

The Database «SPECTR» on Spectral Properties of Atoms And Ions

I. Yu. Skobelev, A. Ya. Faenov, and A. I. Magunov
*Multicharged Ion Spectra Data Center (MISDC) of VNIIFTRI,
Mendeleevo, 141570 Russia*

1 Introduction

The database «SPECTR» has been created in the Multicharged Ion Spectra Data Center (MISDC) of VNIIFTRI as a tool to allow the fast determination of information on spectra of atoms and ions. It is a database containing data on spectroscopic constants of isolated atoms and ions (energy levels, wavelength of spectral lines, radiative probabilities, ionization potentials) and, some collision data (dielectronic recombination rates, electron impact excitation cross sections and rates, electron impact ionization cross sections and rates).

Currently, the database «SPECTR» contains more than 450000 numerical records. The largest part of the data concern the UV and X-ray spectral regions, $l < 100$. Besides published data (experimental and theoretical), the experimental data produced at MISDC for the X-ray spectral band $l < 26$ are used in database «SPECTR».

2 MISDC of VNIIFTRI and Database «SPECTR»

The multicharged Ions Spectra Data Center of VNIIFTRI is a research group, working in the field of X-ray spectroscopy of multicharged ions and its application for the diagnostics of high-temperature plasmas.

Main Fields of Investigations:

- A. creation of Bragg and Bragg-Fresnel optical elements for high-resolution X-ray spectroscopy (see, for example, [1-9])
- B. high-precision X-ray spectroscopy of multicharged ions (emission spectra observations, spectral line identification, accurate wavelength measurements) (see, for example, [6, 10-22])
- C. creation of X-ray spectroscopy diagnostic methods and their application to measurements of different plasma parameters (laser-produced plasmas, Z- and X- pinches, plasma focus) (see, for example, [23-28])
- D. creation of a database on spectra of atoms and ions (database «SPECTR»)

Database «SPECTR»

The database SPECTR (DB «SPECTR»), on one hand, contains a great number of data on characteristics of atoms and ions, and, on the other hand, represents also the software to quickly find the information needed, to browse on the screen and to make a hard copy.

The information stored in DB SPECTR may be divided into two parts. The first part (and now the larger one) is the data on properties of isolated atoms and ions, that is, the data on energy

level structure, wavelengths of radiative transitions and its probabilities. The second part contains the data on characteristics of collision processes. The main difference between these two parts is the following: The first part deals with a set of constants, while the second one deals with a set of functions. That is, for any radiative transition its wavelength, radiative probability, energies of upper and lower levels are numerical quantities, but its collisional characteristics are functions of the relative velocity of the colliding particles. Therefore, the software used to operate on these two different types of data is also somewhat different.

DB “SPECTR” Software

The database “SPECTR” software is based on FoxPro Database Management System. The information is stored in well-known DBF-format and can be transferred easily into another formats.

DB “SPECTR” Data

The quantitative characteristics (4 May 1997):

Data on spectral lines	397 885 records
Data on energy levels	75 100 records
Data on ionization potentials	2 292 records
Data on excitation cross sections and rates	4 932 records
Data on ionization cross sections and rates	276 records
Data on references	504 records
The total number of records	481 134

Qualitative Characteristics

DB “SPECTR” is a database on the characteristics of isolated atoms and ions, i.e., on spectral lines (wavelengths and radiative probabilities) and energy levels. The small number of collisional data were included mainly to test the software developed. Since the MISDC research team works in the field of X-ray spectroscopy, the main part of data (about 75%) refers to the multicharged ions.

Data sources

- ✓ Published experimental data. For the X-ray region, the database contains practically all published experimental data, for the UV and visible regions only some data.
- ✓ Our own experimental data for multicharged ions. The MISDC research group has produced experimental data on the X-ray spectra of multicharged ions for more than 20 years. For example, during last 5 years we have produced new accurate data on satellite lines caused by radiative transitions in He-, Li-, Be-, B-, C-, N-, O-, F-, Na-, Mg- like ions, and on high-n transitions in He- and Ne-like ions. Producing this kind of information is the main field of scientific interest of the MISDC group. For this purpose we create new types of X-ray high-resolution spectrographs (with spherically bent crystals, for example) and develop new methods which improve the accuracy of wavelength measurements.
- ✓ Theoretical data, both published (not all, of course) and calculated especially for DB “SPECTR” in some Russian institutes (see, for example, [29]).

DB "SPECTR" Performance

The search operations are executed fast, and some examples are presented in this table:

Database SPECTR

(4 May 1997)

Total number of records 481 134

Pentium-133, 16 MB RAM

	QUERY	SEARCH TIME	THE NUMBER OF RECORDS SELECTED
1	Lines of copper ions in spectral region 10.1 – 10.11 Å	2 s	9
2	Lines of silver ions in spectral region 10 - 15 Å	5 s	94
3	Lines of H-like and He-like silicon	4 s	3192
4	3d-2p transitions in Ne-like and Na-like silver	2 s	313
5	1s2p 1P_1 - 1s 2 1S_0 transition in He-like uranium	2 s	2
6	2s2p 6 3p - 2s 2 2p 6 transitions in Ne-like ions	1 s	411
7	Lines of OI atom	1 s	441
8	Lines of O-like and N-like iron	3 s	998

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