

Atomic and Molecular Databases and Data Evaluation Activities at NIFS

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The National Institute for Fusion Science (NIFS) has constructed atomic and molecular numerical databases for collision systems and makes them available via the internet at <http://dbshino.nifs.ac.jp/> since 1997. Data compilation was started in the 1970s at the Institute of Plasma Physics, Nagoya University and has a long history. Working groups have been organized to compile and evaluate atomic and molecular collision data and plasma-wall interaction data. Now the NIFS database system has AMDIS (cross sections and rate coefficients of electron collision processes for atoms; 465,991 records as of May 10, 2012), CHART (cross sections of heavy particle collision processes for atoms; 7,054 records), AMDIS-Molecule (cross sections and rate coefficients of electron collision processes for molecules; 1,766 records), CHART-Molecule (cross sections and rate coefficients of heavy-particle collisions for molecules; 1,999 records), SPUTY (sputtering yields for solids; 1,241 records), and BACKS (backscattering coefficients of solid surface; 396 records). The databases are retrievable and numerical data can be shown as a graph or a table. Each data record contains bibliographic information as well as numerical data.

The NIFS databases are used to compare data to evaluate, and evaluated data are also stored in the databases. Evaluated data sets are published as reports in IPPJ-AM series (1977-1989) and NIFS-DATA series (1990 – present). Critical data evaluation was done for electron-impact excitation cross sections (e.g. C and O ions [1] and N-like ions [2]), electron-impact ionization cross sections (e.g. hydrocarbons [3]), and charge exchange cross sections (e.g. Li³⁺ and H [4]). Asymptotic behavior of cross sections at high collision energy was considered to determine analytic formulae for fitting data, and data were fitted to such analytic formulae. Even though reliable energy (temperature) ranges are limited, it is useful to express evaluated data with fitting formulae. Such evaluated data expressed with fitting formulae and parameters are important and useful for plasma simulations and modelings in fusion plasma research. Such evaluation has been done only for limited collision systems. We also selected data sets of electron-impact collision rate coefficients for Fe ions among existing theoretical calculations as recommended data sets for spectral modelings [5]. For the selection, we examined calculation method, number of configurations and ranges of collision energy and partial waves considered in the calculations, and availability of data sets. Such selection is one of evaluation methods for collision processes which experimental measurements are rare or do not exist.

It is important to establish an international collaboration system on data evaluation to evaluate data for many collision systems with systematic way. It is also necessary to have an independent database of evaluated data for easy use for users.

References

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