK NEXT
АГ С2F4 С2F6 С2H4 С2H6 С3F8 С3H8 СF3I СF4 СH4 СHF3 СО СО2 H2 H2O He	Kr N2 N20 Ne O2
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	F3 SF6:CO2 SF6:He
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HOME HOW TO USE CONTRIBUTORS DATA CENTER ONLINE CALCULATIONS data type » databases » first species » second species » databases » first species » second species » databases	DOCS AND LINKS DISCUSSION BOARD e.g. mobility data groups • processes • output
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<ul> <li>e / Air</li> <li>Mobility x gas density (μN)   Frommhold, L, Fortschr. Physik, 1597</li> <li>Mobility x gas density (μN)   Hessenauer, H, Z. Physik 204, 142 (19 Mobility x gas density (μN)   Nielsen et al 1937. Updated: 29 Nove Mobility x gas density (μN)   Nieksen H, Proc. Phys. Soc. London, 85</li> </ul>	7 (1964). Updated: 7 October 2012. 967). Updated: 7 October 2012. mber 2011. , 1283 (1965). Updated: 7 October 2012.		
APLACE (measurements after 1975) 🗵			
Data Group [SwarmGroup11]: Milloy, H. B., Reid, I. D., 231 (1975); Rees, J. A., Aust. J. Phys. 26, 427 (1973); Roznerski, W., Leja, K., J. Phys. D: Appl. Phys. 17, 279 (1 Ruiz-Vargas, G., Urquijo, 29th ICPIG, 12-17 July (2009);	⊕ ⊕ ⊆ Crompton, R. W., Aust. J. Phys. 28, 1984);	2	
OLSIG+ solver ☑			
Data Group [Calculated]: Tgas 300 K EEDF 1 (type of EEDF : 1 = non-Maxwellian) ENmin 0.1 Td ENmax 1000 Td points 100 N2 0.8 Phelps database O2 0.2 Phelps database.			
e / N2 : O2 e / N2 : O2 (0.8 : 0.2) Mobility x gas density (µN)   Updated: 29 September 2014 8:19:3:	3.		



### inter-comparison

- Measurements from different databases
- Calculations using different sets of input data

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• Any combinations of thereof









LX	HOME	HOW TO USE	CONTRIBUTORS	DATA CENTER	ONLINE CALCULATIONS	DOCS AND LINKS	DISCUSSION BOARD	Q e.g. mobility
			data ti	browse and o	download	data groups » processes	» output STEP 1: SELECT DATA TYP	E & CLICK NEXT
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							OSCILLATOR STRENGTHS	
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			scattering	; cross sections	i	first filling	14-Nov-2013	\$ 15:00:00			
			differenti	al scattering cro	oss sections	first filling	up to date				

	interaction potentials	first filling	15-Dec-2013 04:15:00
	swarm / transport data	first filling	15-Nov-2013 11:30:00
Database	Data type	Previous update	Next update
BSR		first filling	up to date
	scattering cross sections	first filling	up to date
	differential scattering cross sections	first filling	up to date
Biagi-v7.1	scattering cross sections	first filling	up to date
Biagi-v8.9	scattering cross sections	first filling	up to date
Bordage	scattering cross sections	first filling	up to date
Bray	scattering cross sections	first filling	up to date
Dutton	swarm / transport data	first filling	up to date
Hayashi	scattering cross sections	first filling	15-Feb-2014 15:30:00
IST-Lisbon		first filling	up to date
	scattering cross sections	first filling	up to date
	swarm / transport data	first filling	up to date
Itikawa	scattering cross sections	first filling	up to date
LAPLACE	swarm / transport data	first filling	15-May-2014 12:30:00
Morgan	scattering cross sections	first filling	up to date
NGFSRDW	scattering cross sections	first filling	up to date
Phelps		first filling	14-Nov-2013 15:00:00
	scattering cross sections	first filling	14-Nov-2013 15:00:00
	swarm / transport data	first filling	up to date
Puech	scattering cross sections	first filling	up to date





This is a forum to share opinions, post doubts and view discussions regarding	ne content of this website. Google discussion group has	s been used for this forum. A 🛛 🛞
request an invitation to join via signing up using a gmail address. All posts are	noderated.	
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Statisical Weights		
Von John - 4 Beiträge - 38 Aufrufe	28. Jun	
Time Machine (previous versions of the website) Von Ixcat.info - 1 Beitrag - 15 Aufrufe	21.11.13	
New Datatype and New Database		
Von Ixcat.info - 1 Beitrag - 10 Aufrufe	13.11.13	
New data type - Differential Cross Sections Von Bhaskar Chaudhury - 1 Beitrag - 6 Aufrufe	08.11.13	
New web interface Von Sergey Pancheshnyi - 6 Beiträge - 31 Aufrufe	23.10.13	
CO2	57,724,774,487 V	
Von bplasma - 4 Beiträge - 56 Aufrufe	10.05.13	
CHEMKIN Format thermal data for excited states of N2 Von Peng Guo - 1 Beitrag - 45 Aufrufe	10 12 12	
Specific heat of different states of O2 and N2	10.12.12	
Von John - 1 Beitrag - 51 Aufrufe		
	https://groups.google.com/forum/#	!forum/lxcat >

![](_page_26_Picture_1.jpeg)

![](_page_27_Figure_0.jpeg)

![](_page_27_Picture_1.jpeg)

http://gaphyor.lpgp.u-psud.fr/gaphyor/

### **GAPHYOR (GAZ-PHYSICS-ORSAY)**

# GAPHYOR

- Five domains of physics, chemical physics and plasma physics are
  - Properties of isolated atoms and molecules.
  - Collisions with photons.
  - Collisions with electrons.
  - Collisions and reactions between atoms and molecules.
  - Macroscopic properties of gases
- Based on a large coverage of the specialized literature in the fields of atomic and molecular physics, chemical physics and plasma physics. After a detailed analysis of papers by a team of scientific experts the information is coded and indexed in a concise and structured way.
- Data include bibliographical, factual and numerical information.
- No longer updated since 2005.

![](_page_28_Figure_10.jpeg)

	Overview Database Handbook Update Fees Help Home C	ontacts
Steward Jr M D (US V <u>Phys. Rev. A, US vol.6</u>	I MA), Chilton J E , Boffard J B , Lin C C 5. <u>p.32704 (2002)</u>	
Ar, e> Ar *, e Excitation (Electronic	collisions)	
Total cross sections (a Medium energies (10 Experimental data <i>energies:</i> 20 - 200 eV <i>notes:</i> 2s2, 2s4, 3d5 le	osolute values) V < E < 10 keV CM system) vels	
Haynes M A (AU QU <u>Phys. Rev. A, US vol.6</u>	VA), Lohmann B 4 <u>p.44701 (2001)</u>	
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http://consult.cern.ch/writeup/magboltz/

# MAGBOLTZ - TRANSPORT OF ELECTRONS IN GAS MIXTURES

### Magboltz - transport of electrons in gas mixtures

Responsible at CERN: Rob Veenhof Manual Type: Source files, cross sections Version: 10.0.4, 2.4 Author: Stephen Biagi Reference: none Created: 20 May 1995 Last Update: 22 Apr 2014 Verified: 17 Jun 2014 Valid until: further notice Support Level: Normal

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#### Magboltz

Magboltz solves the Boltzmann transport equations for electrons in gas mixtures under the influence of electric and magnetic fields.

