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Theoretical Atomic Physics Code Development IV LINES: A Code for Computing Atomic Line Spectra

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THEORETICAL ATOMIC PHYSICS CODE DEVELOPMENT IV

LINES: A Code for Computing Atomic Line Spectra

by

J. Abdallah, Jr. and R. E. H. Clark

ABSTRACT

A new computer program, LINES, has been developed for simulating atomic line emission and absorption spectra using the accurate fine structure energy levels and transition strengths calculated by the (CATS) Cowan Atomic Structure code. Population distributions for the ion stages are obtained in LINES by using the Local Thermodynamic Equilibrium (LTE) model. LINES is also useful for displaying the pertinent atomic data generated by CATS. This report describes the use of LINES. Both CATS and LINES are part of the Theoretical Atomic PhysicS (TAPS) code development effort at Los Alamos.

I. Introduction

Spectroscopic methods are commonly used for plasma diagnostics. The output spectrum provides a fingerprint of the plasma that can be used to determine which ions are present. Sometimes a plasma temperature can be estimated by comparing experimental line ratios to theoretical oscillator strengths.

A large volume of experimental line intensity measurements has been compiled by Kelley and Palumbo.[1] Computer programs have been developed to operate on this data.[2] This data is useful for identifying spectral lines because the positions are usually quite accurate. However, the intensity information is somewhat difficult to interpret because the data often involve different experiments with varying plasma conditions. In addition, the tables do not have entries for all transitions of interest. For some ions, the amount of data available is sparse.

The LINES code has been developed to simulate line spectra as a function of density, temperature, photon energy (or wavelength), and spectrometer resolution. The simulated spectra can be compared to observed spectra to obtain information about the state of the plasma. LINES can also be useful for designing experiments because interesting spectral regions can be predicted before the experiment is performed.

The LINES code uses the accurate atomic energy level and oscillator strength data produced by CATS.[3] Both CATS and LINES are part of the Theoretical Atomic PhysicS (TAPS) project.[4] The theory used by CATS is discussed elsewhere.[5] The level data are used to compute the LTE population distribution by solving the Saha equation[6] for a given plasma density and temperature. The population distribution and oscillator strengths may be appropriately combined to compute emission spectra, absorption coefficients, transmission coefficients, and strengths for individual lines. In addition, configurations, levels, populations, and oscillator strengths can be displayed or written to ASCII files for plotting.[7]

The operation of LINES is discussed in Section II; the various commands are presented in Section III; several examples are presented in Section IV; and the formulas that are used are presented in Appendix I.

II. Operation

A version of LINES that runs on the Los Alamos CRAY/XMP computers can be obtained from the Common File System by using the command:

MASS GET /TAPS/LINES

LINES operates much like the CATS code. Commands to LINES may be entered from input files or directly from the terminal; however, it is usually more convenient to run LINES using an input file. LINES is executed using an input file by entering

LINES I=fname, P=pname

where fname is the input file name, and pname is the print file name. If P=pname is left out, data is written to file P. LINES may be executed interactively from the terminal by entering

LINES I=TTY.

If just

LINES

is entered, then file name I is queried for commands; if I does not exist, control is transferred to the terminal.

Input to LINES is entered in the form of commands that have the format

CNAME v_1 v_2 v_3 ...

where CNAME is the command name, and the v_i are associated values. Command names and values are separated by one or more blanks. All commands and values are entered in lower case. A command may be continued to the next line by using an ampersand (&) as the last character in a line.

A typical sequence of commands may be:

ATOM 30

LOAD ZN

EPLIN 100 1 100

WIDTH EV 1

DNGRD 1.0E18 1.0E19 1.0E20

TEGRD 10

ESPGRD

END

The ATOM command specifies the element of interest.

The LOAD command loads the pertinent atomic physics data from the PARADISE[8] family of files named ZN. These data are generated beforehand using

CATS. Data from all ion stages with atomic numbers equal to 30 are loaded into memory. After loading, a summary display is printed.

The EPLIN command sets up a linear photon energy grid of 100 points between 1 and 100 eV. All spectra will be generated on this grid.

The WIDTH command specifies a 1 eV spectral resolution.

The DNGRD command specifies a number density mesh.

The TEGRD command specifies a temperature grid (in eV).

The ESPGRD command generates emission spectra at the photon energy grid specified for all densities and temperatures specified. All the spectra are written to the specified print file.

The END command terminates the execution of LINES. In the next section we present all the available commands in more detail.

III. Commands

The commands that are available when using LINES are summarized in Table I. Each command appears with its arguments and a reference to a location in this section where a more detailed description can be found. Section III.A describes the parameter setting commands; Sec. III.B describes commands for displaying basic atomic data; Sec. III.C describes the computational commands; and Sec. III.D describes commands that operate on density/temperature grids.

A. Parameter Setting Commands

1. **ATOM z A ρ_0 x_0**

   The ATOM command is used to specify the atomic number (z), the atomic weight (A in grams/mole), initial density (ρ_0 in grams/cubic centimeter), and initial thickness (x_0 in centimeters); values for A, ρ_0, and x_0 need only be entered if transmission calculations are performed.

The ATOM command must be issued before the LOAD command so that data for the desired element are retrieved.

2. SEQ n

   The SEQ command sets the sequence number for use in data retrieval. The default sequence number is 1. The SEQ command must be issued before the LOAD command.

3. LOAD fname

   The LOAD command reads selected data from the family of PARADISE files defined by the family name fname. For example, if fname is ZN, LINES will look for a series of files named ZN, ZN01, ZN01A, ZN01B, ..., ZN02, ZN02A, ZN02B, ..., ZN03, ..., etc., for loading atomic data. Usually it is convenient to have CATS store data for a given ion stage on separate files because these files make the data easier to manage. CATS will create the A, B, C files if more space is needed.

4. FRNG fl fu

   The FRNG command is used to set upper and lower limits on gf values. The default values for fl and fu are 10^{-20} and 10^{300}, respectively. The parameters fl and fu are used by the LOAD command to limit the number of transition strengths read. Often, if fl is set too low, LINES will run out of memory. In addition, any command which displays gf values will be limited to values in the range $fl \leq f \leq fu$. FRNG .01 will modify only fl; FRNG * 1.0 will modify only fu; and FRNG .1 10 will modify both.

5. EPRNG epl epu

   The EPRNG command is used to set the spectral region of interest. The values of epl and epu are specified in eV and these values limit

the amount of transition data used by the LOAD command, and the amount of data printed. Both epl and epu must be entered. The default values for epl and epu are 0 and 10^{300}, respectively.

6. ANGRNG angl angu

   This command is similar to EPRNG except that wavelength in angstroms is specified.

7. IONS iona ionb

   This command limits the range of ion stages used for data loading, displays, and calculations to those having ionicity between iona and ionb. The ion stage numbers are 1 for neutral, 2 for singly ionized, 3 for doubly ionized, etc. If the IONS command is not specified, the limits of the data found by the LOAD command are used.

8. EIRNG eil eiu

   The EIRNG command is used to set lower and upper bounds on individual line strengths. The default values for eil and eiu are 0.0 and 10^{300}, respectively. These parameters are used to limit the number of transitions printed when using the PEI, DEI, PAI, DAI, or PEIGRD commands. The command EIRNG .1 updates only eil, and EIRNG * .8 updates only eiu.

9. INTYPE intype

   If intype is set to NORM (default), all spectra and line intensity information is normalized such that the largest value becomes unity. A value of NONE for intype leaves all spectra in absolute units.

10. EPLIN n el eu

    EPLOG n el eu

    EPLOG n el eu

These commands are used to specify a photon energy grid (in eV) of n points between el and eu. The EPLIN command generates a linear grid, and EPLOG generates a logarithmic grid. The maximum number of photon energies is 1000. The default is a logarithmic grid of 1000 points between 1.0 and 100.0 eV.

11. WIDTH wtype width

The WIDTH command is used to specify line widths (see appendix A). The wtype parameter specifies the width type. Possible values are ANG, EV, or COL. ANG and EV indicate that width is specified in angstroms or electron volts. If COL is specified, LINES uses a hydrogenic collisional line–broadening formula[9] and width is ignored. The default values for wtype and width are EV and 1.0, respectively.

12. DNGRD d_1 d_2 d_3 ...

DNLIN n dl du

DNLOG n dl du

These commands are used to specify a number density mesh (cm^{-3}). DNGRD is used to specify individual densities (d_1, d_2,...). DNLIN and DNLOG construct grids of n points between dl and du, linearly and logarithmically, respectively. The maximum number of densities is 25. The default density grid is 10^{16}, 10^{17}, 10^{18}, 10^{19}, and 10^{20}.

