

COMPILATION OF ATOMIC DATA FOR FUSION
BY THE ORNL CONTROLLED FUSION ATOMIC DATA CENTER

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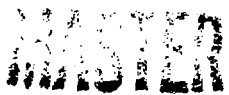
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The Controlled Fusion Atomic Data Center (CFADC) was founded by C. F. Barnett at ORNL in 1959. Its mission is to identify, compile, evaluate and recommend data on atomic and molecular collision processes which are important in fusion energy research. The principal ongoing activities of the CFADC are threefold:

1. Literature searches and maintenance of on-line databases of bibliographic references and numerical collision data,
2. Compilation, evaluation and recommendation of atomic and molecular collision data for fusion applications,
3. Participation in the International Atomic and Molecular Data Center Network, which facilitates the co-ordination of activities, exchange of data, identification of data needs and assessment of the existing database.

On-Line Bibliographic Database

Approximately 120 scientific journals are searched for fusion-relevant publications on a regular basis by a international team of expert consultants. These references are entered daily into an on-line database at ORNL, and updates are sent periodically via diskette to the data centers at the IAEA in Vienna, and at NIFS (Nagoya) and JAERI (Tokai) in Japan. This forms the basis for the semi-annual IAEA *International Bulletin on Atomic and Molecular Data for Fusion*. More than 25,000 indexed bibliographic entries dating to 1978 are retrievable at ORNL using a commercial software package (dBase III+) operating on a local area network of personal computers. On-line searches are routinely performed for specific reactions and reactants for data compilation, as well



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as in response to requests for information. Bibliographies dating to 1950 are available in both indexed hardcopy format and on magnetic tape. Future plans call for reformatting these and making them also available for on-line searching.

Data Compilation and Evaluation

The major vehicle for dissemination of evaluated and recommended data by the CFADC has been the series of ORNL Reports, entitled *Atomic Data for Fusion*, and popularly called the "Redbooks." These reports contain recommended data in graphical and/or tabular format, along with parametrized fits in most cases and references to the original data sources. Collisional data are presented as cross sections and/or rate coefficients, as appropriate. Volumes containing spectroscopic data have been prepared by the NIST Data Centers on Atomic Energy Levels and Transition Probabilities. The volumes published and distributed in this series are listed below:

Collisions of H, H₂, He and Li Atoms and Ions with Atoms and Molecules, C. F. Barnett, ORNL-6086 (1990). [+ ALADDIN Database].

Spectroscopic Data for Titanium, Chromium and Nickel, W. L. Wiese and A. Musgrove (NIST), ORNL-6551 (1989).

Collisions of Carbon and Oxygen Ions with Electrons, H, H₂ and He, R. A. Phaneuf, R. K. Janev and M. S. Pindzola, ORNL-6090 (1987). [+ ALADDIN Database].

Spectroscopic Data for Iron, W. L. Wiese (NIST), ORNL-6089 (1985).

Particle Interactions with Surfaces, E. W. Thomas, ORNL-6088 (1985).

Future plans for this series include a compilation of recommended data for electron collision processes to be prepared in collaboration with the JILA and NIST Data Centers in the U.S.

The CFADC has also been involved in a number of topical database assessments, of which a primary focal points have been the edge plasma and metallic impurities. Reports prepared by the CFADC related to these activities are listed below.

Assessment of Ion-Atom Collision Data for Magnetic Fusion Plasma Edge Modelling, R. A. Phaneuf, (Atomic and Plasma-Material Interaction Data for Fusion, Volume 2, pp. 75-90, Supplement to *Nuclear Fusion* (1992).

Status and Critical Assessment of the Data Base for Collisions of Be⁹⁺ and B⁸⁺ Ions with H, H₂ and He, R. A. Phaneuf, R. K. Janev, H. Tawara,

M. Kimura, P. S. Krstic, G. Peach and M. A. Mazing, (Atomic and Plasma-Material Interaction Data for Fusion, Supplement to *Nuclear Fusion* (to be published, 1992).

Atomic and Molecular Data Requirements for Fusion Plasma Edge Studies, H. Tawara and R. A. Phaneuf, *Comm. At. Mol. Phys.* 21, 177 (1988).

More recently, in collaboration with R. K. Janev of the IAEA and H. Tawara of NIFS, data have been collected and evaluated for state-selective electron capture in collisions of C^{9+} and O^{9+} ions with H, H_2 and He. Such data are important for spectroscopic diagnostics of the edge, and for charge-exchange recombination spectroscopy (CXRS). Cross sections were recommended for 87 reaction channels for $C^{6+} + H$ and $O^{8+} + H$ collisions. Analytical fits were subsequently made to the recommended cross sections by T. Shirai of JAERI, and an ALADDIN database based on these fits will be created for distribution. A manuscript containing the graphical and parametrized representations of these data is being prepared for submission to *Atomic Data and Nuclear Data Tables*. As more data become available, the recommended data will be expanded to include partially stripped C^{9+} and O^{9+} reactants.

The database for collisions of Be and B ions with H, H_2 and He was also reviewed and evaluated as part of an IAEA Consultants' meeting, and a Working Group Report was prepared by the CFADC. Atomic and molecular data needs for edge and divertor plasmas have been the focus of considerable activity during the past several years^{1,2}. In response to these data needs, the CFADC has emphasized data collection and evaluation for edge-relevant processes at low collision energies. The lower temperatures and ionization stages which prevail present a challenge to atomic and molecular data producers, since an entirely new set of theoretical and experimental approaches are required. One important area where almost no data are available is low-energy elastic scattering collisions of impurity ions with hydrogen and helium atoms. The CFADC is currently assessing the available database for such collisions, and evaluating theoretical methods to calculate the needed cross sections. Modelling of helium ash removal and hydrogen recycling will also require accurate low-energy collision data for molecular as well as atomic species.

Data Accessibility and Dissemination

To facilitate a more effective exchange and distribution of recommended data among producers and users, the CFADC has, along with the International

Atomic and Molecular Data Center Network, adopted the ALADDIN format and software³ as the standard. The ALADDIN program is written in FORTRAN-77 and utilizes ASCII data files so that it can operate on virtually any computer system (from personal computer to supercomputer). ALADDIN may be operated in an "on-line" manner in which data files may be scanned, searched and data recovered, or it may be called as a subroutine from other programs. The CFADC has widely distributed the ALADDIN database programs and ORNL "Redbook" ALADDIN data files via diskette and electronic mail. To facilitate wider and more effective access to and distribution of both numerical and bibliographic data, the CFADC is in the process of implementing an "Atomic Data Workstation" to serve as a host for remote on-line access to the CFADC's databases. This workstation will be universally accessible over INTERNET via the TELNET facility.

References

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- # Managed by Martin Marietta Energy Systems, Inc., for the U.S. Department of Energy under Contract No. De-AC05-84OR21400.
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