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KPSEARCH: USER GUIDE
A SYSTEM FOR ONLINE SEARCHING OF ATOMIC LINE SPECTRA

by

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1. INTRODUCTION

The system provides online access to a database containing the gf values for 265,587 atomic lines selected from the line data used by Kurucz, Peytremann, and Avrett[1,2] to calculate line-blanketed model atmospheres. The data are especially useful for line identification and spectral synthesis in solar and stellar spectra.

Except for 10,000 lines taken from the literature, the gf values have been calculated semiempirically by using scaled Thomas-Fermi-Dirac radial wavefunctions and eigenvectors found through least squares fits to observed energy levels. Included in the calculation were the first five or six stages of ionization for sequences up through nickel. Published gf values have been included for elements heavier than nickel. The tabulation is restricted to lines with wavelengths less than 10 μm.

The retrieval system was implemented by the Daresbury Applications Group on the Daresbury Laboratory AS/7000 computer, and may be accessed as described here or via the Atomic Data Bank (K.M. Aggarwal, Queen's University, Belfast). Retrieval of values may be based on wavelength or atomic number (and optionally charge) or both.

2. DISCLAIMER

The contents of the database are those made available by its compilers who have described the constraints on accuracy and content elsewhere[1,2]. Any comments concerning the retrieval system should be addressed to the current authors.

3. ACCESSING THE DATABASE

Log onto a 350K region of TSO (details on how to log onto TSO are included in Appendix I).

The database is stored on a private disk pack which must be mounted before the interactive session may be run. Use the command :

```
MX 'XBZ.CLIST(MOUNT)' 'DL0238'
```

This submits a batch job called IDLIST (where ID is your identifier) to mount the disk pack. On completion of the job it sends the message :

```
IDLIST TERMINATED NORMALLY
```

to your terminal. The retrieval program KPSEARCH should now be run as soon as possible (before the disk is demounted). The command to run it is :

```
MX 'XBZ.CLIST(KPSEARCH)' 'ROUTE()'
```

The ROUTE parameter may be omitted if you do not intend producing lineprinter output or if the lineprinter output is required on the central Daresbury Laboratory printers. Otherwise specify the route name of your local lineprinter inside the brackets.

There will now be a delay while the necessary files are allocated and then the following logo will be displayed.

```
**************************************************************************
*              A DATABASE FOR IDENTIFICATION OF ATOMIC LINES             *
*                          CALCULATED BY                                 *
*                    R.L. KURUCZ AND E. PEYTREMANN                       *
*                  (1975  SAO SPECIAL REPORT NO.309)                     *
*                                                                        *
*                        SMITHSONIAN INSTITUTE                           *
*                    ASTROPHYSICAL OBSERVATORY                           *
*                  CAMBRIDGE, MASSACHUSETTS 02138                        *
*                                                                        *
*               WAVELENGTHS 5.2682 NM TO 9997.2746 NM                    *
*                                                                        *
*                  RETRIEVAL SYSTEM IMPLEMENTED BY                       *
*                    DARESBURY APPLICATIONS GROUP                        *
*                    CONTACT DR. M. ELDER, EXT.350                       *
**************************************************************************
ENTER HELP FOR LIST OF AVAILABLE COMMANDS
*
```


4. RETRIEVAL PROGRAM COMMANDS

The program is capable of retrieving all records in a range of wavelengths, or all records of one element, or all records of one element of a specified charge, or a combination of defined element and wavelength range. The retrieved records may be displayed at the terminal, or on a lineprinter or both. At the end of each search a total of the number of records which have met the supplied conditions is output. It is possible to 'browse' through the selected output, looking only at every n'th record or restrict the output to a total of the retrieved records.

For each record the output lists wavelength in nm, log gf, energy in cm^{-1} for the lower and upper levels, element identification and some associated text. The element identification is the atomic number plus 0.01 times the ionic charge, for example, 23.02 stands for V++, or VIII.

The rest of this section details the available commands with examples. Commands may be entered after the program prompts with a *. If the program is outputting data and the user wishes to stop and return to the prompt, the attention command, usually @y, may be entered.

help

Help requires no parameters and lists the other commands. It may be used at any time. e.g.

```
*
help
```

