Atomic and Molecular Data Activities at NIFS in 2013 – 2015

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Outline

1. NIFS database
2. Satellite databases
3. Research activities related to AM data
4. NIFS–DATA publications
5. Domestic collaborations related to AM data in NIFS
6. Concluding remarks
1. NIFS database
http://dbshino.nifs.ac.jp/

Retrievable numerical database for collision processes

Recent changes
- Data update for AMDIS, CHART, AMOL, CMOL, and SPUTY.
- No new data for ORNL bibliography.
# AM and PWI Numerical Database (http://dbshino.nifs.ac.jp)

<table>
<thead>
<tr>
<th>DB Name</th>
<th>Contents</th>
<th>Period</th>
<th>Records (Oct. 13, 2015)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ION</td>
<td>Electron impact ionization of atoms</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DIO</td>
<td>Electron impact dissociation of simple molecules</td>
<td></td>
<td></td>
</tr>
<tr>
<td>REC</td>
<td>Electron recombination of atoms</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHART</td>
<td>Charge exchange of ion-atom collision</td>
<td>1957–2013</td>
<td>7,616 (7,054)</td>
</tr>
<tr>
<td>AMDIS MOL (AMOL)</td>
<td>Electron collision with molecules</td>
<td>1956–2014</td>
<td>5,295 (3,926)</td>
</tr>
<tr>
<td>CHART MOL (CMOL)</td>
<td>Heavy particle collision with molecules</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SPUTY</td>
<td>Sputtering yield of solid</td>
<td>1931–2007</td>
<td>2,084 (1,241)</td>
</tr>
<tr>
<td>BACKS</td>
<td>Reflection coefficient of solid surface</td>
<td>1976–2002</td>
<td>396</td>
</tr>
<tr>
<td>ORNL</td>
<td>Bibliography on atomic collisions collected at ORNL, USA</td>
<td>1959–2009</td>
<td>78,097</td>
</tr>
</tbody>
</table>
Change of number of data recodes in the database

Number of Data in the Database

- **AMDIS**
- **CHART**
- **MOL**
- **SPUTY**
- **BACKS**
- **ORNL**

Number of Data as of Oct. 13, 2015

- **AMDIS**: 747,001 *
- **CHART**: 7,616 *
- **MOL**: 5,295 *
- **SPUTY**: 2,084 *
- **BACKS**: 396
- **ORNL**: 78,097

- AMDIS Recombination (1998)
- Data Update Working Group (2000–)
- Rate coefficients in AMDIS (2003)
- IAEA GENIE (2002)
- MOL (2001)
- WWW (1997)
- AMDIS Recombination (1998)
- User interface revise for AMDIS EXC (2006)
- User interface revise for AMDIS REC (2007–8)
- NO registration (2007)
Access counts to the database (query counts)

query counts

- AMDIS
- CHART
- SPUTY
- BACKS
- MOL

Counts:

FY1998: 0
FY1999: 1000
FY2000: 2000
FY2001: 3000
FY2002: 4000
FY2003: 5000
FY2004: 6000
FY2005: 7000
FY2006: 8000
FY2007: 9000
FY2008: 10000
FY2009: 11000
FY2010: 12000
FY2011: 13000
FY2012: 14000
FY2013: 15000
FY2014: 16000
FY2015: 17000
FY2016: 18000

Events:

- AMDIS Recombination (1999)
- Data update working group (2000-2001)
- MOL (2001)
- GENIE (2001)
- Rate coefficients (2003)
- No registration (2007)
- User interface revise AMDIS EXC (2006)
- User interface revise AMDIS REC (2007-2008)
Example of data in AMOL (electron collisions)

