NIFS Atomic and Molecular Numerical Database for Collision Processes

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NIFS Atomic and Molecular Numerical Database for Collision Processes

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Abstract: The National Institute for Fusion Science (NIFS) has compiled and developed atomic and molecular numerical databases for various collision processes and makes it accessible from the internet to the public. The database contains numerical data of cross sections and rate coefficients for electron collision or ion collisions with atoms and molecules, attached with bibliographic information on their data sources. The database system provides query forms to search data, and numerical data are retrievable. The graphical output is helpful to understand energy dependence of cross sections and temperature dependence of rate coefficients obtained by various studies. All data are compiled mainly from published literature, and data sources can be tracked by the bibliographic information. We also have data of sputtering yields and back-scattering coefficients for solid surfaces collided by ions in the database. All data in the database are applicable to understand atomic and molecular processes in various plasmas, such as fusion plasma, astrophysical plasma and applied plasma, as well as for understanding plasma–surface interaction in plasmas.

Keywords: atomic and molecular data; collision processes; plasma–surface interaction

1. Introduction

Cross sections of elementary atomic processes, such as electron-impact ionization, are important to describe and understand the behavior of atoms in plasma. Databases for such atomic data are very important and useful for users who need such data for their research on plasma physics and fusion sciences. Data compilations of atomic and molecular data on spectroscopic data and cross sections of collision processes started in the 1960s at the National Bureau of Standards, and Oak Ridge National Laboratory in the United States. In Japan, the data compilation on atomic processes important for fusion plasma was initiated in the early 1970s by the study group organized with Japanese atomic physicists and plasma physicists as the collaboration project at Institute of Plasma Physics (IPPJ), Nagoya University. Compiled data on collision cross sections for hydrogen, the isotopes, and helium were published as IPPJ-DT reports [1,2] in 1975 and 1976. Succeeding studies on data compilation for atomic and molecular collision cross sections and data on plasma-surface interaction were published as IPPJ-AM reports from 1977 to 1989 [3] and NIFS-DATA reports [4] since 1989 when the institution was reorganized from IPPJ to the National Institute for Fusion Science (NIFS).

The retrieval and display system for the atomic and molecular database, named as AMDIS (Atomic and Molecular Data Interactive System), was constructed in the main frame computer at IPPJ using

FAIRS (FACOM Advanced Information Retrieval System) in the early 1980s [5]. Cross sections for electron-impact ionization and excitation, compiled by the collaborative working groups in IPPJ were stored in AMDIS. Later, the database system was extended to include cross sections for charge exchange and ionization processes by ion–atom collision and the new database was named as CHART in the late 1980s. Further extensions of the database, including sputtering yields and back-scattering coefficients of ion collision onto solid surface as SPUTY (Sputtering Yields) and BACKS (Back-Scattering coefficients), respectively, were made in the 1980s [6,7]. These databases are based on the data compilation activities. All data in the databases are taken from publications with their bibliographic information. Data sources can be tracked.

All the databases built in the main frame computer were available only for collaborators visiting IPPJ/NIFS until 1997. In 1997, the database was reconstructed with the ORACLE relational database system in a UNIX computer and the retrieval and display system was changed to use a web browser [8,9]. The database became accessible via the internet. We first required users to be registered in order to use the database until 2007. Since 2007, any researcher can use the database without registration. Meanwhile, the database was extended to have recombination rate coefficients for atomic ions (REC) in 1998, collision cross sections and rate coefficients for molecules (MOL) in 2001, and rate coefficients of electron-impact excitation and ionization in 2003. The database system was again reconstructed in 2016 with PostgreSQL relational database system and Ruby on Rails for web interface to be a secure system [10]. For a simpler data search, tables on available data in the database are newly prepared at the time of access to allow users to find target data simpler and easier than before.

