

## §21. Construction and Update of Atomic and Molecular Database for Light Elements of the 2nd Period

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Atomic and molecular processes play an important role in fusion plasmas. Considerable number of experimental and theoretical cross sections for atomic and molecular collisions have been reported, since the cross-section data concerning atomic and molecular processes are important in the understanding of the fundamental physics of atomic and molecular collisions, which provides the fundamental knowledge in many fields such as electron and ion driven processes in the Earth and planetary phenomena, radiation chemistry, gaseous discharges, weak and strong plasmas, and so on. The cross section data for collision processes including the elements, which consists the plasma facing materials, are crucial demands to model the transport of eroded atoms and molecules. Due to its importance, these cross-section data are also compiled in the atomic and molecular databases around the world, and can be accessed online. The Japanese National Institute of Fusion Science, NIFS, provides one of the most relevant online databases on atomic and molecular cross sections in numerical data and bibliographic information. The database AMDIS for electron collisions and CHART for heavy particle collisions, respectively, were constructed over decades ago, and have been continuously updated from time to time. There also are databases for electron collisions and heavy particle collisions with molecules, so called AMOL and CMOL respectively. Data compilation and evaluation of these databases at NIFS have been continuously proceeding up to now.

The present working group continuously supports the update of the atomic and molecular databases of NIFS by comprehensive data compilation of atomic and molecular cross sections. The collaborations of updates and extension for these NIFS atomic and molecular database had been continuously proceeding by selecting topics, such as atomic process with high Z elements, which were relevant for the LHD peripheral plasma. The collaboration also worked for the comprehensive data mining and compilation of atomic and molecular cross sections for the atomic and molecular processes including hydrogen isotopes and small hydrocarbons, since it was found that atomic and molecular

data for electron impact and heavy particle impact cross section data on hydrogen isotopes and hydrocarbons are the urgent issue, during the previous collaboration for the collection and compilation of atomic and molecular data for high Z elements.

In the present collaboration from 2012, a comprehensive data mining and compilation of atomic and molecular cross sections for light elements of the 2nd period such as Li, Be, B, C, N, O, F and Ne have been attempted. Electron impact cross section data and heavy particle impact cross section data for small atoms and molecules such as hydrogen, hydrogen isotopes, nitrogen, oxygen, hydrocarbons, Water and Carbon Oxide have been continuously surveyed in our previous collaboration and stored into the database, up to year of 2000.<sup>1)</sup> The experimental as well as theoretical data for various processes by electron impact and heavy particle impact on these atoms and molecules reported recently were the target of the present data survey. Optical data such as photoabsorption cross sections for light elements of the 2nd period were also surveyed in the present collaboration. In order to carry out a complete survey for the existing literature, resources of NIFS library have becoming important in now days.

In addition to the survey for the cross section data in the literature, we also have conducted a measurements on electron - atom and molecule collision cross sections in the energy region from 20 eV down to very low energies with very high energy resolution<sup>2,3,4)</sup> in the present project. Our results resolved a number of issues in the literature and assessed various published theoretical results. We also have validated the theoretical electron impact cross sections of He which have been known as "standard" cross sections, to which a majority of experimental cross sections for atoms and molecules reported in the literature were normalized. Total cross section data for electron scattering from He, Ne, Ar Kr, and Xe will be presented in the NIFS-DATA.<sup>5)</sup>

- 1) Kimura M. et al. : NIFS-DATA-98 (2006)
- 2) Kurokawa M. et al. : Phys. Rev. A **84**, 062717 (2011)
- 3) Kitajima M. et al. : Eur. Phys. J. D, (2012) 130.
- 4) Shigemura K. et al. : Phys. Rev. A **89**, 022709 (2014)
- 5) Kitajima M. et al. : NIFS-DATA, to be published.