#### Further information:

- LXCAT cross section compilation;
- The cross sections used by Magboltz 7.1, interfaced with Garfield 9 (current default)
- How to use Magboltz

Magboltz source files:

- Source file for version 7.1 (default since 13/4/2005);
- Source file for version 8.9.1 (edition of 27 Sep 2010, reinstoring GeH<sub>4</sub> and SiH<sub>4</sub> and improving C<sub>2</sub>H<sub>2</sub>F<sub>4</sub>);
- Source file for version 8.9.2 (edition of 14 Nov 2010, hydrogen update);
- Source file for version 8.9.3 (edition of 24 Feb 2011, xenon ionisation cross section corrected);
- Source file for version 8.9.4 (edition of 25 May 2011, xenon ionisation cross section changed at threshold);
- Source file for version 8.9.5 (edition of 12 Jun 2011, TMA);
- Source file for version 8.9.6 (edition of 27 Aug 2011, update of low energy argon excitation cross sections);
- Source file for version 8.9.7 (edition of 25 Sep 2011, krypton update);
- The source file for version 9.0.1 (edition of 12 May 2012) was corrected with version 9.0.3;
- Source file for version 9.0.3 (edition of 28 Aug 2013);

Magboltz Cross sections Cross sections used by Magboltz 7.1 Select your gases argon Update Reset selection **Cross sections Further information** ARGON (2002) Cross section graph in PostScript format. hydrogen deuterium CM\*\*2 BRITANNIC helium Background information from nitrogen Information on the element from oxygen ELAST. M ELAST. TO EXC S EXC. P EXC. D IONS. EXC. SUM 10\*\*-16 ozonefluorine neon × ∉ argon krypton SECTION xenon cæsium mercury × methane deuterated methane ENERGY EV. methanol ethane ethanol ethylene acetylene propane2-propanol o cyclo propane propylene
 isobutane n-butane neopentane n-pentane silane 62 http://jilawww.colorado.edu/~avp/

### A COMPILATION OF ATOMIC AND MOLECULAR DATA, ASSEMBLED AND EVALUATED BY PHELPS AND COLLABORATORS

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### **Arthur V. Phelps**

Fellow Adjoint of JILA

#### **Current Research Interests:**

- Atomic and molecular collision data for modeling electrical discharges in rare gases, air, and so on
  - A compilation of atomic and molecular data, assembled and evaluated by Phelps and collaborators, is available.

![](_page_31_Picture_8.jpeg)

Return to JILA Home Page

### Index of /~avp/collision\_data

?	<u>Name</u>	Last modified	Size Description
?	Parent Directory		-
?	ararnotes/	20-May-2005 14:24	-
?	attachment-detachment/	20-May-2005 14:24	-
?	cathodefalldata/	20-May-2005 14:24	-
?	electronneutral/	21-May-2005 16:52	-
?	hehenotes/	20-May-2005 14:25	-
?	ionneutral/	26-Aug-2005 10:40	-
?	methanenotebooks/	20-May-2005 14:25	-
?	millsnotes/	20-May-2005 14:23	-
?	ndvcr/	20-May-2005 14:25	-
?	neutralneutral/	20-May-2005 14:26	-
?	nitrogen/	20-May-2005 14:26	-
?	readme.txt	20-May-2005 14:23	7.8K
?	temporary/	20-May-2005 14:26	-

Apache/2.2.15 (Red Hat) Server at jilawww.colorado.edu Port 80

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in introduction

COMPILATION OF ELECTRON CROSS SECTIONS USED BY A. V. PHELPS

Please refer to these data using the sources cited for each gas. Please do not refer to any of them as "JILA cross sections", because a) the data shown here for a given gas may come from several sources that should be referred to by the respective authors names; b) in most cases no one else at JILA or NIST has approved the data or even looked at it. Reference to this data as "JILA data" could be interpreted incorrectly as indicating NIST approval and could jepordize my Web site usage.

GASES COMPILED: 02, N2, C0, C02, H2, H2O, N0, SF6, He, Ne, Ar, Xe, Na, and Mg  $\,$ 

Comments are made on cross sections from other sources for some of these and other gases.

WE MAKE NO CLAIMS FOR THESE CROSS SECTIONS BEYOND THOSE STATED IN THE PAPERS WHERE THEY ARE PUBLISHED OR CITED. IN MOST CASES THESE CROSS SECTIONS WERE ASSEMBLED IN THE 1970'S AND 1980'S. IN ONLY A FEW CASES HAVE THEY BEEN MODIFIED OR TESTED SINCE THAT TIME. I DO NOT PLAN ANY UPDATES. ADDITIONS HAVE BEEN MADE WHEN CROSS SECTIONS HAVE BEEN ASSEMBLED FOR OTHER PURPOSES. SINCE THE JILA INFORMATION CENTER WAS CLOSED BY NIST, THERE IS NO ONE THERE TO HELP YOU. OPINIONS EXPRESSED ARE THOSE OF A. V. PHELPS AND DO NOT IMPLY JILA, CU, OR NIST APPROVAL.

The cross sections are in 1E-16 cm2. The two-term Boltzmann code, BACKPRO, used in deriving our cross sections employs linear interpolation between points in the cross section tables. Therefore linear interpolation should be applied when using them. Except as noted below for N2, the cross sections listed in JILA Information Center Reports 26, 27, and 28 for N2, H2, and O2 should be the same as those listed here. (This aspect has not been checked in detail, so please inform me of discrepancies.)

It should be kept in mind that the momentum transfer cross sections tabulated are effective values that include the effects of inelastic collisions as is appropriate for use in the two-tern spherical harmonic expansion. See, for example, Baraff and Buchsbaum, Phys. Rev. 130, 1007 (1963) and Sec. IIB of Pitchford and Phelps, Phys. Rev. A 25, 540 (1982). Where data is available, the effective Qm is set equal to the sum of the inelastic cross sections plus the elastic momentum transfer cross section. This is an approximate relation.

Some of the terms used in the tables and the BACKPRO code are:

#### O2 MOMENTUM-TRANSFER CROSS SECTION

	ENERGY	Effective	Qm	-	Defined
1	0.0000	0.3500			
2	0.0010	0.3500			
3	0.0020	0.3600			
4	0.0030	0.4000			
5	0.0050	0.5000			
6	0.0070	0.5800			
7	0.0085	0.6400			
8	0.0100	0.7000			
9	0.0150	0.8700			
10	0.0200	0.9900			
11	0.0300	1.2400			
12	0.0400	1.4400			
13	0.0500	1.6000			
14	0.0700	2.1000			
15	0.1000	2.5000			
16	0.1200	2.8000			
17	0.1500	3.1000			
18	0.1700	3.3000			
19	0.2000	3.6000			
20	0.2500	4.1000			
21	0.3000	4.5000			
22	0.3500	4.7000			
23	0.4000	5.2000			
24	0.5000	5.7000			
25	0.7000	6.1000			
26	1.0000	7.2000			
27	1.2000	7.9000			
28	1.3000	7.9000			
29	1.5000	7.6000			
30	1.7000	7.3000			
31	1.9000	6.9000			
32	2.1000	6.6000			
33	2.2000	6.5000			
34	2.5000	6.1000			
35	2.8000	5.8000			
36	3.0000	5.7000			
37	3.3000	5.5000			
38	3.6000	5.4500			
39	4.0000	5.5000			
40	4.5000	5.5500			
41	5.0000	5.6000			
42	6.0000	6.0000			
4.2	7 0000	6 6000			

![](_page_33_Picture_0.jpeg)

67

Gaseous Electronics Laboratory Data Centre, University of Belgrade http://mail.ipb.ac.rs/~cep/ipb-cnp/ionsweb/

### A DATABASE ON THE TRANSPORT PROPERTIES OF ELECTRONS, POSITRONS AND IONS

# **GELDC** database

The GELDC database maintains transport and collision data for the following charged particle species: electrons, positrons, positive and negative ions.

