

§47. Atomic and Molecular Numerical Databases and Data Activities

Murakami, I., Kato, D., Sakaue, H.A., Kato, M.

We have constructed and made public atomic and molecular (AM) numerical databases for various collision processes, mainly for fusion plasma research but also for other areas such as astrophysics, applied-science with low temperature plasmas, plasma processing, etc. The AM data activities in Japan were initiated in 1970s.

The first retrieval AM database “AMDIS” was constructed in 1981 for electron impact ionization and excitation cross sections at Institute of Plasma Physics, Nagoya Univ. (IPPJ). Following this, other databases have been built and the database system has expanded to cover a wide variety of collision processes in plasma and also plasma-wall interactions (PWI).

The current web accessible database system¹⁾ has been maintained since 1997. The database system consists of 6 sub databases. Table 1 shows a list of AM and PWI numerical databases as well as a bibliographic database “ORNL” for which original data records are collected by Oak Ridge National Laboratory (USA). Cross references are partly supported between bibliographic and numerical databases. Users can retrieve numerical data through the web form by element, ionic stage, initial states and other constraints.

The databases include: “AMDIS” for cross sections and rate coefficients for electron impact ionization, excitation, recombination, and dissociation; “CHART” for cross sections of heavy particle collisions; “MOL” for numerical data on molecular collision processes, “SPUTY” for numerical data on sputtering yields for mono-atomic solids and “BACKS” for numerical data on reflection coefficients. During the 2010 fiscal year, we mainly updated the data for AMDIS excitation. A working group of Japanese atomic and molecular physicists has been organized to collect data systematically by searching literature. Recently we collected cross sections for electron and atomic collisions with high Z elements²⁾. Figure 1 shows an example of updated data sets³⁾.

In addition to the main databases, we have some small satellite databases which are not retrievable. These satellite databases are linked to the top page of the main database and numerical data are available as a text file. In FY2010, we made the photoabsorption database for 9 atoms and 23 molecules⁴⁾ and open it as a satellite database⁵⁾. The oscillator strength spectra, photoabsorption cross sections, and mass absorption coefficients are evaluated and numerical data tables are available from the web page.

As one of the applications of these databases, we have been constructing a collisional-radiative model of W ions with W atomic data to analyze spectra taken from LHD plasmas to investigate spectroscopic properties of W ions.

- 1) NIFS Database, <http://dbshino.nifs.ac.jp/>
- 2) M. Kitajima et al., in preparation.
- 3) C. P. Ballance and D. C. Griffin, J. Phys. B 40 (2007) 247.
- 4) N. Sakamoto et al., NIFS-DATA-109 (2010).
- 5) Photoabsorption database, <http://dpc.nifs.ac.jp/photoab/>

Table 1. AM and PWI databases

Name	Records*	Period
AMDIS	463,592	1961-2011
CHART	7,054	1957-2010
MOL	3,765	1956-2009
SPUTY	1,241	1931-2000
BACKS	396	1976-2002
ORNL	77,714	1959-2008

* as of Aug. 23, 2011.

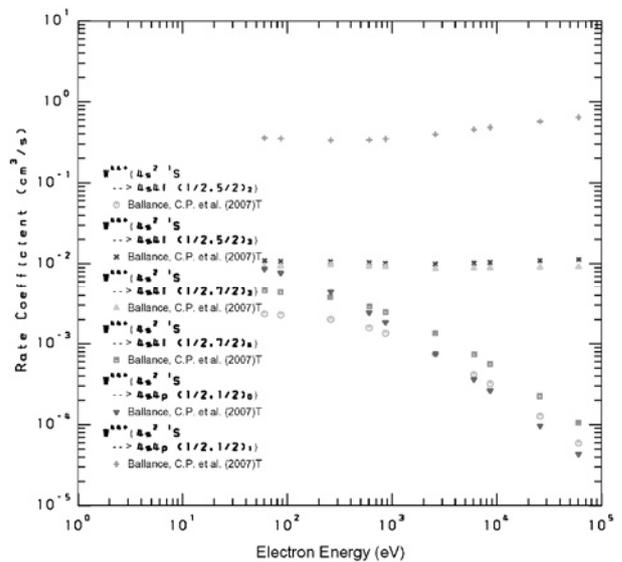


Fig. 1 Example of newly included data of electron-impact excitation rate coefficients for $4s^2 \ ^1S \rightarrow 4s4p, 4s4f$ transitions of W^{4+} ion published in Ref. [3].

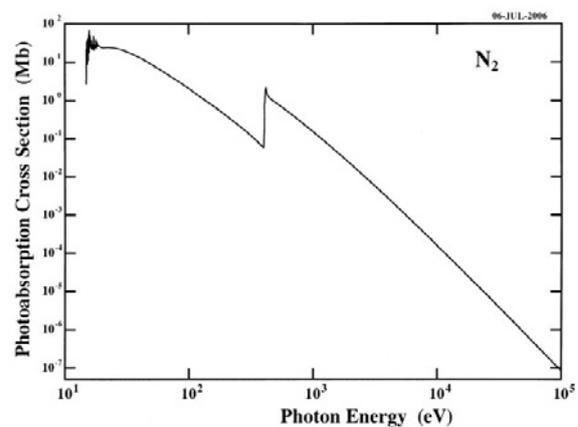


Fig. 2 Photoabsorption cross section for N_2 in Ref.[4].