13. TEGRD t_1 t_2 ...

TELIN n tl tu

TELOG n tl tu

These commands are used to specify a temperature grid (in electron volts). TEGRD is used to specify individual temperatures (t_1, t_2, ...). TELIN and TELOG construct grids of n points between tl and tu,

linearly and logarithmically, respectively. The maximum number of temperatures is 50. The default temperature mesh is 5, 10, 15, 20, and 25 eV.

14. ANGGRD λ_1 λ_2 ...

    ANGLIN n λl λu

    ANGLOG n λl λu

    These commands are used to specify a wavelength grid (in angstroms). The ANGGRD command is used to specify individual wavelengths. ANGLIN and ANGLOG construct grids of n points between λl and λu, linearly and logarithmically, respectively. The maximum number of wavelength values is 1000.

15. TCFGS inc ifc

    This command is used to specify initial (inc) and final (ifc) configuration numbers. These parameters limit printed spectral lines to those transitions occurring between configurations inc and ifc. The default for inc and ifc is 0 (print all lines).

B. Displaying Basic Data

The commands in this section display data from the CATS PARADISE files in various formats. The LOAD command must be issued before any of these commands can be used. The user should exercise caution with regard to the amount of output, especially when requesting terminal displays. The FRNG, EPRNG, ANGRNG, EIRNG, IONS, and TCFGS commands may be used to filter out some of the unwanted data.

1. DSUM

   PSUM

These commands print the load summary. This summary is automatically printed out after the LOAD command. DSUM displays the summary at the terminal and PSUM writes it to the print file.

2. DCFGS il iu

   PCFGS il iu

   These commands display the configurations present for various ion stages according to il and iu. If il and iu are not specified, all ion stages are printed. If just il is specified, only that ion stage is printed. If both il and iu are specified, all ion stages between il and iu are printed. DCFGS generates a terminal display, and PCFGS sends the display to the print file.

3. DCON il iu

   PCON il iu

   These commands display the configurations present including sheil–binding energies for various ion stages according to il and iu. If il and iu are not specified, all ion stages present are printed. If just il is specified, only that ion stage is printed. If both il and iu are specified, all ion stages between il and iu are printed. DCON generates a terminal display, PCON sends the display to the print file.

4. DLEVS il iu

   PLEVS il iu

   These commands display the fine structure atomic energy levels for the various ion stages according to il and iu. If il and iu are not specified, all ion stages are printed. If just il is specified, only that ion stage is printed. If both il and iu are specified, all ion stages between il and iu are printed. DLEVS displays the levels at the terminal, and PLEVS sends the display to the print file.

5. DGF il iu

   PGF il iu

   PEF il iu

   PAF il iu

   These commands display oscillator strengths in various formats for the various ion stages according to il and iu. If il and iu are not specified, all ion stages are displayed; if just il is specified, only that ion stage is displayed; and if both il and iu are specified, all ion stages in that range are displayed. DGF displays gf values at the terminal; PGF sends gf to the print file; PEF sends emission f–values to the print file; and PAF sends absorption f–values to the print file. All line displays are subject to the parameters associated with the EPRNG, ANGRNG, and FRNG commands.

6. DGFC ion j jp

   PGFC ion j jp

   These commands display oscillator strengths for all transitions connecting configuration j to configuration jp for a given ion stage (ion). In addition, configuration–to–configurations totals are printed out. DGFC displays values at the terminal, and PGFC sends the display to the print file. The command DGFC will generate the display for all ion stages and configurations. DGFC ion will generate the display for the specified ion stage and all configurations. DGFC il iu will generate the display for all ion stages in the range il to iu for all configurations. PGFC works in the same manner.

7. DCTE il iu

   PCTE il iu

These commands print configurational transition energies for various ion stages according to il and iu. These commands are useful for finding transitions in the spectral range of interest. CATS only needs to be run in the RCN mode to use DCTE and PCTE. If il and iu are not specified, all ion stages are displayed. If just il is specified, only that ion stage is displayed. If both il and iu are specified, all ion stages in that range are displayed. DCTE sends the display to the terminal, and PCTE sends the display to the print file.

C. Computational Commands

The commands of this section require that the LTE command be issued first.

1. LTE d t

   This command generates the LTE population distribution at the number density d (cm^{-3}) and temperature t (eV) for all levels of all ion stages. The population distribution is stored in an internal array. The number of free electrons is printed at the terminal upon completion.

2. POP

   This command is used to display the population distribution generated by the LTE command. The display is sent to the print file.

3. DEI il iu

   PEI il iu

   DAI il iu

   PAI il iu

   The DEI and PEI display emission intensities of individual lines, and DAI and PAI display the relative absorption strength of individual lines at the density and temperature associated with the last LTE command. The lines displayed are subject to the parameters associated with the

EPRNG, ANGRNG, and EIRNG commands. The parameters il and iu are numbers used to select the ion stages to be displayed. If il and iu are not specified, all ion stages are printed; if just il is specified, then only that ion stage is printed; if both il and iu are specified, all ion stages in the range il to iu are displayed. DEI and DAI display lines at the terminal, and PEI and PAI send the display to the print file.

4. DESP

   PESP

   DASP

   PASP

   DESP and PESP generate emission spectra; DASP and PASP generate absorption spectra. All generate spectra on the specified photon energy or wavelength grid corresponding to the density and temperature of the last LTE command. DESP and DASP present results at the user terminal, and PESP and PASP send results to the print file.

D. Temperature/Density Grid–Oriented Commands

The commands of this section perform spectral calculations on the specified density and temperature grids. All data is written to the print file. Densities are entered using the DNGRD, DNLIN, and DNLOG commands; and temperatures are entered using the TEGRD, TELIN, and TELOG commands (see Sec. III.A).

1. EIGRD

   AIGRD

   The EIGRD and AIGRD commands print emission and absorption intensities, respectively, for individual lines at all density and

temperature points. Values printed are subject to parameters of the EPRNG, ANGRNG, EIRNG, and INTYPE commands.

2. ESPGRD

This command generates line emission spectra on the specified photon energy (wavelength) grid for all density and temperature points using the specified line width (see WIDTH command). Spectra may be normalized according to the INTYPE command.

3. ASPGRD

This command generates line absorption coefficients on the specified photon energy (wavelength) grid for all densities and temperatures using the specified line width (see WIDTH command). Spectra may be normalized using the INTYPE command.

4. OPGRD

This command generates absorption coefficients using both bound–bound and bound–free processes. The bound–free cross sections used are those of the astrophysical opacity[10,11] library. The file GREMDB must be present in the user's local file space. It can be obtained from the /TAPS/CFS directory. Absorption coefficients are generated on the specified photon energy (wavelength) grid for all densities and temperatures using the given line width (see WIDTH command). Results may be normalized according to the INTYPE command.

5. TSPGRD

TOPGRD

These commands generate transmission coefficients. TSPGRD uses just CATS bound–bound transitions, and TOPGRD uses both bound–bound and bound–free contributions as in III.D.4. The A, ρ_o, and x_o

parameters of the ATOM command are required. Spectra may be normalized according to the INTYPE command.

6. POPI

It is often useful to check ion stage populations as a function of temperature for a given density. This data may reveal deficiencies in the configuration sets for a given ion stage. If an ion stage never becomes dominant as a function of temperature in LTE, then some important configurations have probably been left out of the CATS run. POPI generates populations for all ion stages at all specified temperatures at density d_i. CURVES[7] can be used to view the populations.

7. ESPT

ESPT generates the emission spectra for various photon energies as a function of temperature. This function is sometimes useful for estimating the temperature of a plasma by comparing calculations to experiment. No more than 10 photon energies (or wavelengths) should be specified when using this option. Spectra may be normalized at each temperature according to the INTYPE command.

IV. Examples

Examples for using LINES are presented in this section. The examples require the presence of the PARADISE files ZN03, ZN04, ZN05, ZN06, ZN07, ZN08, ZN09, ZN10, ZN11, ZN12, ZN13, ZN14, ZN15, and ZN16 in the user's local file space. These files were generated by the CATS code. File ZN03 contains data for ZnIII; ZN04 contains data for ZnIV, etc. These files can be obtained from the CFS directory /TAPS/ZN. Example A. illustrates some commands of

Sec.III.B and uses only file ZN03. Example B. illustrates some commands of Sec.III.C, and example C. illustrates some commands of Sec.III.D.

