


## Article

# Improvement of the NIFS Atom and Molecular Database

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**Abstract:** The NIFS (National Institute for Fusion Science) Atom and Molecular Database, which has been available online since 1997, is a numerical atomic and molecular database of collision processes that is important for fusion research. This database provides the following: (1) the cross-sections and rate coefficients for ionization, excitation, and recombination caused by electron impact; (2) the charge transfer caused by heavy particle collision and collision processes of molecules; and (3) the sputtering yields of solids and backscattering coefficients from solids. It also offers a bibliographic database. We recently reconstructed the database system. The main purpose of the reconstruction was to migrate the database into an open-source architecture to make the system more flexible and extensible. The previous system used proprietary software and was difficult to customize. The new system consists of open-source software, including PostgreSQL database and Ruby on Rails. New features were also added to the system. The most important improvement is the interface with the Virtual Atomic and Molecular Data Center (VAMDC) portal. Using this interface, researchers can search for data in the NIFS database as well as in various other online databases simultaneously.

**Keywords:** databases; atoms; molecules; VAMDC; web

## 1. Introduction

Since 1975, atomic data have been compiled and published by a working group of atomic and plasma physics researchers from Japanese universities [1,2]. In the 1980s, these data were housed in an atomic database whose data retrieval and display systems were accessible via a mainframe computer system in the Institute of Plasma Physics at Nagoya University [3]. In 1997, the database system was migrated to a relational database, Oracle. The system was also uploaded online and named the NIFS Atom and Molecular Database (NIFS DB), enabling online data retrieval and display [4,5]. However, because of the rapid progress of computer and internet technology, several of the NIFS DB's software components had become obsolete and could not be updated further. Moreover, there was a potential security risk. Therefore, we decided to upgrade the system.

Another motivation for the upgrade was to allow the NIFS DB to be used by a wider range of scientists. The NIFS DB was originally constructed to gather information on electron impact ionization and excitation cross-sections and was later expanded to cover a wide variety of collision processes in plasma and plasma wall interactions. Table 1 shows the available contents of the data as of June 2019. Thus, the NIFS DB was produced mainly for fusion plasma research, but it is also useful in other areas of research, such as in astrophysics.

The Virtual Atomic and Molecular Data Center (VAMDC) Consortium runs an interoperable e-infrastructure to integrate a broad range of online atomic and modular databases. Through the VAMDC portal, a user can cross-search all the heterogeneous databases in the system [6]. By joining

this integrated system, the NIFS DB will be widely accessible to other research groups beyond the plasma fusion research community. In order to join the VAMDC system, databases must conform to VAMDC standards, and the NIFS DB needs to be modified accordingly.

**Table 1.** Contents of the NIFS Atom and Molecular Database (NIFS DB) as of June 2019. The NIFS DB stores numerical and bibliographic data.

Name	Description	Records
	Cross-sections for ionization, excitation, recombination, and dissociation of atoms, ions, and molecules by electron impact	
<i>AMIDIS</i>	<i>ION</i> Ionization cross sections and rate coefficients caused by electron impact	2862
	<i>EXC</i> Excitation cross sections and rate coefficients caused by electron impact	716,452
	<i>REC</i> Recombination cross-sections and rate coefficients caused by electron impact	27,532
	<i>DIO</i> Dissociation cross sections of molecules	202
<i>CHART</i>	Cross-sections for charge transfer and ionization caused by heavy particle collision	7618
<i>AMOL</i>	Cross sections and rate coefficients for electron–molecule collision processes	3180
<i>CMOL</i>	Cross sections and rate coefficients for heavy particle–molecule collision processes	2139
<i>SPUTY</i>	Sputtering yields for solids	2349
<i>BACKS</i>	Energy and particle backscattering coefficients of light ions injected into surfaces	485
<i>ORNL</i>	Bibliography on atomic collision collected at ORNL	78,097

## 2. New System

### 2.1. Overview

Figure 1 shows an overview of the new system. The web interface was built using Ruby on Rails [7], which is a web application framework written in Ruby. The database management system was replaced by PostgreSQL, an open-source relational database system. Currently, ION data are copied into another database, which is dedicated to VAMDC node software [8], and are searchable from the VAMDC portal. Table 2 shows the main software components used in the previous and current systems.