A Data	base on th	e Transp	ort Propertie	es of Electro	ns. Positrons	and		
11 Dutt	.ouse on th	e mansp	Ions	.5 of Licetio	115,1 051010115		1.4. E.S.	
	24.22			에 앉아 아니?	1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1			
		[ <u>home</u> ] <u>ove</u>	<u>erview</u>   <u>data</u>   <u>help</u>	contact   links ]				
nose one of t	he sections and o	lick on one of	the gas below to ge	t a plot of the trans	port and collision dat	a. The	유가 있는	a free and the
operty and/o	r the cross section	ie available by	Fransport parameter	s of the charged pa	ticles include the me	sport an		
ergy, drift ve	elocity and diffu	sion tensor con	nponents and rate co	befficients, presente	d as a function of E/I	N and/or	H VÊ I.	
IN.	1.2631234		2.34.545.53	남편 것을 많을 수 없다.				경양소화했는
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ectron Tran	sport and Colli	sion Data				15 15 10	신간 것이	
lectron Tran	sport and Colli	sion Data	Fa F	Br	N <sub>2</sub> O			
lectron Tran	sport and Colli BF <u>3</u>	sion Data	E <u>a</u> E	<u>Br</u>	<u>N<sub>2</sub>O</u>			
ectron Tran	sport and Colli <u>BF3</u> sport and Colli	sion Data	<u>E4 E</u>	<u>Br</u>	<u>N20</u>			
ectron Tran	sport and Colli <u>BE3</u> sport and Colli	sion Data C sion Data	E4 E	Br	<u>N20</u>			
lectron Tran	sport and Colli BF <u>3</u> sport and Colli Ar	sion Data C sion Data	E4 E		<u>N20</u> N2			
ectron Tran	sport and Colli BF3 sport and Colli Ar	sion Data	<u>Е4</u> <u>Н</u>		<u>N20</u>			
ectron Tran ssitron Tran ssitive Ions '	sport and Colli BF3 sport and Colli Ar Transport and O	sion Data	<u>Е4 Н</u>		<u>N20</u>			
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![](_page_34_Picture_1.jpeg)

# **POTLIB Library**

- Global and semiglobal potential energy surface subprograms for calculating Born-Oppenheimer energies as a function of nuclear geometry.
- The library currently features nearly 300 potential energy routines for a wide range of chemical systems.
- Our goal is to facilitate chemical dynamics research by collecting and disseminating a comprehensive collection of state-of-the-art potential energy routines (developed by a wide, international group of researchers) with systematic and well-defined interfaces for use with chemical dynamics programs.

	Potential energy surface information
System	CH4
ID	ch4T8
Number of bodies	5
Common name	Schwenke-Partridge T8
Functional form	
Interface	Section-2
Number of electronic surfaces	1
Number of derivatives	0
References	D. W. Schwenke and H. Partridge, Spectrochim. Acta A 57, (2001) 887
Notes	The data file (ch4T8datafile.tar) contains two files: ch4pes is a data file read once by the PES routine getpot_ch4t8.f90 is a calling routine that accepts cartesian coordinates, converts them to Radau coordinates (the required input for the T8 PES), calls the surface, zeroes it so that the ZOE is at the global minimum, and returns the energy. There are no derivatives. One should use nuclear rather than atomic masses for the C and H atoms.

72

![](_page_36_Picture_0.jpeg)

73

http://www.nist.gov/pml/data/

### THE NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY (NIST, US)

NIST physical reference data

#### **Atomic Spectroscopy Data**

Contains databases for energy levels, wavelengths, and transition probabilities for atoms and ions and related bibliographic databases.

#### **Molecular Spectroscopic Data**

Includes databases containing spectroscopic data for small molecules, hydrocarbons, and interstellar molecules. In addition, there are two publications containing equations and the underpinning theory for molecular spectroscopy.

#### Atomic and Molecular Data

Contains databases on thermophysical properties of gases, electron-impact cross sections (of atoms & molecules), potential energy surfaces of group II dimers, and atomic weights and isotopic compositions.

#### X-Ray and Gamma-Ray Data

Contains databases on the interaction of x-rays and gamma-rays with elements and compounds.

#### **Radiation Dosimetry Data**

This database calculates stopping-power and range tables for electrons, protons, or helium ions.

#### **Nuclear Physics Data**

Contains a table of the half lives of 65 radionuclides and a database of the isotopic compositions, atomic weights and relative atomic masses of the elements.

#### **Condensed Matter Physics Data**

This database consists of evaluated data for use in total-energy calculations of electronic structure by density-functional theory. It contains total energies and orbital energy eigenvalues for all atoms from hydrogen to uranium.

![](_page_37_Picture_0.jpeg)

![](_page_37_Picture_1.jpeg)

![](_page_38_Picture_0.jpeg)