A. This example of LINES is used to print some of the basic data from the file ZN03 during an interactive session (Fig. 1).

The ATOM command is used to specify zinc as the element of interest.

The LOAD command is used to load data from ZN03.

The DCFGS is used to display the configurations; the energy of the ground configuration is taken to be 0. The parameter IP is the ionization potential (eV).

The DSUM command is issued to redisplay the load summary. NCF is the number of configurations, NLEV is the number of levels, and NGF is the number of level–to–level dipole–allowed transitions.

The DCON command displays more information about the configurations, i.e., the binding energies (in eV) for each shell.

The DLEVS command is used to display the levels. For each level, the level number, ion number, configuration number, configuration, term designator, J–value, and energy (in eV) are printed.

The DGF command prints the gf–values for all level–to–level transitions. For each transition, the wavelength (in angstroms), photon energy (in eV), gf value, lower configuration number, lower level number, lower term designator, lower J-value, upper configuration number, upper level number, upper term designator, and upper J–value are printed. All commands that list individual transitions present the level of lower energy first.

The DGFC command lists the three transitions involving levels of configurations 1 and 3. The parameter e is the average energy (eV) of the levels for configuration 1; ep is the average energy of levels for configuration 3; et is the average transition energy, ANG is the wavelength in angstroms; g is the statistical

```
lines i=tty
? atom 30
atom 30
? load zn03
load zn03
        ***load summary***
   iz  ion  ncf nlev     ngf
   30    3    4   21       7
? dcfgs
dcfgs
1
  ion    3
   cn      ev        configuration       ip =  4.2457e+01
    1       0.0000  1s2  2s2  2p6  3s2  3p6  3d10
    2    1030.9420  1s2  2s2  2p5  3s2  3p6  3d10 4s1
    3    1047.7231  1s2  2s2  2p5  3s2  3p6  3d10 4d1
    4    1209.0008  1s2  2s1  2p6  3s2  3p6  3d10 4p1
? dsum
dsum
        ***load summary***
   iz  ion  ncf nlev     ngf
   30    3    4   21       7
? dcon
dcon
iz     =  30
ion    =   3
configuration no.  1 eav = -4.882937e+04
-----------------------------------------
  n  l  w         ev
  1  0  2.  9.7577e+03
  2  0  2.  1.2559e+03
  2  1  6.  1.0876e+03
  3  0  2.  1.7935e+02
  3  1  6.  1.2729e+02
  3  2 10.  4.2457e+01


configuration no.  2 eav = -4.779843e+04
-----------------------------------------
  n  l  w         ev
  1  0  2.  9.8476e+03
  2  0  2.  1.2990e+03
  2  1  5.  1.1453e+03
  3  0  2.  1.9279e+02
  3  1  6.  1.4039e+02
  3  2 10.  5.4006e+01
  4  0  1.  2.9838e+01


configuration no.  3 eav = -4.778165e+04
-----------------------------------------
  n  l  w         ev
  1  0  2.  9.8529e+03
  2  0  2.  1.3040e+03
  2  1  5.  1.1504e+03
  3  0  2.  1.9776e+02
  3  1  6.  1.4554e+02
  3  2 10.  5.9174e+01
```

```
  4  2  1.  1.2963e+01

configuration no.  4 eav = -4.762037e+04
----------------------------------------
  n  l  w        ev
  1  0  2.  9.8324e+03
  2  0  1.  1.3071e+03
  2  1  6.  1.1324e+03
  3  0  2.  1.9303e+02
  3  1  6.  1.4199e+02
  3  2 10.  5.5870e+01
  4  1  1.  2.2122e+01


? dlevs
dlevs
1
  lev ion  configuration                                        ls  j      energy
   1:  3:  1:1s2  2s2  2p6  3s2  3p6  3d10                  1s) 1s 0.0  0.0000e+00
   2:  3:  2:1s2  2s2  2p5  3s2  3p6  3d10 4s1             2p) 3p 2.0  1.0230e+03
   3:  3:  2:1s2  2s2  2p5  3s2  3p6  3d10 4s1             2p) 1p 1.0  1.0231e+03
   4:  3:  3:1s2  2s2  2p5  3s2  3p6  3d10 4d1             2p) 3p 0.0  1.0398e+03
   5:  3:  3:1s2  2s2  2p5  3s2  3p6  3d10 4d1             2p) 3p 1.0  1.0398e+03
   6:  3:  3:1s2  2s2  2p5  3s2  3p6  3d10 4d1             2p) 3f 4.0  1.0398e+03
   7:  3:  3:1s2  2s2  2p5  3s2  3p6  3d10 4d1             2p) 3f 3.0  1.0398e+03
   8:  3:  3:1s2  2s2  2p5  3s2  3p6  3d10 4d1             2p) 3p 2.0  1.0398e+03
   9:  3:  3:1s2  2s2  2p5  3s2  3p6  3d10 4d1             2p) 1d 2.0  1.0399e+03
  10:  3:  3:1s2  2s2  2p5  3s2  3p6  3d10 4d1             2p) 3d 3.0  1.0399e+03
  11:  3:  3:1s2  2s2  2p5  3s2  3p6  3d10 4d1             2p) 1p 1.0  1.0400e+03
  12:  3:  2:1s2  2s2  2p5  3s2  3p6  3d10 4s1             2p) 3p 0.0  1.0466e+03
  13:  3:  2:1s2  2s2  2p5  3s2  3p6  3d10 4s1             2p) 3p 1.0  1.0467e+03
  14:  3:  3:1s2  2s2  2p5  3s2  3p6  3d10 4d1             2p) 3f 2.0  1.0634e+03
  15:  3:  3:1s2  2s2  2p5  3s2  3p6  3d10 4d1             2p) 3p 2.0  1.0635e+03
  16:  3:  3:1s2  2s2  2p5  3s2  3p6  3d10 4d1             2p) 3f 3.0  1.0635e+03
  17:  3:  3:1s2  2s2  2p5  3s2  3p6  3d10 4d1             2p) 3d 1.0  1.0635e+03
  18:  3:  4:1s2  2s1  2p6  3s2  3p6  3d10 4p1             2s) 3p 0.0  1.2089e+03
  19:  3:  4:1s2  2s1  2p6  3s2  3p6  3d10 4p1             2s) 3p 1.0  1.2089e+03
  20:  3:  4:1s2  2s1  2p6  3s2  3p6  3d10 4p1             2s) 3p 2.0  1.2090e+03
  21:  3:  4:1s2  2s1  2p6  3s2  3p6  3d10 4p1             2s) 1p 1.0  1.2091e+03
? dgf
dgf
start     ion    3
c   lam(ang)       ev       gf-value
       10.26  1.2091e+03  1.2962e-02   1:   1:2s2 2p6 3s2 3p6 3d10(1s) 1s 0.0 --   4:  21:2p6 3s2 3p6 3d104p1 (2s) 1p 1.0
       10.26  1.2089e+03  2.7552e-03   1:   1:2s2 2p6 3s2 3p6 3d10(1s) 1s 0.0 --   4:  19:2p6 3s2 3p6 3d104p1 (2s) 3p 1.0
       11.66  1.0635e+03  1.3701e-02   1:   1:2s2 2p6 3s2 3p6 3d10(1s) 1s 0.0 --   3:  17:2p5 3s2 3p6 3d104d1 (2p) 3d 1.0
       11.85  1.0467e+03  2.0896e-03   1:   1:2s2 2p6 3s2 3p6 3d10(1s) 1s 0.0 --   2:  13:2p5 3s2 3p6 3d104s1 (2p) 3p 1.0
       11.92  1.0400e+03  2.6162e-02   1:   1:2s2 2p6 3s2 3p6 3d10(1s) 1s 0.0 --   3:  11:2p5 3s2 3p6 3d104d1 (2p) 1p 1.0
       11.93  1.0398e+03  4.1954e-04   1:   1:2s2 2p6 3s2 3p6 3d10(1s) 1s 0.0 --   3:   5:2p5 3s2 3p6 3d104d1 (2p) 3p 1.0
       12.12  1.0231e+03  4.3440e-03   1:   1:2s2 2p6 3s2 3p6 3d10(1s) 1s 0.0 --   2:   3:2p5 3s2 3p6 3d104s1 (2p) 1p 1.0
? dgfc 3 1 3
dgfc 3 1 3
start     ion,i,ip=    3   1   3
c   lam(ang)       ev       gf-value
       11.66  1.0635e+03  1.3701e-02   1:   1:2s2 2p6 3s2 3p6 3d10(1s) 1s 0.0 --   3:  17:2p5 3s2 3p6 3d104d1 (2p) 3d 1.0
       11.92  1.0400e+03  2.6162e-02   1:   1:2s2 2p6 3s2 3p6 3d10(1s) 1s 0.0 --   3:  11:2p5 3s2 3p6 3d104d1 (2p) 1p 1.0
       11.93  1.0398e+03  4.1954e-04   1:   1:2s2 2p6 3s2 3p6 3d10(1s) 1s 0.0 --   3:   5:2p5 3s2 3p6 3d104d1 (2p) 3p 1.0
```

```
c    e          0.000000e+00          ep         1.047723e+03          et         1.047723e+03
c    ang        1.183525e+01          g          1.000000e+00          gp         6.000000e+01
c    sumgf      4.028295e-02          sumf       4.028295e-02          sumfp      6.713825e-04
? dcte
dcte
start     configurational transition energies for ion  3
        ang          ev
     738.930       16.781    2:2p5  3s2  3p6  3d10 4s1  --  3:2p5  3s2  3p6  3d10 4d1
      76.886      161.278    3:2p5  3s2  3p6  3d10 4d1  --  4:2p6  3s2  3p6  3d10 4p1
      69.640      178.059    2:2p5  3s2  3p6  3d10 4s1  --  4:2p6  3s2  3p6  3d10 4p1
      12.028     1030.942    1:2s2  2p6  3s2  3p6  3d10 --  2:2p5  3s2  3p6  3d10 4s1
      11.8[illegible]5  1047.723    1:2s2  2p6  3s2  3p6  3d10 --  3:2p5  3s2  3p6  3d10 4d1
      10.256     1209.001    1:2s2  2p6  3s2  3p6  3d10 --  4:2p6  3s2  3p6  3d10 4p1
? end
end
 stop
lines    ctss time    14.139     seconds
cpu=     .170   i/o=    8.388   mem=    5.581

 all done
```