The main reason for this update was that the OS and other software components had become outdated, and the security updates for the software were no longer being accepted. Therefore, we decided to upgrade the system to be compatible with the latest OS and other software. We also decided to use open-source software rather than proprietary software, because we could support it ourselves more easily. We chose Ruby on Rails as the web application framework, which can be used to develop a smoother and more interactive user interface. Now, a user can compose complex and multiple condition queries to search the data via a web browser. The user can also search from the periodic table interface for simplicity (Figure 2). The query results for the numeric data can be obtained in the form of tabular data, coefficients of the fitting curve, or graphic files (Figure 3).

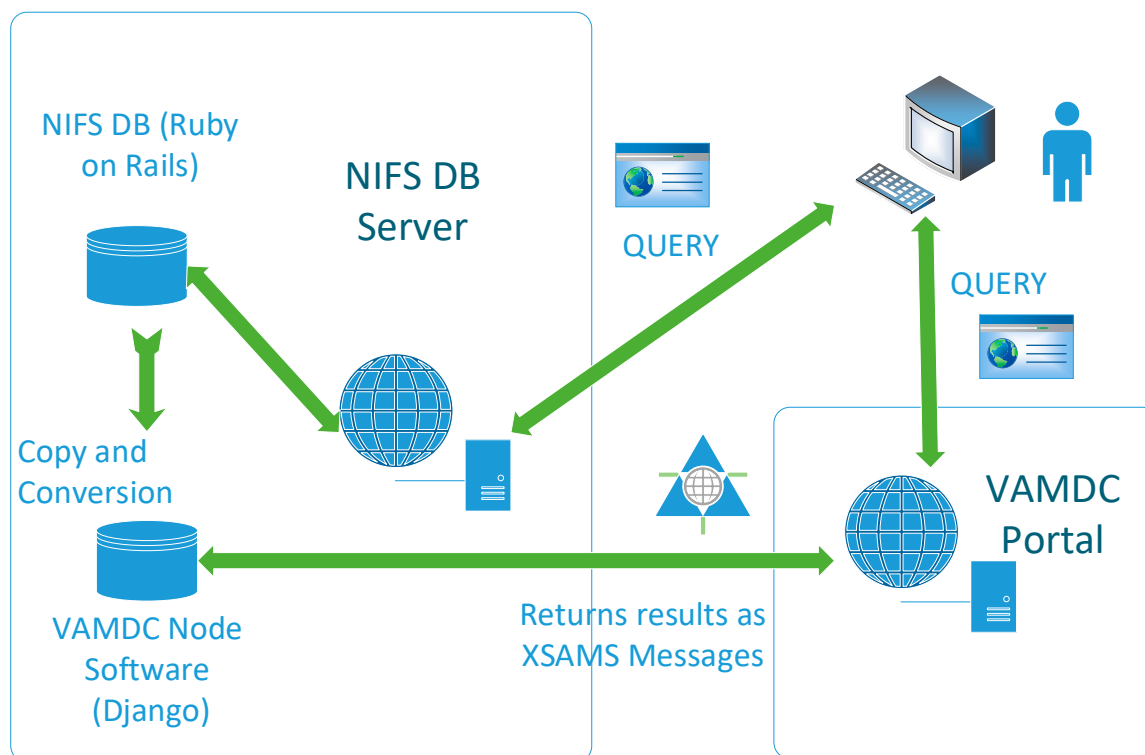
### 2.2. VAMDC Interface

Through the VAMDC portal, a user can search simultaneously across a wide range of integrated databases from all over the world via a web browser. These database systems all comply with VAMDC standards, allowing the user to easily access their data. The standards define several parameters, including data models of atoms and molecules, protocols for queries and data retrieval, and so on. The portal is run via a node system. The VAMDC portal sends out queries and retrieves the results from the

