LTE_LINES — Atomic data for LTE calculations (v2)

C. Simon Jeffery, *Armagh Observatory and Planetarium, College Hill, Armagh BT61 9DG, N. Ireland*

April 1, 2020

Abstract

An 'end-user' oriented data collection 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, electron and van der Waal's damping widths, lower-level excitation potential, ion and multiplet identification and source citations, where available. Whilst much could still be done, this technical report updates the database specification in order to keep it current.

1 Introduction

Analyses of astronomical spectra depend critically on reliable sources of atomic and molecular data. These come from many sources including, while active, two of the UK's Collaborative Computational Projects (CCP's: see `www.ccp.ac.uk`), namely CCP2 (Continuum States of Atoms and Molecules) and CCP6 (Heavy Particle Dynamics). As a part of its mission, CCP7 (1980 - 2001: Analysis of Astronomical Spectra `ccp7.dur.ac.uk`) was concerned with making such data accessible for astronomical applications. Over the years and thanks to the generosity of many authors, CCP7 acquired a number of data collections.

One such, LTE_LINES, attempts to collate and maintain 'recommended' data for LTE analyses of early-type stars. It has been extended with the end user in view and may find practical uses in a variety of applications such as spectrum-synthesis in LTE calculations. Jeffery (1991) provided a guide to the database as originally implemented. As the demand for synthesis of large regions of spectrum including ultraviolet and far ultraviolet wavelengths increased, several changes were introduced. This document updates the technical description.

2 Data

The collection is organised by ion, presenting one record for each line. Each record contains the atom and ion identifier, a wavelength, an oscillator strength (gf), damping widths (γ) for radiative, electron and ion broadening and the excitation energy of the lower level. Where possible, a multiplet identifier and references for these data are give in additional columns (Table 1).

Table 1: Column explanation for LTE_LINES data files.

Col	Format	Contents	Symbol	Units	Example	
1	i3	Atomic Number	Z		6	carbon
2	i3	Ionisation stage			2	singly ionised
3	f9.3	Wavelength	λ	Å	4267.020	one of a doublet
4	f7.3	Oscillator strength	$\log gf$		0.559	
5	f8.3	Electron damping width	$\log \gamma_e$	s^{-1}	-4.686	
6	f8.3	Radiative damping width	$\log \gamma_r$	s^{-1}	9.495	
7	f8.3	van der Waal's damping width	$\log \gamma_V$	s^{-1}	-99.00	not available
8	f8.3	Lower level excitation energy	E_i	eV	18.047	
9	f7.2	Multiplet identifier			6.00	Moore's tables
10	a20	References for 4 – 8			yan87/kon76/jon71	See appendix

Table 2: Ions available and number of lines per ion.

Ion	Sym	Z	I=0	II=+	III=++	IV=+++
Helium	He	2	367	2		
Lithium	Li	3	2			
Carbon	C	6	15	60	27	10
Nitrogen	N	7		220	23	
Oxygen	O	8	6	262	6	
Neon	Ne	10	17	33		
Magnesium	Mg	12		12		
Aluminium	Al	13		10	18	
Silicon	Si	14	1	19	26	14
Phosphor	P	15		24	6	1
Sulphur	S	16		88	32	
Chlorine	Cl	19		33		
Argon	A	20		96		
Calcium	Ca	22		21		
Titanium	Ti	22		45		
Vanadium	V	23				
Chromium	Cr	24		5		
Iron	Fe	26	101	59	12	
Nickel	Ni	28				

3 Sources

The CCP7 library (Jeffery 1990) contains *inter alia* 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 data cited 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.

Since the inception of LTE_LINES several other large and better resourced databases containing atomic data have been established. Briefly (and not exclusively) these include:

CHIANTI:	An atomic database for spectroscopic diagnostics of astrophysical plasmas (Dere et al. 1997, 2019)	`www.chiantidatabase.org`
KURUCZ:	Kurucz linelists	`kurucz.harvard.edu/linelists.html`
NIST:	The NIST[1] atomic spectra database	`www.nist.gov/pml/atomic-spectra-database`
TIPBASE:	The Iron Project database	`cdsweb.u-strasbg.fr/tipbase/home.html`
TMAD:	The Tübingen Model Atom database	`astro.uni-tuebingen.de/~TMAD/`
TOPBASE:	The Opacity Project database	`cdsweb.u-strasbg.fr/topbase/topbase.html`
VALD3:	The Vienna Atomic Line Database (Kupka et al. 1995)	`vald.astro.uu.se`
VAMDC:	The Virtual Atomic and Molecular Data Center	`www.vamdc.org`

4 History

Prior to 1990, Dufton and coworkers at Queen's University of Belfast maintained 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 formed 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. Most data pertained to transitions of light ions in the blue-visible. This list provided 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.