Figure 1: Sample interactive session corresponding to Ex. IV.A using LINES to display basic data.

weight of configuration 1; gp is the statistical weight of configuration 3; sumgf is the sum of gf values; sumf is sumgf/g; and sumfp is sumgf/gp.

The DCTE command displays configuration–to–configuration transition energies.

B. Figure 2 shows an example of LINES using some commands of Sec.III.C. LINES reads the command file EXB and echoes the information back to the terminal during execution. All output is written in file PXB.

The LOAD command specifies zinc as the element of interest.

EPRNG and FRNG are used to limit the amount of transition data LINES will load. Only those transitions with energies between 980 and 1120 eV and gf values greater than or equal to 10^{-3} are loaded.

The LOAD command loads data from the family of ZN files. The load summary is displayed at the terminal.

The LTE command is used to calculate the population distribution at a number density of $10^{19}cm^{-3}$ and a temperature of 20 eV. The calculated number of free electrons per atom is displayed at the terminal.

The POP command is used to print the population distribution.

The EIRNG command is used to set the lower bound on–line strength for printing. Note that the maximum normalized line strength is unity.

The PEI and PAI commands are used to print normalized (INTYPE NORM) line strengths for emission and absorption, respectively. Figures 3 and 4 show the respective printed output. Note that the 1041 eV $2p(^3H_4) - 3d(^2I_4)$ transition of Zn IX is predicted to be the strongest individual line.

The INTYPE forces spectral calculations in default units (see Appendix A).

The WIDTH command forces CATS to use hydrogenic line–broadening widths.

```
lines i=exb,p=pxb
atom 30
eprng 980 1120
frng 1.0e-3
load zn
        ***load summary***
   iz  ion  ncf nlev     ngf
   30    3    4   21       4
   30    4    7  149     107
   30    5    7  603     841
   30    6    7 1494    3583
   30    7    7 2616    5429
   30    8    7 3173    3216
   30    9    7 2860    2992
   30   10    7 2130   64002
   30   11    7 1703   37684
   30   12    8 1211   16960
   30   13    9  840    2531
   30   14   12 1651   19883
   30   15   11 2494   46967
   30   16   11 2717   41078
lte 1.0e19 20
 no free electrons =   7.654867
pop
eirng .2
pei
pai
intype none
width col
eplin 500 980 1120
pesp
pasp
width ev 1
pesp
pasp
end
 stop
lines    ctss time   117.917     seconds
cpu=   68.124   i/o=    4.407   mem=   45.386
```

Figure 2: Execution of LINES for Ex. IV.B.