elect	an	element	of	interest	to	view	its	data	

Hydrogen H	
Indium, In	
Lithium, Li	
Nitrogen, N	_
Oxygen, O	Submit

la	2a	3b		4b	5b	6b	7b		VIII		16	2b	3a	4a	5a	6a	7a	0
1 <u>H</u>																		<sup>2</sup> <u>He</u>
<sup>3</sup> Li	<sup>4</sup> Be												5 <u>B</u>	<u>6С</u>	7 <u>N</u>	<sup>8</sup> 0	<sup>9</sup> F	<sup>10</sup> Ne
<sup>11</sup> Na	<sup>12</sup> Mg												13 <u>Al</u>	<sup>14</sup> Si	<sup>15</sup> P	<sup>16</sup> S	17Cl	<sup>18</sup> Ar
<sup>19</sup> K	<sup>20</sup> Ca	<sup>21</sup> Sc		<sup>22</sup> Ti	<sup>23</sup> V	<sup>24</sup> Cr	<sup>25</sup> Mn	<sup>26</sup> Fe	<sup>27</sup> Co	<sup>28</sup> Ni	<sup>29</sup> Cu	<sup>30</sup> Zn	<sup>31</sup> Ga	<sup>32</sup> Ge	<sup>33</sup> As	<sup>34</sup> Se	<sup>35</sup> Br	<sup>36</sup> Kr
<sup>37</sup> Rb	<sup>38</sup> Sr	<sup>39</sup> Y		<sup>40</sup> Zr	<sup>41</sup> Nb	<sup>42</sup> Mo	<sup>43</sup> Tc	<sup>44</sup> Ru	<sup>45</sup> Rh	<sup>46</sup> Pd	47Ag	<sup>48</sup> Cd	49 <u>In</u>	<sup>50</sup> Sn	<sup>51</sup> Sb	<sup>52</sup> Te	<sup>53</sup> I	<sup>54</sup> Xe
<sup>55</sup> Cs	<sup>56</sup> Ba	<sup>57</sup> La	*	72Hf	<sup>73</sup> Ta	<sup>74</sup> W	<sup>75</sup> Re	<sup>76</sup> Os	<sup>77</sup> Ir	<sup>78</sup> Pt	<sup>79</sup> Au	<sup>80</sup> Hg	<sup>81</sup> Tl	<sup>82</sup> Pb	<sup>83</sup> Bi	<sup>84</sup> Po	<sup>85</sup> At	86Rn
<sup>87</sup> Fr	<sup>88</sup> Ra	<sup>89</sup> Ac	+	<sup>104</sup> Rf	<sup>105</sup> Db	<sup>106</sup> Sg	<sup>107</sup> Bh	<sup>108</sup> Hs	109Mt	110Uun	111Uuu	112Uub		114Uuq				
* Lan	thanid	es		<sup>58</sup> Ce	<sup>59</sup> Pr	<sup>60</sup> Nd	<sup>61</sup> Pm	<sup>62</sup> Sm	<sup>63</sup> Eu	<sup>64</sup> Gd	<sup>65</sup> Tb	<sup>66</sup> Dy	<sup>67</sup> Ho	<sup>68</sup> Er	<sup>69</sup> Tm	<sup>70</sup> Yb	<sup>71</sup> Lu	
+ Act	inides			<sup>90</sup> Th	<sup>91</sup> Pa	<sup>92</sup> U	<sup>93</sup> Np	94Pu	95Am	<sup>96</sup> Cm	97Bk	<sup>98</sup> Cf	99Es	<sup>100</sup> Fm	<sup>101</sup> Md	<sup>102</sup> No	<sup>103</sup> Lr	

#### BEB/BE-scaled References for Atoms\*

Numbe	r	Ioniz	ation Data	Excit	ation Data
Symbo Ionizatio	l on	Reference	Comparison to Experiment	Reference	Comparison to Experiment
1 H	I	[1]	Yes	[21]	3 Yes, 6 No
2 He	I	[1]	Yes	[21]	3 Yes, 6 No
3 Li	I			[21]	1 Yes, 8 No
5 B	I	[18]	No		
6 C	I	[20]	Yes		
7 N	I	[20]	Yes		
8 O	I	[20]	Yes		
13 Al	I	[18]	Yes		
31 Ga	I	[18]	Yes		
49 In	I	[18]	Yes		

\*References to other calculations and experimental measurements for each atom are shown beside the graph for that atom.

*		e	Ele	ec f	tron-li or Ion	mpact ( ization (	Cross Sec and Excite	tions ation
oductio	on and Rei	feren	ces		Table of	Atoms	Table of Mo	lecules
Se	elect a r	nole	ecule BE	of B F	intere: Reference	st to viev <sup>s*</sup>	v its data.	
	Small mol	ecule	s	Atmospheric molecules			s Oxygenates	5
H <sub>2</sub>	H <sub>2</sub> <sup>+</sup> HO <sub>2</sub>	H <sub>2</sub> O	H <sub>3</sub> O <sup>+</sup>		H <sub>2</sub> S N <sub>2</sub>	O NO2	СНО	1
N <sub>2</sub>	N2 <sup>+</sup> NH3	NO	<b>0</b> <sub>2</sub>		0 <sub>3</sub> CS	s cos	CH <sub>2</sub> O	
	co co⁺	CO2			S <sub>2</sub> SC	D <sub>2</sub> CS <sub>2</sub>	C <sub>2</sub> H <sub>3</sub> O	
		_	н	vdr	ocarbon	s		-
<b>C</b> 11		<u></u>		1	C 11	-		
CH <sup>+</sup>		C <sub>3</sub> H <sub>3</sub>	(allono)					.
CHa	CoHo	CoH4	(propyne	6)	СаНе		CeHe (fulvene)	"
CH2+	CH2 <sup>+</sup> C2H3 C3H4 (propyne CH2 <sup>+</sup> C2H4 C2H6				C4H8 (1-b	utene)		
СН3	C <sub>2</sub> H <sub>4</sub> +	C <sub>3</sub> H <sub>6</sub>			C4H8 (trai	ns-2-butene)		
CH3+	CH3 <sup>+</sup> C2H6 C3H8				C <sub>4</sub> H <sub>8</sub> (iso	butene)		
$CH_4$	CH <sub>4</sub> C <sub>2</sub> H <sub>6</sub> <sup>+</sup>							
CH4+								
								_
Si	licon and	Germ	nanium	Hy	drides	SiFx	SFx	
SiH	SiH <sub>2</sub> SiH	3	GeH	Ge	H <sub>2</sub> GeH <sub>3</sub>	SIF SIF	SF SF2 SF	3
SiH4	SI2H6 SI(C	;H <sub>3</sub> ) <sub>4</sub>	GeH <sub>4</sub>	Ge	2 <sup>H</sup> 6	SiF <sub>3</sub> SiF <sub>4</sub>	SF4 SF5 SF	6
Fit	lorocarbo	ns E	Boron C	om	pounds	Fr	eons	[
CF	CF2 CF	3	BCI E	3CI2	BCI3	CCIF3 CO	Cl <sub>2</sub> F <sub>2</sub> CCl <sub>3</sub> F	
CF	4 C <sub>2</sub> F <sub>6</sub> C <sub>3</sub>	F8	BF E	BF <sub>2</sub>	BF3	CHCIF <sub>2</sub> CH	HCI2F CH2CIF	
elect	molecule b	<b>y forr</b> loride	nula:		- OR -	Select m Acetylene -	olecule by nam	ie:
12 – B 13 – B	oron dichlor oron trichlor	'ide ride				Acetylene ion Allene – C3	- C2H2+	
- Bor	on fluoride					Allyl – C3H	5	
: – Bo I – Bo	ron difluoric	ue de				Ammonia – Benzene –	NH3 C6H6	
IF3 -	Freon 13					Boron dichlori	ide – BCl2	
I3F -	Freon 11					Boron fluoride	e - BF	
- Flu	oromethylidy	yne				Boron monocl	nloride – BCl	
	Submit						Submit	
								77

National Institute of Standards and Tec

![](_page_38_Picture_8.jpeg)

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IIST Home > PML > Physical Reference Data > Molecular Spectroscopic Data	
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• Hydrocarbons	
Wavenumber Tables for Calibration of Infrared Spectrometers	
Frequencies for Interstellar Molecular Microwave Transitions	
Photoionization of CO <sub>2</sub> (ARPES)	
Equations & Underpinning Theory:     Diatomic Rotational Calculations	
• Methane Symmetry Operations	
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Microwave Spectral Data: Diatomics, Triatomics, and	Physical Reference Data
Hydrocarbons	
F.J. LOVAS, E. Hemann, and R.D. Suenram These three databases of diatomic, triatomic, and hydrocarbon molecules were o	originally Contact
published as spectral tables in the Journal of Physical and Chemical Reference D	ata. Each of General Information:
the databases covers primarily the microwave region with some data available for irrequency region	or the radio 301-975-4200 Telephone
	100 Bureau Drive, M/S 8400

![](_page_39_Picture_1.jpeg)

http://dbshino.nifs.ac.jp/

ATOMIC AND MOLECULAR DATA RESEARCH CENTER, NATIONAL INSTITUTE FOR FUSION SCIENCE (NIFS, JAPAN)

### Information on the NIFS Bibliographic and Atomic and Molecular Numerical Database

We have Atomic and Molecular (A & M) numerical databases and bibliographic databases on plasma physics and atomic physics:

#### **Bibliographic Database**

ORNL bibliographic information for atomic collisions compiled by Oak Ridge National Laboratory, USA since 1959.

