LTE_LINES — Atomic data for LTE calculations

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Abstract

An 'end-user' oriented database containing atomic data suitable for the LTE analysis of early-type stellar atmospheres has been extended and updated using modern atomic data. Data for each line comprise wavelength, oscillator strength, radiative and electron damping widths, lower-level excitation potential, ion and multiplet identification and source citations. Whilst much remains to be done, this paper reports on work carried out, and invites reaction from potential users and other database compilers.

1 Introduction

Analyses of astronomical spectra depend critically on reliable sources of atomic and molecular data. Amongst the CCP's, the large scale computation and collation of these data remains principally the domain of Collaborative Computational Projects Nos. 2 (Continuum States of Atoms and Molecules) and 6 (Heavy Particle Dynamics). However, CCP7 is concerned with making these data accessible for astronomical applications and has, over the years and thanks to the generosity of their authors, acquired a number of databases.

One such database attempts to collate and maintain 'recommended' data for LTE analyses of early-type stars. It has been extended with, in particular, the end user in view and may find practical uses in a variety of applications such as (eg) the spectrum-synthesis in non-LTE calculations.

2 Available linelists

The CCP7 library (Jeffery 1990) currently contains the Kurucz & Peytremann (1975) list of semi-empirical gf-values, the Kurucz (1990) list of semi-empirical gf-values for iron-group elements, and the Bell (1973) list of gf-vales for atomic and molecular transitions.

A substantial body of new atomic data, gf-values in particular, has been calculated as a result of recent endeavours such as the Opacity Project (Seaton 1987 and subsequent publications). Owing to the number of methods currently used in atomic calculations, the cited data for a given transition may vary substantially according to author. Serious attempts to evaluate the data objectively have been undertaken in a few cases (eg CIII, NIV, OV, Allard et al. 1991). These are invaluable to the spectroscopist whose results depend on reliable data but who cannot afford to frequently reassess the extensive literature.

Dufton and coworkers at Queen's University of Belfast use a linelist containing a restricted number of data for LTE calculations of transitions used frequently in the analysis of main-sequence B-star atmospheres. It forms a part of their LTE line-analysis package (SPECTRUM). Significant features of this linelist are its format, which is sufficiently simple to allow easy identification of all data (including sources), and its small size, which allows for convenient maintenance. The data included were wavelengths, oscillator strengths, electron and radiative damping constants and excitation potentials. Most data pertain to transitions of light ions in the blue-visible.

This linelist was identified as a valuable starting point for establishing a resource of modern atomic data appropriate for LTE analyses of stellar atmospheres, and possibly with more extended applications.

3 LTE_LINES

A project to make spectroscopic abundance analyses of a number of hydrogen-deficient B-type supergiants (eg Jeffery & Heber 1991) demonstrated a number of areas for improvement, particularly with respect to transition identification, source identification and the number of transitions treated.

Therefore a substantial revision to the Belfast linelist was undertaken. Firstly line identification has been improved by the addition of a (Moore) multiplet identification. The number of transitions treated has been increased to include weaker lines (frequently measurable in supergiants and non-rotating B stars) and more ions. The citation of sources has been generalized. A substantial number of data have been updated from Opacity Project data (Yan et al. 1987), recent Munich publications (Becker & Butler 1988, 1989, 1990, Kilian et al. 1991) and from the critical compilation of Allard et al. (1991).

Data for the individual ions are stored separately. For the original application (SPECTRUM), the separate ions are simply combined as required to form a linelist suitable for the spectrum being analysed. Normally, the expanded citation list is appended to the concatenated linelist to ensure the integrity of source identification.

The database is held on-line in the CCP7 data/program library (Jeffery 1990) on the STARLINK microVAX system at St Andrews. Files may be found in the VMS directory:

```
(STARLINK/SPAN)     SASTAR::CCP7DISK:[CCP7.LTE_LINES]
(Internet/Janet)    UK.AC.ST-AND.STAR::CCP7DISK:[CCP7.LTE_LINES]
```

The ion data are stored in files with a simple naming convention such that lines due to CII (ie C^+) are in `C2.DAT`, CIII in `C3.DAT`, SiIV in `SI4.DAT`, etc. By way of example, the appendices show data for some low excitation lines in the spectrum of CII (file `C2.DAT`). An explanation of the columns and an abstract from the file which amplifies the source citations are also shown. With varying degrees of completeness and mainly in the blue visible, data have been compiled for several ions listed in the appendix.

