



ATBASE User's Guide

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1. Introduction

ATBASE is a suite of FORTRAN 77 computer codes used for generating large-scale high quality basic atomic data. It includes the following eight codes:

(1) ATBASE: This is the main segment of the package. It is a configuration-interaction code with Hartree-Fock wavefunctions. It computes atomic radial wavefunctions, atomic energy levels, transition oscillator strengths, photoionization cross sections, and autoionization rates.

(2) STATE: This code sets up the input table of configurations for the ATBASE calculation.

(3) DWBORN: This code computes collision strengths for electron-impact excitation by using a distorted wave Born method.

(4) ATTABLE: This code does data organization for the basic data outputted from ATBASE and/or DWBORN, computes all related rate coefficients, and creates an atomic model (i.e., detailed formatted atomic data tables) for applications.

(5) MICPSSR: This code computes ion impact ionization cross sections (for both single and multiple ionization processes).

(6) BEAMTAB: This code generates a formatted data table for ion impact ionization cross sections.

(7) CKFYED: This code does large scale calculations for fluorescence yields.

(8) CKFTAB: This code generates a formatted data table for fluorescence yields.

In order to generate an atomic model for a specific problem, these codes must be run in a chain in one of the following combinations:

(1) STATE/ATBASE/ATTABLE

(2) STATE/ATBASE/DWBORN/ATTABLE

(3) STATE/ATBASE/ATTABLE/CKYED/CKFTAB

(4) STATE/ATBASE/DWBORN/ATTABLE/CKYED/CKFTAB

(5) STATE/ATBASE/ATTABLE/MICPSSR/BEAMTAB/CKYED/CKFTAB

(6) STATE/ATBASE/DWBORN/ATTABLE/MICPSSR/BEAMTAB/CKYED/CKFTAB

This report is intended to be a “user’s guide” for the ATBASE package. Thus, the focus here will be on the structure of the relevant codes and how to use them in setting up an atomic model for applications (e.g., for CRE calculations, or equations of state and opacity calculations). Detailed discussions of the relevant theoretical models can be found elsewhere [1,2].

Sections 2 through 9 of this report provide detailed descriptions for programs ATBASE, STATE, ATTABLE, DWBORN, CKFYED, MICPSSR, CKFTAB, and BEAMTAB. Section 10 presents step by step demonstrations for how to run the codes in a chain manner to set up formatted atomic data tables.

2. Computer Code ATBASE

2.1. Program Outline

This is a code for the calculations of atomic structure (radial wavefunctions $P_{nl}(r)$ and energy levels) and radiative transition properties (oscillator strengths, photoionization cross sections, and autoionization rates). Atomic data of four different level structures are calculated simultaneously:

- (1) fine structure (nlLSJ),
- (2) term structure (nlLS),
- (3) configuration average structure (nl),
- (4) complex average structure (n).

Depending on the specific problem, the user can make a selection for level structures. Before doing atomic structure calculations, the user should determine what kind of level structure is suitable for the application. For example, if the purpose of atomic structure calculation is for generating data tables for equation of state and opacity calculations, then configuration average structure is usually a proper structure. However, for detailed spectral analyses, LS term structure or even fine structure is required.

This code is based on the modification of three of Cowan's atomic physics codes (RCN, RCN2, and RCG) [2,3] and Fischer's multiconfiguration Hartree-Fock program (MCHF) [4]. The fine structure levels (nLSJ) of a many-electron atomic system are evaluated within the framework of a configuration interaction (CI) treatment, while the term structure levels (nLS) are calculated by taking a proper averaged summation over the relevant fine structure levels.

As shown in Figure 1, ATBASE consists of four blocks: primary input, self-consistent-field calculation, CI calculation with intermediate-coupling scheme, and primary output. There are 53 data files involved in the whole calculation. These files can be classified into three groups: input files, intermediate data files, and final output files. A detailed classification for these files is given in Table 1.

2.2. Primary Input

To run ATBASE, the user needs to provide the following information:

- (1) specify atomic system,
- (2) specify physical models,
- (3) specify calculation parameters.

The basic input structure for ATBASE is shown in Figure 2. The primary input consists of four input files:

- (1) `atbase.inp` — a namelist input file which contains all computation switches and parameters.
- (2) `config.inp` — a formatted data input file which specifies atomic system to be calculated. This file can be generated by running STATE.
- (3) `hygen_cfg` — a formatted data file which contains all the hydrogenic states for the system. This file can also be generated by running STATE.
- (4) `ev.expdat` — a formatted data input file which contains experimental data for atomic energy levels. This is an optional input. This file should be provided only if the user wants to incorporate experimental data in the calculation.