#### A & M numerical Database

AMDIS	Ionization, excitation, and dissociation cross sections by electron impact and recombination cross sections and rate coefficients by
	electron impact
	Examples from AMDIS
CHART	Charge transfer cross sections of ions with atoms and molecular hydrogen
	Examples from CHART
SPUTY	Sputtering yields for monatomic solids
BACKS	Backscattering coefficients of light ions from solid
AMOT	Cross sections and rate coefficients for electron - molecule collision processes
AMOL	Examples from AMOL
CMOI	Cross sections and rate coefficients for heavy particle - molecule collision processes
CMOL	Examples from CMOL

These databases are available for research purposes. You can use them now without registration.

Please note these databases are copyrighted: ORNL by ORNL AMDIS, CHART, SPUTY and BACKS by NIFS.

When you use numerical data extracted from our database in your publication, we request you to refer to our database.

[Help]

#### **OutPut Data in AMDIS IONIZATION**

#1 [Ar  $(3p^6)$  + e --> Ar<sup>+</sup> + 2e]

Record Number = 020701 Process = ION **Theory or Experment** = T Method = Coulomb-Born approximation with exchange Atomic Number = 18 Element = Ar Ionic State = 0 **#Of Electrons** = 18 Initial State = Ar +0 Initial State Ion Conf = 3p^6` Final State = Ar +1 Final State Ion Conf = Data Producer : # of Data Points = 17Author(s) = Povyshev, V.M.\$Sadovoy, A.A.\$Shevelko, V.P.\$Shirkov, G.D.\$Vasina, E.G.\$Vatulin, V.V. Title = ELECTRON-IMPACT IONIZATION CROSS SECTIONS OF H.He.N.O.Ar,Xe,Au,Pb ATOMS AND THEIR IONS IN THE ELECTRON ENERGY RANGE FROM THE THRESHOLD UP TO 200 keV Journal Name = Commun. Joint Inst. Nucl. Res. Dubna Volume and Issue No = Page of Publication = Date of Publication = 2001 **Comment** = Table5.1. Atom code Sub Comment = AM Record No. = ORNL Record No. =

 $#2 [Ar (3s^23p^6) + e --> Ar^+ (3s3p^6) + 2e]$ 

![](_page_41_Picture_0.jpeg)

Atomic Molecular Data Services Provided by the Nuclear Data Section

https://www-amdis.iaea.org/

### ATOMIC AND MOLECULAR DATA UNIT, INTERNATIONAL ATOMIC ENERGY AGENCY (IAEA)

	I Atomic Energy Agency c Molecular Data Services	NDS Mission   About Us
Provide	by the Nuclear Data Section	Go
Databases » AMB	DAS ALADDIN OPEN-ADAS GENIE On-line Computing » HEAVY AAEXCITE RATES LANL Codes FLYCHK	FAC Data
Abome A&M Data Unit Home	Atomic and Molecular Data Unit Activities	☆ IAEA Meetings July 7-9, 2014
♠ News News Calendar	The Atomic and Molecular Data Unit operates within the Nuclear Data Section of the International Atomic Energy Agency, Vienna, Austria. The primary objective of the Atomic and Molecular Data Unit is to establish and maintain internationally recommended numerical databases on atomic and molecular collision and radiative processes, atomic and molecular structure characteristics, particle-solid surface interaction processes and physico-chemical and thermo-mechanical material properties for use in fusion energy research and other processes.	Joint IAEA-ITAMP TM on Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data,Cambridge,
Overview AMBDAS ALADDIN OPEN-ADAS	Databases on Atomic and Molecular Data for Fusion.	Aug 18-19, 2014 Aug 18-19, 2014 2nd RCM of CRP on Data for Erosion and Tritium Retention in Bendlium Placema
GENIE KNOWLEDGE BASE	Atom, Molecule ALADDIN AMBDAS GENIE OPENADAS Kovipronic Plasma-Surface Database Database Database Search Engine Search Triplet D <sub>2</sub>	Facing Materials Aug 20, 2014 CM on Plasma
© On-Line Computing Overview HEAVY	FC Factors & A-values of H <sub>2</sub> & Isotopes	Interaction with Steel Surfaces Sep 29- Oct 3, 2014 16th International
ATES	Online Computing Capabilities	Conference on Radiative Properties
ANL Codes LYCHK AC Data	Code Centres PortalLANL Atomic PhysicsFLYCHK Non-LTE KineticsHeavy Particles CollisionsAveraged e- Impact Cross-sectionEffective e- Inpact Rates	of Hot Dense Matter (RPHDM) October 8-10, 2014 3rd RCM of CRP on
Activities FRC Subcommittee RP	ATOM-AKM e - Collision Data	AMO/PSI Meetings May 26-30, 2014 21th
leetings /orkshops	Knowledge Base for Atomic, Molecular and Plasma-Material Interaction Data for Fusion	International Conference on Plasma-Surface Interaction Conference,
Data Centre Network Code Centre Network (SAMS Contacts	Our Unit achieves its objectives by coordinating the activities of the International Atomic and Molecular Data Center Network (DCN) and Code Center Network (CCN), initiation and conducting international Coordinated Research Projects (CRP), organization of various types of Expert's Meetings, publication of technical reports on meetings and research activities and using other forms (research contracts, research agreements, consultancies) for stimulation of the generation, collection and critical assessment of the required atomic and critical intermediation (DMI) data informations.	Kanazawa, Japan Jun 1-5, 2014 22nd International Conference on Spectral Line shapes, Tullahoma, TN, USA Jun 2-4, 2014 12th

tomic and Molecular Data	Particle-Surface Interactions
Electron Collisions Photon Collisions Heavy Particle Collisions	Erosion, Sputtering, Sublimation Reflection Trapping, Penetration
Data presented here are IAEA recon Data are mostly compiled from the <u>Co-ordinated research projects (CRI</u> IAEA Atomic and Molecular Data U The Author's Units for heavy particl publications (NUC-FUS-SUPP/87 ( 6086 (1990)) were given incorrectly Author's Units are eV/amu. This wa	Note Immended at their time of compilation. AEA APID series, published results of and from consultancies inside the init. e collision cross-sections from 3 (987), ORNL-6090 (1987), ORNL- in ALADDIN as eV. The correct a fixed on 2010-Feb-10.