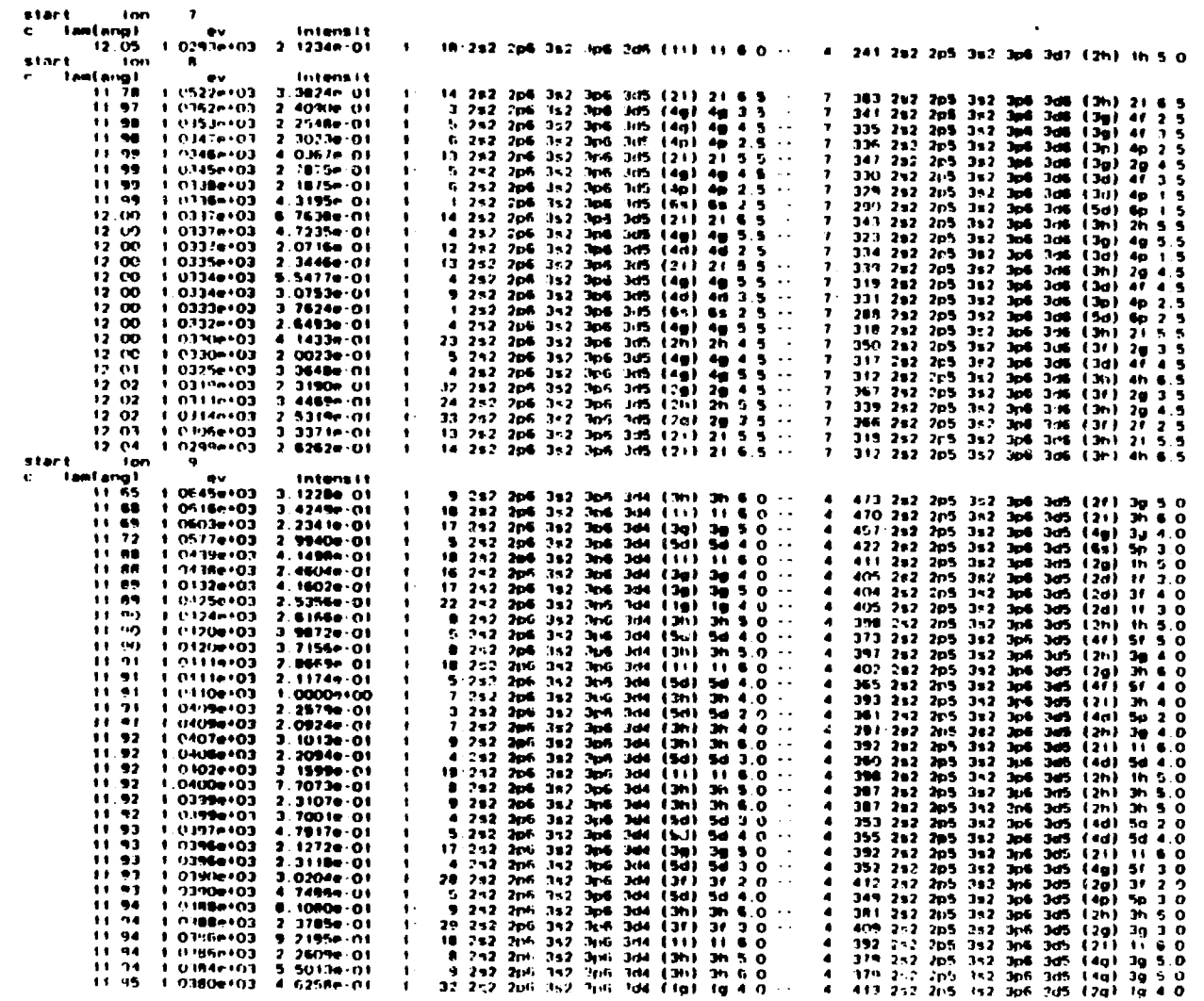

Figure 3: Normalized emission line strengths corresponding to Ex. IV.B.

```
11.95  1.0379e+03  2.6064e-01  1:  20:2s2 2p6 3s2 3p6 3d4 (3d) 3d 2.0 --   4: 388:2s2 2p5 3s2 3p6 3d5 (4d) 3p 2.0
11.95  1.0377e+03  2.5057e-01  1:   8:2s2 2p6 3s2 3p6 3d4 (3h) 3h 5.0 --   4: 370:2s2 2p5 3s2 3p6 3d5 (4g) 3g 4.0
11.95  1.0376e+03  3.9034e-01  1:   9:2s2 2p6 3s2 3p6 3d4 (3h) 3h 6.0 --   4: 371:2s2 2p5 3s2 3p6 3d5 (2h) 3i 7.0
11.95  1.0375e+03  2.0653e-01  1:   7:2s2 2p6 3s2 3p6 3d4 (3h) 3h 4.0 -    4: 368:2s2 2p5 3s2 3p6 3d5 (4g) 3g 3.0
11.95  1.0373e+03  3.8325e-01  1:  11:2s2 2p6 3s2 3p6 3d4 (3f) 3f 3.0 --   4: 370:2s2 2p5 3s2 3p6 3d5 (4g) 3g 4.0
11.96  1.0371e+03  2.7660e-01  1:  16:2s2 2p6 3s2 3p6 3d4 (3g) 3g 4.0 --   4: 376:2s2 2p5 3s2 3p6 3d5 (2i) 1h 5.0
11.96  1.0369e+03  2.6171e-01  1:  12:2s2 2p6 3s2 3p6 3d4 (3f) 3f 2.0 --   4: 368:2s2 2p5 3s2 3p6 3d5 (4g) 3q 3.0
11.96  1.0367e+03  2.7806e-01  1:   7:2s2 2p6 3s2 3p6 3d4 (3h) 3h 4.0 --   4: 362:2s2 2p5 3s2 3p6 3d5 (2i) 3i 5.0
11.97  1.0358e+03  2.4814e-01  1:  22:2s2 2p6 3s2 3p6 3d4 (1g) 1g 4.0 --   4: 376:2s2 2p5 3s2 3p6 3d5 (2i) 1h 5.0
11.97  1.0358e+03  2.2815e-01  1:  13:2s2 2p6 3s2 3p6 3d4 (3f) 3f 4.0 --   4: 359:2s2 2p5 3s2 3p6 3d5 (4g) 5f 3.0
11.97  1.0357e+03  2.9020e-01  1:   8:2s2 2p6 3s2 3p6 3d4 (3h) 3h 5.0 --   4: 354:2s2 2p5 3s2 3p6 3d5 (2i) 3i 6.0
11.98  1.0352e+03  2.7496e-01  1:  17:2s2 2p6 3s2 3p6 3d4 (3g) 3g 5.0 --   4: 360:2s2 2p5 3s2 3p6 3d5 (4d) 5d 4.0
11.98  1.0352e+03  2.0863e-01  1:  13:2s2 2p6 3s2 3p6 3d4 (3f) 3f 4.0 --   4: 355:2s2 2p5 3s2 3p6 3d5 (4d) 5d 4.0
11.98  1.0349e+03  2.0064e-01  1:  29:2s2 2p6 3s2 3p6 3d4 (3f) 3f 3.0 -    4: 397:2s2 2p5 3s2 3p6 3d5 (2h) 3g 4.0
11.99  1.0340e+03  2.2500e-01  1:  18:2s2 2p6 3s2 3p6 3d4 (1i) 1i 6.0 --   4: 358:2s2 2p5 3s2 3p6 3d5 (2i) 1k 7.0
11.99  1.0339e+03  3.2074e-01  1:  32:2s2 2p6 3s2 3p6 3d4 (1g) 1g 4.0 --   4: 398:2s2 2p5 3s2 3p6 3d5 (2h) 1h 5.0
```

Figure 3, continued

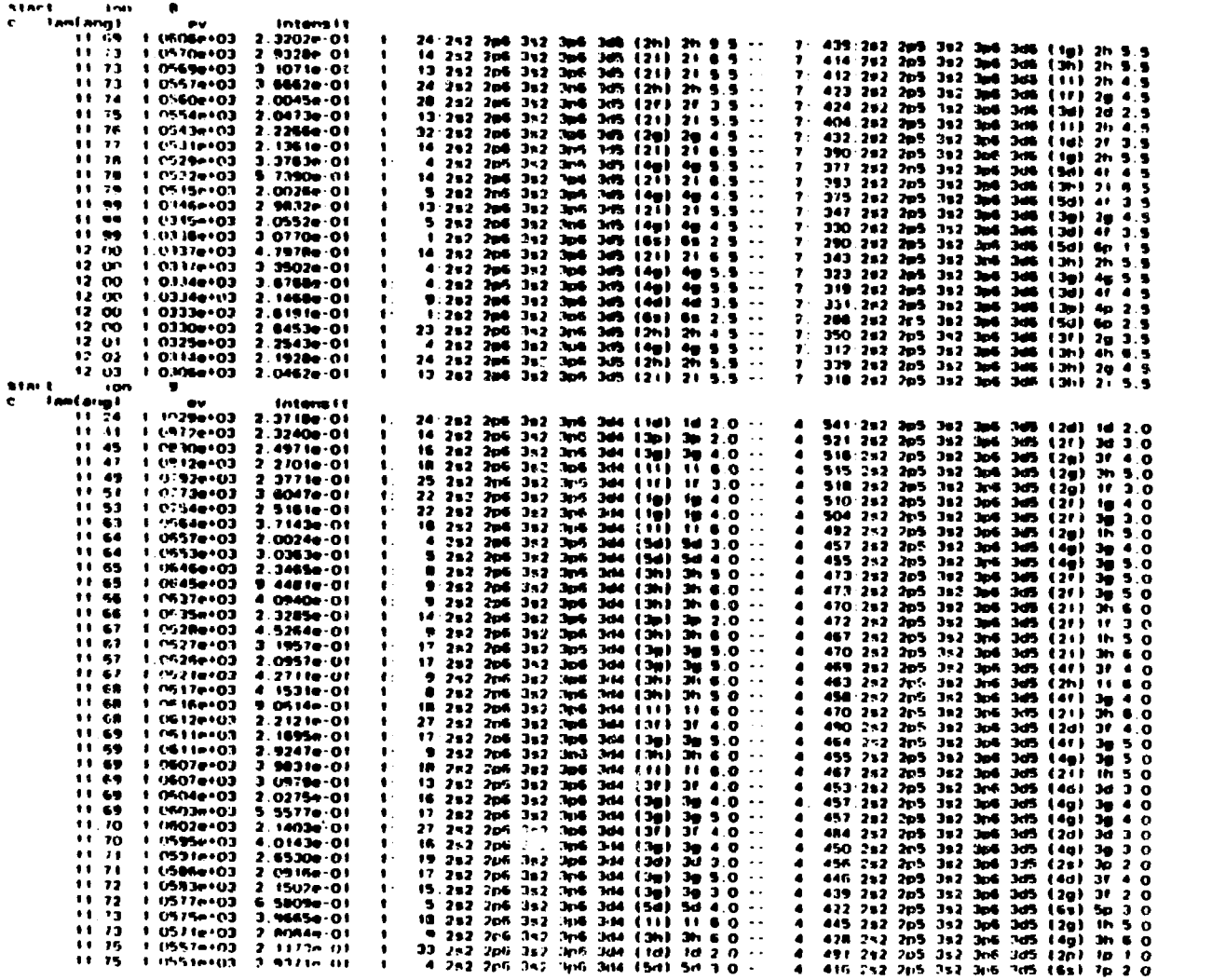

Figure 4: Normalized absorption line strengths corresponding to Ex. EV.B.