COMMAND	PARAMETERS	ACTION
LIST	ON/OFF	SWITCH TERMINAL DISPLAY ON/OFF (DEFAULT = ON)
PRINT	ON/OFF	SWITCH PRINTER ON/OFF (DEFAULT = OFF)
SHOW	N	WRITE OUT ONLY EVERY N TH RECORD (DEFAULT = 1)
WRANGE	W	SET VALUE OF W FOR WAVE COMMAND (DEFAULT = 0.05)
HELP		LISTS AVAILABLE COMMANDS
SETTING		DISPLAYS CURRENT SETTINGS
WAVE	P1	SEARCH FOR WAVELENGTHS IN RANGE P1-W TO P1+W
"	P1 P2	SEARCH FOR WAVELENGTHS IN RANGE P1-W TO P2+W
ELEM	J	SEARCH FOR ELEMENT WITH ATOMIC NUMBER J
"	J C I	SEARCH FOR ELEMENT WITH ATOMIC NUMBER J AND CHARGE I (THE LETTER C IS A KEYWORD)

ELEM J C I N1 N2 SEARCH FOR ELEMENT WITH ATOMIC NUMBER J, CHARGE I AND WAVELENGTHS BETWEEN N1 AND N2

STOP EXIT FROM INTERACTIVE SESSION

COMMANDS MAY BE ABBREVIATED TO FIRST 4 LETTERS

list

This command controls whether the full output is sent to the terminal (list on) or only the counted totals sent (list off). On entering the program list is set as on.

To switch list off type :

```
*
list off
```

To switch list on type :

```
*
list on
```

print

This command controls whether output for a retrieval is sent to the lineprinter or not at the end of the session. On entering the program print is set as off.

To switch print on type:

```
*
print on
```

To switch print off type :

```
*
print off
```

Note that any combination of List on/off and print on/off may be used.

show

Show has one integer parameter. The command gives the user the option to sample the output by only showing every n'th record which meets the retrieval conditions. On entry n is set as 1 i.e. showing every record. To show only every 10'th record the command would be :

```
*
show 10
```

wrange

Wrange has one real parameter which is used to control the permissable

error range when searching on wavelength. The command which retrieves records of a certain wavelength has a margin for error (set at 0.05 on entry) in its search for records. That is, if asked to search for wavelengths of value 100 nm, the program will search between 99.95 (100-0.05) and 100.05 (100+0.05). This range of values searched outside the specified limits may be reset by the wrange command.

e.g.

To set to zero

```
*
wrange 0.0
```

To set to 5 nm

```
*
wrange 5.0
```

setting

Setting has no parameters and displays the current values of the four variables described above. Thus if used just after entering the system

e.g.

```
*
sett
 SHOW    WRANGE  LIST  PRINT
   1    0.05000   ON    OFF
```

wave

Wave may have one or two parameters either integer or real (but not mixed integer and real). The command searches the database for records with the wavelengths specified by wave (plus and minus the wrange) and then displays them (if list on) and gives a total count. In the next example the wrange value was at 0.05.

e.g

```
*
wave 1030
```

WAVELENGTH(NM)	LOGGF	E LOWER(/CM)	E UPPER(/CM)	ELEM	TEXT
1029.9680	-4.470	328818.070	319111.700	10.01	0707S2P4P N=4 S2P4G N=6
1029.9700	-3.000	328818.070	319111.710	10.01	0709S2P4P N=4 S2P4G N=6
1029.9711	-3.140	328818.050	319111.700	10.01	0507S2P4P N=4 S2P4G N=6
1029.9876	-4.027	44551.325	54257.520	26.00	0604 (D+S)7 4P-D7 4D
1030.0028	-6.861	7255.369	16961.420	22.00	0406 (D+S)4-(D+S)3 4P
1030.0401	-4.390	125072.600	115366.900	18.00	0202S2P5P N=9 S2P5P N=3
1030.0428	-3.924	20062.980	29768.655	22.00	0204 (D+S)4-(D+S)3 4P

TOTAL OF 7 RECORDS BETWEEN WAVELENGTH 1029.95000 & 1030.05000

The following examples demonstrate uses of wrange, show and setting as well as wave.

```
*
wrange 0.01
*
wave 1030
```

WAVELENGTH(NM)	LOGGF	E LOWER(/CM)	E UPPER(/CM)	ELEM	TEXT
1030.0028	-6.861	7255.369	16961.420	22.00	0406 (D+S)4-(D+S)3 4P

TOTAL OF 1 RECORDS BETWEEN WAVELENGTH 1029.99000 & 1030.01000

```
wave 1030.03 1030.11
```

WAVELENGTH(NM)	LOGGF	E LOWER(/CM)	E UPPER(/CM)	ELEM	TEXT
1030.0401	-4.390	125072.600	115366.900	18.01	0202S2P5P N=9 S2P5D N=3
1030.0428	-3.924	20062.980	29768.655	22.00	0204 (D+S)4-(D+S)3 4P
1029.0581	-4.462	51638.170	41932.640	25.00	0507 (D+S)7-(D+S)6 4P
1030.0794	-3.029	4513.220	54818.550	24.00	0604 (D+S)5 4P-D4S 5S
1030.0942	-2.332	99442.860	109148.050	28.01	0909 (D8 4D-4P+5P+4SP
1030.1177	-2.249	31489.451	41194.420	22.00	0806 (D+S)3 4P-D2S 4D