![](_page_42_Figure_1.jpeg)

#### Electron collisions / N Cross Sections

Reset page Complete restart

		Cı	OSS S	ections all data			Go to n	umerical data			Units in Energy origin ev Apply unit conversion
1	2	<u>3</u>	4	Reactants	Products	<u>7</u>	Comment	Authors	Year	Publication	Validity Limits in eV
۷	ION	A	DER	<b>e</b> , <b>N</b> [G]		BELI		M.A. Lennon et al.	1988	JPCRD, 17/3 (1988)	1.45000e+01 (E <sub>P</sub> )
☑	ION	A	DER	<b>e</b> , <b>N</b> <sup>+</sup> [G]		BELI		M.A. Lennon et al.	1988	JPCRD, 17/3 (1988)	2.96000e+01 (E <sub>P</sub> )
☑	ION	A	DER	$\mathbf{e}, \mathbf{N}^{2+}[G]$		BELI		M.A. Lennon et al.	1988	JPCRD, 17/3 (1988)	4.75000e+01 (E <sub>P</sub> )
☑	ION	A	DER	$\mathbf{e}, \mathbf{N}^{3+}[G]$		BELI		M.A. Lennon et al.	1988	JPCRD, 17/3 (1988)	7.75000e+01 (E <sub>P</sub> )
☑	ION	A	DER	$e, N^{3+}$ [*]		BELI	comment	M.A. Lennon et al.	1988	JPCRD, 17/3 (1988)	6.91000e+01 (E <sub>P</sub> )
≤	ION	A	DER	$\mathbf{e}, \mathbf{N}^{4+}[G]$		BELI		M.A. Lennon et al.	1988	JPCRD, 17/3 (1988)	9.79000e+01 (E <sub>P</sub> )
☑	ION	В	DER	$\mathbf{e}, \mathbf{N}^{5+}[G]$		BELI		M.A. Lennon et al.	1988	JPCRD, 17/3 (1988)	5.52100e+02 (E <sub>P</sub> )
≤	ION	A	DER	$\mathbf{e}, \mathbf{N}^{6+}[G]$		BELI		M.A. Lennon et al.	1988	JPCRD, 17/3 (1988)	6.67000e+02 (E <sub>P</sub> )

Fitting Function Sources | BELI |

				Output options	
		Boundaries	2	Plot options:	Fitting coefficients
	minimal X	maximal X	Number of points	PNG and PDE file: yes of X log: of X log:	show table
l	1.45000e+01	2.e+4	50	The and The nice yes V A log. V Thog. V	show table

Go to numerical data Reset page Complete restart

87

![](_page_43_Picture_7.jpeg)

http://esther.ist.utl.pt/

### EUROPEAN SHOCK-TUBE FOR HIGH-ENTHALPY RESEARCH, INSTITUTE FOR PLASMAS AN NUCLEAR FUSION

### ESTHER team

- ESTHER is part of the Gaseous Electronics Group of the Institute for Plasmas an Nuclear Fusion, an Associated Laboratory of Instituto Superior Técnico.
- The team hosts the European Shock-Tube for High Enthalpy Research, where experimental research on plasma radiation of high-speed (>10km/s) shocked flows is carried out.
- The team also carries theoretical and numerical research on non-equilibrium kinetics and radiation in hypersonic shocked flows.

![](_page_44_Picture_4.jpeg)

![](_page_45_Picture_0.jpeg)

![](_page_45_Picture_1.jpeg)

Software packages with databases

# EMISSION/ABSORPTION SPECTRAL SIMULATIONS

![](_page_46_Figure_2.jpeg)

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### specair: spectral fitting made easy

![](_page_46_Figure_5.jpeg)

specair is the leading software for calculating and fitting plasma spectra

A demo version of Specair is available here:

download specair

![](_page_46_Picture_9.jpeg)

global fitting

#### **SRI** International Products News Blog Careers Contact 日本支社 R&D Capabilities View Our Work About Us Work With Us Q Search Products + Solutions LIFBASE Spectroscopy Tool LIFBASE is a free software program to chart the spectroscopy of diatomic molecules that is available as freeware from SRI. The software is compatible with all 32-bit Windows T = 10 K versions. No support is available. Download Software Features include: **Comprehensive Database Capabilities** • Absolute rovibrational emission and absorption coefficients Variation of transition probabilities taking into account rovibrational wavefunctions and electronic transition moments • Rotational radiative lifetimes and tabulated predissociation rates 2240 2250 2270 2260 • Frequencies for all rovibrational transitions Wavelength (Å) **Spectral Simulation** Optical emission, absorption, excitation laser-induced fluorescence Thermal and non-thermal population distributions 95

### **PLASMA CHEMICAL KINETICS**

# bad news

- In the majority of cases, plasma kinetic models are not freely available. Some of them are (partly) published, e.g.
  - 02: Annemie Bogaerts, Modeling of plasmas
  - MC 05: Daniil Marinov, New perspectives on surfacekinetics
  - MC 06: Vasco Guerra, Kinetic modeling of air plasmas: selfconsistency, bottlenecks, successes

![](_page_48_Picture_5.jpeg)

### **Planetary Entry Integrated Models**

http://users.ba.cnr.it/imip/cscpal38/phys4entry/

see MC03: Annarita Laricchiuta, The state-of-the-art description of vibrational-electronic excitations

Atmospheres S All T	pecies Classes All + All	▼)	Processes All	Sear
Class & Process	Reagents and Products \$	Intermediate state	Reference	Action
<ul> <li>electron-molecule proces</li> <li>electron-diatom</li> <li>resonant vibrational excitation</li> </ul>	s $e+CO(^{1}\Sigma^{+}) \implies e+CO(^{1}\Sigma^{+})$	СО <sup>-</sup> ( <sup>2</sup> П)	V. Laporta, C.M. Cassidy, J. Tennyson, R. Celiberto, Plasma Sources Sci. Technol. 21 (2012) 045005	۹ 📕 🕻
<ul> <li>electron-molecule proces</li> <li>electron-diatom         <ul> <li>dissociative attachment</li> </ul> </li> </ul>	s $e+H_2(X \ ^1\Sigma_g^+) \implies H(n=2)+H^-(^1S)$	$H_2^{-}(^{2}\Sigma_{g}^{+})$	R. Celiberto, R.K. Janev, J.M. Wadehra, A. Laricchiuta, Physical Review A 80 (2009) 012712. R. Celiberto, R.K. Janev, J.M. Wadehra and J. Tennyson, Chemical Physics 398 (2012) 206–213.	۹ 🖬 🕻
<ul> <li>electron-molecule proces</li> <li>electron-diatom</li> <li>resonant vibrational excitation</li> </ul>	s e+NO(X <sup>2</sup> П) 🛶 e+NO(X <sup>2</sup> П)	NO <sup>-</sup> ( <sup>3</sup> Σ <sup>-</sup> , <sup>1</sup> Δ, <sup>1</sup> Σ <sup>+</sup> )	V. Laporta, R. Celiberto, J.M. Wadehra, Plasma Sources Sci. Technol. 21 (2012) 055018	۹ 📕 🕻
electron-molecule proces     electron-diatom     resonant vibrational     excitation	s $e+N_2(X \ ^1\Sigma_g^+) \Longrightarrow e+N_2(X \ ^1\Sigma_g^+)$	N <sub>2</sub> <sup>-</sup> ( <sup>2</sup> Π <sub>g</sub> )	V. Laporta, R. Celiberto, J.M. Wadehra, Plasma Sources Sci. Technol. 21 (2012) 055018	۹ 📕
		₿ € 1/5 ₽ ₽		