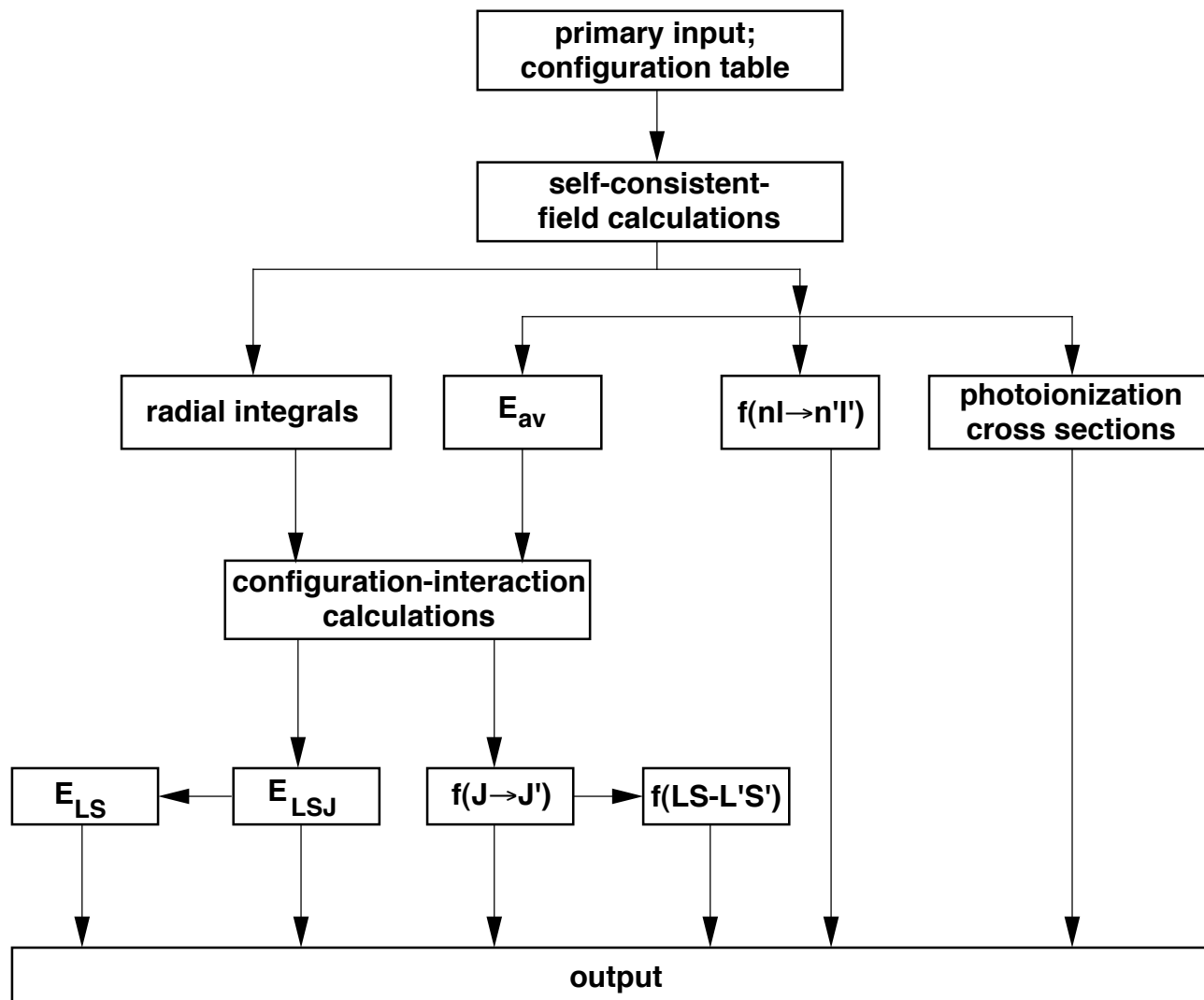


Figure 1. Flow diagram for ATBASE calculations.

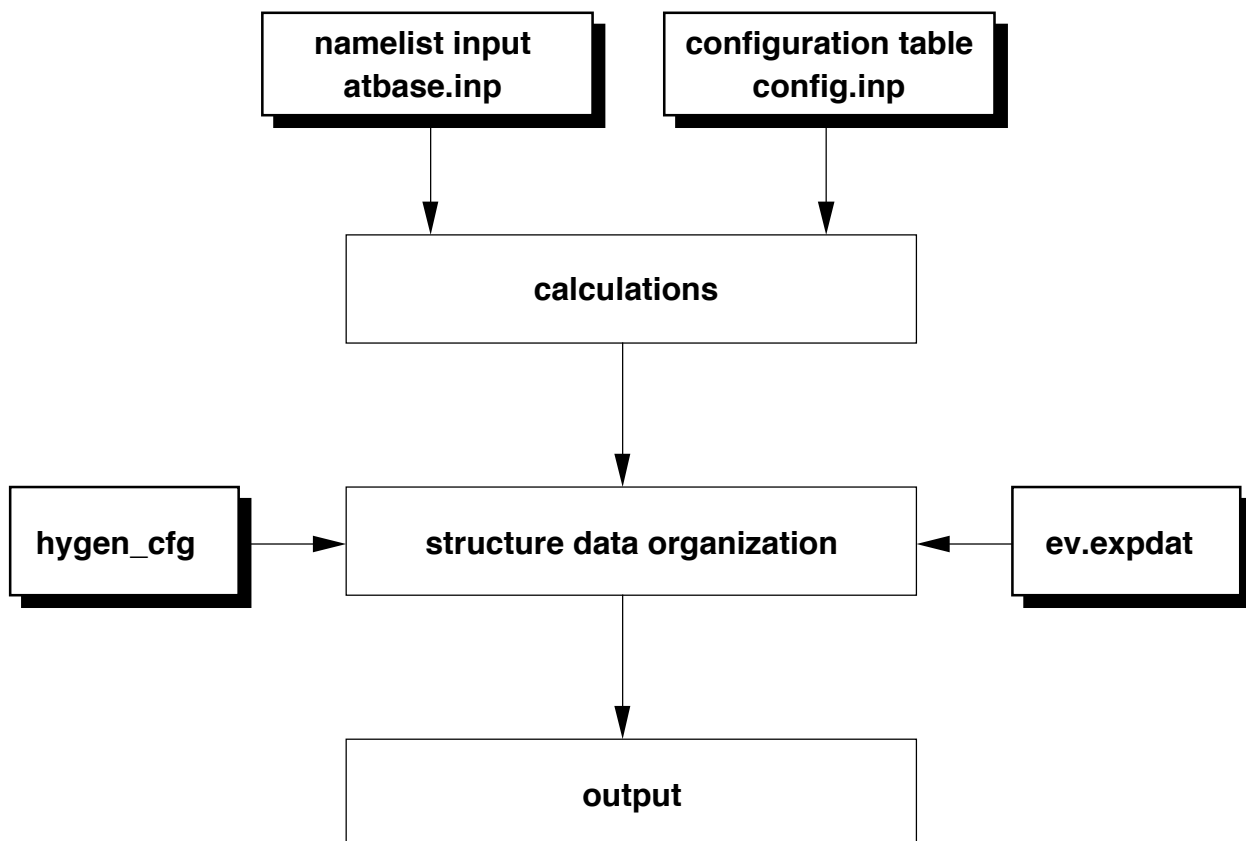


Figure 2. ATBASE input structure.