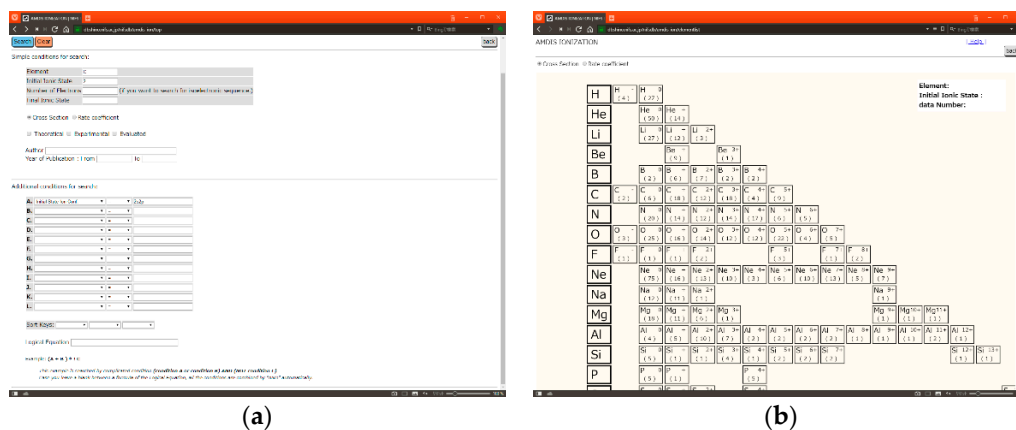
nodes by exchanging XML messages. To integrate the NIFS DB into the VAMDC node system (thereby making the NIFS DB a node), there were two possible courses of action, plan A and B (Figure 4). Plan A was to build a VAMDC interface on the present system. The web interface of the NIFS DB is implemented by Ruby on Rails, and it is possible to interpret XML using the Rails application to exchange messages between the NIFS DB and the portal. The advantage of this approach is that it is easy to maintain the consistency of the database. When the original data are updated, the changes in the NIFS DB are reflected in the VAMDC portal simultaneously. However, the necessary development required to implement Plan A would be complicated.

Plan B was to build another system dedicated only to the VAMDC portal using VAMDC node software—an application of Django, which is a python-based web application framework [9]. Adding little to no code, the system could easily become a node without modifying the original system. However, the database structure that the node software requires is different from that of the NIFS DB, and it would be necessary to synchronize data between the two databases.

