ATLAS9 atomic and opacity data in the CCP7 library

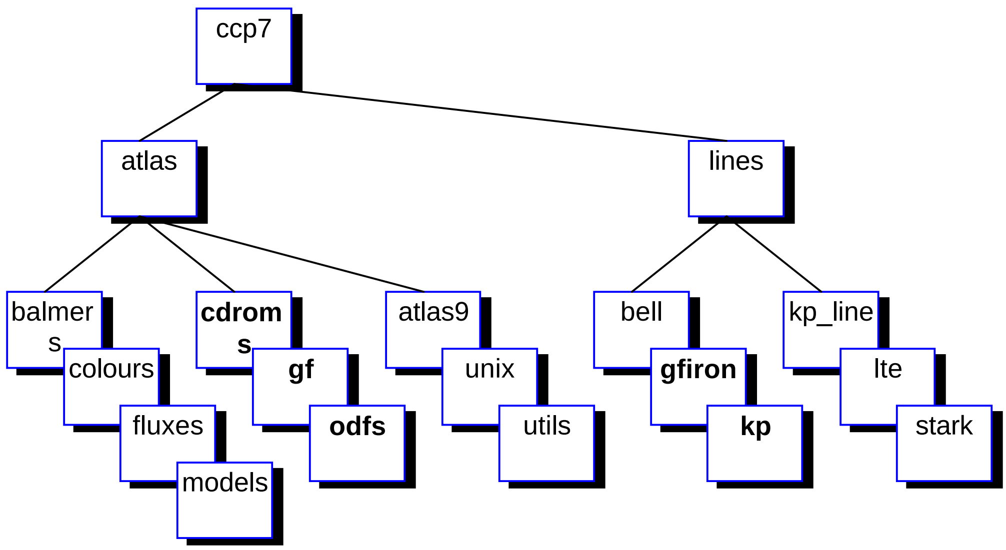
C.S.Jeffery, *Dept of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, Fife KY16 9SS, Scotland*

23 February, 1994
CCP7 User Note 13.0

1. Introduction

Kurucz (1991, in ‘Stellar Atmospheres: Beyond Classical Models’, NATO ASI Series C 341, p. 441 eds. Crivellari, Hubeny & Hummer) presented a substantial compilation of oscillator strengths for some 58,000,000 atomic and molecular transitions. These were employed in the construction of opacity distribution functions in order to calculate an extensive grid line-blanketed plane-parallel stellar atmospheres in LTE. Kurucz has kindly made this data available to CCP7 in a number of formats; the Project is attempting to make these data available to the community in as convenient a form as possible. This document describes some of the datasets available.

The volume of Kurucz data (especially gf-values and opacity distribution functions) means that it is not possible to store all of it on-line. Some tools and holders for data subsets are defined on the the CCP7 Sun SPARCstation: Kurucz’ opacity and atomic data files are stored in a folders marked by **bold** labels in the structure shown. The diagram also illustrates some of the other atomic data stored in the library.



However, the bulk of Kurucz data is stored on-line in a variety of media, including 1/2” tape (VAX format), Exabyte tape (VMS BACKUP and tar format) and CD-ROMS (VAX format). The remainder of this document describes what is available.

2. atlas.cdroms

CCP7 holds two copies of the complete set of Kurucz' CD-ROMs. The CD's are available for loan to astronomers for genuine research programmes. Individuals wishing to borrow one or more CD's from CCP7 should approach the author (C.S.Jeffery).