http://dpc.nifs.ac.jp/amata/amol.html

<table>
<thead>
<tr>
<th>target</th>
<th>Data sets</th>
<th>target</th>
<th>Data sets</th>
<th>target</th>
<th>Data sets</th>
<th>target</th>
<th>Data sets</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>599</td>
<td>C₂H₄</td>
<td>37</td>
<td>NH₃</td>
<td>4</td>
<td>D₃O</td>
<td>2</td>
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<tr>
<td>DBr</td>
<td>305</td>
<td>C₂H₂</td>
<td>31</td>
<td>GeH₄</td>
<td>4</td>
<td>CH₃Cl</td>
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<tr>
<td>O₂</td>
<td>131</td>
<td>NO</td>
<td>29</td>
<td>HD₂O</td>
<td>3</td>
<td>C₂H₂Cl₄</td>
<td>2</td>
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<tr>
<td>C₃H₈</td>
<td>107</td>
<td>c-C₄F₈</td>
<td>25</td>
<td>CD</td>
<td>3</td>
<td>C₂H₃Cl₃</td>
<td>2</td>
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<tr>
<td>H₂O</td>
<td>165</td>
<td>SF₆</td>
<td>17</td>
<td>CD₂</td>
<td>3</td>
<td>C₂H₄Cl₂</td>
<td>2</td>
</tr>
<tr>
<td>CH₄</td>
<td>69</td>
<td>Si₂H₆</td>
<td>13</td>
<td>CD₃</td>
<td>3</td>
<td>H</td>
<td>1</td>
</tr>
<tr>
<td>CO</td>
<td>74</td>
<td>BCl₃</td>
<td>12</td>
<td>H₃O</td>
<td>2</td>
<td>H₂⁺</td>
<td>1</td>
</tr>
<tr>
<td>C₂H₆</td>
<td>66</td>
<td>CH</td>
<td>15</td>
<td>H₂S</td>
<td>2</td>
<td>H₃O⁺</td>
<td>3</td>
</tr>
<tr>
<td>CO₂</td>
<td>51</td>
<td>C₂H₃</td>
<td>11</td>
<td>HCl</td>
<td>3</td>
<td>HBr</td>
<td>1</td>
</tr>
<tr>
<td>D₂</td>
<td>676</td>
<td>CH₃</td>
<td>17</td>
<td>HI</td>
<td>2</td>
<td>BF</td>
<td>1</td>
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<tr>
<td>N₂</td>
<td>40</td>
<td>C₂H₅</td>
<td>10</td>
<td>D₃</td>
<td>2</td>
<td>BF₂</td>
<td>1</td>
</tr>
</tbody>
</table>
### Example of data in CMOL (heavy particle collisions)

[http://dpc.nifs.ac.jp/amdata/cmol.html](http://dpc.nifs.ac.jp/amdata/cmol.html)

<table>
<thead>
<tr>
<th>Projectile</th>
<th>target</th>
<th>Data sets</th>
<th>Projectile</th>
<th>target</th>
<th>Data sets</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>H₂</td>
<td>805 (cs 31; rc774)</td>
<td>Ar</td>
<td>C₃H₄</td>
<td>16 (cs)</td>
</tr>
<tr>
<td>H</td>
<td>H₂</td>
<td>244 (cs)</td>
<td>Kr</td>
<td>CO</td>
<td>15 (cs)</td>
</tr>
<tr>
<td>He</td>
<td>H₂</td>
<td>63 (cs 59; rc 4)</td>
<td>C</td>
<td>C₂H₆</td>
<td>14 (cs)</td>
</tr>
<tr>
<td>T</td>
<td>H₂</td>
<td>45 (rc)</td>
<td>H</td>
<td>D₂</td>
<td>16 (cs)</td>
</tr>
<tr>
<td>He</td>
<td>CH₄</td>
<td>35 (cs 1; rc 4)</td>
<td>H</td>
<td>CO₂</td>
<td>15 (cs)</td>
</tr>
<tr>
<td>He</td>
<td>CO</td>
<td>22 (cs 18; rc 4)</td>
<td>C</td>
<td>H₂</td>
<td>12 (cs)</td>
</tr>
<tr>
<td>He</td>
<td>O₂</td>
<td>21 (cs 17; rc 4)</td>
<td>H₂</td>
<td>Kr</td>
<td>11 (cs)</td>
</tr>
<tr>
<td>He</td>
<td>CO₂</td>
<td>20 (cs 16; rc 4)</td>
<td>O</td>
<td>N₂</td>
<td>11 (cs 9; rc 2)</td>
</tr>
<tr>
<td>H</td>
<td>CO</td>
<td>19 (cs)</td>
<td>H₂</td>
<td>Xe</td>
<td>10 (cs)</td>
</tr>
<tr>
<td>H</td>
<td>CH₄</td>
<td>23 (cs)</td>
<td>Ne</td>
<td>C₃H₄</td>
<td>10 (cs)</td>
</tr>
<tr>
<td>H₃</td>
<td>H₂</td>
<td>16 (cs)</td>
<td>H₂</td>
<td>Ar</td>
<td>9 (cs)</td>
</tr>
<tr>
<td>C</td>
<td>CH₄</td>
<td>16 (cs)</td>
<td>D</td>
<td>H₂</td>
<td>9 (cs)</td>
</tr>
</tbody>
</table>

Including ion as projectile

Cs = cross sections; rc= rate coefficients
Working group has been organized to update data with Japanese atomic and molecular physicists.

