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*Theoretical Atomic Physics
Code Development I
CATS: Cowan Atomic Structure Code*

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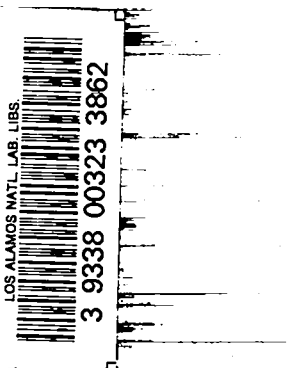
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ABSTRACT

An adaptation of R. D. Cowan's Atomic Structure program, CATS, has been developed as part of the Theoretical Atomic Physics (TAPS) code development effort at Los Alamos. CATS has been designed to be easy to run and to produce data files that can interface with other programs easily. The CATS produced data files currently include wave functions, energy levels, oscillator strengths, plane-wave-Born electron-ion collision strengths, photoionization cross sections, and a variety of other quantities. This paper describes the use of CATS.

I. Introduction

A. TAPS

Level energies are required to calculate the level populations for ions present in a plasma that can be described by Local Thermodynamic Equilibrium (LTE). In addition, if line spectra or opacities are desired, then oscillator strengths and photoionization cross sections consistent with the level energies are also required. If the plasma is not in LTE (NLTE), then populations are described by a set of rate equations whose coefficients involve all the atomic processes present. Usually the rate coefficients or cross sections are calculated from semi-empirical formulas or

simple models. Sometimes a small amount of experimental data or theoretical results is available. These data are usually not complete, consistent, or in a conveniently usable form for a NLTE rate code. The purpose of the Theoretical Atomic Physics (TAPS)¹⁻⁴ code development effort at Los Alamos is to bridge the gap between simple models and sparse sets of more accurate data by providing a collection of computer programs for conveniently calculating the quality atomic data needed by LTE opacity codes and NLTE rate codes.

The programs being developed under the TAPS project have the following common requirements:

- 1) The codes should be easy to run. Users need not be experts in atomic physics to run the codes. All codes are command driven and can be run interactively from terminals or from input files. Required input is minimized with many default values provided.

- 2) All codes operate on a common easy access data file structure. The TAPS codes use PARADISE files⁵ to store and retrieve atomic data. A standard file format facilitates code interfacing.

- 3) TAPS codes generate atomic physics data in the greatest detail possible. When such detail is not necessary, programs are provided to perform averages. For example, TAPS programs (CATS and ACE) store data based on fine structure levels; if quantities based on multiplet terms or configurations are desired, then the fine structure data is averaged.

- 4) The source coding for the programs will not be released, thus reducing the proliferation of individual versions. Instead, the developers will work with users to provide the options that are needed.

- 5) All TAPS programs are primarily intended for use on Los Alamos supercomputers. We have made use of local software for memory managing and random access file capabilities. Although these dependencies have made the codes less portable, we are able to use the local computers efficiently and conveniently both

for small jobs and very large ones that produce megawords of data. The future generations of computers will make the TAPS programs even more appealing because increased speed and memory may allow plasmas to be modeled entirely by rigorous atomic structure calculations.

6) The initial atomic methods chosen for TAPS produce the large volume of data required for plasma modeling using a realistic amount of computer time. As TAPS evolves, more sophisticated methods may be incorporated.

The following codes are currently being developed under the TAPS project:

The CATS code is an adaptation of R. D. Cowan's atomic structure programs.⁶⁻⁸ CATS is the foundation of the TAPS system because it supplies data to the other components. The detailed use of CATS is described in the remainder of this manual.

The ACE (Another Collisional Excitation) code is used to generate more accurate (and more expensive) electron-ion collision strengths than can be obtained from CATS. However, ACE still requires atomic structure data from CATS for bound wavefunctions and energy levels. ACE is described in a separate paper.²

The TAPS code is used to display data generated by CATS and ACE. Graphical displays, terminal displays, and print files are available. The use of TAPS is described in a separate paper.³

The LINES code uses the energy levels and oscillator strengths produced by CATS to predict line emission and absorption spectra based on LTE population distributions. The use of LINES is described in a separate paper.⁴

The NERD code is being developed to solve the NLTE rate equations in time-dependent and in steady state modes using CATS and ACE data. NERD is not yet available for general use.