TOTAL OF 6 RECORDS BETWEEN WAVELENGTH 1030.02000 & 1030.12000

```
*
show 2
*
wave 1030.03 1030.11
```


WAVELENGTH(NM)	LOGGF	E LOWER(/CM)	E UPPER(/CM)	ELEM	TEXT
1030.0428	-3.924	20062.980	29768.655	22.00	0204 (D+S)4-(D+S)3 4P
1030.0794	-3.029	45113.220	54818.550	24.00	0604 (D+S)5 4P-D4S 5S
1030.1177	-2.249	31489.451	41194.420	22.00	0806 (D+S)3 4P-D2S 4D

TOTAL OF 6 RECORDS BETWEEN WAVELENGTH 1030.02000 & 1030.12000

```
*
sett
```

SHOW	WRANGE	LIST	PRINT
2	0.01000	ON	OFF

element

Element has three different styles of use and up to 4 integer parameters. The command searches the database for records with the specified atomic number, charge, and range of wavelengths. The first parameter is the atomic number of the element, for instance, a search on all records of beryllium (at.no.=4):

```
*
show 2
*
elem 4
```

WAVELENGTH(NM)	LOGGF	E LOWER(/CM)	E UPPER(/CM)	ELEM	TEXT
249.4600	0.150	21980.000	62066.587	4.00	0000
332.1200	-0.510	21980.000	52089.599	4.00	0000
351.5540	-0.910	42565.000	71010.132	4.00	0000
381.3400	-0.600	42565.000	68788.318	4.00	0000
457.2670	-0.240	42565.000	64434.061	4.00	0000
103.6270	-0.794	0.000	96499.947	4.01	0000
177.6200	-0.399	31933.000	88232.966	4.01	0000
324.7700	-0.888	96498.000	127289.021	4.01	0000
436.0900	0.493	96498.000	119429.046	4.01	0000
527.0700	-0.093	96498.000	115470.812	4.01	0000
6426.6000	-0.314	96498.000	98054.033	4.01	0000
10.0250	-0.258	0.000	997506.234	4.02	0000
58.3010	-0.122	956496.000	1128019.645	4.02	0000
74.6700	0.329	997466.000	1131388.593	4.02	0000
614.1200	-0.827	981187.000	997470.463	4.02	0000

30 RECORDS WITH ELEMENT VALUES 4.00 TO 4.09 AND WAVELENGTHS 0 TO 9999

To search for an element with a specific charge the format is element, atomic number, c(harge), charge value. Where c is left as the letter c. For instance, a search for beryllium with charge 1 is as follows (note show=2):

```
*
elem 4 c 1
```

WAVELENGTH(NM)	LOGGF	E LOWER(/CM)	E UPPER(/CM)	ELEM	TEXT
151.2400	0.592	31933.000	98053.074	4.01 0000	
313.0600	0.004	0.000	31942.759	4.01 0000	
327.4640	-0.860	88231.000	118768.708	4.01 0000	
467.3460	1.006	98053.000	119450.423	4.01 0000	
1209.4000	0.225	88231.000	96499.563	4.01 0000	

11 RECORDS WITH ELEMENT VALUES 4.01 TO 4.01 AND WAVELENGTHS 0 TO 9999

The last two parameters are used to specify records of set element and charge between two defined wavelengths. So beryllium with charge 1 and between wavelengths 200 nm and 500 nm is as follows (note show=2):

```
*
elem 4 c 1 200 500
```

WAVELENGTH(NM)	LOGGF	E LOWER(/CM)	E UPPER(/CM)	ELEM	TEXT
324.7700	-0.888	96498.000	127289.021	4.01 0000	
436.3460	0.493	98053.000	119429.046	4.01 0000	

5 RECORDS WITH ELEMENT VALUES 4.01 TO 4.01 AND WAVELENGTHS 200 TO 500

stop

Stop has no parameters and ends the retrieval session. The output sent to the print queue is now printed out under the user name.

5. DATA ELEMENTS

(a) Wavelength

Wavelength in nanometres of the line

(b) Log gf

The Logarithm (Base 10) of the generalised oscillator strength of the line.

(c) E Lower

The energy of the lower level in cm^{-1} (relative to the ground state).