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 revision to the Belfast linelist was made. Firstly line identification was improved by the addition of a (Moore) multiplet identification. The number of transitions treated was increased to include weaker lines (frequently measurable in supergiants and non-rotating B stars) and more ions. The citation of sources was generalized. A substantial number of data were 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). With varying degrees of completeness and mainly in the blue visible, data have been compiled for several ions (Table 2). Data for individual ions were stored separately. For the original application (SPECTRUM), the separate ions were simply combined as required, using a VAX/VMS script, to form a linelist suitable for the spectrum being analysed. Normally, the expanded citation list was appended to the concatenated linelist to ensure the integrity of source identification.

4.1 Version 1

The original files forming this collection were held on-line in the CCP7 data/program library (Jeffery 1990) on the STARLINK microVAX system at St Andrews and could be accessed over the UK academic network JANET. This collection constituted version 1 (Jeffery 1991).

Following increased access to the internet, the database migrated to a web-based interface on the CCP7 website – whilst it was maintained in St Andrews and later Armagh. Data for specific ions could be requested online, and later concatenated as required by the user. When the CCP7 website moved to Durham, the LTE_LINES pages stayed in Armagh and can currently (2020 April 1) be found at

`193.63.77.2:2805/~SJeffery/linelists/lte/html/lines.lte.html`

The ion data are stored in files with a simple naming convention such that lines due to CII (ie C^+) are in `C2.d`, CIII in `C3.d`, SiIV in `Si4.d`, and so on. By way of example, appendices show data for the spectrum of CII (file `C2.d`).

4.2 Version 2

Soon after its release through CCP7, radiative transfer components within SPECTRUM came to be used for studies of cooler stars (Unruh et al. 1992) and thus required inclusion of ion-broadening data. The spectrum synthesis tools within SPECTRUM were also enhanced, and used extensively in the semi-automatic spectral fitting software SFIT (Jeffery et al. 2001), either by means of pre-computed grids or by real-time adjustment of abundances in the formal solution. Spectral synthesis requires that, as far as possible, the contributions of all lines be computed, particularly including contributions from weak and blended lines.

A comprehensive master list of lines was collated by Woolf et al. (2000), starting with the original LTE_LINES list and supplemented with data from MOOG (Sneden 1973) for the wavelength range 3700 – 5200 Å. This list has acquired additional data for the ultraviolet and into the green-red parts of the spectrum; data have been collated from a variety of source, including Kurucz original linelists (op cit.) and more recent compilations, and from VALD (Kupkka et al. 1995) and NIST. Changes were also required for precision: logarithmic forms were preferred for all atomic data except energy levels.

5 Data quality and completeness

For spectral synthesis methods to work well, linelists must be as complete as possible, as well as accurate as possible. This creates a tension; ideally it can be ameliorated by maintaining quality flags, as well as close attention to maintaining the source references. Whilst a conscious choice has always made when selecting data to include in LTE_LINES, reasons for choices and quality indicators have not been preserved. Many databases now do this better (see Section 3).

The original intention has always been that xLTE_LINES 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 are as follows:

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

Oscillator strengths are given for about 1000 lines, mostly in the blue-visible ($\lambda 4000 - 5000$ Å). Calculated damping widths are available for $\sim 20\%$.

6 Future

There is now a symbiosis between a reference list distributed with the LTE_CODES package, which includes SPECTRUM, a live master list which is augmented as required for specific projects, and the constituent ion-by-ion data files. The data held on line in the LTE_LINES collection represent the latter.

On inception, additional developments were anticipated. This version realises some of the format changes for higher density and precision. The linelist format remains compatible with the Armagh version of the LTE line formation code SPECTRUM. Utilities for restricting and sorting the lines in wavelength or by ion and multiplet would be useful, Further identification of the atomic transitions (*e.g.* electron configurations) would be helpful. A high priority is greater completeness for ultraviolet transitions and for damping widths in the blue-visible.