4 Data quality and completeness

It is intended that the database should contain 'recommended' data for LTE analyses of stellar atmospheres. This does not necessarily mean that they are the 'best' data, or are based on the most accurate atomic calculations. It does mean that where more than one value for a datum is available, an assessment of data quality should have occurred. At present, the criteria for selection is as follows:

1. Objectively evaluated data (eg Allard et al. 1991)
2. Opacity Project oscillator strengths (where available)
3. Modern theoretical oscillator strengths
4. Experimental lifetimes
5. Other data (eg semi-empirical values)

Oscillator strengths are given for about 1080 lines, mostly in the blue-visible ($\lambda 4000 - 5000 \mathring{A}$). Calculated damping widths are available for $\sim 20\%$.

One objective is to contain the size of the database for maintainability and not to duplicate the efforts of data producers. Therefore completeness over a large wavelength range would be counter-productive, since (eg) for B stars, many lines in the red show large departures from LTE. In general, data should only be incorporated if they are useful for the analysis of astronomical spectra. Semi-empirical oscillator strengths are only useful as a last resort for estimating abundances.

5 Future

At present, a number of additional developments are being considered. Utilities for restricting and sorting the lines in wavelength or by ion and multiplet will become available. One simple format change would allow greater precision and higher data density, whilst it has been suggested that ion damping widths should be tabulated separately. Further identification of the atomic transitions (ie electron configurations) would be helpful. A high priority, from the author's point of view, is greater completeness for ultraviolet transitions and for damping widths in the blue-visible.

At present, the linelist format is compatible with the Belfast LTE line formation code SPECTRUM. In order to maintain this compatibility, format changes will have to be reviewed carefully. However it may be desirable to work towards a format which is common across many codes and institutions in order, ultimately, to reduce the effort of maintaining this (or other) databases.

Comments from potential users or contributors would be welcomed by the author. Since it is likely that this effort is being duplicated in many institutions, interaction with other data compilers would be valuable.

Acknowledgments

I am grateful to Philip Dufton for being so understanding when I first rearranged his linelists, and to Uli Heber, Keith Butler and Mike Seaton, who have transmitted many of the data currently stored.

References

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Becker S.R. & Butler K. 1988. A&A 201, 232
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Becker S.R. & Butler K. 1990. A&A 235, 326
Bell R.A. 1973. MNRAS 164, 197
Jeffery C.S. 1990. CCP7 Newsletter No. 14, 43
Jeffery C.S. & Heber U. 1991. A&A (submitted)
Kilian J., Montenbruck O., & Nissen P.E. 1991. A&AS 88, 101
Kurucz R.L. 1990. Trans. IAU XXB, 168
Kurucz R.L. & Peytremann E. 1975. SAO Spec.Rep.No. 362
Seaton M.J. 1987. J.Phys.B. 20, 6363
Yan Y., Taylor K.T. & Seaton M.J. 1987. J.Phys.B. 20, 6399

A Database contents

A.1 Example data file

File: C2.DAT

```
  6  2  1323.91 1.32E+00 7.30E-04 7.30E-05  9.290  -1.00  Tob 84/      /
  6  2  1334.53 5.25E-01 2.30E-04 2.30E-05  0.000  -1.00  Tob 84/      /
  6  2  6578.10 9.13E-01 2.64E-03 5.11E-04 14.445   2.00  Yan 87/Jon 71/Nus 81
  6  2  6582.90 4.57E-01 2.64E-03 5.11E-04 14.445   2.00  Yan 87/Jon 71/Nus 81
  6  2  3918.98 2.85E-01 3.70E-03 2.50E-04 16.333   4.00  Yan 87/Gol 82/Nus 81
  6  2  3920.69 5.70E-01 3.70E-03 2.50E-04 16.334   4.00  Yan 87/Gol 82/Nus 81
  6  2  4267.02 3.62E+00 9.97E-03 1.51E-03 18.047   6.00  Yan 87/Kon 76/Jon 71
  6  2  4267.27 5.42E+00 9.97E-03 1.51E-03 18.047   6.00  Yan 87/Kon 76/Jon 71
  6  2  4637.63 5.80E-02 1.00E-02 1.50E-04 21.150  12.01  Yan 87/      /
  6  2  4638.91 1.16E-02 1.00E-02 1.50E-04 21.150  12.01  Yan 87/      /
  6  2  4306.33 2.05E-02 1.00E-02 1.50E-04 21.150  12.02  Yan 87/      /
  6  2  4307.59 4.11E-02 1.00E-02 1.50E-04 21.150  12.02  Yan 87/      /
  6  2  4802.70 3.88E-01 2.85E-01 1.69E-04 22.000  17.08  Yan 87/      /Yan 87
  6  2  4313.10 4.19E-01 3.36E-03 3.41E-04 23.120  28.00  Yan 87/Sah 69/Yan 87
  6  2  4317.26 9.79E-01 3.36E-03 3.41E-04 23.120  28.00  Yan 87/Sah 69/Yan 87
  6  2  4318.60 3.90E-01 3.36E-03 3.41E-04 23.120  28.00  Yan 87/Sah 69/Yan 87
  6  2  4321.65 1.25E-01 3.36E-03 3.41E-04 23.120  28.00  Yan 87/Sah 69/Yan 87
  6  2  4323.10 7.83E-02 3.36E-03 3.41E-04 23.120  28.00  Yan 87/Sah 69/Yan 87
  6  2  4325.83 4.22E-01 3.36E-03 3.41E-04 23.120  28.00  Yan 87/Sah 69/Yan 87
  6  2  4326.16 3.91E-01 3.36E-03 3.41E-04 23.120  28.00  Yan 87/Sah 69/Yan 87
  ...etc.
```