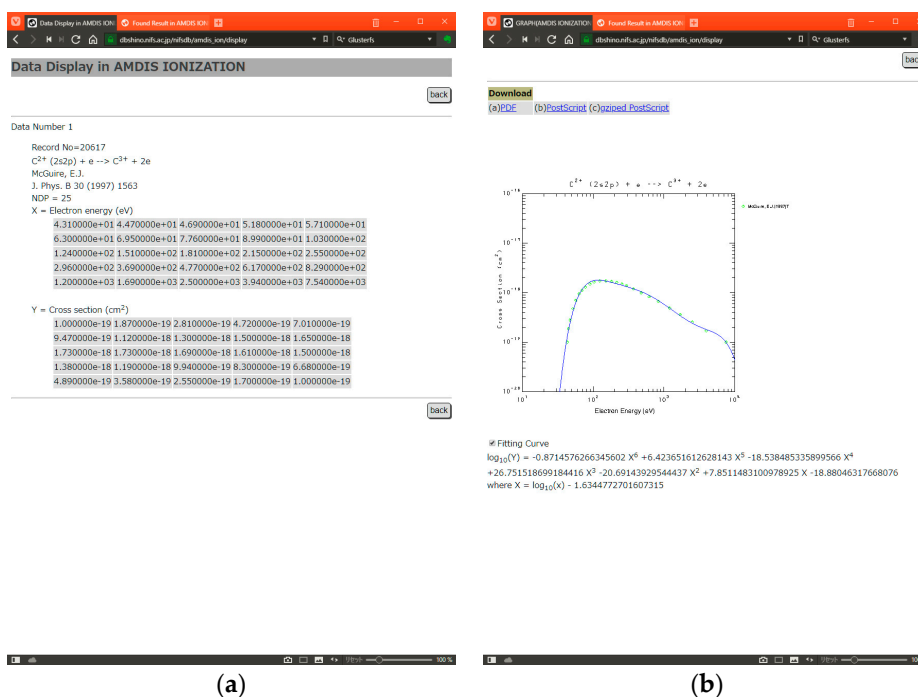
After weighing these plans, we adopted Plan B, because the implementation of Plan A would have required huge modifications. Because updates of the NIFS DB are not frequent, real-time synchronization between the NIFS DB and the VAMDC database is not necessary, and it can be executed occasionally or manually. In the first step, only the ION table was copied into the VAMDC database, and currently, these are the only NIFS DB data available to be searched through the VAMDC portal.



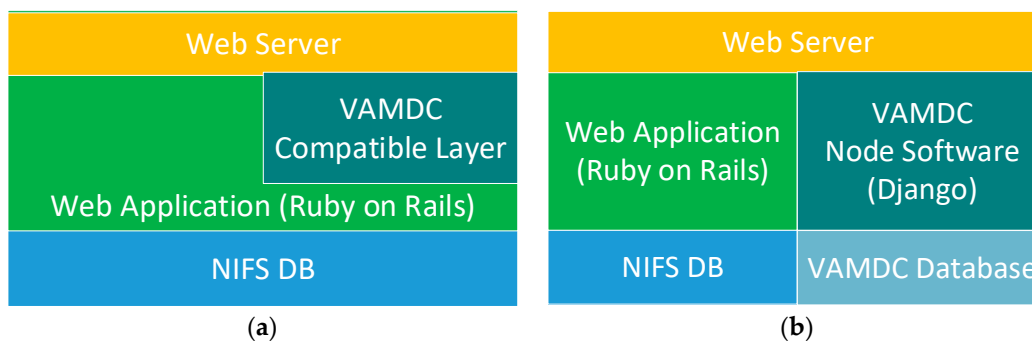
**Figure 1.** An overview of the new system. The contents of the NIFS DB are provided by the Ruby on Rails application. In order to communicate with the Virtual Atomic and Molecular Data Center (VAMDC) portal, VAMDC node software runs in the same server.



**Figure 2.** The graphical user interface (GUI) of the NIFS DB. (a) The user can search data by constructing complex queries in the web browser. (b) For simplicity, the user can obtain the expected data of the atoms from the periodic table interface.



**Figure 3.** The results of the search can be obtained in the form of (a) numerical data, (b) images (PostScript, PDF, PNG), or the coefficients of fitting curve.



**Figure 4.** The two possible integration plans. (a) Plan A was to implement the VAMDC standards in the NIFS DB by building node compatibility into the existing system. (b) Plan B was to build another NIFS DB system dedicated to the VAMDC portal, which was compatible with the VAMDC node software, Django.

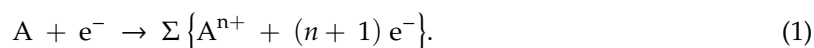
**Table 2.** The major software components used for the old and current systems.