There have been several databases on collision processes available via the internet since the 1990s. For example, the International Atomic Energy Agency (IAEA) maintains IAEA ALADDIN (A Labelled Atomic Data Interface) database [11] which has evaluated cross sections and rate coefficients for atomic and molecular collision processes and particle-surface interaction data stored with ALADDIN format [12]. All data were evaluated but restricted for fusion relevant processes. National Institute of Standards and Technology (NIST) has electron-impact cross sections for ionization and excitation database [13] based on the Binary-Encounter-Bethe model calculations for some selected atoms and molecules [14]. OPEN-ADAS [15] is the database of basic data and some derived data from ADAS (the Atomic Data and Analysis Structure) on spectroscopic diagnostics for fusion and astrophysical plasmas including electron-impact excitation and ionization rate coefficients and charge-exchange cross sections of ion–atom collisions [16]. All data are obtained by theoretical calculations or evaluation using available theoretical data. The NIFS database contains theoretical and experimental data as well as evaluated data from publications. Experimentally obtained data are useful to evaluate theoretically-calculated data. These databases and some others are mainly from the fusion community and are searchable at once via the search engine GENIE (a General Internet Search Engine for Atomic Data) since 2001 [17].

There are many other databases in different communities, such as astrochemistry, atmospheric science, lighting, application plasmas, etc. The Virtual Atomic and Molecular Data Centre (VAMDC) is the project to establish the e-infrastructure to access many various atomic and molecular databases developed in various communities from one portal site simultaneously [18]. Many atomic and molecular databases on spectroscopy and collision processes join to VAMDC. Data accessed from VAMDC web portal are provided with the same format described with the XML Schema for Atoms, Molecules, and Solids (XSAMS) and are useful for any application. XSAMS was developed as an XML-based standard for the exchange of atomic, molecular, and particle–solid interaction data by the working group organized under the Atomic and Molecular Unit, IAEA from 2006 to 2011 [19]. Based on this first version of XSAMS, VAMDC developed their own schema as VAMDC-XSAMS [20]. We implemented one of the databases, AMDIS-ION, to VAMDC for wider user communities in 2018 [10,21].

The concepts of the database system were maintained during the reconstructions. Atomic and molecular data on collision processes, which are important for plasma physics and fusion science are

primarily compiled from publications in refereed journals. Target atoms and molecules to be included in the database have been extended to other fields, such as astrophysics and plasma applications. Data in the database are retrievable by queries on element, charge state, initial and final electronic states, and other conditions, such as authors or publication year. Retrieved numerical data are displayed in a tabular form and in a graphic form. All attached information, such as a theoretical or experimental method used to obtain the data, energy range, and bibliography are also shown. Data compilations are continued with the help of Japanese atomic and molecular physicists under the NIFS collaboration program and data updates are regularly performed. The list of publications, whose data are newly included in the database, is shown in the entry page of the database.

In the following sections, details of the database system are described and data evaluation activities using the database are introduced.

2. NIFS Database

2.1. Main Database

The NIFS atomic and molecular numerical database consists of nine sub-databases currently. Table 1 shows the list of sub databases with the number of data records stored in the database. All data are retrievable using the database system. AMDIS EXC (electron-impact excitation rate coefficients and cross sections) has the largest number of data records among them.

Table 1. List of sub databases in the NIFS Atomic and Molecular Numerical Database.

Name		Description	Number of Data Sets [1]
AMDIS	ION	Electron-impact ionization cross sections and rate coefficients for atoms	806,493
	EXC	Electron-impact excitation cross sections and rate coefficients for atoms	
	REC	Electron recombination rate coefficients for atoms	
	DIO	Dissociation cross sections for molecules	
CHART		Charge exchange and ionization cross sections for ion–atom collisions	7646
MOL	AMOL	Cross sections and rate coefficients of electron-molecule collision processes	5405
	CMOL	Cross sections and rate coefficients of atom-molecule collision processes	
SPUTY		Sputtering yields by atomic ions for solid surface	2349
BACKS		Energy and particle back-scattering coefficients of light ions from solid surface	485

[1] As of 11 August 2020.