B. CATS

Bob Cowan's computer programs⁶⁻⁸ for computing the electronic structure of atoms and ions have been recognized for many years. The programs compute wavefunctions, energy levels, oscillator strengths, photoionization cross sections, plane-wave Born (PWB) collision strengths and autoionization rates for arbitrary ions and configurations. These programs calculate multiconfiguration Hartree-Fock wave functions, including relativistic corrections and vector coupling of angular momentum. CATS was developed to adapt these programs to the supercomputers at Los Alamos in the TAPS environment while preserving the atomic physics. CATS is the backbone of the TAPS system.

First, the three separate codes RCN, RCN2, and RCG were incorporated as overlays in CATS. RCN calculates the atomic self-consistent-field radial wavefunctions. RCN2 computes various integrals from these functions. These integrals are passed to RCG which performs the angular momentum algebra and configuration interaction to calculate the atomic structure data. The file interfaces between these codes were replaced by common blocks. The large memory available did not justify having three separate programs.

The column oriented input was replaced by blank delimited commands. Many parameters that required specification were given default values. Consequently, only a few commands are necessary to run CATS.

Output was made more convenient for interfacing with other codes by storing atomic data on PARADISE files.⁵ These files are random access binary files that also contain directory information. Data are stored and retrieved by specification of keywords. Data records have been conveniently formatted for use by other programs.

A memory managing package⁹ was implemented to avoid dimension changes and subsequent code recompilation for different problems. Memory managing subroutines make it possible to calculate array sizes at execution time and then to allocate the

exact amount of space needed. Memory managing in CATS is exceedingly important because it is difficult to estimate array sizes in Cowan's code for a given set of configurations before the code runs. This memory management also allows CATS to run at optimum size for a given problem.

Several hand operations were automated in CATS. CATS automatically separates configurations by parity. The user need not worry about the order in which configurations are entered. CATS computes the powers needed for PWB calculations. Blocked output was introduced so that dimensions do not restrict the number of oscillator strengths or PWB cross sections that could be calculated. Scale factors for radial integrals are estimated¹⁰ by CATS for a given atomic number and charge.

A typical example of running CATS is presented in Section II. Section III describes the more commonly used commands. Appendix A presents rarely used commands, most of which update default values of parameters in Cowan's original programs.

Appendix B describes the PARADISE file data records generated by CATS. The theoretical methods used have been discussed elsewhere⁶ and will not be presented here.

II. A Typical Example

A version of CATS that operates on the Los Alamos Cray XMP computers may be obtained from the Common File System (CFS) by using the command:

```
MASS GET /TAPS/CATS
```

Although CATS may be run interactively it is usually more convenient to run it using an input file because a list of configurations must be typed. CATS is executed using an input file by entering:

```
CATS I=IN3
```


where IN3 is a CATS input file. IN3 must be present in the users local file space. A sample CATS input file is presented below. If an interactive session is desired then

CATS I=TTY

is entered. If just

CATS

is entered, the program looks for a file named I for input, if none is found control is transferred to TTY.

A typical input file consists of a set of commands with optional parameter settings. Each command has the format

CNAME val₁ val₂ ...

where CNAME is the command name and the val_i are associated values. Command names and values are separated by one or more blanks. A command may be continued to the next line by entering an & as the last character of the current line.

The following sample input file may be used to run CATS.

```
ION 7 3
PWB
RCF
1S2 2S2 2P1
1S2 2S1 2P2
1S2 2P3
1S2 2S2 3S1
1S2 2S2 3P1
1S2 2S2 3D1
/
DEST N3
OPEN N3
RUN
CLOSET
END
```

The ION command specifies doubly ionized nitrogen as the ion stage of interest. Note that detailed descriptions of all commands are given in Sec. III. The PWB command tells CATS to calculate plane-wave Born collision strengths. The RCF command is used to enter configurations. Configurations are entered one per line.

