

§7. Atomic and Molecular Numerical Databases and Data Activities

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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 it, 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 opened and 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 2011 fiscal year, we mainly updated the data for AMDIS. Fig.1 shows an example of recombination rate coefficient for a tungsten ion^{2,3)}. A working group has been organized to collect data systematically, and data on collision processes for hydrogen isotopes were searched in FY2011.

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 FY2011, we have prepared a web page for a bibliographic database of electron – molecule collision processes, compiled by M. Hayashi. Some bibliographic databases are already published as NIFS-DATA series⁴⁾. Recommended cross section data sets for some molecules by Hayashi, such as cross section data for C₂H₂ shown in Fig.2, will be open in a web page as well.

Table 1. AM and PWI databases

Name	Records*	Period
AMDIS	465,991	1961-2011
CHART	7,054	1957-2010
MOL	3,765	1956-2009
SPUTY	1,241	1931-2000
BACKS	396	1976-2002
ORNL	78,097	1959-2009

* as of May 10, 2012.

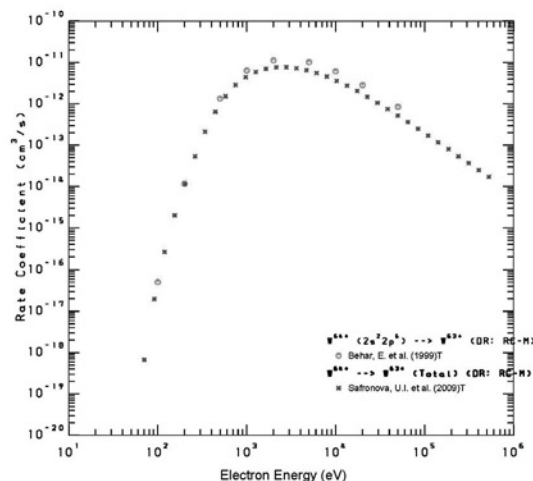


Fig. 1 Example of newly included data of dielectronic recombination rate coefficients for W⁶⁺ ion published in Ref. [2] (crosses) compared with data in Ref.[3] (circles).

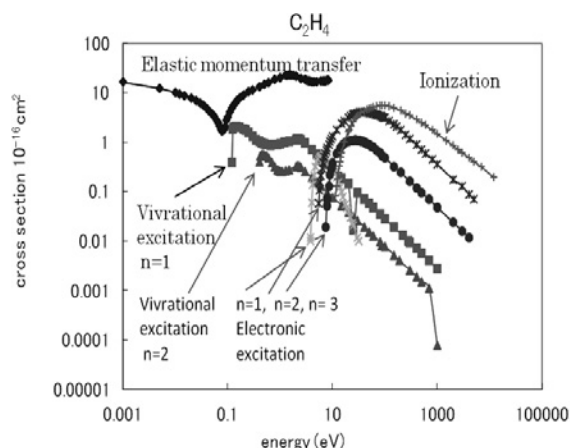


Fig. 2 Cross sections of electron-impact processes for C₂H₂. Data are compiled by M. Hayashi.

- 1) NIFS Database, <http://dbshino.nifs.ac.jp/>
- 2) U. I. Safronova et al., ADNDT **95** (2009) 751.
- 3) E. Behar et al., Phys. Rev. A **59** (1999) 2787.
- 4) M. Hayashi, NIFS-DATA 72 ; 74 ; 76 ; 77 (2003) ; 79 ; 80 ; 81 ; 82 ; 83 ; 87 ; 90 (2004).