One record in the data, for example, in AMDIS EXC, consists of element, charge state, initial and final states, numerical data table of electron temperature and rate coefficients of electron-impact excitation, transition energy, theoretical or experimental method used to obtain the data, and bibliographic information of data source such as author names, title of the paper, journal name, volume, page, and published year, as shown in Table 2. Additional information on table number or figure number in the original paper and name of the atomic code used to calculate data is also stored in the record. Initial and final states are given in the same notation of the original papers. That is, *LS* coupling or *jj* coupling notations are used to describe the states of atoms and ions, depending on the papers. When ionization or excitation cross sections are given in the original paper, we calculate collision strengths from the cross sections and store them in the database, and vice versa. When ionization or excitation rate coefficients are given in the original paper, effective collision strengths are calculated

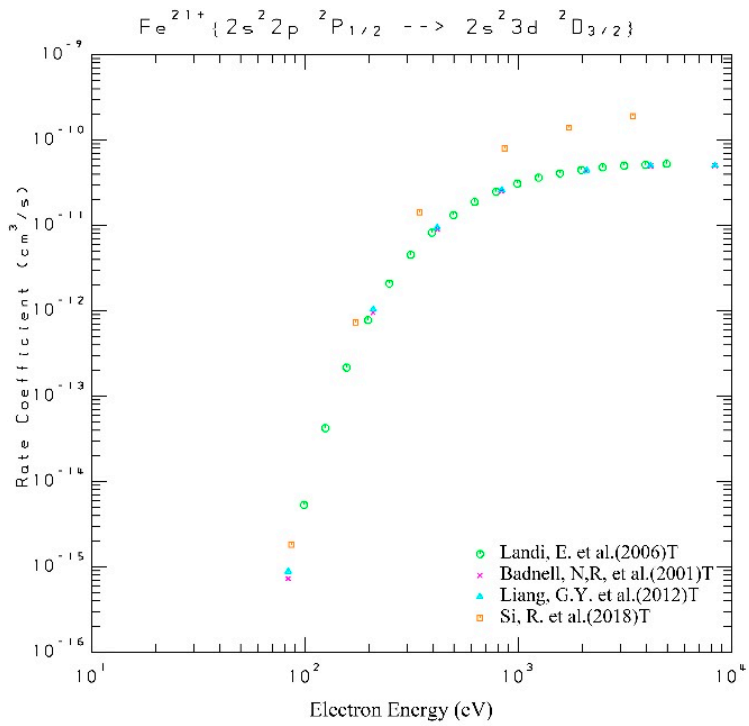
and stored in the database, and vice versa. These values can be displayed in a table or in a graph. Figure 1a shows an example of a graph for AMDIS-EXC. There are four theoretical data sets shown for the same electron-impact excitation process. Users can compare these data to examine the validity. Three data sets calculated with R-matrix method [22–24] agree with each other, and one calculated with distorted wave method by Si et al. [25] shows larger values than others.

Table 2. An example of one data record stored in AMDIS EXC.

