24th DCN meeting, IAEA, Sep. 4-6, 2017

## Atomic and Molecular Data Activities at NIFS in 2015 – 2017

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### Outline

- 1. NIFS database
- 2. Satellite databases
- 3. Research activities related to AM data
- 4. Concluding remarks

### 1. NIFS database http://dbshino.nifs.ac.jp/

#### Nifs database information

What's

New:

- 1. Lindsay, B.G. J.Phys.B 38 p1977-1986 (2005) [CHART molecule] H in CH<sub>4</sub> 2. Sanders, J.M. J.Phys.B 36 p3835-3846 (2003) [CHART molecule] H in H<sub>2</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>2</sub>H<sub>6</sub>
  - 3. Seredyuk, B. Phys.Rev.A 71 022713 (2005) [CHART molecule] He<sup>2+</sup> in CH.
  - 4 Kimura M Phys Rev A 32 p802-809 (1985) [CHART molecule] H<sup>+</sup> + H.

### NIFS DATABASE

National Institute for Fusion Science

#### Atomic & Molecular Numerical Databases

Cross Sections and Rate Coefficients for Ionization, Excitation, and Recombination by Electron Impact, Charge Transfer by Heavy Particle Collision, and Collision Processes of Molecules, Sputtering Yields of Solids, and Back Scattering Coefficients from Solids

#### **Bibliographic Databases**

Fusion and Plasma Sciences, Atomic and Molecular Physics, and Atomic Collision Processes

#### Made by <u>A&M and PWI data research section</u>

More detailed information is here. Samples on Numerical Data are here. We welcome your data submission. Details are here. We welcome your comments and suggestions. Please send email to dbadmin@dbshino.nifs.ac.jp

#### **Please Logon Free**

Logon Free

#### Information on Database Service

Please used the URL http://dbshino.nifs.ac.jp/ to connect to the NIFS database. Thank you for your cooperation.

Free Access Databases on Atomic and Molecular Data provided by NIFS

Retrievable numerical database for collision processes

### **Recent changes**

[Japanese]

- Database managing system is changed from Oracle to PostgreSQL and the whole system was rebuilt in 2016.
- New functions are added.
- New "simple search" entry pages are available for all sub databases.
- Some bugs in BACKS displaying system are fixed.
- New data added for AMDIS, CHART, AMOL, and CMOL.

### AM and PWI Numerical Database (http://dbshino.nifs.ac.jp)

DB Name		Contents	Period	<b>Records</b> (Aug.3, 2017)		
EXC		Electron impact excitation of atoms				
	ION	Electron impact ionization of atoms	tion of atoms			
	DIO	Electron impact dissociation of simple molecules	1961-2015	(747,001;		
	REC	Electron recombination of atoms		Oct. 2015)		
СНА	RT	Charge exchange of ion-atom collision	1957-2013	<b>7,618</b> (7,616)		
AMDIS MOL (AMOL)		Electron collision with molecules	1050 0015	5.326		
CHART MOL (CMOL)		Heavy particle collision with molecules	1950-2015	(5,295)		
SPUTY		Sputtering yield of solid	1931-2007	<b>2,084</b> (2,084)		
BACKS		Reflection coefficient of solid surface	1976-2002	396 (396)		
(AM Bibliographic database)						
ORNL		Bibliography on atomic collisions collected at ORNL, USA	1959–2009	78,097		

### Change of number of data recodes in the database

Number of Data in the Database

■AMDIS ■CHART ■MOL ■SPUTY ■BACKS ■ORNL



### Access counts to the database (query counts)

query counts

#### ■AMDIS ■CHART ■SPUTY ■BACKS ■MOL



## New "simple search" entries for each sub database

NIFS DATABASE

#### Welcome to NIFS DATABASE

Please select the database. Atomic and Molecular Research Center, NIFS is making the Atomic and Molecular Numerical databases for various collisional processes and the Bibliographic Databases. You can access the databases only which you applied for at the registration. Information on each database will be found from 1.