Further details of these input files are given in Table 2 through Table 5. It should be noted that only a few parameters in ‘atbase.inp’ are dependent on atomic system. In the following, step by step guidance is given for how to prepare input for ATBASE calculations.

STEP 1: Determine the purpose for running ATBASE. For the current version of ATBASE, make the following choices:

(a) do large scale calculations to obtain atomic energy levels, transition oscillator strengths, and photoionization cross sections for a specific atomic system;

(b) do detailed calculations to obtain atomic physics data for a few specific atomic states of an atom (with the inclusion of a large number of configurations to account for correlation effects).

(c) do detailed calculations to obtain autoionization rates and/or dielectronic recombination rate coefficients for a specific electronic configuration.

STEP 2: In all cases, first determine the nuclear charge Z and the number of bound electrons in the atomic system of interest.

STEP 3: For choice (a), run STATE to generate electronic configurations for the system. Two files, ‘config.inp’ and ‘hygen_cfg’ will be generated by running STATE (see Section 3 for running STATE). For choice (b), edit ‘config.inp’ by typing in all relevant electronic configurations in the sequence as indicated in Table 3. For choice (c), figure out all the possible exit channels for the specific autoionizing configuration and edit ‘config.inp’ by typing in all relevant electronic configurations in the sequence as indicated in Table 5.

STEP 4: Edit namelist input file ‘atbase.inp’. Since most of the parameters in ‘atbase.inp’ have been set as defaults, in most cases the user only needs to change the following nine parameters:

(1) switch parameters (on=1, off=0):

ISWICH(1) = 1, compute energy levels and f-values. This switch should be always on.

ISWICH(2) = 1, compute photoionization cross sections. If there is interest in obtaining photoionization cross section data, turn off this switch by setting the parameter to 0.

SWICH(3) = 0, compute electron impact excitation cross sections. This option has not been completed yet.

ISWICH(4) = 0, compute autoionization rates. If autoionization rates for a specific electronic configuration are to be calculated, turn this switch on by setting the parameter to 1.

ISWICH(5) = 0, compute dielectronic recombination rate coefficients. If dielectronic recombination rate coefficients for a specific electronic configuration are to be calculated, turn this switch on by setting the parameter to 1.

(2) physical model selections:

IHF = 2, choose Hartree-Fock model by setting 'IHF=2', choose HX model by setting 'IHF=1'. It is suggested that the user choose 'ihf=2'.

IREL = 1, if 'IREL=0' ATBASE does non-relativistic self-consistent-field calculations, if 'IREL=1' ATBASE does relativistic self-consistent-field calculations. For elements with $Z \leq 20$, IREL should be set equal 0, while for elements with $Z > 20$, IREL should be set equal to 1.

(3) output criteria:

FVMIN= 1.0e-5, only consider those transitions with oscillator strength values larger than 'fvmin'. In most cases, 1.0e-5 is appropriate.

(4) incorporating experimental data:

IEXPSW = 0, if the user wants to incorporate experimental data in the calculation, set IEXPSW equal 1, otherwise set IEXPSW equal 0. If 'IEXPSW=1', a formatted data table, 'ev.expdat', which contains experimental energy data must be provided by the user.

STEP 5: Check the following files to see whether they are consistent with the problem:

(1) config.inp:

Are all electronic configurations of your interest in the table? If this is for a large scale calculation, there must be at least one Rydberg state type configuration in the table.

(2) hygen_cfg:

Do configurations in this table belong to the same atomic system as those in ‘config.inp’? If not, delete this file.

(3) atbase.inp: Double-check the parameters.

(4) ev.expdat: If the user does not intend to incorporate experimental data in the calculation, delete this file.

Now, the user is ready to run ATBASE.

2.3. Computational Procedure

First of all, ATBASE reads in all electronic configurations from ‘config.inp’, and calls subroutine STRUCT to calculate the single-configuration wavefunctions $P_{nl}(r)$ for each configuration. Also calculated for each configuration are various radial integrals ($\langle r^m \rangle$, F^k , G^k , ζ), and the configuration-average energy (E_{av}) including approximate relativistic and correlation energy corrections. If IREL is set equal to 1, relativistic terms will be included in the potential function of the radial differential equation to give approximate relativistic corrections to the radial wavefunctions, as well as improved relativistic energy corrections in heavy atoms. The single-configuration structure data calculated in STRUCT are stored in a binary data file WFUNT_DAT. With these basic single-configuration structure data, ATBASE can then perform various atomic physics calculations depending on the options selecting by the user.

2.3.A. Calculating Atomic Energy Levels and Spectra of an Atomic System

ATBASE calls subroutine RINTG1 to calculate various multiple-configuration radial integrals: overlap integrals $\langle P_{nl} | P_{n'l'} \rangle$, configuration-interaction coulomb integrals R^k and spin-orbit integrals $\zeta_{nl,n'l'}$, and radial electric-dipole and electric-quadrupole integrals. These data along with the single-configuration average energy and radial integrals will be transferred to subroutine CILSJ via a data file CILSJ_INP. Subroutine CILSJ calculates all relevant angular factors of various matrix elements in the theory of atomic structure and spectra [2] by employing Racah-algebra technique. These angular factors include

(a) the trivial (unit-matrix) coefficient of E_{av} , the center-of-gravity energy of each configuration;

(b) the coefficients f_k, g_k , and d of the single-configuration direct and exchange Coulomb-interaction (F^k and G^k) and spin-orbit-interaction (ζ) radial integrals, and the coefficients r_d^k and r_e^k of the direct and exchange configuration-interaction Coulomb radial integrals R^k , which are involved in the calculation of the Hamiltonian (energy-level) matrix elements;

(c) the magnetic-dipole matrix elements, and the angular coefficients of the electric-dipole and electric-quadrupole reduced matrix elements

$$P_{l,l'}^{(t)} = \langle l || r^t || l' \rangle. \quad (2.1)$$

Combining these angular coefficients with the radial integrals in the data file CILSJ_INP, energy levels and intermediate-coupling eigenvectors are computed. And finally the energy levels and eigenvectors are used for computation of spectrum-line wavelengths and the associated oscillator strengths and radiative transition probabilities.