The "/" is used to indicate the end of the configuration list. The DEST command is used to destroy any existing N3 file. The OPEN command specifies N3 as the PARADISE output file. The RUN command executes the atomic structure code for the specified configurations. The CLOSET command closes and truncates the PARADISE file N3. The END command terminates execution of CATS.

Upon completion N3 contains the atomic structure data that may be displayed using TAPS³ or LINES.⁴ Reference 3 presents some of the data generated by this example. The N3 file can be used to calculate distorted-wave collision strengths using ACE² or to compute atomic spectra with the LINES code.⁴ All printed information is written to CATSOUT. Also several files named TAPEnn may be used during the execution of CATS where nn = 31, 32, 20, 41, 72, 73, 74, 3, 19, 69, and 13.

III. Commands

A. Parameter Setting Commands

1. ION z i

The ION command is used to specify the ion stage of interest, where z is the atomic number and i is the ionicity (1 = neutral, 2 = singly ionized, etc.) For example, ION 7 3, specifies doubly ionized nitrogen. The ION command also invokes computation of the radial integral scale factors; these values are then displayed at the user's terminal. The ION command must be entered before any execution commands.

2. SEQ n

The SEQ command is used to set the sequence number. Each execution command generates data sets that are referenced by z, i, and n. The sequence number was introduced to distinguish data for the same z and i on the same PARADISE file. The sequence number is set to 1 each time

an ION command is invoked and incremented by every execution of a RUN command. The SEQ command is used only if another sequencing scheme is desired.

3. FACT $s_1 s_2 s_3 s_4 s_5$

The FACT command is used to override the radial integral scale factors calculated by the ION command. An * may be entered for any scale factor the user wishes to remain the same. The FACT command is useful for fitting energy levels to experimental data. FACT * 0 * * 0 sets the spin orbit and CI scale factors to 0. See Ref. 7 for more details.

4. DFACT

The DFACT command displays the current radial integral scale factor values.

5. RCF

The RCF command is used to specify configurations. The RCF command must be invoked before an execution command. Configurations are specified one per line after the RCF line:

1S2 2S2 2P1

1S2 2S1 2P2.

Each orbital is separated by blanks and given by nLw, where n is the principal quantum number, L is the character designation (S, P, D, F, ...) for orbital angular momentum, and w is the occupation number. Continuum orbitals are specified by

1S2 2S2 99L1 e

where e is the free electron energy in Rydbergs. If e is not specified, then a set of continuum configurations

1S2 2S2 99L1 e_i

is generated where the e_i is specified using the EC, ECLIN, and ECLOG commands below. The default e_i values are 0.1, 0.5, 1.0, 5.0 and 10 eV. A record with a / in column 1 terminates the configuration list.

6. EC $e_1 e_2 e_3 \dots$

The EC command specifies continuum electron energies. Energy is specified in eV. The maximum number of energies is 10.

7. ECLIN n ecl ecu

The ECLIN command sets up linear grid of n continuum energies between ecl and ecu. Energy is specified in eV, and the maximum value of n is 10.

8. ECLOG n ecl ecu

The ECLOG command sets up a log grid of n continuum energies between ecl and ecu. Energy is specified in eV and the maximum value of n is 10.

9. PWB

The PWB command is used to signal CATS to perform plane-wave Born collision strengths. PWB 0 turns these calculations off. The PWB command must be entered before entering an execution command. PWB calculations are not done by default.

B. Data File Management Commands

1. OPEN fname

The OPEN command opens the PARADISE file fname for CATS output. An OPEN or OPEND command must be invoked before an execution command if PARADISE files are desired. If fname exists in the users local file space, then data is added to fname. If fname does not exist, it is created. If the data generated exceeds the length of the file, a new file

is created by appending the letter A to fname. Additional files may be created by appending letters in alphabetical order to fname. This set of files is called a family.

2. DEST fname

The DEST command destroys the family of files specified by fname.

3. OPEND fname

The OPEND command is a combination of DEST and OPEN. The user is insured of getting a fresh copy of fname on successive runs of CATS.

4. LDAT lin

The LDAT command is used to specify the length in words of PARADISE file data space. The default is 6,000,000 words.

5. CLOSE

The CLOSE command is used to close a PARADISE file. The file is not truncated to its actual data size so that other data may be added on subsequent executions of CATS. All execution commands invoked after the OPEN or OPEND commands and before the CLOSE or CLOSET command are added to that file.