[Help]

	Atomic and Molecular Numer	rical Databases 🚺	Simple search	
	AMDIS EXC I ION II	REC DIO	EXC ION REC	DIO
			HART AMOL CMO	<u>L</u>
	BACKS SPUTY		BACKS SPUTY	
	Bibliographic Data	base 🚺		
C				

- Easy to select initial ionic state / projectile and target elements.
- Especially, it is easy to find molecules in the databases.
- Total number of data records in the databases are shown.

### New "simple search"



- Users can select an initial ionic state from the table matrices for ION, EXC, REC, and AMOL.
- The table can expand to see well.
- The matrix is built dynamically from the data tables in the database.

New "simple search"

#### CHART

													-	Dack
Sort ◉ by ele	ement A (pro	jectile) or C	) by element	B (target)										
H> Ar (18)	H> C (14)	H> C2F6 (1)	H> C2H2 (3)	H> C2H4 (2)	H> C2H6 (4)	H> C2H8 (1)	H> C3H6 (1)	H> C3H8 (3)	H> C4F8 (1)	H> C4H10 (1) Ele	mentA:D	IH> САНЯ	)[H> CF4	H
D> C8F16	(1) D> CH4	(1) D> CO	(1) D> D	(2) D> H	(2) D> H2O	(1)	(1)	(2)	(1)	dat	mentB:H2 a Number	20		
(1) H3> H2O (1)	(1) H3> NH3 (1)	] (1)	(1)	(2)										
He> Ar ( 10 )	He> C2F6	He> C2H2	He> C2H4	He> C2H6 (5)	He> C3F8 (1)	He> C3H6	He> C3H8 (4)	He> n-C4F10 (1)	He> c-C4F8	He> C4F8 (1)	He> n-C4H10 (1)	He> C4H8 (1)	He> CF4	Н
Li> H ( 369 )	Li> H2 (16)	Li> He (47)	Li> Li (1)											
Be> H (3)	Be> H (185)	Be> H2 (3)	Be> He (46)											
B> H (3)	B> H ( 206 )	B> H2 (17)	B> He (64)											
C> Ar (1)	C> Ar (8)	C> C2H2 (3)	C> C2H4 (3)	C> C2H6 (13)	C> C3H8 (9)	C> n-C4H10 (3)	C> (CH3)2NH	C> CH4 (13)	C> CO (4)	C> CO2 (8)	C> D (2)	C> D2 (1)	C> H (1)	С
N> Ar (1)	N> CO (2)	N> CO2 (3)	N> H (1)	N> H (495)	N> H2 (54)	N> H2O (1)	N> He (27)	N> Kr (2)	N> Li (8)	N> N2 (1)	N> NO (1)	N> Ne (25)	N> O2 (1)	N
0> 1 (1)	O> Ar (10)	O> CO (3)	O> CO2 (6)	O> H (1)	O> H (598)	O> H2 (1)	O> H2 (83)	O> H2O (8)	O> He (63)	O> N2 (5)	O> NO (1)	O> Ne (19)	0> 02 (1)	
E NH2	E > No	1												

- Initial projectile and target elements are shown as matrix element for selection for CHART, CMOL, SPUTY and BACKS.

V

[Help]

(In a stall )

### New function

#### AMDIS MOLECULE

#### [Simple search]



#### Simple conditions for search:

Initial State M	lolecular form	nula			or		
N	folecular nam	1e	(CF3)2	CO			
Ic	nic State		(CH3)2 1-C3H7				
1	ine state		1-C4H9	i			
Final State			2-C3H7	'CI			
			2-C4H9	)CI			
			2-methy BCI	yiproper	le		
Process :			BCI2				
			BCI3				
Data Type : @	Cross Section	on C	BF			e	r
51			BF3				
Theoretica	1 🗆 Experin	nenta	C2CI4				
			C2CI6				
			C2F6				~
Author(s)			C2H2				$\sim$
			C2H2+				
Year of Public	ation : From		C2H2C	12			
			C2H2C	14			
			C2H3C	13			
			C2H3O				
Additional condition	is for search:		C2H4				
			C2H4+	12			
<b>A</b> .	~	=	C2H5	-			
<b>B</b> .	~	=	C2H5C	1		$\sim$	
<b>C</b> .	~	=					
D	~	=	~				
Б Г		-					
E	¥		<b>•</b>	L			
r	<b>`</b>	-	×				
G	<b></b>	<u> </u>					
H	~	=	~				
I	~	=	~				
J.	~	=	~				
K.	~	=	~				
L.	~	=	~				
Sort Keys:	~			Image: Second		$\checkmark$	
							_
Logical Equat	ion						

