

# Development of an Atomic Spectroscopy Reference Implemented on a PC Platform under Windows 95

K. Visser and G.E. Hattingh  
*Physics Department*  
*University of Stellenbosch*  
*STELLENBOSCH*  
*Republic of South Africa*  
*e-mail: kv@maties.sun.ac.za*

## 1 Introduction

Atomic Spectroscopic reference data comprising the characteristic energy levels and their associated eigenstate descriptions, wavelengths, and transition probabilities are available mostly in printed format. The major computerized databases implemented on the Personal Computer (PC) platform for Atomic Spectroscopy consist of the NIST Standard Reference Database 38 “*Spectroscopic Properties of Atoms and Atomic Ions*” and the NIST Standard Reference Database 61 “*Database for Atomic Spectroscopy*”. On the World Wide Web the NIST Atomic Spectroscopy Database, version 1.1, is currently available at [http://aeldata.nist.gov/nist\\_atomic\\_spectra.html](http://aeldata.nist.gov/nist_atomic_spectra.html)

Our objectives are to develop software providing

- a comprehensive database integrating the available critically evaluated Atomic Spectroscopic information,
- a search engine serving as input filter to selectively retrieve user-specified information from the database,
- user-specified custom-designed formatting of the output data both as tabular alphanumeric text and in graphical format,
- appropriate calculations using the primary data as input to derive secondary parameters.

For the initial phase of the project we decided to develop the software for the IBM and compatible PC platform under the Windows 95 operating system and used Borland’s Delphi 3 compiler to generate a 32 bit application program. The program is developed in a modular way with each module representing a particular application, which can be activated by clicking on its named tab. Presently available and operational modules are:

- Energy level tables;
- Wavelength and Multiplet tables;
- Wavelengths calculated from the energy level data and applying user-selectable subsets of the selection rules for the various radiative transition types.

Upon initiation the program searches for all associated data files (one per element) present. For each file found it uses an efficient blockread procedure to transfer the file's available data records as a single block at high speed into memory. These data records are kept memory resident to avoid repetitive reading and swapping of the database information in and out of memory during subsequent searches. Adding more elements to the program is a simple matter of making their correctly formatted data files available in the assigned directory. An array of indices referring to the first and last record for each elemental ionization stage is kept for quick searches in the appropriate subset of the memory resident list of data records.

The database files for the program use an internal encoding format to decrease their size compared to the original ASCII text files, thereby increasing the efficiency of the program in terms of speed and smaller data file size. Each variable is enumerated and mapped onto the smallest integer type which covers its range. For instance, instead of storing the name or chemical symbol of the element and its ionization stage as ASCII fields in the data records, the hundred plus elements and possible ionization stages are mapped onto a subset of the integers ranging from 0 to 127 and declared as variables of type Byte. By packing variables of lesser range bit-wise together, to optimally fit into the range of the smallest suitable integer type, memory and mass storage space are conserved. Strings, such as are used for the description of the electron configuration and parent term, the term value, the multiplet number, line codes and references to the original source of the data, are variables which occur repetitively in the database records. They are also enumerated and the 2 Byte variable, serving as referencing index into the stringlist, is stored in the appropriate record fields of the database file instead of repetitively storing the longer string of text itself. This enumeration and internal formatting of the database files led to a 7.2 times reduction of the comparative ASCII text file size for energy levels and a 5.1 times reduction for wavelength files. The ASCII text files containing the stringlists for configurations, etc., have a size of 80 kb.

The displayed tables can be dynamically reformatted according to the user's choice with respect to which columns of data are currently visible and which are hidden from view so as to remove information which the user might consider unnecessary for his current needs. The displayed data columns/rows in the scrollable tabular list can also be dragged and dropped to change their vertical and horizontal ordering. The widths of the displayed columns are also dynamically resizable.

## 2 Energy Levels Module and Wavelength & Multiplet Module

The database currently includes energy level data for 417 atomic/ionic species from 20 elements (O, Na, Mg, Al, Si, P, S, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Ni, Co, Cu, Kr & Mo) consisting of 33,004 energy level records. It also contains wavelength data for 47 atomic/ionic species from 4 elements (O, Mg, Al, Sc) with 11,320 wavelength records. Expansion for the energy levels of another 123 ionic species from 17 more elements and 17,785 energy level records are underway, as well as wavelength data for another 186 ionic species from 10 more elements and 23,648 wavelength records.