(d) E Upper

The energy of the upper level in cm^{-1} (relative to the ground state).

(e) Element

The element identification is the atomic number of the element producing the line plus 0.01 times the ionic charge (i.e. 6.03 is C+++ or CIV).

(f) Text

Permits further description of a particular line where required.

ACKNOWLEDGEMENTS

We would like to thank Dr. A. Linas-Gray of University College London and Dr. A.E. Kingston of Queen's University Belfast for introducing us to the problem and for their encouragement and suggestions while the system was being developed.

1. R.L. Kurucz, E. Peytremann and E.H. Avrett, Blanketed Model Atmospheres for Early-Type Stars (Washington: Smithsonian Institution Press, 1974).

2. R.L. Kurucz and E. Peytremann, A table of semiempirical gf values. Research in Space Science SAO Special Report No.362 Smithsonian Institution Astrophysical Observatory, Cambridge, Massachusetts 01238 (1975).

3. User Support Group. Computer User's Guide, Daresbury Laboratory, Daresbury, Warrington WA4 4AD

This appendix of the manual has been split into two subsections. Sub-section A is a description of what a TSO session is and sub-section B describes how to set up a TSO section. Throughout the documentation CR has been used to mean carriage return (use the return key on the VDU).

A. The TSO session

A TSO session is set up when a user logs onto the Daresbury AS/7000 at a terminal. During the session the computer will respond to commands which the user issues from that terminal. Each user has a unique identifier so that the system can keep each session separate from any other users.

The commands issued from the terminal may be standard TSO commands, or commands which have been created for a particular application. Documentation for the full range of TSO commands available is in the computer users guide[3].

The TSO session is terminated when the user logs off. Please note however that there are other ways in which a session may be terminated, for instance a computer failure or in situations where no command has been issued from a terminal for a considerable length of time.

If the user's terminal is not connected directly to the Daresbury AS/7000, or is a Daresbury workstation, then a network call must be made. For further details on accessing the AS/7000 via the SERC networks, see Daresbury Computer Notice 116.

B. Logging on

Once the terminal has been switched on and the green bar has appeared at the bottom left of the screen you may commence typing your commands. If the terminal has been used for a previous session you will see the message:-

```
DARESBURY LABORATORY TERMINAL SYSTEM (DARESBURY NEW-NODE)
ENTER NAME OF SERVICE REQUIRED OR LOCAL COMMAND OR HELP
```

The cursor (green bar) will again be positioned at the bottom left of the screen.

The name of the service you require is TSO so type

TSO CR
and a message appears of the form

```
CALLING REQUESTED SERVICE
CALL ESTABLISHED (USE @Q TO DISCONNECT)
DARESBURY TSO SYSTEM - ENTER LOGON OR LOGOFF -
```

now type

LOGON ID REG(350) CR

where ID is your identifier,
the computer should respond with several lines of information starting
ID LOGON IN PROGRESS .....

The end of the logon messages is indicted by a READY (or MVS) prompt. The prompt is TSO's way of indicating when you may type in commands. Commands may be stacked to a depth of 4.

If you are accessing the database via the Daresbury Terminal Concentrator (TCON) you may at this stage wish to set the line limit for the terminal. The line limit is the number of lines which will be output to the terminal before a prompt to continue from the user is required - for instance if a file of 100 lines is being listed it may be useful to display it in blocks of 20 lines. If the line limit has been set to 20 then after 20 lines of output have appeared on the screen a line of three asterisks (***) will appear and the listing will halt until the user has pressed the carriage return key.

If the line limit is set to 0 then no halts wil occur in the listing. It is suggested that a line limit of 20 is used.

The commands used to set the line limit are:-


```
@L      CR      (enter local command mode)
PL  20  CR      (or PL 0 - the line limit)
```

(the computer should reply with OK at this point)

```
CR  }           (return to normal command mode)
CR
```

The session is now ready for you to enter commands - either the commands specific to the Kurucz-Peytremann database or standard TSO commands. Details of the commands for online interrogation of the database are given in Sections 3 & 4 of this manual.

In summary the commands covered so far are:-

```
TSO   CR
LOGON ID REG(350)  CR
@L     CR
PL  20 CR          Optional - indeed these commands may be entered at
       CR          any point in a TSO Session
       CR
```

Please note that logon may be prevented by

a) A network or host failure (computer not working)
b) Maximum number of users already logged on
   (no more than 50 users may be logged on to TSO at any one time)
c) Not an authorised user (this message usually occurs when you try to logon during a system development session)
d) it is less than half an hour since you finished a TSO session during prime session time (2 pm - 5 pm)

When you have completed your TSO session the command LOGOFF should be used.