#### AMDIS MOLECULE

#### [Simple search]

#### Search Clear

Simple conditions for search:

Initial State Molecular for	mula	or
Molecular nar	ne	or
Ionic State		1-butene
Final State		Acetylene
		Boron dichloride
		Boron difluoride
Process :		Boron fluoride
		Boron trichloride
Data Type :      Cross Secti	on C	Boron trifluoride
		C1 monochlorocarbon
□ Theoretical □ Experim	ment?	C2 chlorocarbon
		C2 monochlorocarbon
		C4 monochlorocarbon
Author(s)		Carbon monoxide ion
		Carbon tetrafluoride
Vear of Publication - From		Cisplatin
real of r doncation : From	·	Deuterium
		Deuterium bromide
		Dichlorodifluoro methane
onal conditions for search		Difluoromethylene Ethono.ion
Shortone for Sturen.		Ethylene ion
A. 🗸	=	Fluoromethylidyne
n		Formaldehyde
в	<u> </u>	Formyl radical
C. 🗸	=	Hydrogen molecule
D. 🗸	=	
E. 🗸	=	✓
F. 🗸	=	✓
G. ~	=	✓
н. 🗸 🗸	=	✓
I. 🗸 🗸	=	×
J. 🗸 🗸	=	~
к. 🗸 🗸	=	✓
L. 🗸	=	✓

- A candidate list of molecules for formula and name are shown for AMOL and CMOL.

^

Logical Equation	

Example: (A + B) \* ! C

### Working group for data update

- Working group has been organized to update data with Japanese atomic and molecular physicists.
- Main targets to search data of last two years tungsten and heavy elements (FY2015 -).
- New data on heavy elements have been searched for update.

### Examples of newly registered data



Excitation cross sections for  $26 \le Z \le 92$  B-like, C-like, N-like, O-like ions By C. J. Fontes & H. L. Zhang, ADNDT 100 (2014) 802; ADNDT 100 (2014) 1292, ADNDT 101 (2015) 143; H. L. Zhang & C. J. Fontes, ADNDT 101 (2015) 41

### 2. Satellite databases

Free Access to Databases on Atomic and Molecular Data provided by NIFS:

ALADDIN (Ionization Cross Sections and Excitation Rate Coefficients by Electron Impact) Data for Autoionizing States (Energy Levels of Autoionizing States and Satellite Lines by Dielectronic Recombination) Differential Cross Sections of Ionization for Atomic Hydrogen by Proton Impact Electron Dissociative Attachment to Molecular Hydrogen Hayashi's bibliographic database for electron and photon collision cross sections with atoms and molecules ION FRACTION (Ion Abundance Tables in Ionization Equilibrium) Photoabsorption database (Oscillator strength spectra and related quantities of 9 atoms and 23 molecules over the entire energy region) Recommended data set of electron collision cross sections of atoms and molecules (compiled by The Institute of Electrical Engineers of Japan) Sputtering yield, Reflection coefficient and Range value of solid surfaces (Calculated by Dr. W. Eckstein)

<u>IPPJ-AM publications</u> (Reports on atomic data for fusion research published by the Institute of Plasma Physics, Nagoya University from 1977 to 1989) NIFS-DATA publications

Links to Other Atomic and Molecular Databases

By the <u>Atomic and Molecular Process Research Section</u>, Fusion System Research Division, Department of Helical Plasma Research, <u>NIFS</u>

- Various small databases are linked at the database top page, such as rate coefficients of electron dissociative attachment to molecular hydrogen.
- No new entries during last 2 years

## 3. Research activities related to AM data under collaboration

- Experimental and theoretical study on tungsten ions have been carried out continuously.
- EUV and visible spectra of Tungsten ions measured with Tokyo-EBIT, CoBIT, and LHD.
- Atomic data calculations and CR model constructed for Tungsten ions have been conducted to compare with spectra.
- EUV spectra measurements of high Z elements such as lanthanides, tungsten, and bismath with LHD have been done.
- Atomic structure and opacity calculations on low-charged high Z elements are on going for astrophysical purpose.
- Isotope effect in dissociation processes of deuterated molecules from doubly excited states are studied.