A.2 Column explanation

File: COLS.TXT

```
Column   Explanation                                    Example

 1       Atomic number                                  6       Carbon
 2       Ionisation stage                               2       Singly ionised
 3       Wavelength (Angstroms)  Moo 48, etc.           4267.2
 4       Oscillator strength    g.f
 5       Electron damping width:
              FWHM/PI/4 * WL**2/C * 1.E15
              WL is wavelength in Angstroms
              C  is speed of light (Angstroms/second)
 6       Radiative damping width:
              FWHM/PI/4 * WL**2/C
 7       Excitation energy of lower level (electron Volts)
 8       Multiplet identification   Moo 48, etc
              -ve numbers indicate a UV multiplet
 9       References for 4, 5 and 6.
```

A.3 Source citation

File: REFS.DAT

```
All wavelengths, ionization potentials and energy levels are taken from:
    Wiese et al. NBS publications.
    C.E.Moore , Selected tables of atomic spectra : NSRDS - NBS3 sections 1-10.

Effects of ion broadening also included in the electron width
Major compilations are shown by a '+'

All 90. + Allard,M., Artru,M.-C., Lanz,T., \& Le Dourneuf,M., 1990.
         Astr.Astrophys.Supp. 84, 563.
Art 81. Artru,M.C., Jamar,C., Petrini,D., & Praderie,F., 1981.
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...
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Bec 89. Becker,S.R., & Butler,K., 1989. Astr.Astrophys. 209, 244.       N II
Bec 90. Becker,S.R., & Butler,K., 1990. Astr.Astrophys. 235, 326.       Si II/III/IV
...
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...
Jon 71. Jones,W.M., Benett,S.M., & Griem,H.R., 1971,
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...
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...
Nus 81. Nussbaumer,H., & Storey,P.J., 1981. Astr.Astrophys., 96,91.
...
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...
Tob 84. Tobin & Kaufmann 1984. Mon.Not.R.astr.Soc., 207, 369.
...
Yan 87. Yan,Y., Taylor,K.T. & Seaton,M.J., 1987. J.Phys.B. 20, 6399.
...
```

A.4 Ions with data available

File: IONS.TXT

```
LI1.DAT                                                     Li I
C1.DAT     C2.DAT    C3.DAT    C4.DAT                       C  I/II/III/IV
           N2.DAT    N3.DAT                                 N    II/III
O1.DAT     O2.DAT    O3.DAT                                 O  I/II/III
NE1.DAT                                                     Ne I
           MG2.DAT                                          Mg   II
           AL2.DAT   AL3.DAT                                Al   II/III
           SI2.DAT   SI3.DAT   SI4.DAT                      Si   II/III/IV
           P2.DAT    P3.DAT                                 P    II/III
           S2.DAT    S3.DAT                                 S    II/III
           CL2.DAT                                          Cl   II
           A2.DAT                                           A    II
           CA2.DAT                                          Ca   II
           TI2.DAT                                          Ti   II
           CR2.DAT                                          Cr   II
FE1.DAT    FE2.DAT   FE3.DAT                                Fe I/II/III
           NI2.DAT                                          Ni   II
```