![](_page_49_Picture_1.jpeg)

![](_page_50_Figure_0.jpeg)

#### ZDPLASKIN: ZERO-DIMENSIONAL PLASMA KINETICS

http://www.zdplaskin.laplace.univ-tlse.fr/

about	how to use	download	examples	publications	google				
Laplace				N <sub>2</sub> -O <sub>2</sub> MIXT	URE				
A ready-to-use Ferreira, B.F. Ge	complete list of plasmacher ordiets and A.I. Osipov "Plas	nical processes in nitrog ma Kinetics in Atmosphe	en-oxygen mixtures taker ric Gases" (2000) Springe	n mainly from the book M. Ca er is available.	apitelli, C				
version 1.02									
This is the vers improve this dat	This is the version 1.02 and we encourage you to test it for your cases and send us your suggestions and contributions in order to improve this data.								
This state-speci molecules N <sub>2</sub> (X positive ions N <sup>+</sup>	fic model of N <sub>2</sub> -O <sub>2</sub> mixture <sup>1</sup> , v = 0 - 8), N <sub>2</sub> (A <sup>3</sup> , B <sup>3</sup> , a <sup>-1</sup> , N <sub>2</sub> <sup>+</sup> , N <sub>3</sub> <sup>+</sup> , N <sub>4</sub> <sup>+</sup> , O <sup>+</sup> , O <sub>2</sub>	includes a set of about $^{I}$ , $C^{3}$ ), $O_{2}(X^{3}, v = 0 - 4)$ $_{4}^{+}$ , $NO^{+}$ , $O_{2}^{+}N_{2}$ , negative	430 chemical reactions w O <sub>2</sub> (a <sup>1</sup> , b <sup>1</sup> , 4.5eV), O <sub>3</sub> , N e ions O <sup>-</sup> , O <sub>2</sub> <sup>-</sup> , O <sub>3</sub> <sup>-</sup> , O <sub>4</sub> <sup>-</sup> , N	ith the participation of 44 sta NO, atoms N( <sup>4</sup> S, <sup>2</sup> D, <sup>2</sup> P), O( O <sup>-</sup> and electrons E.	tes, name <sup>3</sup> P, <sup>1</sup> D, <sup>1</sup> \$				
The model also $N_2(W^3,B^{\prime3}) \Longrightarrow N_2(W^3,B^{\prime3}) \longrightarrow N_2(W^3,B^{\prime3$	accounts the excitation of $I_2(B^3)$ , $N_2(a^1,w^1) \Rightarrow N_2(a^{(1)})$	of other electronic states and $N_2(E^3,a^{"1}) \Rightarrow N_2(C^3)$	of nitrogen and oxyger <sup>3</sup> ). The generalized level (	, but assumes instantaneou $O_2(4.5eV)$ corresponds to $O_2(4.5eV)$	is relaxati (A <sup>3</sup> , C <sup>3</sup> ) ai				
O <sub>2</sub> (c <sup>1</sup> ) states.	$O_2(c^1)$ states.								
Transport paran The density of including super- function.	neters and constant rates for 20 species, namely $N_2(X^1, elastic collisions with above$	r electron-neutral interact $v = 0 - 8$ ), $O_2(X^3, v = 0)$ e-mentioned states are us	ons are calculated using $-4$ ), N <sub>2</sub> (A <sup>3</sup> ), O <sub>2</sub> (a <sup>1</sup> ), N, sed solving the Boltzmann	build-in into the package BOL O, NO, O <sub>3</sub> and 78 collisiona n equation for electron energy	SIG+ solve al processe / distributio				
Requred cross the present exa <b>Phelps</b> (NO) da O <sub>3</sub> species avai	sections for electron proces imple, these electron cross labases. This cross-section lable at Kinema Research &	ses with species indicate sections were retrieved database has to be com Software, Humid air che	d in section <b>BOLSIG</b> hav from ELECTRON SCAT pleted with the cross sec mistry database, http://ww	e to be stored in <i>bolsigdb.dat</i> FERING DATABASE, <b>SIGLO</b> tions for N, O atoms and N <sub>2</sub> (. w.kinema.com/download.htm	t data file. (N <sub>2</sub> ,O <sub>2</sub> ) ai A3), O <sub>2</sub> (a <sup>-</sup>				
The constant ra was built with co	tes of VT relaxation were ap onstant rates obtained using	plied for all vibrational lev the principle of detailed b	rels using the harmonic os balance.	cillator model. A set of revers	e process				
version 1.03									
A work-in-progre N <sub>2</sub> O, NO <sub>2</sub> , NO <sub>3</sub>	ess version 1.03 is also ava , N <sub>2</sub> O <sub>5</sub> , N <sub>2</sub> O <sup>+</sup> , NO <sub>2</sub> <sup>+</sup> , N <sub>2</sub> O <sup>-1</sup>	ilable for downloading. Tl NO <sub>2</sub> - NO <sub>3</sub>	ne following NxOy species	with corresponding reactions	s are adde				
You can downlo	ad all these files in a zin arc	hive							

### **CHEMICAL KINETICS**

![](_page_51_Picture_1.jpeg)

### **NIST Chemical Kinetics Database - Gas-Phase**

http://kinetics.nist.gov/kinetics/

![](_page_52_Figure_0.jpeg)

### Task Group on Atmospheric Chemical Kinetic Data Evaluation, IUPAC (International Union of Pure and Applied Chemistry)

http://iupac.pole-ether.fr/

![](_page_52_Picture_4.jpeg)

### NASA Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies

http://jpldataeval.jpl.nasa.gov/

![](_page_53_Picture_0.jpeg)

### **OTHER SOURCES**

### http://plasma-gate.weizmann.ac.il/directories/

![](_page_54_Picture_1.jpeg)

