Data Evaluation Activities at NIFS

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Development for Atomic and Molecular Numerical Database in NIFS

### Reports

- **1977—1989**
  - IPPJ-AM (64 reports)

- **1990—present**
  - NIFS-DATA (113 reports)

### Organization

- **1978—1989**
  - Nagoya Univ.
  - Institute of Plasma Physics

- **1989—2004**
  - NIFS
  - Data Planning Center

- **2004—2009**
  - NIFS
  - Coordination Research Center

- **2010 - present**
  - NIFS
  - Fusion Systems Research Division

### Working groups

- **1973—1977**
  - Nagoya Univ. IPP
  - Atomic Processes WG
  - IPPJ-DT-48 ('75), 50('76)

### International A&M database activities

- **1977 — present**
  - IAEA Advisory Group Meeting of A&M Data for Fusion; Data Center Network

### Data Compilation for nearly 40 Years (Data Bank)

Retrievable databases in computer:
- 1981 AMDIS
- 1985 CHART SPUTY BACKS
- 1990s ALADDIN
- 1997 WWW
- 1998 AMDIS Rec.
- 2001 AMOL CMOL
- 2001 AMDIS to GENIE
- 2002 - [satellite databases]

### Additional notes:

- 1973—1977
  - Nagoya Univ. IPP
  - Atomic Processes WG
  - IPPJ-DT-48 ('75), 50('76)

- 1997
  - WWW

- 2001
  - GENIE

- Search engine
2. NIFS AM Numerical Database
http://dbshino.nifs.ac.jp/
<table>
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<th>DB Name</th>
<th>Contents</th>
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<td>DIO</td>
<td>Electron impact dissociation of simple molecules</td>
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<td>77,714</td>
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</table>
Data Evaluation by working group

• “Filtering” by the data-update working group for data to be put into the database for update: excluding “strange” data

• The working group consisted with Japanese atomic and molecular physicists search publications and compile AM data with some specific targets every 3 years.
  FY2009-2011: hydrogen isotopes
  FY2012-: light elements

• Reports:
  -NIFS-DATA-98 (2006) for $\text{H}_2$, hydrocarbon, and other molecules
  -preparing one report for high Z elements.
Data evaluation by collaboration

- Domestic/international collaborations work on data evaluation for AM / PWI data.
- Evaluation are mainly done for electron-impact excitation cross sections and rate coefficients, and charge transfer cross sections for some ions.
- Old evaluated data are stored with ALADDIN format, which can be seen from our satellite database, “ALADDIN”.
- Results are published as NIFS-DATA reports as well as in journals.
- NIFS Databases are used to evaluate data.
AM data evaluation in NIFS-DATA


Satellite databases

• Small databases are linked at the database top page, such as rate coefficients of electron dissociative attachment to molecular hydrogen.

Database of Photo-absorption cross sections becomes available recently (since 2010).
ALADDIN database in NIFS

- Data files are described with ALADDIN format.
Search for excitation, C, with KATO

[Excitation] e + C^1 (2s2p^2 2D) → (2s2p^2 2P)

Electron Temperature (eV) | Rate Coefficient (cm^3/s)
--- | ---
2.371374e-01 | 3.758610e-16
2.738420e-01 | 4.247286e-15

program (F77 source)
Each evaluation work

- Electron-impact excitation cross sections for N-like ion and N atom.
- Cross sections of ionization, excitation, and charge transfer for C atom and ions.
- Electron-impact excitation rate coefficients for Fe ions.
- Electron-impact ionization cross sections for hydrocarbon molecules.
- Excitation, ionization, and electron capture cross sections for Li\(^{3+}\) and H collision.
- Proton-impact excitation rate coefficients for Fe ions.
Data assessment meeting in Abindgon in March 1992


- Data assessment from H-like to F-like atom and ions, Si ions, S ions, Fe ions.