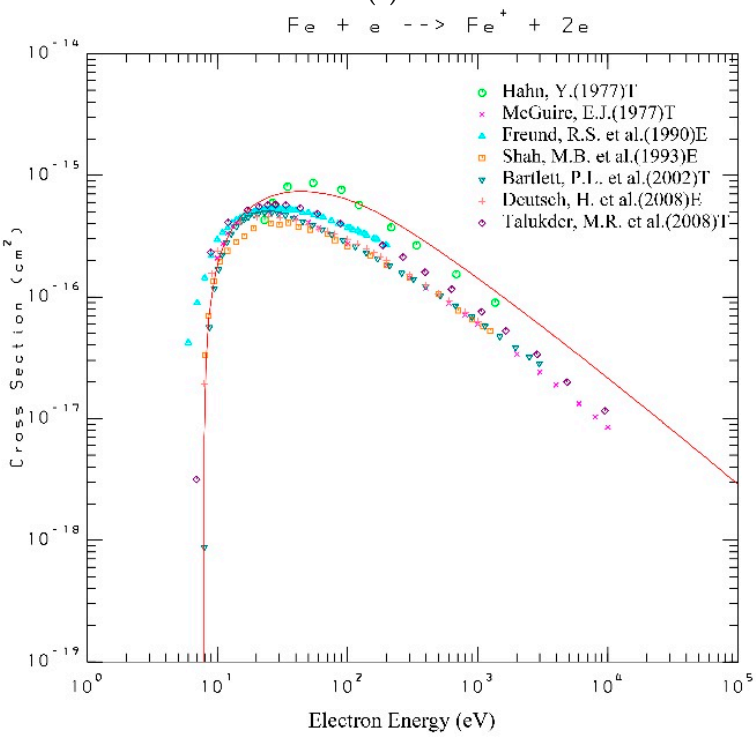
Items	Values	Remarks
Process	ERC	EXC (excitation cross sections) or ERC (excitation rate coefficients)
Theory or Experiment	T	T (theory) or E (experiment) or V (evaluated)
Method	Relativistic distorted-wave	Theoretical or experimental method to obtain the data
Atomic number	24	
Element	Cr	
Ionic state	7	Charge state
Number of electrons	17	
Initial state	$3s^2 3p^5\ ^2P^O{}_{3/2}$	Based on the notation in original source
Final state	$3s^2 3p^4\ (^1S)\ 3d\ ^2D_{3/2}$	The same as above
Transition energy	54.508	(eV)
No. of data point	9	
SEE	1	Original unit of x data: 1 (eV), 2 (Ryd), 4 (E/ΔE), 6 (K)
CSS	A	Original unit of y data: A (cm^2), B ($\pi\ a_0{}^2$), D (collision strength), F (cm^3/s), G (effective collision strength)
X1	8.617320×10^0 $1.365845 \times 10^1 \ldots$ [1]	Electron temperature (eV)
Y1	3.923830×10^{-13} $3.470539 \times 10^{-12} \ldots$	Rate coefficients (cm^3/s)
X2	1.000×10^5 $1.5845 \times 10^5 \ldots$	Electron temperature (K)
Y2	3.213×10^{-2} $3.465 \times 10^{-2} \ldots$	Effective collision strength
Authors	Aggarwal, K.M., Kato, T., ...	
Title	Radiative rates and electron	
Journal name	Astronomy and Astrophysics	
Volume	506	
Page numbers	1501–1509	
Date of publication	2009	
Comment	Table 6. (1–25). FAC code	Additional information on data source and name of theoretical code used.

AMDIS-ION has a similar data structure to AMDIS-EXC. Figure 1b shows an example of single ionization cross section of a Fe atom, taken from AMDIS-ION. There are plotted seven data sets obtained theoretically or experimentally [26–32] and an empirical curve calculated with Lotz's formula [33]. Users can draw the formula in a graph for elements with atomic numbers smaller than 30.

When fitting formula and fitting coefficients are given in the original papers, we calculate cross sections or rate coefficients using the fitting formula to store in the database. Dielectronic recombination rate coefficients are often given as fitting formulae and fitting coefficients in the original papers. Therefore, such formulae and coefficients are also stored in the database AMDIS-REC as the items "FITEQ" and "FITP" and can be shown in results of query. In the case of AMDIS-REC, rate coefficients in Maxwellian electron velocity distribution for thermal plasma and non-Maxwellian electron velocity distribution, such as in merged beam experiments, are stored with "RC-M" and "RC-NM" for the item "YTP" (y-type), respectively.



(**a**)



(**b**)

Figure 1. (**a**) Electron-impact excitation rate coefficients as a function of electron temperature in eV for Fe^{21+} $2s^2$ 2p $^2P^o_{1/2}$–$2s^2$ 3d $^2D_{3/2}$ transition, as a graphic output from AMDIS-EXC. Four data sets from 4 publications are plotted [22–25], where T means theoretical calculations; (**b**) Electron-impact single ionization cross sections as a function of collision energy in eV for Fe, taken from AMDIS-ION. Seven data sets from 7 publications are plotted [26–32], where T and E represent theoretical and experimental results. Red line: Lotz's empirical formula [33].

CHART, the database of charge exchange and ionization cross sections for heavy particle collisions has additional items—e.g., mass of incident and target particles in the database. Collision energies in laboratory frames are stored with the unit of eV/u, where u is the unified atomic mass unit. In many publications, as well as in outputs of CHART database, unit eV/amu is used conventionally, where amu means atomic mass unit and 1 amu = 1 u.

AMOL and CMOL, the databases of electron and heavy particle collisions with molecules, respectively, have similar items to AMDIS-REC in the database. For CMOL, mass of projectile and target particles are stored as similarly to CHART. Collision energies in laboratory frame are displayed.