### http://plasma-gate.weizmann.ac.il/directories/ Recombination Collisional Ionization and Autoionization Charge Transfer Auger Processes Energy Levels, Wavelengths, Transition Probabilities Collision Strengths, Excitation Rates Stark Broadening Opacities Atomic Line List Atomic databases • Opacity Project Database, Strasbourg, France: Opacity Project Database, Strasbourg, France: TOPbase telnet to TOPbase (password Seaton+) and USA Web interface TOPbase user manual tp to TOPbase (Dopacities) Data for OD Opacities NIFS Database, Nagoya, Japan: registered users only feaccess AMDIS, IAEA, Vienna, Austria AMDIS, Bibliognaphic Database Stark Urodzehing Opacities Stark Urodzehing Observatory of Paris-Meudon, France Bibliography Database on Atomic Line Shapes and Shifts STARK-B: Database for Stark broadening of isolated lines of atoms and ions in the impact approximation Stark Broadening Parameters for Neutral and Singly Charged Ions VALD: Vienna Atomic Line Database, Vienna, Austria MCHF/R/COHF Collection CHIANTI: A Database for Astrophysical Emission Line Spectroscopy CDS Catalogues, Strasbourg, France Molt F/R/COHF Collection EHLIANTI: A Database for Astrophysical Emission Line Spectroscopy CDS Catalogues, Strasbourg, France Molt F/R/COHF Collection EHLIANTI: A Database of programs and data for physics, Masaryk University, Czech Republic ETAM Database, University of Helsinki, Finland Interactive Elaste, Photon-Atom Scattering Database, Lawrence Livermore National Laboratory, CA Laboratory, CA Los Alamos National Laboratory, NM Los Alamós National Laboratory, NM o Opacities of Mixtures Database o Atomic Structure and Cross Sciences DABAX, DAtaBAse for X-rays, European Synchrotron Radiation Facility, France CCC Database, Curtin University of Technology, Perth, Australia AMODS, Taejon, Korae Energy levels and transition probabilities (orthogonal operator technique), Amsterdam, Th Netherlands JEAMDL – Japanese Evaluated Atomic and Molecular Data Library, JAERI, Japan DREAM, Database on Rare Earths At Mons University, University of Mons-Hainaut, BejpertDavid Database Search R.L.Kurdicz adomic lineitist (<u>UD-YCW i re</u> and y European mirror of CD-ROM 23 diabase Search R.L.Kelly atomic and ionic linelist Chandra X-Ray Center: Atomic Database ATOMDB Energy Levels of Hydrogen and Deuterium Uppsala University, Sweden COREX Database Electron binding energies Henke scattering factors Beigium SPECTR-W<sup>2</sup> – Database on Spectral Properties of Atoms and Ions, Snezhinsk, Russia CAMDB, Beijing, China Energy levels and atomic spectra of actinides, Paris, France Time-Dependent Ionization in Radiative Cooling Gas, TAU, Israel . LAPLACE, CNRS and University of Toulouse, France <u>LXcat - electron scattering dat</u> <u>ICEcat - ion scattering databas</u> base ORNL Controlled Fusion Atomic Data Center, Oak Ridge, TN ORNL Controlled Fusion Atomic Data Center, Oak Ridge, TN ORAL Collibliographic Database Electron-Impact Excitation of Multicharged Ions at ORNL Electron-Impact Data for Advertised Ions at ORNL University of Kentucky, KY Advertise Data for Advertised Plasma Databases Goddard SFC Databases Goddard SFC Databases Heliospheric Field and Plasma Data OMNWeb OCHOWeb Agnetic Field NASA/Goddard: Atomic Data for Astrophysics Photoionization COHOWeb Magnetic Fusion Energy Database, University of Texas at Austin ITER Databases and Modeling Activities 110

# VAMDC consortium: www.vamdc.eu (development phase)

VAMDC				8 8 8
Consortium				
		ABOU	T US NEWS	JOB ADVERTS
SUP@VAMDC Final Annual Me	eting: 17 Sept. IST-Africa Confere	nce May 2014		
Final SUP@VAMDC Project Annual	Meeting: 17 Sept. IST-Africa 2014 is the	ninth in an Annual Conference		
2014 This meeting will be held at the News I Admin Admin I Friday, 20 Ju	ne 2014 News   Admin Admin	getner senior represent		
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Standards	Welcome to \	AMDC Consortium	-	
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<ul> <li>Standards</li> <li>Software</li> <li>User Support</li> </ul>	Welcome to N Atomic and molecular (A+I	AMDC Consortium	Partners	
Standards     Software     User Support     Contacts	Welcome to V Atomic and molecular (A+I applications such as ast	/AMDC Consortium M) data are critical for a range of rophysics, atmospheric physics,	Partners	
<ul> <li>Standards</li> <li>Software</li> <li>User Support</li> <li>Contacts</li> <li>Meetings</li> </ul>	<u>Welcome to N</u> Atomic and molecular (A+1 applications such as ast fusion, environmental scien	AMDC Consortium M) data are critical for a range of rophysics, atmospheric physics, ces, combustion chemistry, health line codietocony.	Partners	
<ul> <li>Standards</li> <li>Software</li> <li>User Support</li> <li>Contacts</li> <li>Meetings</li> <li>Links</li> </ul>	<u>Welcome to N</u> Atomic and molecular (A+I applications such as ast fusion, environmental scien and clinical science incluc industries ranging from tect	AMDC Consortium M) data are critical for a range of rophysics, atmospheric physics, ces, combustion chemistry, health ding radiotherapy. They underpin nological plasmas to lighting. The	Partners	
<ul> <li>&gt; Standards</li> <li>&gt; Software</li> <li>&gt; User Support</li> <li>&gt; Contacts</li> <li>&gt; Meetings</li> <li>&gt; Links</li> <li>&gt; Gallery</li> </ul>	<u>Welcome to N</u> Atomic and molecular (A+l applications such as ast fusion, environmental scien and clinical science incluc industries ranging from tect Virtual Atomic and Molec	AMDC Consortium M) data are critical for a range of rophysics, atmospheric physics, ces, combustion chemistry, health ding radiotherapy. They underpin nological plasmas to lighting. The ular Data Center (VAMDC) is a	Partners	
<ul> <li>Standards</li> <li>Software</li> <li>User Support</li> <li>Contacts</li> <li>Meetings</li> <li>Links</li> <li>Gallery</li> </ul>	<u>Welcome to N</u> Atomic and molecular (A+l applications such as ast fusion, environmental scient and clinical science incluc industries ranging from tect Virtual Atomic and Molec Consortium of Databases	AMDC Consortium M) data are critical for a range of rophysics, atmospheric physics, ices, combustion chemistry, health ding radiotherapy. They underpin nological plasmas to lighting. The ular Data Center (VAMDC) is a & Services Providers that has	Partners	

# software packages with databases

- Boltzmann solvers:
  - BOLSIG (predecessor of BOLSIG+ and SIGLO)
  - MAGBOLTZ (http://consult.cern.ch/writeup/magboltz/)
  - ELENDIF (Kinema Research, USA)
  - EEDF code (http://www.lxcat.net/download/EEDF/)
- Emission/absorption spectra:
  - SPECAIR (http://www.specair-radiation.net/)
  - LIFBASE (http://www.sri.com/engage/products-solutions/lifbase)
- Gas/liquid/solid thermodynamics (LTE composition):
  - CANTERA & NASA database (code.google.com/p/cantera/)

# don't forget "old-fashion" regular publications, reports & private communications

AIP Journal of Physical and Chemical Reference Data

![](_page_56_Picture_1.jpeg)

ISSN: 0047-2689 E-ISSN: 1529-7845

*Journal of Physical and Chemical Reference Data* is the authoritative resource for critically evaluated reference data for physical science and engineering disciplines. Th journal publishes papers which report the best available measurements for the relevar properties.

### CONCLUSIONS

# Where do I get data, finally?

- Step 1: check specific plasma databases
   LXCAT, GAPHYOR, MAGBOLTZ, ESTHER, GELDC, etc.
- Step 2: check general-purposes databases
   NIST, NIFS, IAEA, IUPAC, NASA, etc.
- Step 3: search in the Internet and publications — Libraries, Google Scholar, Research Gate, etc.
- Step 4: ask colleagues
  - e.g. LXCAT discussion board
- Step 5: be critical

![](_page_57_Picture_7.jpeg)