- Recommended data are fitted to analytic formulae.
\[ \Omega = A + B/X + C/X^2 + D/X^3 + E \ln X, \]  
\[ \text{where } X = E_0/\Delta E, \text{ } E_0 \text{ the energy of the incident electron, } \Delta E \text{ the excitation energy. Correspondingly then, the effective collision strength } \gamma \text{ is given as} \]
\[ \gamma = y \left\{ (A/y + C) + (D/2)(1 - y) + e^y E_1(y)(B - Cy + Dy^2/2 + E/y) \right\} \]
\[ \text{where } y = \Delta E/kT_e, T_e \text{ is the electron temperature, and} \]
\[ E_1(y) = \int_y^\infty \frac{e^{-t}}{t} dt \]

- Evaluation for atomic data for carbon atom and ions.
- Recommended data are fitted to analytic formula in which cross section behavior at high energy is considered.

**Excitation: (J unresolved)**

Two types of formulae have been used for the fit procedures. The formula of Type 1 is defined by

\[
\Omega_{ef}(X) = A + \frac{B}{X} + \frac{C}{X^2} + \frac{D}{X^3} + E \ln X,
\]

whereas for Type 2 we have

\[
\Omega_{ef}(X) = \frac{A}{X^2} + B e^{-FX} + C e^{-2FX} + D e^{-3FX} + E e^{-4FX}.
\]

Here, \(\gamma\) is the effective collision strength and is defined by

\[
\gamma = y e^y \int_1^\infty \Omega_{ef} e^{-ux} dX.
\]

We have

\[
\gamma = y \left\{ \left( \frac{A}{y} + C \right) + \frac{D}{2} (1 - y) + e^y E_1(y) \left( B - C y + \frac{D}{2} y^2 + \frac{E}{y} \right) \right\}
\]

for Type 1 and by

\[
\gamma = A y \{ 1 - e^y E_1(y) y \} + \left( \frac{B e^{-F}}{F + y} + \frac{C e^{-2F}}{2F + y} + \frac{D e^{-3F}}{3F + y} + \frac{E e^{-4F}}{4F + y} \right) y
\]

for Type 2, with

\[
E_1(y) = \int_y^\infty \frac{e^{-t}}{t} dt.
\]
The recommended cross section for electron-impact ionization is parametrized by the expression

$$
\sigma [\text{cm}^2] = \frac{10^{-13}}{IE} \left\{ A_1 \ln(E/I) + \sum_{i=2}^N A_i \left(1 - \frac{I}{E}\right)^{i-1}\right\},
$$

(17)

where the collision energy $E$ and ionization potential $I$ are expressed in eV units and $A_i$ are fitting coefficients. Note that the coefficient $A_1$ can be related to the continuum oscillator strength $df/d\epsilon$ by

$$
A_1 = 8.39 \times 10^{-2} I [\text{eV}] \int_0^\infty \frac{1}{E + \epsilon} \frac{df}{d\epsilon} d\epsilon
$$

(18)

where $\epsilon$ is the energy of ejected electrons. However, we do not use this equation to derive $A_1$ value. The values of $A_i$ in Eq. (17) are given in Table VII, together with the ionization energy.

Charge exchange

analytic functions:

\[
\sigma [\text{cm}^2] = 10^{-16} \times \left( \frac{a_1 \exp\left[-(a_2/E)^{a_2}\right]}{1 + (E/a_4)^{a_4} + (E/a_6)^{a_6} + (E/a_8)^{a_8}} + \frac{a_9 \exp\left[-(a_{10}/E)^{a_{10}}\right]}{1 + (E/a_{13})^{a_{13}} + (E/a_{15})^{a_{15}}} \right),
\]

where the collision energy \(E\) is expressed in eV/amu units and \(a_i, i = 1-14\) are fitting parameters. The values of \(a_i\) in Eq. (19) are given in Tables VIII and IX, together with the

![Graph 1](image1)

FIG. 157: Cross section for charge exchange.

![Graph 2](image2)

FIG. 158: Cross section for charge exchange.