### **Experiments with Large Helical Device**



- Toroidal magnetic field < 3 T</li>
- Major radius = 3.6 m
- Averaged minor radius = 0.64 m
- Toroidal period number = 10
- Poloidal mode number = 2



## 3.1 Observation of ground-state M1 lines of W<sup>q+</sup> HCI in LHD core plasmas and its application to ion density analysis

D. Kato et al., IAEA FEC2016.

Visible and near-UV emission lines of tungsten ions are useful for analysis of tungsten ion distributions at ITER because the radiation shielding of detectors is not basically necessary by using optical fibers.



q+	gr	upper	lower	LHD	EBIT	MCDF	RMBPT
27+	4f	<sup>2</sup> F <sub>7/2</sub>	<sup>2</sup> F <sub>5/2</sub>	337.73(2)	337.743(26)	339.3 338.18	338.4
261	A.£2	30	${}^{1}G_{4}$	335.73(2)	335.758(11)		
20+	41-	-r <sub>4</sub>	${}^{3}F_{3}$	333.70(2)	333.748(9)		

#### 11 visible lines of W<sup>q+</sup> identified in 330 – 390 nm



## 3.2 Collisional-radiative model with recombining processes for W<sup>27+</sup> ion

Murakami et al. (2017) accepted in EPJD (ICAMDATA proceedings).

- Recombining processes are included for a collisional-radiative model of W<sup>27+</sup> ion.
- Atomic data are calculated with HULLAC code.
- 226 Electron configurations are considered: 4d<sup>10</sup> 4f, 4d<sup>10</sup> nl (n=5-9, l=0-5), 4d<sup>9</sup>4f<sup>2</sup>, 4d<sup>9</sup> 4fnl (n=5-9, l=0-5), 4d<sup>9</sup>5ln'l' (n=5-8, l,l'=0-5), 4d<sup>9</sup>6lnl' (n=6-7, l,l'=0-4), 4p<sup>5</sup>4d<sup>10</sup>4f<sup>2</sup>, 4p<sup>5</sup>4d<sup>10</sup>4fnl (n=5-6, l=0-5). In total 25,632 J-resolved levels are considered in the model.



## 3.4 Collaboration with Univ. Electro-Communications using Compact EBIT (CoBIT)





e-beam energy 100 - 2500 eV e-beam current 20 mA (max) B-field 0.2 T (max) @77 K (High-Tc SCM)

### W EUV spectra: e-beam energy dependence

N. Nakamura (Univ. Electro-Comm.), ICPEAC XXX 2017



### EUV spectra: e-beam energy dependence



### EUV spectra: comparison with CRM



### Benchmarking atomic structure calculations

M1 transitions between FS splitting in the ground state configuration of W<sup>7+</sup>



### EUV spectrum of Tm ions

Plasma Phys. Control. Fusion 59 (2017) 014009



C Suzuki et al

C. Suzuki, F. Koike, et al. PPCF 59 (2017) 014009

**Table 1.** List of the isolated lines identified experimentally for the first time in the LHD.

Ion	Transition	Wavelength (nm)	References
Ni-like			
$Nd^{32+}$	3d <sub>3/2</sub> 4p <sub>1/2</sub> -3d <sub>3/2</sub> 4d <sub>3/2</sub>	7.413	[25]
Cu-like			
$Tb^{36+}$	3d <sup>10</sup> 4p <sup>2</sup> P <sub>1/2</sub> -3d <sup>10</sup> 4d <sup>2</sup> D <sub>3/2</sub>	7.203	[26]
$Tb^{36+}$	3d <sup>10</sup> 4d <sup>2</sup> D <sub>3/2</sub> -3d <sup>10</sup> 4f <sup>2</sup> F <sub>5/2</sub>	8.796	[26]
$Ho^{38+}$	3d <sup>10</sup> 4p <sup>2</sup> P <sub>1/2</sub> -3d <sup>10</sup> 4d <sup>2</sup> D <sub>3/2</sub>	6.614	
$Tm^{40+}$	3d <sup>10</sup> 4p <sup>2</sup> P <sub>1/2</sub> -3d <sup>10</sup> 4d <sup>2</sup> D <sub>3/2</sub>	6.072	
Ag-like			
$Tm^{22+}$	$4d^{10}4f {}^2F_{7/2}$ - $4d^94f^2 {}^2G_{9/2}$	5.933	
$Tm^{22+}$	$4d^{10}4f\ ^2F_{5/2}-4d^94f^2\ ^2G_{7/2}$	5.986	