2.3.B. Calculating Photoionization Cross Sections

The calculations of photoionization cross sections are performed in subroutine BFDATA. BFDATA first calls subroutine INPUT3 to read in all bound configuration structure data from data file WFUNT_DAT and to determine the electronic configurations of a residual ion after ionization. Then BFDATA calls subroutine EKMESH to construct a universal kinetic energy mesh for an ejected electron in threshold unit. Photoionization cross sections for each subshell are calculated in 50 kinetic energy points ranging from threshold to 500 times the threshold. In order to obtain a detailed shape of the cross sections (e.g., Cooper minimums, etc.), the whole kinetic energy region is divided into 5 sub-regions as shown in Table 6. The mesh points are distributed over each sub-region in a logarithm manner. In the calculation of photoionization cross sections, continuum wavefunctions are calculated by using a frozen core approximation, i.e., all bound wavefunctions are assumed to be unchanged before and after ionization. Configuration-interaction and autoionization resonance structure are not included.

2.3.C. Calculating Autoionization Rates and Dielectronic Recombination Rate Coefficients

First of all, it should be mentioned that the calculation of autoionization rates and dielectronic recombination rate coefficients in ATBASE is not done in an automatic manner, the user must do some hand calculations to set up the input properly. The following information must be supplied by the user as input for ATBASE to calculate autoionization rates and dielectronic recombination rate coefficients:

- (1) Doubly excited (autoionizing) configuration.
- (2) All possible stable configurations of residual ion after autoionization.
- (3) All possible stable configurations of the ion after radiative decay from the autoionizing configuration.
- (4) Threshold correction for doubly excited configuration. In some cases, not all the levels of the doubly excited configuration are autoionizing levels, only a few levels lie above the ionization limit of the ion. For this kind of configuration, the configuration-average energy E_{av} may be below the ionization limit. In such cases, the user must first calculate atomic energy levels for configurations in both (1) and (2) to determine the kinetic energies of a free electron via autoionization. These actual kinetic energies are assigned to the array element GODEPS (i) relative to the *i*th configuration of the residual ion.
- (5) EIONRY, the ionization energy (in Ry) from the ground level of the recombined ion to the center of gravity energy of the ground configuration of the recombining ion. If EIONRY=0, the reference point is taken as the center of the gravity energy of the ground configuration of the recombined ion instead of the ground level.
- (6) AEDGE, this is an edge value for excluding the non-physical autoionization. Only those levels with energy $E_j > AEDGE$ can autoionize. AEDGE is in units of 1000 cm^{-1} referenced to the same E_{min} as E_j does.

2.4. Output

All the output results from ATBASE are stored in 19 data files. There are three different types of output data files which serve different application purposes.

(1) Atomic data tables in conventional expressions of spectral symbols. This type of file can be used for table lookup or data checking. There are seven files in this category:

- ev_nl.table — configuration-average atomic energy levels;
- ev_ls.table — LS term energy levels;
- ev_final.tab — energy levels in final structure specified by the user;
- fv_nl.table — the array oscillator strengths (configuration-average);
- fv_ls.table — oscillator strengths for transitions between terms;
- fv_final.tab — oscillator strengths between levels;
- autoii.rate — autoionization rates.

(2) Atomic data files in numerical formats. This type of file is used as formatted data input files for the ATTABLE code or other applications. There are eight files in this category:

- ev_nl.dat — configuration-average atomic energy levels;
- ev_ls.dat — LS term energy levels;
- ev_final.dat — energy levels in final structure specified by the user;
- fv_nl.dat — the array oscillator strengths (configuration-average);
- fv_ls.dat — oscillator strengths for transitions between terms;
- fv_final.dat — oscillator strengths between levels;
- photoionization_x — subshell photoionization cross sections.
- wfunt_dat — radial wavefunctions (in binary format).

(3) Complete output files. This type of file contains detailed information of the whole calculation.

- outpt_scf — complete output for self-consistent-field calculations;
- outpt_integl — complete output for radial integral calculations;
- outpt_lsj — complete output for atomic data calculations
(energy levels, spectra, dielectronic recombination rate coefficients).
- ev.dat — energy levels
- fv.dat — oscillator strengths

All relevant data of dielectronic recombination rate coefficients are written in ‘outpt_lsj’.

3. STATE

3.1. Program Outline

This is a code for generating input configuration tables for ATBASE calculations. Strictly speaking, STATE only functions as a convertor. It first takes the specifications for the atomic level structure from the user, and then goes into two pre-supplied electronic configuration tables, CONFIG.TAB and AUTOST.TAB, to dig out the proper configurations and outputs them to the files CONFIG.INP and HYGGEN_CFG in the format accepted by ATBASE. There are 4 files involved in running STATE. These files are listed in Table 7, along with the default logical unit numbers, names, types, and a brief description of their contents.

3.2. Input

STATE takes the input parameters in an interactive manner. In running STATE, the user must be able to answer the following questions about the level structure of an atomic system:

(1) what is the atomic number of the atomic system (atom/ion)? — input atomic nuclear charge Z .

(2) how many bound electrons are there in the atomic system? — input the number of bound electrons, the difference of (1) and (2) is the charge state of the atomic system.