Single or multiple elements can be selected/deselected via mouse clicks on the element name buttons arranged to resemble the periodic table, as shown in Fig. 1, with the selected state being indicated by a change of color. Unavailable elements are grayed out.

For ease of element selection an element list is also provided which can either contain the elements arranged alphabetically by name or chemical symbol and atomic number. A command button to toggle the selected state for all available elements is also provided.

Single or multiple ionization stages can be selected/deselected by clicking on their individual buttons. Different ionization stages for each individual element or ionization stages common to all elements can be selected for all actively selected elements. A similar *"Select/deselect All"* command

button is also provided for the ion selection. Additional search criteria that can be specified are the energy/wavelength range; the electron configuration; the term values; parity; total angular momentum quantum number  $J$ ; orbital angular momentum symbol  $L$  and spin multiplicity  $m_s$ .

Figure 1: Selection of elements from the periodic table.

### 3 Calculated Wavelength Module

In this module theoretically expected wavelengths can be calculated from the energy levels by applying the Ritz combination principle

$$\lambda_{vac} = \frac{hc}{|E_i - E_f|}$$

to pairs of levels  $E_i$  and  $E_f$  that might be radiatively connected. Both the energy levels of a single element and ionization stage can be selected at a time. The user can specify the following criteria that pairs of levels must meet for selection in the derived wavelength calculation:

- a transition mode from:
  - absorption from a single lower state, or
  - emission from a single excited state, or
  - transitions involving all states;

(For absorption and emission the initial state can be picked from the applicable energy level list of the selected atom/ion.)

- a wavelength interval in terms of its upper and lower wavelength limits;
- LS-coupling can be activated or ignored to prevent or allow intercombination lines;
- electric dipole (E1), magnetic dipole (M1) and electric quadrupole (E2) radiation types or combinations thereof can be checked to activate their respective selection rules;
- combinations of changes in the total angular momentum  $\delta J$  can be checked.

For the interval ( $2 \mu\text{m} > \lambda > 2000 \text{ \AA}$ ) wavelengths in air are calculated from

$$\lambda_{air} = \frac{\lambda_{vac}}{n(\lambda)}$$

with the refractive index of air calculated from the Edlen formula[1]

$$n(\lambda) = 1 + 8.34213 \times 10^{-5} + \frac{2.406030 \times 10^6}{(1.30 \times 10^{10} - \sigma^2)} + \frac{1.5997 \times 10^4}{(3.89 \times 10^9 - \sigma^2)}$$

with the wavenumber  $\sigma$  in  $\text{cm}^{-1}$ . The displayed table of calculated wavelengths can be sorted according to wavelength, or energy of the upper or lower state.

The module can be used for such applications as theoretical prediction of suitable transitions for a multi-step laser excitation scheme, identification of the states involved in experimentally observed wavelengths and selection of closely grouped wavelengths from largely different excitation states suitable for spectroscopic temperature determination.

## 4 Future Development

We plan to develop the program further to include modules for

- transition probability tables,
- Grotrian diagram creation from the energy levels and selection rules,
- calculation of simulated spectra,
- hyperfine structure,
- line profiles and convolution,
- Zeeman splitting.

Other future developments planned, include: expansion of the number of available elements, allowance for editing of the data fields and insertion of data records by a user which are to be saved as overlay files so as not to corrupt the original data files, saving and retrieving of the last used options and configurations. We also envision making a demonstration version of the program available on the World Wide Web.

## References

- [1] B. Edlén, *Metrologia* **2**, 71 (1966)

H	Selected Elements																He					
Li	Be	Unselected Elements																				
Na	Mg	Unavailable Elements																				
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	B	C	N	O	F	Ne					
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	Al	Si	P	S	Cl	Ar					
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Ga	Ge	As	Se	Br	Kr					
Fr	Ra	Ac	Rf	Ha	Mercury (80)												In	Sn	Sb	Te	I	Xe
		Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Tl	Pb	Bi	Po	At	Rn	
		Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr							
		Ok		Select From List				Deselect All				Cancel										