6. CLOSET

The CLOSET command is used to close a PARADISE file. The file is truncated to its actual data size. If a CLOSE or CLOSET command is not invoked, the END command closes and truncates the current PARADISE file.

7. MBGF mbgfd mbgfb

The MBGF Command specifies the number of transitions per block (record) for output on PARADISE files. The factor mbgfd is used when only dipole oscillator strengths are calculated, and mbgfb is used when PWB computations are performed. The default value for mbgfd is 50,000, and the default value for mbgfb is 2,000.

8. GFLOW gfl

The GFLOW command specifies the lowest gf value to be stored on the PARADISE files. The option is exercised only when PWB calculations are not being performed. The default value for gfl is 10^{-30} .

C. Execution Commands

1. RCN

The RCN command runs the RCN segment of CATS.

2. RCN2

The RCN2 command runs the RCN and RCN2 segments successively.

3. RCG

RUN

These commands run the complete sequence of RCN, RCN2, and RCG segments.

D. Photoionization Commands

1. RUNPI

The RUNPI command initiates a photoionization calculation for each configuration entered by means of the RCF command. RUNPI ionizes one electron from each shell going to all possible continua. The photon energy grid is determined from values of x , specified by commands below. The photon energy ($h\nu$) is related to x by

$$x = \frac{h\nu}{\phi}, \quad h\nu > \phi$$

where ϕ is the ionization energy. The default for x is a logarithmic grid of 10 points between 1.1 and 100. The maximum number of x values is 10. The photoionization calculations can get into trouble for values of x

near unity and for large values of x . Cross sections based on initial fine structure levels are obtained.

2. XPI $x_1 x_2 \dots$

Specify x values for photoionization calculations.

3. XPILIN $n x_l x_u$

Specify a linear grid of n x -values between x_l and x_u .

4. XPILOG $n x_l x_u$

Specify a logarithmic grid of n x -values between x_l and x_u .

E. Miscellaneous Commands

1. BUFTTY

Holds messages from CATS to TTY in a buffer that gets flushed when full. This command saves time when CATS is run from a controller.

2. ISHELL mode

A new shell ordering scheme was introduced in RCN2 to correct a problem in Cowan's code. The ISHELL OLD command will force CATS to use Cowan's shell ordering. This forcing command may be useful for comparison runs. The ISHELL NEW command will revert CATS back to using the new shell ordering scheme. NEW is default.

3. REFC yon

When sets of configurations only differ in principle quantum numbers between RUN commands, the angular factors do not change and need not be recalculated. The REFC NO command is used to prevent the recalculation of coefficients. The REFC YES command is used to revert CATS back to calculating the coefficients. YES is default.

4. SAMPON

SAMPOFF

The SAMPON and SAMPOFF commands are used to perform timing studies in CATS. Sampling begins when the SAMPON command is issued and terminates when the SAMPOFF command is issued. The sampling information is written to disk file CATSTL which can be used by the TALLY utility to find out where computer time was spent.

5. IRRU yon

If the command IRRU YES is invoked, the starting potential is taken from the internal data statement for each configuration. IRRU NO forces CATS to use the final potential from the previous configuration as the starting potential. NO is default.

Appendix A: More Commands

Commands described in this section correspond to input parameters for Cowan's original code. Explanations of these parameters have been extracted from Refs. 7 and 8. Please consult these references for more information.

1. ITPOW itpow

If itpow =1 or ≥ 3 , print SCF iteration information,
 ≥ 2 , call POWER to print $\langle r^m \rangle$.

The default value for itpow is 2.

2. IPTVU iptvu

If iptvu ≥ 1 , print F^k and G^k ;
 ≥ 2 , print Coulomb interaction energies;
 ≥ 3 , print wavefunction overlap integrals;
 ≥ 4 , print HFS potentials (RU, RUEE, etc.);
 ≥ 5 , print HX potentials ($V^{n\ell}$);
 ≥ 6 , in SCHEQ, print relativistic contribution to potential.

The default value for iptvu is 0.