References

Allard M., Artru M.-C., Lanz T., & Le Dourneuf M., 1990. A&AS 84, 563
Becker S.R. & Butler K. 1988. A&A 201, 232
Becker S.R. & Butler K. 1989. A&A 209, 244
Becker S.R. & Butler K. 1990. A&A 235, 326
Behara N.T. & Jeffery C.S. 2006 A&A 451, 643
Bell R.A. 1973. MNRAS 164, 197
Dere K.P., et al., 1997. A&AS 125, 149
Dere K.P., et al., 2019. ApJS 241, 2
Jeffery C.S. 1990. CCP7 Newsletter No. 14, 43
Jeffery C.S. 1991. CCP7 Newsletter No. 16, 17
Jeffery C.S. & Heber U. 1992. A&A 260, 133
Jeffery C.S., Woolf V.M. & Pollacco D. 2001. A&A 376, 497
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
Sneden, C. A. 1973. PhD thesis, The University of Texas at Austin
Collier Cameron A., Unruh, Y.C., & Jeffery C.S. 1991. In Jeffery C.S. & Griffin R.E.M., eds, Stellar Chromospheres, Coronae and Winds. Institute of Astronomy, Cambridge, p. 81
Woolf V.M. & Jeffery C.S. 2000. A&A 358, 1001.
Yan Y., Taylor K.T. & Seaton M.J. 1987. J.Phys.B. 20, 6399

A Database examples

A.1 Data file

File: C2.d

```
 -6  2 1323.910  0.121  -4.804  10.129 -99.000   9.290  -1.00 tob84/     /hub95
 -6  2 1334.530 -0.280  -5.313  10.122 -99.000   0.000  -1.00 tob84/     /hub95
  6  2 1323.860 -1.130 -99.000  10.129 -99.000   9.290   0.00 hub95/hub95/hub95
  6  2 1323.910 -0.170 -99.000  10.129 -99.000   9.291   0.00 hub95/hub95/hub95
  6  2 1323.950  0.021 -99.000  10.130 -99.000   9.290   0.00 hub95/hub95/hub95
  6  2 1324.000 -1.130 -99.000  10.130 -99.000   9.291   0.00 hub95/hub95/hub95
  6  2 1334.530 -0.620  -5.410   9.529 -99.000   0.000   0.00 hub95/hub95/hub95
  6  2 1335.660 -1.320  -5.411   9.529 -99.000   0.008   0.00 hub95/hub95/hub95
  6  2 1335.710 -0.360  -5.411   9.539 -99.000   0.008   0.00 hub95/hub95/hub95
  6  2 6578.100 -0.040  -5.639   8.648 -99.000  14.445   2.00 yan87/jon71/nus81
  6  2 6582.900 -0.340  -5.639   8.648 -99.000  14.445   2.00 yan87/jon71/nus81
  6  2 3918.980 -0.545  -5.042   8.788 -99.000  16.333   4.00 yan87/gol82/nus81
  6  2 3920.690 -0.244  -5.043   8.787 -99.000  16.334   4.00 yan87/gol82/nus81
  6  2 4267.020  0.559  -4.686   9.495 -99.000  18.047   6.00 yan87/kon76/jon71
  6  2 4267.270  0.734  -4.686   9.495 -99.000  18.047   6.00 yan87/kon76/jon71
 -6  2 4802.700 -0.394  -4.787   8.389 -99.000  18.050   7.08 heb83/      /
  6  2 4637.630 -1.237  -4.757   8.420 -99.000  21.150  12.01 yan87/      /
  6  2 4638.910 -1.936  -4.757   8.419 -99.000  21.150  12.01 yan87/      /
  6  2 4306.330 -1.688  -4.692   8.484 -99.000  21.150  12.02 yan87/      /
  6  2 4307.590 -1.386  -4.692   8.484 -99.000  21.150  12.02 yan87/      /
  6  2 4802.700 -0.411  -3.332   8.441 -99.000  22.000  17.08 yan87/      /yan87
  6  2 4313.100 -0.378  -5.167   8.839 -99.000  23.120  28.00 yan87/sah69/yan87
  6  2 4317.260 -0.009  -5.168   8.838 -99.000  23.120  28.00 yan87/sah69/yan87
  6  2 4318.600 -0.409  -5.168   8.838 -99.000  23.120  28.00 yan87/sah69/yan87
  6  2 4321.650 -0.903  -5.169   8.837 -99.000  23.120  28.00 yan87/sah69/yan87
  6  2 4323.100 -1.106  -5.169   8.837 -99.000  23.120  28.00 yan87/sah69/yan87
  6  2 4325.830 -0.375  -5.170   8.837 -99.000  23.120  28.00 yan87/sah69/yan87
  6  2 4326.160 -0.408  -5.170   8.837 -99.000  23.120  28.00 yan87/sah69/yan87
  6  2 4074.480  0.204  -4.623   9.644 -99.000  24.370  36.00 yan87/      /yan87
  6  2 4074.520  0.408  -4.623   9.644 -99.000  24.370  36.00 yan87/      /yan87
  6  2 4074.850  0.593  -4.623   9.644 -99.000  24.370  36.00 yan87/      /yan87
  6  2 4075.400 -0.194  -4.623   9.643 -99.000  24.370  36.00 yan87/      /yan87
  6  2 4075.850  0.756  -4.623   9.643 -99.000  24.370  36.00 yan87/      /yan87
  6  2 4075.940 -0.076  -4.623   9.643 -99.000  24.370  36.00 yan87/      /yan87
  6  2 4076.530  0.604  -4.623   9.643 -99.000  24.370  36.00 yan87/      /yan87
  6  2 4411.200  0.517  -4.580   9.328 -99.000  24.500  39.00 yan87/      /yan87
  6  2 4411.520  0.672  -4.580   9.328 -99.000  24.500  39.00 yan87/      /yan87
  6  2 4413.260 -0.629  -4.580   9.328 -99.000  24.500  39.00 yan87/      /yan87
  6  2 4291.820 -0.236  -4.513   9.390 -99.000  24.600  42.00 heb83/      /
  6  2 4285.700 -0.428  -4.512   9.391 -99.000  24.600  42.00 heb83/      /
  6  2 4289.880 -1.383  -4.513   9.390 -99.000  24.600  42.00 heb83/      /
  6  2 4287.720 -1.383  -4.512   9.391 -99.000  24.600  42.00 heb83/      /
  6  2 4368.260 -0.967  -4.437   9.403 -99.000  24.650  45.00 yan87/      /yan87
  6  2 4369.860 -0.745  -4.438   9.402 -99.000  24.650  45.00 yan87/      /yan87
  6  2 4372.350  0.057  -4.438   9.402 -99.000  24.650  45.00 yan87/      /yan87
  6  2 4372.490  0.272  -4.438   9.402 -99.000  24.650  45.00 yan87/      /yan87
  6  2 4374.270  0.634  -4.439   9.401 -99.000  24.650  45.00 yan87/      /yan87
  6  2 4375.010 -0.043  -4.439   9.401 -99.000  24.650  45.00 yan87/      /yan87
  6  2 4376.560  0.354  -4.439   9.401 -99.000  24.650  45.00 yan87/      /yan87
  6  2 4734.600 -0.199  -4.474   9.225 -99.000  24.790  48.00 heb83/      /
  6  2 4727.410 -0.330  -4.472   9.227 -99.000  24.790  48.00 heb83/      /
```

```
  6  2 4736.750 -1.631  -4.474   9.225 -99.000  24.790  48.00 heb83/     /
  6  2 4725.360 -1.631  -4.472   9.227 -99.000  24.790  48.00 heb83/     /
  6  2 4618.400  0.737  -4.439   9.213 -99.000  24.790  50.00 wie66/     /
  6  2 4619.230  0.854  -4.439   9.213 -99.000  24.790  50.00 wie66/     /
  6  2 4627.440 -0.708  -4.441   9.211 -99.000  24.790  50.00 wie66/     /
  6  2 5640.500 -0.682 -99.000   7.814 -99.000  20.695  15.00 wie66/     /wie66
  6  2 5648.080 -0.381 -99.000   7.813 -99.000  20.698  15.00 wie66/     /wie66
  6  2 5132.960 -0.244 -99.000   7.935 -99.000  20.695  16.00 wie66/     /wie66
  6  2 5133.290 -0.210 -99.000   7.935 -99.000  20.698  16.00 wie66/     /wie66
```