There are two databases for properties of plasma–surface interaction. SPUTY is the database of sputtering yields of solid surface by ion bombardment. As similarly to CHART, mass of incident ion and solid element are stored in the database. BACKS has energy and particle back scattering coefficients as functions of colliding energies and scattering angles. For graphical output, either energy or angle can be selected for the x-axis, and some values of the other can be selected to be plotted.

When drawing a graph in AMDIS-ION, CHART, SPUTY, and BACKS, users can draw data calculated by empirical formulae to compare with other data. The formulae are given for ionization cross section [33] for AMDIS-ION, charge exchange cross sections with H, H_2, and He targets for CHART, sputtering yields for simple solid target for SPUTY [34] and number- or energy-backscattering coefficients for BACKS [35]. Figure 1b shows an example of a graph with Lotz's empirical formula for a singly ionization cross section of a Fe atom.

2.2. Satellite Database

In addition to the main database constructed with the retrieval system described above, we have several small databases which do not fit to the main databases. We call them satellite databases. They are compilations of various processes and most of them are results of research collaborations, published in NIFS-DATA reports or in refereed journals. The list of the satellite databases is found at the entrance page of the NIFS database, as shown in Table 3. Some of them have a retrieval system and others give a list of ascii data files.

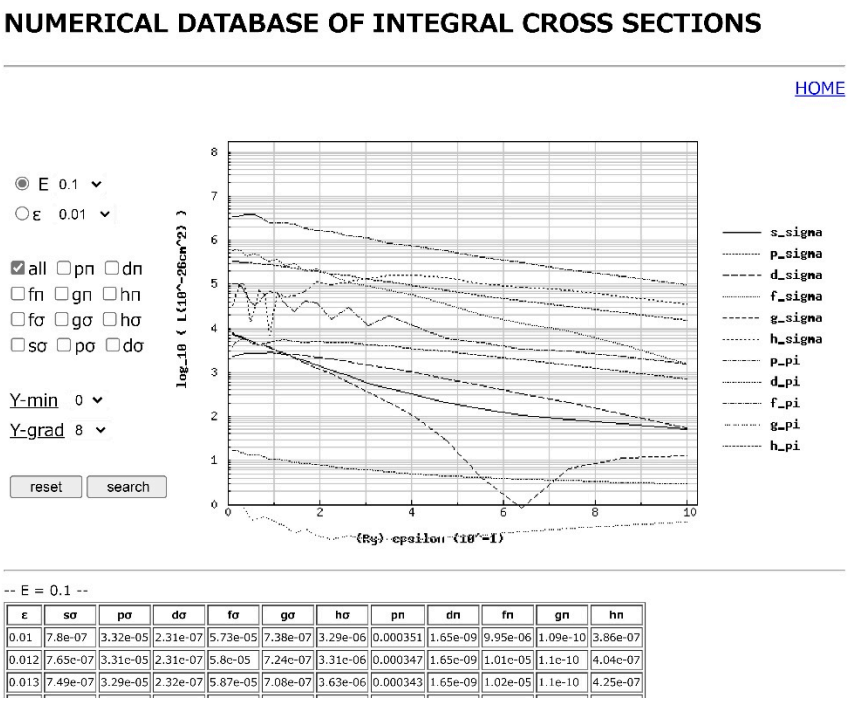
Table 3. List of satellite databases [1].

Name	Remarks
ALADDIN (Ionizing cross sections and excitation rate coefficients by electron-impact)	Calculate with evaluated formulae in ALADDIN format [12]
Data for autoionizing states	Collaboration with Y. J. Rhee
Differential cross sections for molecules by electron impact	Collaboration with Y. J. Rhee
Differential cross sections of ionization for atomic hydrogen by proton impact	Collaboration with L. Pichl [36,37]
Electron dissociative attachment to molecular hydrogen	Collaboration with J. Horachek [38]
Hayashi's bibliographic database for electron and proton collision cross sections with atoms and molecules	Compiled by M. Hayashi—e.g., in [39]
Photoabsorption database	Collaboration with N. Sakamoto et al. [40]
Recommended data set of electron collision cross sections of atoms and molecules	Compiled by the Institute of Electrical Engineers of Japan [41]
Sputtering yields, reflection coefficients and range values of solid surface	Calculated by W. Eckstein [42]

[1] URL = http://dbshino.nifs.ac.jp/.