3. IPTEB ipteb

If ipteb ≥ 1 , print EE, JJJ, R(JJJ), AZ;
 ≥ 2 , print E_{kin} , et.

The default value for ipteb is 0.

4. NORBPT norbpt

If norbt < 0 , do not print wavefunctions;
 > 0 , print first two and last NORBPT wavefunctions
at every fifth mesh point.
 ≥ 6 , print continuum wavefunctions at every mesh point.

(for configurations 1, 5, 10, 15, ... only, if $0 < \text{NORBPT} < 6$
any, write on tape 2 or 7 the last $|\text{NORBPT}|$ wavefunctions)
(at least 2; if $|\text{NORBPT}|=9$, write all wavefunctions)

The default value for norbpt is -9.

5. IHF ihf

If ihf =0, signifies RCN calculation only; do not load HF8 program;
=1, skip all RCN calculations of radial integrals if $\text{IREL} > 1$; if
 $\text{IREL} = 0$ and $\text{TOLEND} < 1.0\text{E-}4$, call only ZETA1 (to
calculate relativistic energy correction for HF E_{av});
=2, carry out a HF calculation within RCN.

The default value for ihf is 2.

6. IBB ibb

If ibb $\neq 0$, sets the outer boundary of the atom at mesh point ibb;
do not use this option!

The default value for ibb is 0.

7. TOLSTB tolstb

The default value for tolstb is 1.0.

8. TOLKM2 tolkm2

Tolerance for switching from HFS to HF or HX.

The default value for tolkm2 is 1.0.

9. TOLEND tolend

The parameter tolend is the maximum permissible value of DELTA (change in
the absolute value of RU) for ending the SCF iteration (RCN32, statements
number 530-550, 700-780).

10. THRESH thresh

The parameter thresh is the maximum permissible fractional change in the value of the eigenvalue E to end the eigenvalue iteration (SCHEQ, 805 and 205).

The default value for thresh is 10^{-11} .

11. EXF10 exf10
KUT kut
KUTD kutd
EXFM1 exfm1
CAO cao
CA1 ca1

The parameter exf10 is the coefficient of Slater's exchange term for an HFS calculation with no tail cutoff (KUT = 1) or with tail cutoff (KUT = 0). Slater's original value is exf10 = 1.5; exf10 = 1.0 is Kohn and Sham's modified value.

The parameters exfm1, cao, and ca1 are values of k_1 , k_2 , k_3 , respectively, for KUT = -1 [HX calculation; Phys. Rev. 163, 54 (1967) eqs. (13) - (14) or Cowan's book, eqs. (7.49) - (7.50)]; exfm1 = 0.0 will give a Hartree calculation for kut = -1; kut = -2 gives an HS calculation.

Default values for exf10, kut, kutd, exfm1, cao, and ca1 are 1.0, 0, -2, .65, .5, and .7, respectively.

12. IREL irel

If irel = 0, relativistic terms are omitted from the differential equations (HX and HF); if irel = 1 or 2 or 3, they are included (HXR and HFR); if irel > 3, some diagnostic printouts will occur. A value of irel = 3 is supposedly better than irel = 1 for HX, but it sometimes leads to instabilities present in HXR that are not present with irel = 1; the difference lies only in numerical

methods used in calculating dV/dr . If $irel = 2$, approximate Briet magnetic and retardation energies will be included (provided the dimensions of QNL are the same as those of PNL). The default value for $irel$ is 1.

13. MAXIT maxit

The parameter maxit is the maximum allowable number of SCF iterations; if convergence is not obtained, the calculation is continued for 4 more cycles with diagnostic printout if $npr \geq 0$.

The default value for maxit is 30.

14. NPR npr

IF $npr \neq 0$, diagnostic potentials and diagnostic wavefunctions are printed during the course of the RCN SCF iteration.

The default value for npr is 0.

15. EMAX emax

EVMAX evmax

A continuum wavefunction is computed when the last orbital defined on the configuration card is singly occupied and specified by "99S", "99P", "99D", etc., followed by a positive eigenvalue (in Rydbergs).