KURUCZ CD-ROMS

No. 1 Atomic data for opacity calculations.
No. 2 Opacities for Stellar Atmospheres: [+0.0],[+0.5],[+1.0].
No. 3 Opacities for Stellar Atmospheres: [-0.5],[-1.0],[-1.5].
No. 4 Opacities for Stellar Atmospheres: [-2.0],[-2.5],[-3.0].
No. 5 Opacities for Stellar Atmospheres: [+0.1],[+0.2],[+0.3].
No. 6 Opacities for Stellar Atmospheres: [-0.1],[-0.2],[-0.3].
No. 7 Opacities for Stellar Atmospheres: [-3.5],[-4.0],[-4.5].
No. 8 Opacities for Stellar Atmospheres: [-5.0],[+0.0,noHe],[+0.3,.31He].
No. 9 Opacities for Stellar Atmospheres: [+0.5a],[+0.0a],[-0.5a] +.4 alpha
No. 10 Opacities for Stellar Atmospheres: [-1.0a],[-1.5a],[-2.0a] +.4 alpha
No. 11 Opacities for Stellar Atmospheres: [-2.5a],[-3.0a],[-3.5a] +.4 alpha
No. 12 Opacities for Stellar Atmospheres: [-4.0a],[-4.5a],[-5.0a] +.4 alpha
No. 13 ATLAS9 model atmosphere programs and 2 km/s grid.
No. 14 Opacities for Stellar Atmospheres: abundance sampler
No. 15 Diatomic molecular data for opacity calculations.
No. 16 Limb darkening for 2 km/s...[+0.0]-[-5.0]
No. 17 Limb darkening for 2 km/s...[+1.0]-[-1.0]
No. 18 SYNTHE spectrum synthesis programs and line data

Mounting and reading the disks ...

OpenVMS V.1.5:

```
MOUNT /MEDIA=CDROM <device> <label>
```

Unix:

```
mount -r -t cdfs [-v] /dev/r---  /folder

-r         ...  read only
-t cdfs    ...  type of filesystem (cdfs for CDROM)
-v         ...  verbose output in case of errors (optional)
/dev/r---  ...  SCSI device connected to CDROM drive
/folder    ...  root folder for the CDROM
```

If the CDROM label is (eg) CDROM1, and "folder" is ../myfolder, then the CD files will appear in ../myfolder/CDROM1/..

After mounting one can use the CDROM like a write protected subdirectory. If others require access, remember to modify the protections of /myfolder and /myfolder/CDROM1 to 755. For unmounting set your current directory above the mounting point, and type

```
umount [-v] /dev/rz4c
```

before removing.

3. atlas.gf

Semi-empirical gf values for iron-group transitions compiled by R.Kurucz. (Kurucz, 1991. In 'Stellar atmospheres: beyond classical models' p. 441, eds L.Crivellari, I.Hubeny & D.G.Hummer, Kluwer) were distributed on ~20 1/2 inch VAX tapes. A set of copies was kindly supplied to CCP7 by Dr Kurucz. These have been read and compiled onto one Exabyte tape by the author; copies are available for distribution.

The Exabyte tape contains 11 files in 'tar' format. Each tar file contains all the files comprising one group of gf values in Kurucz' compilation. The files on the tape, with their sizes in Mbytes, are:

Tar file	Size (Mbytes)	Notes
gf20	39.8	
gf21	53.0	
gf22	83.1	
gf2200	35.7	update of gf2200.* files
gf23	124.0	
gf24	140.2	
gf25	168.9	
gf26	252.9	
gf27	318.8	
gf28	339.0	
gfiron	53.6	quality assessed gf values

Each tar file 'gf<nn>' contains the following ASCII files:

Bnn0jE.OUT	least squares file for even levels
Bnn0jO.OUT	least squares file for odd levels
Cnn0jE.OUT	all even eigenvalues
Cnn0jO.OUT	all odd eigenvalues
GFnn0j.GAM	Ws, WLS,GLandes, Damping
GFnn0j.LIN	WLs, gfs, indices in GFnn0j.GAM
GFnn0j.POS	lines between known E levels

where <j> refers to the ionisation level of species <nn>. The file 'gfiron' contains all the lines from the .POS files with the damping constants added. SAO special report No. 390 should be consulted for a further explanation of the file contents, if one is needed. However, the report itself is obsolete.
Copies of the tape are available upon request from CCP7 via the author. However, note that copies of CD-ROMS containing these data are also available on loan from CCP7.

gf_tape

A C shell script providing utilities for listing the tar file contents, making copies of the GF tape, and unpacking the GF tape. It is available in the ccp7 library via anonymous ftp in the file ' gf.tar.Z '. The following commands are supported:

gf_tape -t dev0	Make a listing of tape GF on device 0
gf_tape -c dev0 dev1	Copy tape GF from device 0 to device 1
gf_tape -x dev0 file	Unpack tar file from tape GF on device 0 to disk

4. atlas.odfs

ATLAS9 odfs on 1/2" tape

Bob Kurucz supplied the grid of ATLAS9 odfs (Kurucz 1991 op. cit.) to CCP7 in early 1991. The medium consisted of 42 1/2 " tapes at 6250 bpi in VMS BACKUP format. These tapes may be borrowed if required.