(3) what kind of spectrum do you want to calculate? x-ray spectrum or thermal spectrum?

— x-ray spectrum and thermal spectrum are associated with two completely different energy level structures, x-ray spectrum is associated with inner-shell transitions, while the thermal spectrum is not. If the user is interested in the x-ray spectrum, those configurations with inner-shell holes must be included in the table.

(4) what is the maximum principal quantum number (n_{\max})? — to set up an atomic data table, the user must set a cutoff boundary for the bound states. This parameter limits the configuration table by only including the configurations with principal quantum number

not larger than n_{\max} . For carbon atom, for example, if the input parameter is 4, only the following configurations will be included in CONFIG.INP:

$$1s^2 2s^2 2p^2,$$

$$1s^2 2s^1 2p^3,$$

$$1s^2 2s^2 2p^1 3s^1,$$

$$1s^2 2s^2 2p^1 3p^1,$$

$$1s^2 2s^2 2p^1 3d^1,$$

$$1s^2 2s^2 2p^1 4s^1,$$

$$1s^2 2s^2 2p^1 4p^1,$$

$$1s^2 2s^2 2p^1 4d^1,$$

$$1s^2 2s^2 2p^1 4f^1.$$

In most cases, $n_{\max} = 10$ is a proper selection.

(5) what is the boundary for hydrogenic approximation (n_{hy})? — most users are usually only interested in spectra being associated with low excited levels. However, in order to take account of the influence of highly excited states on ionization balance and low excited state occupation numbers, it is necessary to include highly excited states in the calculation. Since no detailed spectrum information is required for these highly excited states, a hydrogenic approximation can be used to describe their average properties. It should be noted that n_{hy} must be bounded by n_{\max} , i.e., $n_{\text{hy}} \leq n_{\max}$. A general guideline for setting this parameter is that if the outer shell principal quantum number of the ground configuration is n_g , then $n_{\text{hy}} \geq n_g + 2$.

(6) do you want to consider LS term structure? — if no, input 1, if yes, input 2.

(7) do you want to consider fine structure splitting? Specify the outer shell principal quantum number (n_f) and orbital quantum number (l_f) for the configurations you would like to consider fine structure. — Fine structure splitting will be considered for those

configurations with $n \leq n_f$ and $l \leq l_f$. If the user is not interested in fine structure levels, just set $n_f = 0$ and $l_f = 0$.

3.3. Output

Two output files, CONFIG.INP and HYGEN_CFG, are generated from running STATE. CONFIG.INP contains all non-hydrogenic configurations, while HYGEN_CFG contains all hydrogenic configurations. Further details of these two files are described in Tables 3 and 4.

4. ATTABLE

4.1. Program Outline

ATTABLE serves as an interface between raw atomic data and applications (e.g., CRE and/or equations of state and opacity calculations). ATTABLE first reads in all the raw atomic data from atomic data files for each ion, then it calculates rate coefficients for all related atomic processes in the temperature and density region specified by the user, and finally creates an atomic model for applications. An atomic model is actually two formatted data tables, ATOMIC.DAT and PIXFIT.DAT, containing the information of atomic energy levels, oscillator strengths, photoionization cross sections, and rate coefficients of all related atomic processes for ions of an element.

There could be as many as 95 files involved in running ATTABLE. These files are listed in Table 8, along with the default logical unit numbers, names, types, and a brief description of their contents.

4.2. Input

There are two types of input for ATTABLE. One is for atomic model specification, and the other provides raw atomic data.

Two files, ATTABLE.INP and LEVELS.INP, are used for atomic model specification. Further details of these two files are given in Tables 9 and 10, respectively.

Atomic raw data files are arranged in the sequence of ionic state. There are four different raw data files for each ion. Each file is designated by the number of bound electrons in the ion and an extension specifying data property. `#.LEV` is a data file which contains atomic structure data such as energy levels, number of shells, binding energy of each shell and the radius of each shell, etc., where `#` represents the ion with `#` bound electrons, `#.FDA` is a data file contains all the oscillator strengths, `#.PDA` is a data file containing photoionization cross sections, and `#.STRENG` is a data file containing collision strengths of electron impact excitations. Data files `#.LEV`, `#.FDA`, and `#.PDA` are generated from ATBASE calculations, while `#.STRENG` is generated from DWBORN calculations. If `#.STRENG` is not supplied, the collisional coupling between levels will not be complete; only electric-dipole-allowed couplings are considered.

4.3. Rate Coefficient Calculations

Rate coefficients for the following atomic physics processes are calculated in ATTABLE. A Maxwellian distribution is assumed for free electrons in all cases.

- (1) Spontaneous decay. Spontaneous decay rates are deduced from the corresponding transition energies and oscillator strengths.
- (2) Electron impact excitation. For electric dipole allowed transitions, electron impact excitation rate coefficients are calculated by using a semiclassical impact parameter method [5], while for forbidden transitions, collision strengths must be supplied from data file `#.STRENG` which is generated from DWBORN calculations.
- (3) Electron collisional deexcitation. Deexcitation rate coefficients are obtained from the detailed balance relationship with excitations.
- (4) Electron impact ionization. Rate coefficients are calculated by using Burgess' semiempirical formula [6].
- (5) Electron collisional recombination (three body recombination). Rate coefficients are obtained from the detailed balance relationship with ionizations.
- (6) Radiative recombination. Rate coefficients are obtained by integrating Hartree-Fock photoionization cross sections weighted by a Maxwellian distribution.

(7) Dielectronic recombination. Rate coefficients are calculated by using Burgess-Mert semiempirical formula [7].

4.4. Output

Two output files, ATOMIC.DAT and PIXFIT.DAT, are generated from running ATTABLE.