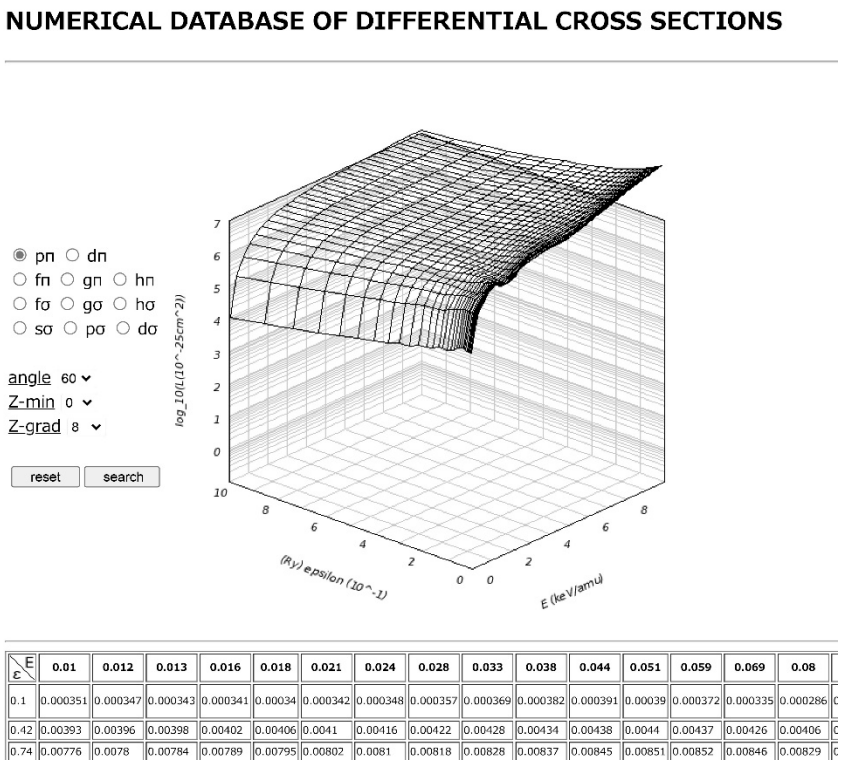
Our ALADDIN database has data in ALADDIN format, as in the IAEA-ALADDIN database, but is simpler and more restricted than the IAEA-ALADDIN database. Electron-impact ionization and excitation cross sections and rate coefficients are only available for some selected atoms.

Figure 2 shows examples of results shown as a 2D graph of integral cross sections and a 3D graph of differential cross sections for atomic hydrogen by proton impact, which are drawn interactively using data from the database. Numerical tables are also shown at the same time.



ε	sσ	pσ	dσ	fσ	gσ	hσ	pn	dn	fn	gn	hn
0.01	7.8e-07	3.32e-05	2.31e-07	5.73e-05	7.38e-07	3.29e-06	0.000351	1.65e-09	9.95e-06	1.09e-10	3.86e-07
0.012	7.65e-07	3.31e-05	2.31e-07	5.8e-05	7.24e-07	3.31e-06	0.000347	1.65e-09	1.01e-05	1.1e-10	4.04e-07
0.013	7.49e-07	3.29e-05	2.32e-07	5.87e-05	7.08e-07	3.63e-06	0.000343	1.65e-09	1.02e-05	1.1e-10	4.25e-07

(**a**)



ε \ E	0.01	0.012	0.013	0.016	0.018	0.021	0.024	0.028	0.033	0.038	0.044	0.051	0.059	0.069	0.08
0.1	0.000351	0.000347	0.000343	0.000341	0.00034	0.000342	0.000348	0.000357	0.000369	0.000382	0.000391	0.00039	0.000372	0.000335	0.000286
0.42	0.00393	0.00396	0.00398	0.00402	0.00406	0.0041	0.00416	0.00422	0.00428	0.00434	0.00438	0.0044	0.00437	0.00426	0.00406
0.74	0.00776	0.0078	0.00784	0.00789	0.00795	0.00802	0.0081	0.00818	0.00828	0.00837	0.00845	0.00851	0.00852	0.00846	0.00829

(**b**)

Figure 2. T (**a**) 2D graph of integral cross sections for ionization of atomic hydrogen by proton impact; (**b**) 3D graph of differential cross sections of atomic hydrogen by proton impact [36,37].