The quantity emx should have a value equal (approximately) to the largest value of e (see RCF command) contained on any of the configuration lines. The action of emx is to change the radial integration mesh $R(I)$ which is set up: instead of

$$\Delta R \equiv R(I) - R(I-1)$$

being doubled at mesh points 41, 81, 121, 161, ..., no further doubling is done after ΔR becomes $\geq (2.5\sqrt{emx})^{-1}$. This insures that the mesh interval will not become so large but that there will still be about 10 mesh points within each half-wavelength of the continuum function, even at large R .

It is necessary, of course, that the dimension of the integration mesh be great

enough, or that `emx` be small enough, so that sufficiently large radii can be reached: the value of "F" printed via Format 97 of SCHEQ should not differ from unity by more than about 0.1. The required dimension is usually quite large: In place of the 561, 601, or 641 that is sufficient for bound functions, RCN uses 1801.

Use of an inappropriate value of `emx` usually causes convergence failures or causes execution to terminate on an overflow. If `emx` is not specified, CATS will choose a default value equal to the largest input value of `e` on configuration lines.

EVMAX allows the user to enter `emax` in electron volts.

16. ALFMIN `alfmin`

ALFMAX `alfmax`

The parameters `alfmin` and `alfmax` are iteration control variables⁷.

Default values for both are 1.0.

17. NBIGKS `nbigks`

The number of momentum transfer values for plane-wave-Born calculations.

The default value for `nbigks` is 41.

18. EAV11 `eav11`

The parameter `eav11` is the value desired for the center-of-gravity energy E_{av} of the first configuration (in units of 1000 cm^{-1}). It merely shifts the energy scale of all energy levels calculated by RCG.

The default value for `eav11` is 0.

19. IQUAD `iquad`

The parameter `iquad` causes electric-quadrupole radial integrals to be computed for configurations of the first, second, or both parities according as `equad` = 1, 2, or 3; its value is also transferred to RCG.

The default value for `iquad` is 0. Electric quadrupole transitions are calculated only when `ispecc` ≥ 0 . These transition strengths are not currently stored on PARADISE files.

20. `IMAG imag`

If `imag` > 0 , calculate magnetic-dipole transitions for the first, second or both parities, according as `imag` = 1, 2, or 3.

The default value for `imag` is 0. Magnetic dipole transitions are calculated only when `ispecc` ≥ 0 . These transitions are not currently stored on PARADISE files.

21. `IENGYD iengyd`

IF `iengyd` = 0, print full energy matrix;
= 1, do not print matrix;
= 2, print first `nevmas` rows and columns;
 > 2 , print first $11 \cdot iengyd$ rows and columns.

The default value for `iengyd` is 1.

22. `ISPECC ispecc`

if `ispecc` = 1, 3, 5, or 7, print spectrum lines sorted by levels of first parity;
= 2, 3, 6, or 7, print lines sorted by levels of second parity;
= 4 to 8, print lines sorted by wavelength;
 ≥ 8 , call `lvdist` and `wndist` (wavelength-sort printed if 8, no line-list printed if 9);
(must be 2, 3, 6, 7, 8, or 9 to obtain values of `BRNCH`).
= -1 to obtain spectral and PWB information on PARADISE files.
For this case the `ispecc` ≥ 0 printouts are not generated.

The default value for `ispecc` is -1.

23. ISLI isli

- If isli = 0, print all SLI2 output;
- = 1, omit restore and most printout;
- = 2. omit all but final parameter values that are printed unscaled as well as scaled;
- = 3, omit all printout.

The default value for isli is 2.

24. IDIP idip

- If idip = 7, values of R^k and dipole integrals in Rydberg series will be modified appropriately for pseudodiscrete calculations.
- = 8, modifications are automatically made for simple photoionization calculations in RCG.
- ≥ 9 , values of E_{av} , R^k , and dipole integrals involving continuum functions will be modified appropriately for perturbation calculation of autoionization transition probabilities in program RCG.

The default value for idip is 9.

25. KCPLD kcpld(1) kcpld(2) ... kcpld(9)

kcpld(I) If > 0 , do not print eigenvectors in the representation I (I = 1 to 7). See Ref. 7.

kcpld(9) \equiv IPRINT: If ≥ 7 , delete energy matrix print;
if ≥ 8 , delete all eigenvector and purity prints;
if = 9, delete eigenvalue and A^a prints;

The default value for kcpld(1) through kcpld(7) is 1 and the default value for kcpld(9) is 9.