A.2 Citation extract

```
File: refs.d

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 '+'

all90. + Allard,M., Artru,M.-C., Lanz,T., \& Le Dourneuf,M., 1990.
         Astr.Astrophys.Supp. 84, 563.
art81. Artru,M.C., Jamar,C., Petrini,D., & Praderie,F., 1981.
         Astr.Astrophys.Supp. 44, 171.
...
bec88. Becker,S.R., & Butler,K., 1988. Astr.Astrophys. 201, 232.       O II
bec89. Becker,S.R., & Butler,K., 1989. Astr.Astrophys. 209, 244.       N II
bec90. Becker,S.R., & Butler,K., 1990. Astr.Astrophys. 235, 326.       Si II/III/IV
...
gol82. Goly & Weniger 1982. J.Quant.Spectrosc.Radiat.Transfer, 28,389.
...
jon71. Jones,W.M., Benett,S.M., & Griem,H.R., 1971,
         University of Maryland, Tech.report #71-128.
...
kon76. Konjevic,N., & Wiese,W.L., 1976. J.Phys.chem.ref.Data, 5,(No.2),259.
...
nus81. Nussbaumer,H., & Storey,P.J., 1981. Astr.Astrophys., 96,91.
...
wah69. Sahal-Brechot,S., 1969. Astr.Astrophys., 2, 322.
...
tob84. Tobin & Kaufmann 1984. Mon.Not.R.astr.Soc., 207, 369.
...
yan87. Yan,Y., Taylor,K.T. & Seaton,M.J., 1987. J.Phys.B. 20, 6399.
...
```