*Note*:The uncertainty of the wavelengths measured in the LHD is estimated to be less than  $\pm 0.005$  nm. The details of the lines from Ho and Tm ions will be reported soon in a separate paper.

**Figure 10.** Comparison between the measured and modelled spectra from Tm ions at a temperature of 2.2 keV: (a) spectrum measured in LHD, (b) synthesised spectrum with assuming the abundance ratio of 0.625:1.0:1.521:1.5 for Tm<sup>37+</sup>:Tm<sup>38+</sup>:Tm<sup>39+</sup>:Tm<sup>40+</sup> and (c)–(f) calculated spectra for each ion.

• Emission lines of Tm ions measured in LHD plasma are newly identified and compared with synthesized spectrum of CR model.

# 3.6 New collaboration on atomic structure and opacity calculations for low-charged high-Z elements for neutron star merger.

M. Tanaka (NAOJ), D. Kato (NIFS). G.Gaigalas (Vernius Univ.), et al., submitted to Ap.J (2017)

- Neutron star merger is expected to emit "gravitational wave".
- Spatial resolution of measurements for gravitational wave is about 1400 degree<sup>2</sup> => too wide to identify the object.
- Identification by light curve is important to search for a source of gravitational wave.
- Opacity data are required to calculate light curve from "kilonovae" as a result of neutron star merger.





### **Atomic structure calculations**

### HULLAC code (relativistic, local radial potential, Bar-Shalom+99)

Se I-III (Z=34, p) Ru I-III (Z=44, d) Te I-III (Z=52, p) Nd I-III (Z=60, f)Er I-III (Z=68, f)

Ion	Configurations	Number of levels	Number of lines
HULLAC			
Se 1	$4s^{2}4p^{4}, 4s^{2}4p^{3}(4d, 4f, 5-8l), 4s4p^{5}, 4s4p^{4}(4d, 4f), \\ 4s^{2}4p^{2}(4d^{2} + dd^{2} + 4f^{2}), 4s4p^{3}(4d^{2} + dd^{4} + 4f^{2})$	3076	973,168
Se II	$4s^{2}4p^{3}, 4s^{2}4p^{2}(4d, 4f, 5-8l), 4s4p^{4}, 4s4p^{3}(4d, 4f),$	2181	$511,\!911$
Se III	$ 4s^{-4}p^{-2}(4a^{-},4a^{-}), 4s^{-4}p^{-1}(4a^{-},4a^{-}), 4s^{-4}p^{-1}(4a^{-},4a^{-}), 4s^{-4}p^{-1}(4d^{-},4f^{-1}) $	922	92,132
Ru I	$4s^{-}(4a^{-}, 4a4f, 4f^{-}), 4s4p(4a^{-}, 4a4f, 4f^{-})  4d^{7}5s, 4d^{6}5s^{6}, 4d^{8}, 4d^{7}(5p, 5d, 6s, 6p), $	1,545	250,476
Ru II	$4d^{\circ}5s(5p, 5d, 6s)$ $4d^{7}, 4d^{6}(5s - 5d, 6s, 6p)$	818	76.592
Ru III	$4d^6, 4d^5(5s-5d, 6s)$	728	49.066
Те і	$5s^2 5p^4,  5s^2 5p^3 (4f, 5d, 5f, 6s-6f, 7s-7d, 8s),$	329	$14,\!482$
Te II	$5s5p^{\circ}$ $5s^{2}5p^{3}$ , $5s^{2}5p^{2}(4f, 5d, 5f, 6s - 6f, 7s - 7d, 8s)$ ,	253	9,167
Теш	$5s5p^*$ $5s^25p^2$ , $5s^25p(5d, 6s - 6d, 7s)$ , $5s5n^3$	57	419
Nd I	$4f^46s^2, 4f^46s(5d, 6p, 7s), 4f^45d^2, 4f^45d6p,$	31,358	70,366,259
Nd 11	$4f^{\circ}5acs^{\circ}, 4f^{\circ}5a^{\circ}(6s, 6p), 4f^{\circ}5acsop$ $4f^{4}6s, 4f^{4}5d, 4f^{4}6p, 4f^{3}6s(5d, 6p),$	6,888	3,951,882
Nd III	$4f^35d^2, 4f^35d6p$ $4f^4, 4f^3(5d, 6s, 6p), 4f^25d^2, 4f^25d(6s, 6p),$	2252	458,161
Er 1	$4f^{2}6s6p$ $4f^{12}6s^{2}$ , $4f^{12}6s(5d, 6p, 6d, 7s, 8s)$ ,	10,535	9,247,777
Er 11	$\begin{array}{l} 4f^{11}6s^2(5d,6p), \dot{4}f^{11}5\dot{d}^26s, 4f^{11}5\dot{d}6s(6p,7s)\\ \mathbf{4f^{12}6s}, 4f^{12}(5d,6p), 4f^{11}6s^2, 4f^{11}6s(5d,6p), \end{array}$	5,333	$2,\!432,\!665$
Er III	$\begin{array}{l} 4f^{11}5d^2,  4f^{11}5d6p \\ \mathbf{4f^{12}},  4f^{11}(5d, 6s, 6p) \end{array}$	723	42,671