ATOMIC.DAT contains the following information for a specific atom:

- (1) atomic nuclear charge Z ;
- (2) total number of atomic energy levels included in the model;
- (3) energy level structure for each ion;
- (4) oscillator strengths and spontaneous decay rates for all transitions;
- (5) rate coefficients for b-b transitions at a specially designed plasma temperature grid;
- (6) rate coefficients for b-f transitions at a specially designed plasma temperature and density grid.

PIXFIT.DAT contains subshell photoionization cross sections for all states in the model. Photoionization cross sections are fit to

$$\sigma(\nu) = \sigma(\nu_1) \left\{ \beta \left(\frac{\nu_1}{\nu} \right)^\phi + (1 - \beta) \left(\frac{\nu_1}{\nu} \right)^{\phi+1} \right\} \quad (4.2)$$

where ν_1 is the ionization threshold value. Four fitting parameters, $\sigma(\nu_1)$, ν_1 , β and ϕ are listed in PIXFIT.DAT for each subshell of all atomic states.

5. DWBORN

5.1. Program Outline

DWBORN is a code for computing electron impact excitation cross sections by using a distorted wave Born method [8]. The calculations of this code may serve two purposes:

- (1) as a benchmark for the calculated results of semiclassical impact parameter method;

(2) to provide large scale collision strength data for forbidden transitions. In large scale calculations DWBORN should be run in a chain with ATBASE so that all the energy levels are in the same indexing order. There are 15 I/O data files involved in DWBORN calculations. These files are listed in Table 11, along with the default logical unit numbers, names, types, and a brief description of their contents.

5.2. Input

The input of DWBORN consists of three input files:

(1) `dwborn.inp` — this is a namelist input file which contains information on target atom, incident electron, computational switches and parameters for a specific problem.

(2) `dwborn.sts` — this file contains a list of atomic states of the target atom. DWBORN will calculate electron impact excitation cross sections for transitions between these states.

(3) `wfunt.dat` — this is a binary data file which contains radial wavefunctions for all states listed in `DWBORN.STS`. It is generated from ATBASE calculations.

Further details on `DWBORN.INP` and `DWBORN.STS` are described in Tables 12 and 13. If DWBORN is not run in a chain with ATBASE, all radial wavefunctions will be calculated within DWBORN and the data file `WFUNT.DAT` will not be needed.

5.3. Output

DWBORN generates 4 output files:

(1) `eaout.read` — formatted output for cross sections and collision strengths;

(2) `eaout.rate` — formatted output for rate coefficients and average collision strengths;

(3) `eaout.plot` — plotting data file:

x - incident electron kinetic energies,

y1 - electron impact excitation cross sections,

y2 - collision strengths;

(4) `streng.dat` — fitting parameters for collision strengths in the format accepted by `ATTABLE`. If there are more than three atomic states involved in the calculation, the calculation is viewed as a ‘large scale’ calculation. Output files `EAOUT.READ`, `EAOUT.PLOT`, and `EAOUT.RATE` will not be generated in large scale calculations.

6. MICPSSR

6.1. Program Outline

MICPSSR is a code for calculating ion-impact ionization cross sections for both single and multiple ionization processes. This code employs a modified plane-wave Born method (MPWBA) [9] which incorporates binding effect, Coulomb-deflection effects, and relativistic corrections for target wavefunctions. This method has been shown [9,10] to produce much better results than the conventional plane-wave Born approximation. The calculation for the multiple ionization cross section is based on a formulation of the single-electron ionization probability with the binomial distribution [11]. This code is usually run in a chain with another code, `BEAMTAB`, to generate data tables for analyzing inner-shell emission spectra of ion beam heated plasmas.

There are 5 I/O data files involved in MICPSSR calculations. These files are listed in Table 14, along with the default logical unit numbers, names, types, and a brief description of their contents.

6.2. Input

To run MICPSSR, the user needs to provide the following information:

- (1) Target ion properties — nuclear charge, atomic weight, number of bound electrons, electronic configuration.
- (2) Ionization process specification — specify principal quantum (n), orbital quantum number (l) for each ionizing shell.
- (3) Projectile ion properties — nuclear charge, atomic weight, net charge, beam energy.

(4) Calculation controlling parameters — most parameters have been set by default. The user only needs to specify one debugging switch and a mesh for beam energies.

All the inputs for MICPSSR calculations are contained in a namelist input file ‘mi_cpssr.inp’. Further details on ‘mi_cpssr.inp’ are described in Table 15.

6.3. Output

MICPSSR generates 3 output files:

- (1) Xsecton.tab — an output table for ion impact ionization cross sections.
- (2) Xsecton.dat — data file for ionization cross sections in the format accepted by computer code BEAMTAB as input.
- (3) debug.out — debugging output information.

7. BEAMTAB

7.1. Program Outline

BEAMTAB does data organization to generate a data table for analyzing inner-shell emission spectra of ion beam heated plasmas. BEAMTAB first reads all energy levels from data files #.lev which are the same as those for ATTABLE calculations. Then it searches for the upper and lower levels connected by ion impact ionizations and couples them with the proper cross sections.

7.2. Input

The inputs for BEAMTAB include atomic energy levels and ion impact ionization cross sections. Hence, the input for BEAMTAB consists of the following files:

- (1) beamtab.inp — general input file to specify target atom and beam ion properties. This file includes four parameters: atomic nuclear charge Z of the target, the number of ionization states included in the model, nuclear charge of the beam ion, and the net charge of the beam ion.

- (2) `levels.inp` — the same as that for `ATTABLE`;
- (3) `#.lev` — the same as those for `ATTABLE`;
- (4) `#.iics` — ion impact ionization cross sections for the target ion with `#` bound electrons. `#.iics` is in the same format as data file `'Xsecton.dat'` of `MICPSSR`.

7.3. Output

The output file of `BEAMTAB` is `'beams.dat'`. `'beams.dat'` is in the format accepted by the `CRE` code. Data file `'beams.dat'` along with `'atomic.dat'`, `'pixfit.dat'`, and `'ackf.table'` form a complete *atomic model* for studying inner-shell emission spectra of ion beam heated plasmas.