• Recommended data are fitted to analytic formulae.

\[ f_1(x, p_1, p_2, p_3, p_4, p_5, p_6, p_7) = p_1 \frac{\exp(-(p_2/x)p^3)}{1+(x/p_4)p^5 + (x/p_6)p^7} \]

\[ f_2(x, p_1, p_2, p_3, p_4, p_5, p_6, p_7) = p_1 \frac{\exp(-(p_2/x)p^3)}{1-(x/p_4)p^5 + (x/p_6)p^7} \]

\[ f_3(x, p_1, p_2, p_3, p_4, p_5, p_6, p_7) = p_1 \exp(-(p_2/x)p^3)(1+(p_4/x)p^5 + (x/p_6)p^7) \]

Figure 7. Comparison of effective collision strengths, calculated for transitions \(3s^23p^5\)
\(2P_{3/2} \rightarrow 3s^23p^4(1D)3d \, ^2S_{1/2}\) and \(3s^23p^5\)
\(2P_{1/2} \rightarrow 3s^23p^4(1D)3d \, ^2S_{1/2}\) of Fe X:
solid line – [4], dashed line – [2], solid line with \(\triangle\) - [3], solid line with \(\Box\) - [12].
Skobelev et al. (2009)

- Theoretical excitation rates are compared with experimental data which are available.

Figure 12. Comparison of experimental and theoretical excitation rates for transition \(3s^23p^5\,2P_{1/2,3/2}\) - \(3s^23p^4(1D)3d\,2S_{1/2}\) of Fe X: solid line – [4], dotted line – [2], solid line with * - experiment [13].

Fig. 29. Comparison of experimental [27] and theoretical [16-19] values of excitation rates for some levels of Fe XI.
Effective collision strengths of the Fe XIII $3s^23p^2\,^3P_0 \rightarrow 3s^23p^2\,^3P_1$ (open symbols) and the $3s^23p^2\,^3P_0 \rightarrow 3s^23p^2\,^3P_2$ (filled symbols) transitions obtained by Gupta and Tayal (1998) (squares), Tayal (2000) (circles), and Aggarwal and Keenan (2005) (triangles) as a function of electron temperature.

Effective collision strengths of the Fe XXII $2s^22p\,^2P_{1/2} \rightarrow 2s^22p\,^2P_{3/2}$ (open symbols) and the $2s^22p\,^2P_{1/2} \rightarrow 2s2p^2\,^4P_{1/2}$ (filled symbols) transitions obtained by Zhang and Pradhan (1997) (squares), Badnell et al. (2001) (circles), and Landi and Gu (2006) (triangles) as a function of electron temperature.
Recommended data are selected for electron-impact excitation

<table>
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<tr>
<th>Ion</th>
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<th>Number of levels included</th>
<th>Principal quantum number of levels</th>
<th>Log Te (K)</th>
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<td>5.0 – 6.8</td>
<td>CDS</td>
<td>[53]</td>
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Examining high energy behavior and scaling:

\[ \sigma_i = \frac{4\pi \alpha^2 Ry}{E} M_i^2 \ln(C_i E) \] (2)
• Checking branching ratio for dissociated fragments.
Janev et al. (2001)

- Recommended data are fitted to analytic formulae

\[ \sigma = \frac{10^{-13}}{EI_p} \left[ B_1 \ln \left( \frac{E}{I_p} \right) \right. \]
\[ \left. + \sum_{i=1}^{N-1} B_{1+i} \left( 1 - \frac{I_p}{E} \right)^i \right] \text{ (cm}^2\text{)} \quad (15) \]

\[ \sigma_{B-B} = \frac{10^{-13}}{EI_p} \left[ B_1 \ln \left( \frac{E}{I_p} \right) + B_0 \right] \text{ (cm}^2\text{)}. \quad (16) \]

- \( \text{Li}^3+ + \text{H}(n_0 \geq 1) \rightarrow \text{Li}^3+ + \text{H}(n>n_0) \), \\
  \( \text{Li}^3+ + \text{H}(n_0 \geq 1) \rightarrow \text{Li}^3+ + \text{H}^+ + \text{e} \), \\
  \( \text{Li}^3+ + \text{H}(n_0 \geq 1) \rightarrow \text{Li}^2+ (n’l’) + \text{H}^+ \),

- Excitation:

- \( 1s \rightarrow n \) transition scaling
  \( \sigma_{n}^{(q)} \sim q \chi(q) \sigma_{n}^{(2)}(E/q), \quad E/q \geq 10 \, \text{keV/amu} \)
  \( \sigma_{n}^{(q)} \sim q \chi(q) \sigma_{n}^{(2)}(E), \quad E/q \leq 10 \, \text{keV/amu} \)

- where \( \chi(q)=2^{0.52381-\sqrt{2/q}} \), and \( \sigma_{n}^{(2)}(E) \) is the cross section for \( 1s \rightarrow n \) transition induced by He2+ (given in Ref.[11]).
Janev (Murakami et al. (2008))

- Fitting to analytic formulae and scaling low
- Excitation

\[ \sigma^{(q)}_n(n) = a_1 \left[ \frac{\exp(-a_2/E)\ln(1+a_3E)}{E} + \frac{a_4\exp(-a_5E)}{E^{a_6}} + \frac{a_7\exp(-a_8/E)}{1 + a_9E^{a_{10}}} \right] \]

\[ \sigma_{exc}(n) = b_1 \left[ \frac{\exp(-b_2/E)\ln(1+b_3E)}{E} + \frac{b_4\exp(-b_5E)}{E^{b_6} + b_7E^{b_8}} \right] \]

\[ \sigma_{exc}(n \geq 7) = \left( \frac{6}{n} \right)^3 \sigma_{exc}(1s \rightarrow n = 6) \]

\[ \sigma_{exc}(2 \rightarrow n) = c_1 \left[ \frac{\exp(-c_2/E)\ln(1+c_3E)}{E} + \frac{c_4\exp(-c_5E)}{E^{c_6}} \right] \]

\[ \sigma_{exc}(2 \rightarrow n = 6 - 10) = c_{2-n} \sigma_{exc}(2 \rightarrow 5) \]

\[ \sigma_{exc}(2 \rightarrow n = 6 - 10) = c_{2-n} \sigma_{exc}(2 \rightarrow 5) \]

\[ \sigma_{exc}(n_0 \rightarrow n) = 2.769 \frac{n_0^4}{\epsilon} [ADL + FGH] \]

\[ A = \frac{8}{3s} \left( \frac{n}{sn_0} \right)^3 \left( 0.184 - 0.04 \frac{s^{2/3}}{\sqrt{s}} \right) \left( 1 - \frac{0.2s}{n_0n} \right)^{1+2s} \]

\[ D = \exp \left[ -\frac{1}{n_0n^2} \right] \]

\[ L = \ln \left( 1 + 0.53\epsilon^2n_0(n-2/n) \right) \]

\[ F = \left( 1 - \frac{0.3sD}{n_0n} \right)^{1+2s} \]

\[ G = \frac{1}{2} \left( \frac{s}{n-1/n} \right)^3 \]

\[ H = \left[ c_2(z^c, y) - c_2(z^c, y) \right] \]

\[ c_2(z, y) = \frac{z^2\ln(1 + 2z/3)}{2y + 3z/2} \]
Janev (Murakami et al. (2008))

- Ionization

\[ \sigma_{ion}(n_0) = a_1 \left[ \frac{\exp\left(\frac{-a_2}{E}\right)\ell n(1 + a_3 E)}{E} + \frac{a_4 \exp\left(\frac{-a_5 E}{E}\right)}{E^{a_6} + a_7 E^{a_8}} \right] \]

\[ n_0=1 \quad \frac{\sigma_{ion}(q, n_0)}{q n_0^4} = f \left( n_0^2 E/q \right) \]

\[ n_0=3 \quad \frac{\sigma_{ion}(Li^{3+}; n_0 = 3)}{\sigma_{ion}(Li^{3+}; n_0 = 2)} = \frac{\sigma_{ion}(He^{2+}; n_0 = 3)}{\sigma_{ion}(He^{2+}; n_0 = 2)} \]

\[ n_0=4 \quad \sigma_{ion}(n_0; E_{n_0}) = \left( \frac{n_0}{3} \right)^4 \sigma_{ion}(n_0 = 3; E) \quad E_{n_0} = \left( \frac{3}{n_0} \right)^2 E \]
Murakami et al. (2008)