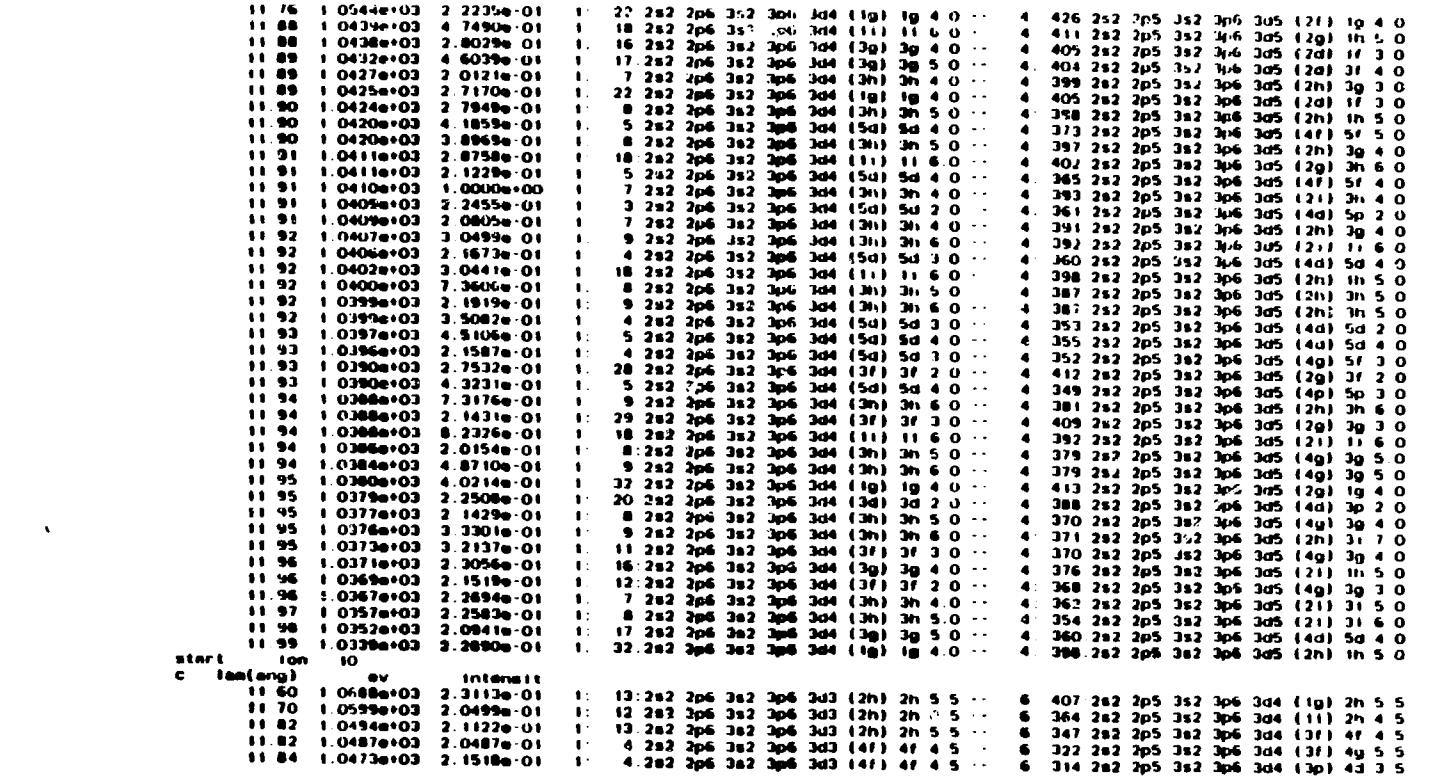

Figure 4, continued

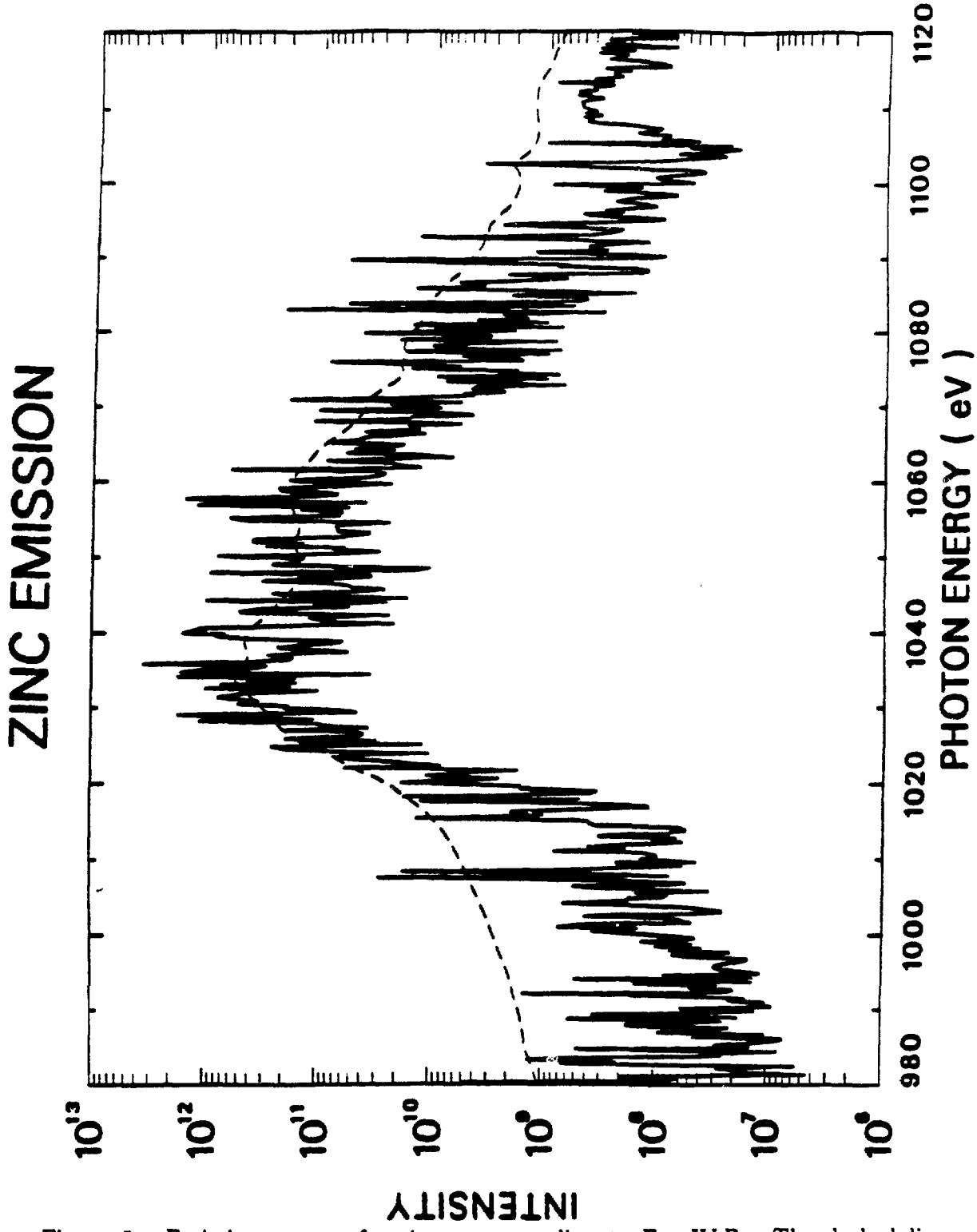

Figure 5: Emission spectra for zinc corresponding to Ex. IV.B. The dashed line corresponds to the 1 eV line width case, and the solid line corresponds to line widths calculated using the hydrogenic collision–broadening formula.