8. CKFYED

8.1. Program Outline

`CKFYED` is a code for doing large-scale calculations for both configuration-averaged and term-dependent fluorescence yields. `CKFYED` does the calculation ion by ion. There are 14 I/O data files involved in running `CKFYED`. These files are listed in Table 16, along with the default logical unit numbers, names, types, and a brief description of their contents.

8.2. Input

To calculate fluorescence yield for an autoionizing state, one must specify the electronic configuration of the autoionizing state, all possible Auger and/or Coster-Kronig exit channels, and radiative decay channels. In `CKFYED`, all the radiationless and radiative exit channels are set up automatically. The user only needs to specify a list of autoionizing configurations and the corresponding 'hole' transitions.

The input for `CKFYED` consists of two files:

- (1) `yields.inp` — a namelist input file containing calculation switches and parameters;

(2) `ckf.state` — a data file containing all autoionizing configurations to be considered. Further details of these two input files are described in Tables 17 and 18.

8.3. Output

The output of CKFYED consists of four data files:

(1) `Auger_CK_fyield.tab` — a readable data table which contains Auger rates, Coster-Kroning rates, radiative decay rates, and fluorescence yields for each LS term of all input autoionizing configurations.

(2) `fyield_term.dat` — a data file containing term-dependent fluorescence yields in the format accepted by computer code CKFTAB.

(3) `fyield_config.dat` — a data file containing configuration-averaged fluorescence yields in the format accepted by computer code CKFTAB.

(4) `debug.out` — debugging output file.

Since CKFYED is run ion by ion, every time one finishes running CKFYED for a specific ion, one should remember to copy data files (1), (2), and (3) to other files with special designed names. When the calculations for all ions are done, all the ‘`fyield_term.dat`’ or ‘`fyield_config.dat`’ files should be combined together in one file ‘`fyield.dat`’ which is the input data file for code CKFTAB. As an example, a step by step guide for generating a K_α fluorescence yield data table for carbon system is shown as follows.

STEP 1: edit ‘`yields.inp`’ by setting

<code>Z = 6</code>	—	atomic nuclear charge
<code>klmno = 1</code>	—	initial hole is in K-shell
<code>nih = 1</code>	—	principal quantum number of the K-shell
<code>lih = 0</code>	—	orbital quantum number of the K-shell
<code>nfhole = 1</code>	—	only consider 2p - 1s radiative transition, hence there is only one hole created by radiative transition
<code>nfh(1) = 2</code>	—	principal quantum number of the final hole in 2p shell
<code>lfh(1) = 1</code>	—	orbital quantum number of the final hole in 2p shell
<code>jjcog = 0</code>	—	only consider LS coupling.

STEP 2: figure out autoionizing configurations for each ion CI, CII, CIII ...

STEP 3: type in all the autoionizing configurations for one ion (e.g., CI).

STEP 4: run CKFYED

STEP 5: copy Auger_CK_fyield.tab to CI.ACKF.tab

copy fyield_term.dat to CI_term.dat

copy fyield_config.dat to CI_config.dat

Repeat step (2) to (5) for all ions

STEP 6: Combine CI_term.dat, CII_term.dat, ..., CV_term.dat together into a file C.fyield_term.dat.

Combine CI_config.dat, CII_config.dat, ..., CV_config.dat together into a file C.fyield_config.dat

Data file C.fyield_term.dat or C.fyield_config.dat is accepted by computer CKFTAB as input.

9. CKFTAB

9.1. Program Outline

CKFTAB does data organization to generate a data table for analyzing x-ray spectra. CKFTAB first reads all energy levels from data files #.lev which are the same as those for ATTABLE calculations. Then it searches for all autoionizing levels and assigns them with corresponding fluorescence yields.

9.2. Input

The inputs for CKFTAB include atomic energy levels and fluorescence yields. Hence, the input for CKFTAB consists of following files:

(1) levels.inp — the same as that for ATTABLE;

- (2) #.lev — the same as those for ATTABLE;
- (3) fyield.dat — fluorescence yield data file.

9.3. Output

The output file of CKFTAB is 'ackf.table'. 'ackf.table' is in the format accepted by the CRE code. data file 'ackf.table' along with 'atomic.dat', 'pixfit.dat', and 'beams.dat' form a complete *atomic model* for studying inner-shell emission spectra of ion beam heating plasmas.

10. Running Codes in a Chain Manner

In order to generate an atomic model for plasma spectroscopy analysis and/or equation of state and opacity calculations, atomic data for atomic structure and different types of atomic processes are needed. These data are usually calculated by using different codes. Depending on what atomic model the user wants to create, the computer codes in the ATBASE package should be run in a chain in one of the following combinations:

- (1) STATE/ATBASE/ATTABLE
- (2) STATE/ATBASE/DWBORN/ATTABLE
- (3) STATE/ATBASE/ATTABLE/CKYED/CKFTAB
- (4) STATE/ATBASE/DWBORN/ATTABLE/CKYED/CKFTAB
- (5) STATE/ATBASE/ATTABLE/MICPSSR/BEAMTAB/CKYED/CKFTAB
- (6) STATE/ATBASE/DWBORN/ATTABLE/MICPSSR/BEAMTAB/CKYED/CKFTAB

Details of these combinations are described in this section.

10.1. Simple Atomic Model

To create a simple atomic model for analyzing emission/absorption thermal spectra for a plasma or calculating equations of state and opacities, the user should run program chain STATE/ATBASE/ATTABLE.

