

§39. Atomic and Molecular Database of Hydrogen-isotopes and Hydro-Carbons

Kitajima, M. (Tokyo Inst. Tech.), Kusakabe, T. (Kinki Univ.), Moribayashi, K. (JAERI), Igarashi, A. (Miyazaki Univ.), Motohashi, K. (Toyo Univ.), Imai, M., Tsuchida, H. (Kyoto Univ.), Okuno, K. (Tokyo Metropolitan Univ.), Soejima, K., Shimakura, N. (Niigata Univ.), Pichl, L. (ICU), Suzuki, R. (Hitotsubashi Univ.), Morishita, T. (Univ. Electro-Comm.), Ishi, K. (Nara Women's Univ.), Suno, H. (Earth Simulator Center, JAMSTEC), Hoshino, M. (Sophia Univ.), Kato, D., Sakaue, H.A., Murakami, I., Goto, M., Morita, S., Sato, K., Funaba, H., Ido, T., Peterson, B.J.

Cross-section data concerning atomic and molecular processes are of great importance in understanding the fundamental physics of atomic and molecular collisions and 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. Considerable number of experimental cross section data for atomic and molecular collisions has been reported. Compilation of these data sets has been published as review articles, such as references. 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.

Atomic and molecular processes play an important role in fusion plasmas. The cross section database for collisions processes of elements consists the plasma facing materials are needed to model the transport of eroded atoms and molecules. Data compilation and evaluation of atomic and molecular cross section data for fusion research at NIFS have been continuously proceeding. 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.

On the course of the continuous update of the atomic and molecular databases of NIFS, a working group has been organized for comprehensive data compilation of atomic and molecular cross sections. In the previous collaborations, updates and extension of these NIFS atomic and molecular database, especially for the data for atomic process with high Z elements, which were relevant for the LHD peripheral plasma, have been carried out by the working group.¹⁾ It was found that most of the absolute cross section data for high-Z elements, a part from rare gas atoms, were obtained theoretically. Experimental cross

sections are strongly demanded for reliability for the data for high-Z elements, which will be highly required for the plasma modeling in fusion science. Recent literature research for cross section data also shows that number of experimental reports providing electronic state selective data, which will help to make a more realistic model for plasma diagnostics, are increasing for rare gas targets. However, the data are often relative quantities and most of these data were difficult to be included in AMDIS or CHART. In addition to these literature researches, we also have conducted a new measurement on absolute total cross section for electron scattering from Ar, Kr and Xe in the energy range from 20 eV down to around 10 meV with very narrow electron energy width of 10–12 meV.^{2,3)}

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. Electron impact cross section data for small hydrocarbons, together with heavy particle impact cross sections on small hydrocarbons have been continuously surveyed our collaboration and stored into the database, up to year 2000.⁴⁾ However, new experimental as well as theoretical data for various processes by electron impact and heavy particle impact on hydrocarbons have been reported from since we have carried out data survey. In addition, extensive compilation and evaluation of electron impact cross sections for molecular hydrogen has been reported recently.⁵⁾

In the present collaboration, a comprehensive data mining and compilation of atomic and molecular cross sections for the atomic and molecular processes including hydrogen isotopes and small hydrocarbons have been attempted. A complete survey for the existing literature and extraction of the cross section data sets were carried out in the present project. Including the evaluated data, comprehensive sets of electron hydrogen molecule are stored in AMOL. We also have conducted a new measurement on electron - hydrogen molecule collision cross sections in the energy region at low energies and very low energies with very high energy resolution.

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- 4) Kimura M. et al., NIFS-DATA-98 (2006)
- 5) Yoon J.-S. et al. : J. Phys. Chem. Ref. Data **37** (2008) 913