26. FLB flbdn flbdx

The variables flbdn and flbdx specify the minimum and maximum wavelengths (in Å) of spectrum lines to be retained. These values are used for ispecc \geq 0 only. The default values are .001 and 500,000 respectively.

27. DELEKEV delekev

The parameter delekev is used in subroutine WNDIST. Its default value is .00025 keV. WNDIST is used only if ispecc \geq 8.

Appendix B: Data Structure

Each data record stored on PARADISE files produced by CATS is referenced by

- z = integer atomic number,
- i = integer ion stage,
- s = integer sequence number,
- c = 1 word character descriptor,
- q = optional qualifier.

The following table describes the various stored data and the associated character descriptor and qualifier.

| <u>c</u> | <u>q</u> | <u>description</u> |
|----------|----------------------|---|
| CONFIG | configuration number | Configuration energy (eV), principal quantum numbers, orbital angular momentum quantum numbers, occupation numbers and binding energies (eV) for all shells. |
| MESH | | Number of radial mesh points. |
| RMESH | | Radial mesh array (bohr). |
| WF | configuration number | Radial wavefunction for each shell and mesh point. |
| KS | | Dimension of stored shell arrays. |
| SHELLORD | | Principal quantum number and orbital angular momentum quantum number for all participating shells, of all configurations. The size is $2 \times NC \times KS$, where NC is the number of configurations. |

| | |
|--------|---|
| NLSJ | The total number of levels. |
| E | Energy level array in increasing order of energy (eV). The size is NLSJ. |
| CFG | The dominant configuration number for each level. |
| L | The total orbital angular momentum L of the dominant term for each level. |
| S | The total spin S of the dominant term for each level. |
| J | The total angular momentum quantum number J for each level. |
| DES | A one-word character description for each level. |
| DQ | Index to the dominant basis level for each energy level. |
| NOSUBC | The total number of participating subshells. |
| NCFG | Configuration number for each basis level. |
| SCRL | Script L values for each shell of each basis level (size is NOSUBC*NLSJ). |
| SCRS | Script S value for each shell of each basis level. |
| BLL | Block L value for each shell of each basis level. |
| BLS | Block S value for each shell of each basis level. |
| BLV | Block v or seniority number for each shell of each basis level. |

| | | |
|---------|---------------|---|
| MEIGV | | Order of each eigenvector matrix. The number of matrices is the number of J and parity combinations. |
| EIGVEC | matrix number | Eigenvector matrix. |
| LEVEIGV | | Points to the energy level corresponding to each eigenvector (size is NLSJ). |
| BLOCKS | | Contains blocking information for transition records, including the blocking factor, the total number of blocks, the total number of transitions, and the starting block number for dipole gf values. |
| LEV | block number | Array of initial level numbers. |
| LEVP | block number | Array of final level numbers. |
| PWBCS | block number | Array of collision strength values. |
| GF | block number | Array of gf values. |
| XPWB | | Array of energies (in threshold units) for PWB calculations. |
| RDIPOLE | | Array of configuration-to-configuration reduced dipole matrix elements. |
| NCDIP | | Array of initial configuration numbers corresponding to RDIPOLE. |
| NCDIPP | | Array of final configuration numbers corresponding to RDIPOLE. |

The following data records are generated for the RUNPI command.

| <u>c</u> | <u>q</u> | <u>description</u> |
|----------|----------------------|--|
| PICB | configuration number | Array containing control information, i.e., the number of photon energies, the number of shells for the configuration, and the number of initial levels. |
| XPI | | Array of photon energies in threshold units. |
| SJPIL | configuration number | Array of J values for each initial level. |
| EIL | configuration number | Ionization energy from each shell for each level. |
| EIC | configuration number | Ionization energy from each shell. |
| PICSL | configuration number | Cross sections for photoionization from each shell and initial level at all photon energies. |
| PICSC | configuration number | Cross section for photoionization from each shell of the configuration at all photon energies. |

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