Main targets to search data of last two years are (1) light elements from Li to Ne (– FY2014) and (2) tungsten and heavy elements (FY2015 –).

New data on light elements are included to ION, CHART, and CMOL so far. Some data for EXC are prepared to be included.

New data on heavy elements will be searched for update this year.
Examples of newly registered data: CMOL

\[ \text{H}^+ + \text{D}_2 \rightarrow \text{D}_2^+ + \text{H} \quad \ldots \ (1) \]
\[ \rightarrow \text{D}^+ + \text{HD} \quad \ldots \ (2) \]
\[ \rightarrow \text{H} + \text{D}_2^+ \quad \ldots \ (3) \]
\[ \rightarrow \text{HD}^+ + \text{D} \quad \ldots \ (4) \]

Data found by the working group

![Graph showing cross-section vs. energy with data points and reactions](image-url)
Examples of newly registered data: AMDIS ION

Distorted wave
Crossed beam
Coulomb Born
Beam
Examples of newly registered data: CHART

\[ \text{C}^6^+ + \text{H}(1s) \rightarrow \text{C}^5^+ (n=8) + \text{H}^+ \]

CVI (n=8–7; \(\lambda\)520.09nm) is used for charge exchange recombination spectroscopy
2. Satellite databases

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
Experimental and theoretical study on tungsten ions have been carried out.
EUV and visible spectra of Tungsten ions measured with Tokyo-EBIT, CoBIT, and LHD
Atomic structure calculations for Tungsten ions
CR model for Tungsten ions
Sputtering experiments for Tungsten target

EUV spectra measurements of high Z elements such as lanthanides, tungsten, and bismuth with LHD have been done.
Experiments with Large Helical Device

- Toroidal magnetic field $< 3$ T
- Major radius = 3.6 m
- Averaged minor radius = 0.64 m
- Toroidal period number = 10
- Poloidal mode number = 2
Tungsten pellet injection experiment in LHD

- **Tungsten pellet injection**
  - Coaxial structure of a thin tungsten wire inserted into a polyethylene or carbon cylindrical tube
  - Tungsten wire: l0.6 mm x φ0.15 mm, ~7 × 10^{16} tungsten atoms
  - Accelerated by pressurized He gas of 10–20 atm with speed of ~200 m/s.

- **Plasma conditions**
  - H discharges
  - \( R_{ax} = 3.60 \text{ m}, B_t = -2.75 \text{ T.} \)
  - Three n–NBI beams with total port–through power of 10 MW

- The measurement of tungsten WIV–WVII line emissions was carried out by changing the central wavelength for each shot in the wavelength range of 495–1475 Å.
visible spectrometer (Jobin Yvon HR320)
gas injector

collaboration with Univ. Electro–Communications: Experiments setup for CoBIT


Top view

flat field grazing incidence
EUV spectrometer with a HITACHI grating

CoBIT
Charge analysis system based on the time of flight method

Side view

![Diagram of the charge analysis system showing MCP and Einzel lenses.]

- MCP
- Einzel lenses
- Bender
- CoBIT

![Graph showing normalized voltage vs. time of flight for different energies: Ee=340eV, Ee=320eV, Ee=300eV, Ee=280eV, Ee=260eV.]

- $W^{q+}$
- q=15, 14, 13, 12, 11, 10
Charge state identification

Nd-like

Pm-like

Sm-like

W(Z=74)

$E_e$ (eV)

340

320

300

280

260
Visible spectra of tungsten ions for the 340-600nm range

Nd-like

Pm-like

Sm-like
Observation of the M1 transitions between the fine structure levels in the metastable state

\[ \text{W}(Z=74) \]

\[ [4f^{13}5s^2]\text{ J}=^7/2 - ^5/2 \]

<table>
<thead>
<tr>
<th>Ion</th>
<th>( \lambda_{exp}(\text{nm}) )</th>
<th>( \lambda_{th}(\text{nm}) )</th>
<th>( A(s^{-1}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>\text{W}^{13+}</td>
<td>560.25</td>
<td>567.8(^a)</td>
<td>552(^d)</td>
</tr>
</tbody>
</table>