GRASP2K code (relativistic, e-e correlation, Jonsson+07)

Nd II-III, Er II-III

### **Energy levels of Nd II**



MT+ in prep

Kasen+13 (Autostructure code)

### Line expansion opacity of Nd II

T = 5,000 K,  $\rho = 10^{-13}$  g cm<sup>-3</sup>, t = 1 day



Opacities from two codes agree very well

### Line expansion opacity (for each element)



MT+ in prep.

к (p shell) << к (d shell) << к (f shell)

see Kasen+13, Fontes+17

3.7 Isotope effect in dissociation processes of deuterated molecules from doubly excited states

Y. Sakai (Toho Univ.) et al., AMPP2016 in Chengdu, China NIFS-PROC-103 (2017), p.26

 Generalized oscillator strength distribution (GOSDs) for ionization of H<sub>2</sub> and D<sub>2</sub> were measured by electron energy-loss spectra of scattered electron and ion coincidence measurements.

$$e + H_2 \rightarrow e_s + H_2^+ + e_e$$

$$H^+$$

$$e + D_2 \rightarrow e_s + D_2^+ + e_e$$

$$D^+$$

**Scattered electron – ion coincidence (SEICO) measurements** 



### **Determination of absolute DDCS and GOSD**

### Mixed gas method

Electron energy-loss spectra of  $D_2$ -He mixture and  $D_2$  (200 eV, 6 deg)

Absolute differential cross  
section for 
$$x : (d\sigma/d\Omega)_x$$
  
 $\left(\frac{d\sigma}{d\Omega}\right)_x = \frac{I_x}{I_2^{1P}} \left(\frac{d\sigma}{d\Omega}\right)_{2^{1P}} \times C$   
 $I : \text{Inteisnty}$   
 $\left(\frac{d\sigma}{d\Omega}\right)_{2^{1P}} : \text{DCS of He 2}^{1P} \text{ state}_{9}$ 

: Correlation term From mixing ratio and number density

[9] T. Y. Suzuki *et al. Phys. Rev. A*, **57**, 1832 (1998).

### 4. Concluding remarks

### • A&M database activities:

The server is replaced in 2016 and the database system is running with PostgreSQL.
Implementation to VAMDC is still pending.

• A & M data related activities:

 LHD experimental group on AM processes continues to measure various spectra of W and high Z ions and activate our AM related research.
 Domestic collaboration projects are progressed.

• No NIFS-DATA publication since 2014.