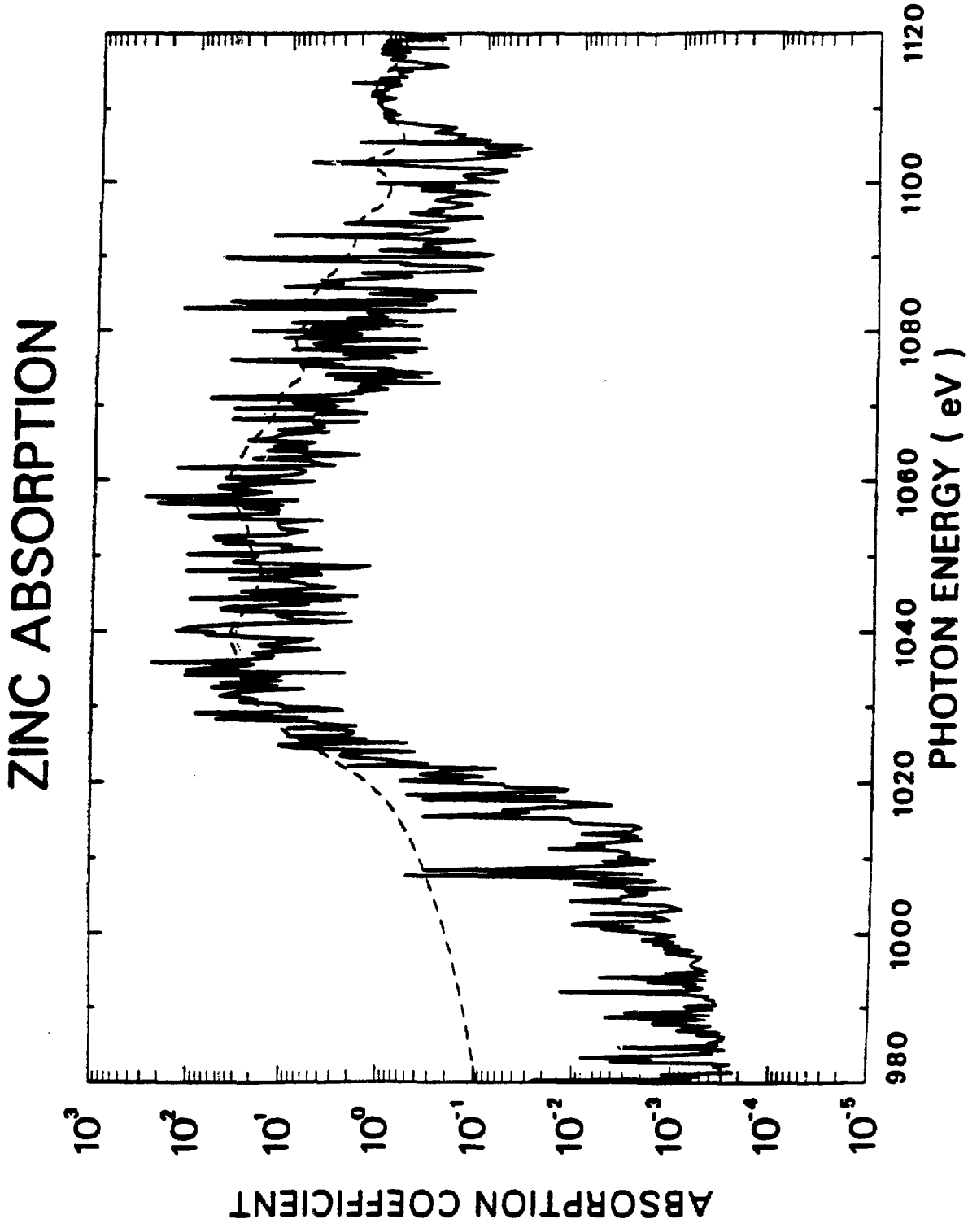

Figure 6: Absorption spectra for zinc corresponding to Ex. IV.B. The dashed line corresponds to the 1 eV line width case, and the solid line corresponds to line widths calculated in the hydrogenic collision–broadening formula.

```
lines i=exc,p=pxc / 10 1
atom 30
eprng 980 1120
eplin 500 980 1120
intype none
frng 1.0e-3
load zn
        ***load summary***
   iz  ion  ncf nlev     ngf
   30    3    4   21       4
   30    4    7  149     107
   30    5    7  603     841
   30    6    7 1494    3583
   30    7    7 2616    5429
   30    8    7 3173    3216
   30    9    7 2860    2992
   30   10    7 2130   64002
   30   11    7 1703   37684
   30   12    8 1211   16960
   30   13    9  840    2531
   30   14   12 1651   19883
   30   15   11 2494   46967
   30   16   11 2717   41078
telin 50 1 50
dngrd 1.0e19
popi
tegrd 10 20 30 40 50
aspgrd
espgrd
end
 stop
lines     ctss time    177.533      seconds
cpu=    99.248    i/o=     8.339    mem=    69.946
```

Figure 7: Execution of LINES for Ex. IV.C.

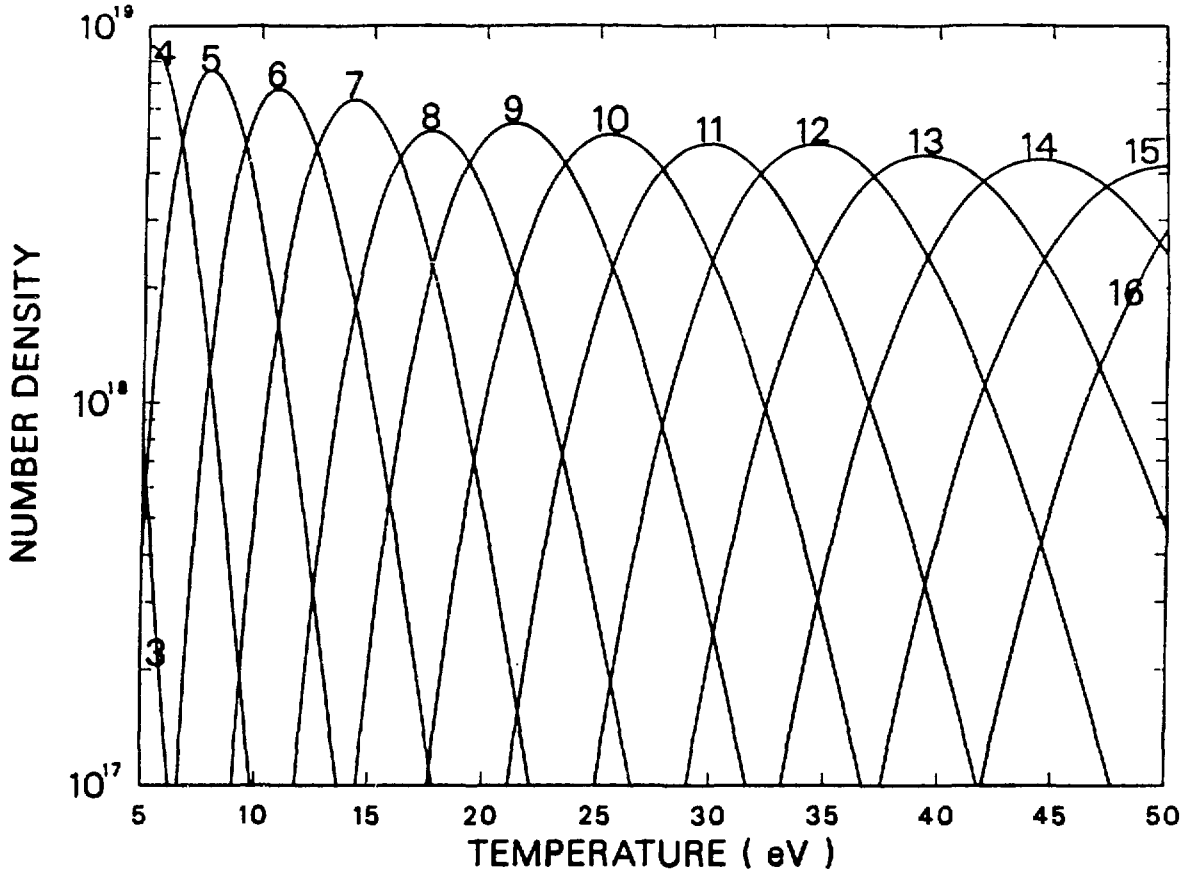

Figure 8: Number densities of the various ion stages as a function of temperature as generated by Ex. IV.C. Each curve is labeled by ionicity.