\(^a\) Present result with GRASP2k
\(^b\) Hatree-Fock relative calculation with COWAN
\(^c\) Relativistic many-body perturbation theory with the FAC
\(^d\) Relativistic configuration interaction with FAC
### Wavelength of the observed visible transitions in tungsten ions in the wavelength range of 380-680nm

<table>
<thead>
<tr>
<th>Ion</th>
<th>Wavelength(nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W^{12+}$ Sm-like</td>
<td>388.19, 399.81, 451.68, 483.26, 496.55, 527.27, 535.90, 540.53, 549.33, 660.30</td>
</tr>
<tr>
<td>$W^{13+}$ Pm-like</td>
<td>401.38, 429.03, 457.26, 459.08, 472.68, 495.16, 537.49, 542.11, 547.22, 553.81, 560.25, 561.46, 563.99, 593.28, 678.20</td>
</tr>
<tr>
<td>$W^{14+}$ Nd-like</td>
<td>431.75, 462.59, 486.57, 506.40, 508.39, 517.74, 527.70, 546.22, 549.93, 583.23, 595.70, 620.62, 638.63</td>
</tr>
</tbody>
</table>
We have constructed a collisional–radiative (CR) model for W ions to analyze spectra taken by LHD and CoBIT.

The CR model calculates population densities of excited states $n(p)$ with quasi-steady state assumption for given electron temperature and density.

Spectral line intensities are obtained from the population densities:

$$I(p, q; T_e, n_e) = n(p; T_e, n_e) A(p, q) \Delta E(p, q)$$

Atomic data used in the CR model are calculated by HULLAC code.

Fine structure levels are considered including inner–shell excitation states. Up to 23,000 levels for one ion are included in the model.

Excitation rate coefficients $C(p, q) = \langle \sigma_{ex} v \rangle$. Maxwellian velocity distribution is assumed for LHD plasma, and mono–energy is used for CoBIT plasma.

Recombination processes are ignored.
Fitting synthesized spectra to the LHD spectra

- Synthesized spectra reproduce the measured spectra of LHD.
- We obtain the charge state distributions, which are resemble to the distribution of ADAS.
We estimate the radiation power rate of tungsten ions. Total line emission power for each ion is calculated with the CR model and estimated ion abundance is used. Our obtained power rate is consistent with models within factor 2.

- NIFS–DATA–115
  G. Gaigalas, D. Kato, P. Jönsson, P. Rynkun, L. Radžiūte,
  “Energy Level Structure of Er3+ Free Ion and Er3+ Ion in Er2O3 Crystal”
  June 20, 2014

![Energy level structure of Er3+ in crystal by using the Multiconfiguraton Dirac- Hartree-Fock method.](image)

Energy levels are carefully calculated and convergent.
5. Domestic collaborations related to AM data in NIFS

- Measurements of absolute cross sections for electron capture processes of low energy multiply charged heavy metal ions in diverter region (K. Soejima et al.) \( W^{q+} + \text{He}; q=6 \text{ and } 7; W^{q+} + \text{H} \) (FY2014)

- Isotope effect in dissociation processes of deuterated molecules (Sakai et al.) (FY2015–FY2017)

- Atomic and Molecular database of Light Elements (M. Kitajima et al.) (FY2014)

- Update of Atomic and Molecular Database for tungsten and high Z elements (M. Kitajima et al.) (FY2015–)

- Spectroscopy of highly charged tungsten ions using Electron Beam Ion Trap (N. Nakamura et al.)

- Systematic study on spectra and atomic structures for highly charged rare earth elements (F. Koike et al.) (FY2015–)

- Improvement of diagnostic capability for solar high-temperature non-equilibrium plasmas by using LHD (T. Watanabe et al.) (FY2015–)
Measurements of absolute cross sections for electron capture processes of low energy multiply charged heavy metal ions in diverter region (K. Soejima et al. (Niigata Univ.)) \( W^{q+} + \text{He}; \ q=6 \text{ and } 7; \ W^{q+} + \text{H} \) (−FY2014)

Collision energy dependence: \( W^{8+} - \text{He} \)
A&M database activities:
- slowly but updated with new data
- The server is needed to be replaced in near future.
- Implementation to VAMDC is pending.

A & M data related activities:
- LHD experimental group on AM processes continues to measure various spectra especially W ions and activate our AM related research.
- Domestic collaboration projects are progressed.