	Old	Current
OS	RedHat Enterprise 5	CentOS 7.5
RDB	Oracle 8.5	PostgreSQL 9.5
Web Application	CGI	Ruby on Rails, JavaScript, Django

### 3. Discussion

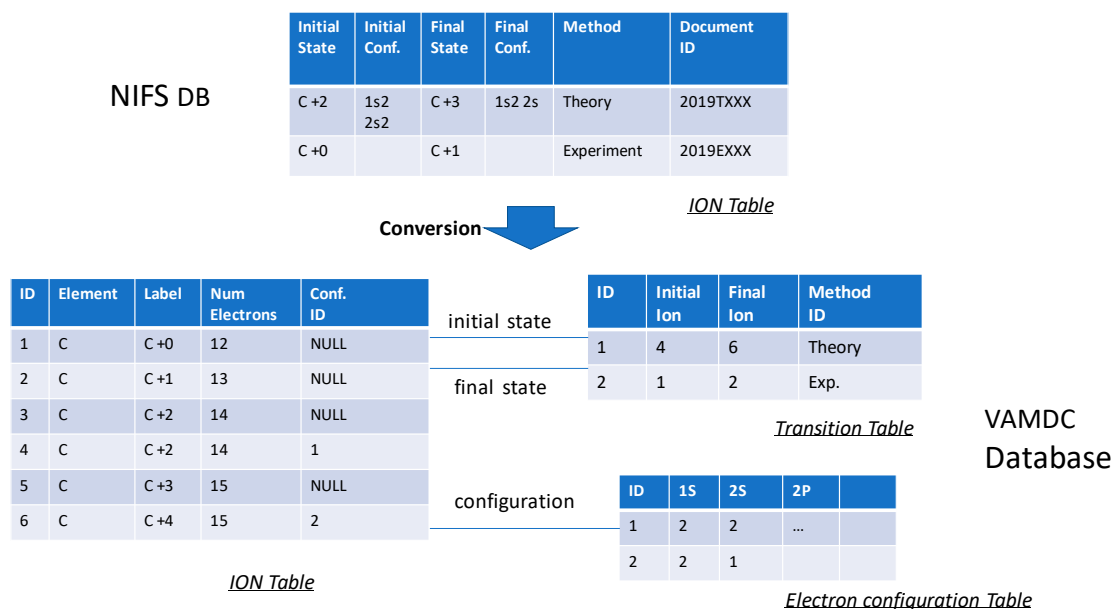
Because the initial design of the NIFS DB and the structure of the VAMDC database differed, the NIFS DB data could not be integrated into the VAMDC database in a straightforward way. For example, the original NIFS DB system compiles data of experiments and theories from published materials, and the database stores the tag of the original resource, to which the user can easily refer. In contrast, the VAMDC database treats atoms, molecules, transitions, and so on as objects. Thus, we decided to develop another NIFS DB system using the VAMDC node software. The conversion from the NIFS DB to the VAMDC database was executed by splitting the ION table into subparts (Figure 5).

In order to record as much published information as possible, the treatment of the data in the NIFS DB is neither consistent nor complete. Certain ION data have attributes of electron configuration, but some data do not. There are also some data that treat multiple reactions as a single reaction, such as the following:



In such cases, only one set of numerical data for a single reaction is provided.

Currently, these data have been ignored and have not been copied into the VAMDC database. In order to access these data from the VAMDC portal, the modification of the VAMDC standards is required.



**Figure 5.** Conversion of the ION table from the NIFS DB to the VAMDC database. The original ION table in the NIFS DB is divided into three tables in the VAMDC database.

### 4. Conclusions

NIFS maintains the NIFS Atom and Molecular Database. Initially, the database was constructed to facilitate fusion plasma research, but it has also become useful in other areas of research, such as astrophysics. The data are now available online, and as a result of our recent updates, the data are

now beginning to be available via the VAMDC portal. Currently, only the ION table has been made compatible with the VAMDC database, but work on making the other tables compatible is in progress.

**Author Contributions:** M.E. designed the new database system and managed the project. I.M. was the supervisor of the project. M.Y. and S.I. were the programmer. D.K. and M.K. helped us to build the database.

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**Conflicts of Interest:** The authors declare no conflict of interest.

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