A substantial fraction of these tapes were written close to and possibly below specification, with the consequence that the only available VMS tape reader in St Andrews, that of the STARLINK VAXcluster and now relatively aged, could not read them. Attempts to do so crashed the VAXcluster. More modern tape readers are more tolerant. After several attempts to concatenate the tapes onto Exabyte, including the use of the STARLINK VAXcluster in Edinburgh, it was decided to process the tapes using the University of St Andrews's Sun system.

ATLAS9 odfs on Exabyte

All odfs on 3 Exabyte tapes: copies available on request (blanks appreciated). Format is VMS BACKUP. See the postscript file odfs_exa.ps for more information

A Fortran procedure was written to make block-by-block copies of the VMS 1/2" tapes onto Exabyte tape, omitting only the label field from the beginning of all (except the first) 1/2" tapes copied to each Exabyte tape. The new tapes have been copied for distribution using the Unix ' dd ' facility on the CCP7 Sun workstation. The tape labels and their corresponding Exabytes are given in Appendix A. The odfs are listed in Appendix B.

Inevitably there were still some read errors on the 1/2" tapes. Because 14 tapes had to be copied in one go, it was not practical to attempt to correct individual casualties. The result is that a few odfs on each Exabyte may not be usable. The project now has the odf grid on CD-ROM; so this gaps can be made good if necessary.

Exabyte tape structure.

The Exabyte tapes are in VMS backup format. Their contents can be inspected under VMS either by

```
$ BACKUP/LIST/IGNORE=LABEL M___:*.*
```

to identify the contents of each file, where ' M___ ' is the name of the tape device, or by

```
$ MOUNT/OVER=ID M___
$ DIR/SIZ=ALL M___:[*]
```

to list the files on each tape. Each file represents a VMS BACKUP saveset, and contains one odf only. An individual odf is recovered by

```
$ BACKUP/IGNORE=LABEL/LOG M___:odf_name []
```

I have not found a way of recovering the odfs on Unix-based systems. The public domain utility 'vmsbackup' cannot deal with the large block sizes (20480 bytes) used for the odfs. However, my inexperience with Unix utilities may account for this. If anyone finds a way to do it ... please let CCP7 know about it.

Since it was necessary to know the physical tape structure in order to copy the tapes, it may be useful to describe it here.

>	start of tape
3 * 80 byte blocks	tape label and first file header
512 * 20480 byte blocks	odf file (BIG intervals)
2 * 80 byte blocks	end of file mark
2 * 80 byte blocks	file header
512 * 20480 byte blocks	odf file (BIG intervals)
2 * 80 byte blocks	end of file mark
....	
2 * 80 byte blocks	file header
1890 * 20480 byte blocks	odf file (LIT intervals)
2 * 80 byte blocks	end of file mark
....	
>	end of tape

When copying the tapes using ' dd ', it was apparent that the number of recored in some odf files varied from the numbers given here. It is suspected that their may be problems with these odfs. Complete details of the Exabyte tape contents are given in Tables 1 and 2.

Table 1. Correspondence between 1/2" and Exabyte tape savesets

Exabyte	1/2" tape	Exabyte	1/2" tape	Exabyte	1/2" tape
ODF1	P00BIG	ODF2	PPPBIG2	ODF3	NOHEBIG
	P00LIT		MMMBIG2		NOHELIT
	P10BIG		P05BIG		P01BIG
	P10LIT		P05LIT		P01LIT
	M10BIG		M05BIG		P02BIG
	M10LIT		M05LIT		P02LIT
	M20BIG		M15BIG		P03BIG
	M20LIT		M15LIT		P03LIT
	M30BIG		M25BIG		M01BIG
	M30LIT		M25LIT		M01LIT
	M40BIG		M35BIG		M02BIG
	M40LIT		M35LIT		M02LIT
	M50BIG		M45BIG		M03BIG
	M50LIT		M45LIT		M03LIT
Number of files	69		80		?70?