- Electron capture

\[
\sigma^{(n,\ell)}_{\text{CX}} = \frac{a_1 \exp \left[ -\left( \frac{a_2}{E} \right)^{a_3} \right]}{1 + \left( \frac{E}{a_4} \right)^{a_5} + \left( \frac{E}{a_6} \right)^{a_7} + \left( \frac{E}{a_8} \right)^{a_9}}
\]

\[
\sigma^{(n,\ell)}_{\text{CX}} = \frac{a_1 \exp \left[ -\left( \frac{a_2}{E} \right)^{a_3} \right]}{1 + \left( \frac{E}{a_4} \right)^{a_5} + \left( \frac{E}{a_6} \right)^{a_7} + \left( \frac{E}{a_8} \right)^{a_9}} + \frac{a_{10} \exp \left[ -\left( \frac{a_{11}}{E} \right)^{a_{12}} \right]}{1 + \left( \frac{E}{a_{13}} \right)^{a_{14}}} + \frac{a_{10} \exp \left[ -\left( \frac{a_{11}}{E} \right)^{a_{12}} \right]}{1 + \left( \frac{E}{a_{13}} \right)^{a_{14}} + \left( \frac{E}{a_{15}} \right)^{a_{16}}}
\]
Proton-impact excitation rate coefficients for M- and L-shell Fe ions

Collisional excitation rate coefficients for transition $2s^22p^2 \ ^3P_1 - ^3P_2$ in C-like Fe ions (Fe XXI): solid thick line – formula (1) for protons, solid thin line – electrons [Butler & Zeippen 2000], ▲ data [Faucher 1977], □ - data [Ryans et al. 1999; relativistic treatment].
Skobelev et al. (2010)

• Analytic formula

\[ C_{ij}(T_p)[\text{cm}^3\text{s}^{-1}] = 10^{-10} p_1 \exp\left(-\left(\frac{p_2}{T_p}\right)^{p_3}\right) \frac{(T_p/p_6)^{p_7}}{1+(T_p/p_4)^{p_5}} \]

Fig. 2. Proton collision rate coefficients for transitions $3s23p4 \, 3PJ - 3PJ$ in S-like Fe XI: solid, dashed and dot lines – formula (3), diamonds – Bhatia & Doschek (1995) and triangle – Landman (1980) - data for $3P2 - 3P1$ transition, $\times$ – Bhatia & Doschek (1995) and $+$ – Landman (1980) - data for $3P2 - 3P0$ transition, $\circ$ – Bhatia & Doschek (1995) - data for $3P1 - 3P0$ transition; solid thin lines with diamonds, $\times$, $\circ$ – electron rate coefficients of Gupta & Tayal (1999) for transitions $3P2 - 3P1$, $3P2 - 3P0$ and $3P1 - 3P0$, respectively.
PWI empirical formulae in NIFS-DATA

Summary

• In order to evaluate data,
  1. Collect data and compare them using database,
  2. Select good data, and
  3. Fit with proper formulae which have correct asymptotic behavior

• For electron-impact excitation cross sections/rate coefficients, mostly data are theoretically calculated and it is almost impossible to fit data because of huge data set.

• Problem is that it takes long time to finish one work.
原子分子データベース活動（1996－）
（2）データ収集・評価、推奨データの作成

• データの計算方法や実験方法を検討し、もっとも信用できるデータを選び、解析式でフィッティング、利用しやすいデータセットを作成する。
  • リチウムイオンと中性水素の電離・荷電交換断面積の評価
    Murakami, Yan, Sato, Kimura, Janev, Kato (ADNDT, 94, 161 (2008))
  • 炭化水素の電子衝突電離断面積データの収集・評価
  • 鉄イオンと陽子の衝突励起断面積の評価
    (NIFS-DATA-95(2006), 99(2007))
  • 鉄イオンの電子衝突励起速度係数の評価

Proton collision rate coefficients for transition 3s^23p^2P_{1/2} - 2P_{3/2} in Al-like Fe XIV: solid line – formula (1), ○ – data [12], ▲ – data [19], + – data [10], ◊ – data [26], □ and × – data [25] for different methods of consideration of small impact parameter region; thin solid line – electron rate coefficient of [32].