3. Data Evaluation Using NIFS Database

As described above, NIFS Atomic and Molecular Numerical Databases have several data sets taken from literature for the same collision processes and we can compare them to evaluate. Critical data evaluation on various collision processes have been done and published in IPPJ-AM and NIFS-DATA reports since the 1970s. Data are compiled first and stored in the database. Next, theoretical or experimental methods and accuracy of data are examined, and then, recommended data are selected or determined among available data. Recommended data are often fitted to a formula and fitting coefficients are given. Fitting formulae are determined according to known physical behavior or with polynomial functions. Such evaluations have been done using data available at the time of evaluation. When new data are published, recommended data might be changed. Such an example was shown for electron-impact excitation cross sections in [43].

The traditional methods on data evaluation need to compare all existing data sets one by one and it becomes difficult for larger data sets, such as excitation rate coefficients for highly charged ions. As one example, calculated data on excitation rate coefficients for all Fe atom and ions, published by 2008, were compiled and the theoretical methods were examined and compared [44]. Most of them were calculated with an R-matrix method, but there were some differences between them. One data set was selected as recommended data for each Fe ion. Data evaluation for each excitation process was not done in this case.

As a next step, the validation of data is required using experiments. For example, measured spectra should be explained by calculated spectra using an atomic data set. Extreme ultraviolet spectra of Fe ions have been measured in laboratory plasmas using the compact electron beam ion trap (CoBIT) [45] and the Large Helical Device (LHD) [46] and compared with theoretical calculations using collisional-radiative models. We examined Fe^{q+} ions with q = 9–16, 20, and 21, using their line intensities [47–62]. We continue to compile data for Fe ions, and the data evaluation using laboratory experiments is ongoing.

Our database is useful for other data compilers. CHIANTI is an atomic database and calculation package on spectroscopy for solar physics [63]. They must evaluate atomic data to be included in the database and they use our NIFS database to check available atomic data [64].

Recently, we have become interested in heavy elements, especially tungsten, since tungsten is used for divertor plates for magnetically confined fusion devices, such as JET-ILW, ASDEX Upgrade, EAST, and ITER, and the atomic data are needed to examine tungsten behavior in plasmas using spectroscopy, to avoid accumulation in the core plasma. Tungsten is partially ionized in plasmas and causes large radiation power loss in the core plasma. Many theoretical and experimental studies on tungsten atomic data, spectroscopy, and collisional-radiative models have been carried out in recent years. Many tungsten atomic data are still lacking and collisional-radiative models for mid- and low-charged tungsten ions are still immature. However, the data compilation and critical evaluation, as in [65], for dielectronic recombination rate coefficients, should be carried out in future.

4. Concluding Remarks

Numerical atomic databases are useful for various users and the progress on computers, database systems, and computer network can provide more convenient tools for uses to find necessary data for their research. The NIFS atomic and molecular databases have numerical data on collision processes, which are important for various form of plasma research, not only for fusion but also for astrophysics and plasma applications. Electron-impact ionization and excitation cross sections and rate coefficients for atoms, recombination rate coefficients for atomic ions, charge exchange and ionization cross sections by ion–atom collision, cross sections and rate coefficients for electron-molecule and atom-molecule collisions, and sputtering yields and backscattering coefficients for atom-solid surface collisions are stored with information on the bibliography of data sources, methods of data production, etc. The database system is accessible via internet and is retrievable. Data are displayed in a table and a graph. We also have satellite databases as results of various collaboration works with the

help of collaborators. The database is useful for data evaluation by comparing data, and laboratory experiments are important for data validation. We continuously work on iron ions for data evaluation and validation and will continue to compile data on heavy elements, especially on tungsten for future data evaluation.

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