Table 2. Contents of Exabyte tapes.

The following table shows the detailed contents of each tape. Those odfs which are simply missing, are marked by spaces. Those which may be corrupted are marked in italics. Please advise me of any errors in this listing.

ODF1

p00big0	p00big1	p00big2	p00big4	p00big8	p00lit0	p00lit1	p00lit2	p00lit4	p00lit8
p10big0	p10big1	p10big2	p10big4	p10big8	p10lit0	p10lit1	p10lit2	p10lit4	p10lit8
m10big0	m10big1	m10big2	m10big4	m10big8	*m10lit0*	m10lit1	m10lit2	m10lit4	m10lit8
m20big0	m20big1	m20big2	m20big4	m20big8	m20lit0	m20lit1	m20lit2	m20lit4	m20lit8
m30big0	m30big1	m30big2	m30big4	m30big8	m30lit0	m30lit1	m30lit2	m30lit4	*m30lit8*
m40big0	m40big1	m40big2	m40big4	m40big8	m40lit0	m40lit1	m40lit2	m40lit4	m40lit8
m50big0	m50big1	m50big2	m50big4	m50big8	m50lit0	m50lit1	m50lit2	m50lit4	*m50lit8*

ODF2

p10big2	p05big2	p03big2	p02big2	p01big2	p00big2	m01big2	m02big2	m03big2	m05big2
m10big2	m15big2	m20big2	m25big2	m30big2	m35big2	m40big2	m45big2	m50big2	
p05big0	p05big1	p05big2	p05big4	p05big8	p05lit0	p05lit1	p05lit2	p05lit4	p05lit8
m05big0	m05big1	m05big2	m05big4	m05big8	*m05lit0*	m05lit1	m05lit2	m05lit4	m05lit8
m15big0	*m15big1*	m15big2	*m15big4*	m15big8	*m15lit0*	m15lit1	m15lit2	m15lit4	m15lit8
m25lit1	m25lit2	*m25lit4*	*m25lit8*	m25big0	m25big1	*m25big2*	*m25big4*	*m25big8*	*m25lit0*

m35big0	*m35big1*	m35big2	m35big4	m35big8	*m35lit0*	*m35lit1*	*m35lit2*	m35lit4	m35lit8
m45big0	*m45big1*	m45big2	m45big4	m45big8	m45lit0	m45lit1	m45lit2	m45lit4	m45lit8

ODF3

nohebig0	nohebig1	nohebig2	nohebig4	nohebig8	nohelit0	nohelit1	nohelit2	nohelit4	nohelit8
p01big0	*p01big1*	p01big2	p01big4	p01big8	p01lit0	p01lit1	p01lit2	p01lit4	p01lit8
p02big0	p02big1	p02big2	p02big4	p02big8	p02lit0	*p02lit1*	*p02lit2*	*p02lit4*	*p02lit8*
p03big0	p03big1	p03big2	p03big4	p03big8	p03lit0	p03lit1	p03lit2	*p03lit4*	p03lit8
m01big0	m01big1	m01big2	m01big4	m01big8	m01lit0	m01lit1	m01lit2	m01lit4	m01lit8
m02big0	m02big1	m02big2	m02big4	m02big8	m02lit0	m02lit1	m02lit2	m02lit4	m02lit8
m03big0	m03big1	m03big2	m03big4	m03big8	m03lit0	m03lit1	m03lit2	m03lit4	m03lit8

Acknowledgments: CCP7 is indebted to Dr J.T.Henderson of the the University of St Andrews Computing Laboratory for writing the tape copying procedure, and to the Computing Laboratory operators for processing many manual tape operations. Bob Kurucz' generosity in continuing to donate invaluable data to the astronomical community, and to CCP7, is also gratefully acknowledged.