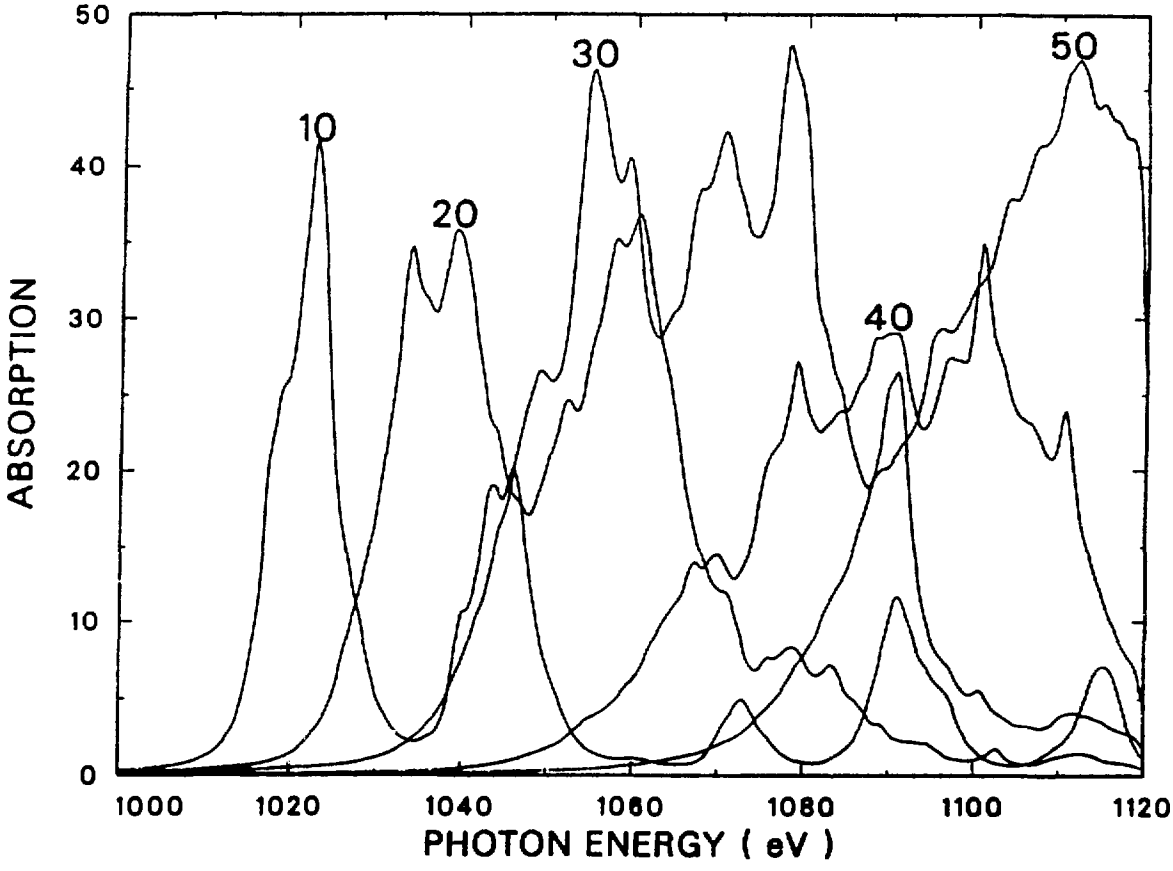

Figure 9: Absorption coefficient as a function of photon energy for various temperatures corresponding to Ex. IV.C.

The PESP and PASP calculate and print the emission and absorption spectra, respectively.

The WIDTH command changes all line widths to a constant 1 eV.

The PESP and PASP commands are used again to compute and print the spectra with the new width. Figure 5 compares the resulting emission spectra for both resolutions, and Fig. 6 compares the same for absorption.

C. Figure 7 shows an example of LINES using some commands of Sec.III.D. Input is read from file EXC and output is written to file PXC. The ATOM, EPRNG, EPLIN, INTYPE, FRNG, and LOAD commands have the same effect as in example B.

The TELIN command is used to define a temperature grid of 50 points between 1 and 50 eV.

The DNGRD command is used to set the desired number density.

The POPI command computes the ion stage populations as a function of temperature (as defined by the TELIN command) for the specified number density. The results of this calculation are shown in Fig. 8. Each curve is labelled by ion stage.

The TEGRD command is issued to redefine the temperature mesh.

The ASPGRD and ESPGRD commands calculate the absorption and emission spectra as the specified number density (10^{19}) and temperatures (10, 20, 30, 40, and 50 eV). The results obtained from the ASPGRD command are presented in Fig. 9. Each curve is labelled by temperature.

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Appendix I

A. Emission Spectra

The number of photons emitted per unit time, per unit volume, per unit energy interval for a transition at given photon energy is given by:

$$U_{nn'} = N_n \frac{8\pi^2 e^2}{h^2 c^2 m} (h\nu_o)^2 \frac{g_{n'}}{g_n} f_{n'n} \frac{W/\pi}{(h\nu - h\nu_o)^2 + W^2} \quad (1)$$

where n labels the upper level, n′ labels the lower level, N_n is the number density of the upper level, e is the electron charge, h is the Planck constant, c is the speed of light, m is the electron mass, $h\nu_o$ is the transition energy, $g_{n'}$ is the statistical weight of the lower level, g_n is statistical weight of the upper level, $f_{n'n}$ is the oscillator strength for the n′ to n transition, $h\nu$ is the photon energy, and W is the line width. For the present purpose, we use line widths as discussed in III.A.11. The total energy emitted per unit time, per unit volume, per unit energy interval is obtained by multiplying $U_{nn'}$ by the transition energy and summing over all transitions of all ion stages. The quantity calculated by LINES is

$$S_e(h\nu) = 1.380845 \times 10^7 \sum_{nn'} N_n \frac{g_{n'}}{g_n} f_{n'n} (h\nu_o)^3 \frac{W}{(h\nu - h\nu_o)^2 + W^2} \quad (2)$$

which has units eV per cm^3, per second, per unit energy interval eV with photon energies and widths given in eV.

B. Individual Emission Line Intensity

The intensity of an individual line is obtained by multiplying $U_{nn'}$ by $h\nu_o$ and integrating over photon energy. Using the normalization

$$\int_o^\infty \frac{(W/\pi)dh\nu}{(h\nu - h\nu_o)^2 + W^2} = 1 \quad (3)$$

the line intensity is given by

$$I_{nn'} = 4.338053\times10^{17}\ (h\nu_o)^3\ \frac{g_{n'}}{g_n}\ f_{n'n}\ \left(\frac{eV}{cm^3\cdot sec}\right) \tag{4}$$

where $h\nu_o$ is specified in eV.

C. Absorption Coefficient

The probability of absorbing a photon of energy $h\nu$ for a given transition is proportional to

$$\mu_{n'n} = N_{n'}\ \frac{he^2\pi}{mc}\ f_{n'n}\ \frac{W/\pi}{(h\nu-h\nu_o)^2 + W^2} \tag{5}$$

where $N_{n'}$ is the number density of the lower state. The unit for $\mu_{n'n}$ is inverse distance (cm^{-1}). The total probability is obtained by summing over all absorbers

$$S_a(h\nu) = 3.49426\times10^{-17}\sum_{n'n} N_{n'}f_{n'n}\ \frac{W}{(h\nu-h\nu_o)^2 + W^2}\ (cm^{-1}) \tag{6}$$

where $N_{n'}$ is specified in units of cm^{-3}, and widths and photon energies are specified in eV.

D. Absorption Strength for Individual Lines

Eq. 5 can be integrated over photon energy to obtain the strength of an individual transition:

$$I_{n'n} = 1.0977554\times10^{-16}N_{n'}f_{n'n}\ (eV\ cm^{-1}). \tag{7}$$

E. Transmission

When light of intensity I_o is passed through a layer of plasma of thickness x, the resulting intensity may be expressed as

$$I = I_o\ \exp(-S_a x)\ . \tag{8}$$

The transmission is then given by

$$T = I/I_o = \exp(-S_a x)\ .$$

The thickness x of the plasma is estimated from the number density N using the 1–D hydrodynamic relationship

$$xN = x_o N_o$$

where x_0 is the initial thickness of the sample, and N_0 is the initial number density.

Appendix II

Table I

LINES COMMANDS

AIGRD	D.1
ANGGRD λ_1 λ_2 λ_3...	A.14
ANGLIN n $\lambda\ell$ λu	A.14
ANGLOG n $\lambda\ell$ λu	A.14
ANGRNG angl angu	A.6
ASPGRD	D.3
ATOM z A ρ_o x_o	A.1
DAI iℓ iu	C.3
DASP	C.4
DCFGS iℓ iu	B.2
DCON iℓ iu	B.3
DCTE iℓ iu	B.7
DEI iℓ iu	C.3
DESP	C.4
DGF iℓ iu	B.5
DGFC ion j jp	B.6
DLEVS iℓ iu	B.4
DNGRD d_1 d_2 d_3...	A.12
DNLIN n dℓ du	A.12
DNLOG n dℓ du	A.12
DSUM	B.1
EIGRD	D.1
EIRNG eiℓ eiu	A.8

LINES COMMANDS, Cont'd.

EPLIN n eℓ eu	A.10
EPLOG n eℓ eu	A.10
EPRNG epℓ epu	A.5
ESPGRD	D.2
ESPT	D.7
FRNG fℓ fu	A.4
INTYPE intype	A.9
IONS iona ionb	A.7
LOAD fname	A.3
LTE d t	C.1
OPGRD	D.4
PAF iℓ iu	B.5
PAI iℓ iu	C.3
PASP	C.4
PCFGS iℓ iu	B.2
PCON iℓ iu	B.3
PCTE iℓ iu	B.7
PEF iℓ iu	B.5
PEI iℓ iu	C.3
PESP	C.4
PGF iℓ iu	B.5
PGFC ion j jp	B.6
PLEVS iℓ iu	B.4
POP	C.2
POPI	D.6

LINES COMMANDS, Cont'd.

PSUM	B.1
SEQ n	A.2
TCFGS inc ifc	A.15
TEGRD t_1 t_2 t_3...	A.13
TELIN n tℓ tn	A.13
TELOG n tℓ tn	A.13
TOPGRD	D.5
TSPGRD	D.5
WIDTH wtype width	A.11