STEP 1: run STATE to generate CONFIG.INP and HYGEN_CFG for a specific ionization state;

STEP 2: run ATBASE to generate atomic energy levels, oscillator strengths and photoionization cross sections;

STEP 3: if the user wants an atomic model in configuration-average structure, then

copy ev_nl.dat to #.lev,

copy fv_nl.dat to #.fda,

copy photoionization_x to #.pda;

if the user wants an atomic model in LS term structure, then

copy ev_ls.dat to #.lev,

copy fv_ls.dat to #.fda,

copy photoionization_x to #.pda;

if the user wants an atomic model in fine structure, then

copy ev_final.dat to #.lev,

copy fv_final.dat to #.fda,

copy photoionization_x to #.pda,

where # is the number of bound electrons of the ion (e.g., #=6 for neutral carbon, #=5 for CII #=4 for CIII, etc.).

Repeat STEP (1), (2), and (3) for all ions of the element.

STEP 4: check all the `#.lev` files, writing down the number of energy levels of each ion to ATTABLE input file LEVELS.INP.

STEP 5: run ATTABLE to generate ATOMIC.DAT and PIXFIT.DAT.

The atomic model created in this way is a simple model which does not include electron collisional coupling for forbidden transitions. It should be noted that complete electron collisional coupling between levels (including both electric dipole allowed and forbidden transitions) is very important for the occupations of metastable levels. If one wants to do very detailed spectrum analysis for some specific lines, all related levels should be coupled in a complete manner.

10.2. Complete Coupling Atomic Model

To create a complete coupling atomic model for detailed spectroscopy analysis, one should run program chain STATE/ATBASE/DWBORN/ATTABLE.

STEP 1: run STATE to generate CONFIG.INP and HYGEN_CFG for a specific ionization state;

STEP 2: run ATBASE to generate atomic energy levels, oscillator strengths and photoionization cross sections;

STEP 3: if the user wants an atomic model in configuration-average structure, then

copy `ev_nl.dat` to `#.lev`,

copy `fv_nl.dat` to `#.fda`,

copy `photoionization_x` to `#.pda`,

copy `wfunt.dat` to `#.wfunt`;

if the user wants an atomic model in LS term structure, then

copy `ev_ls.dat` to `#.lev`,

copy `fv_ls.dat` to `#.fda`,

copy photoionization_x to #.pda,

copy wfunt_dat to #.wfunt;

if the user wants an atomic model in fine structure, then

copy ev_final.dat to #.lev,

copy fv_final.dat to #.fda,

copy photoionization_x to #.pda,

copy wfunt_dat to #.wfunt,

where # is the number of bound electrons of the ion (e.g., #=6 for neutral carbon, #=5 for CII #=4 for CIII, etc.).

Repeat STEP (1), (2), and (3) for all ions of the element.

STEP 4: Determine ionization states of your particular interest, then

copy #.lev to dwborn.sts,

copy #.wfunt to wfunt.dat,

where #.lev is atomic structure data table for the ion you would like to have complete coupling.

STEP 5: run DWBORN. Then copy streng.dat to #.streng

Repeat STEP (4) and (5) for all ions of interest.

STEP 6: Run ATTABLE to create ATOMIC.DAT and PIXFIT.DAT

10.3. Atomic Model for Analyzing X-ray Line Emission Spectra From High Energy Density Plasmas

The intensities of x-ray line emissions are determined by fluorescence yields instead of spontaneous decay rates. Hence, to create an atomic model for analyzing x-ray line

emission spectra, one needs to provide fluorescence yields for all autoionizing levels. This can be done by running program chain

```
STATE/ATBASE/ATTABLE/CKYED/CKFTAB
```

or

```
STATE/ATBASE/DWBORN/ATTABLE/CKYED/CKFTAB.
```

In this case, the atomic model consists of three data tables: ATOMIC.DAT, PIXIFT.DAT, and ACKF.TABLE.

10.4. Atomic Model for Analyzing X-ray Line Emission Spectra of Ion Beam Heated Plasmas

For ion beam heated plasmas, x-ray line emissions are produced by inner-shell ion impact ionizations. The atomic model should include inner-shell ion impact ionization processes. To create such an atomic model, the user should run program chain

```
STATE/ATBASE/ATTABLE/CKYED/CKFTAB/MICPSSR/BEAMTAB
```

or

```
STATE/ATBASE/DWBORN/ATTABLE/CKYED/CKFTAB/MICPSSR/BEAMTAB.
```

In this case, the atomic model consists of four data tables: ATOMIC.DAT, PIXIFT.DAT, ACKF.TABLE, and BEAMS.TAB.

Acknowledgment

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Table 1
ATBASE Data Files

Default Unit No.	Default Name (UNIX)	Type	Description
1	ev.dat	intermediate output	energy level data to be organized
2	tape2e	intermediate data	data transfer
3		SCRATCH	scratch file
4	fv.dat	intermediate output	oscillator strength data to be organized
5		SCRATCH	scratch file
7	autoii.rate	output	autoionization rates
9	outpt_lsj	output	complete output for spectrum calculations
10	input_lsj	intermediate input	constraint parameters for spectrum calculation. This file is automatically generated within the calculation.
11	outgine	intermediate data	data transfer
12		SCRATCH	scratch file
13		SCRATCH	scratch file
18	tape19	intermediate data	data transfer
19		SCRATCH	scratch file
20		SCRATCH	scratch file
21	atbase.inp	input	primary namelist input file
22	config.inp	input	configuration table input file
31	SCRATCH	SCRATCH	scratch file
32		SCRATCH	scratch file
41		SCRATCH	scratch file

Table 1 (Continued)

Default Unit No.	Default Name (UNIX)	Type	Description
50	input_scf	intermediate input	constraint parameters for SCF calculation. This file is automatically generated within the calculation.
51	outpt_scf	output	complete output for SCF calculations
52	param_scf	intermediate output	configuration-average structure data
53	wfunt_dat	output	radial wavefunctions in binary format
54	input_integl	intermediate input	constraint parameters for SCF calculation. This file is automatically generated within the calculation.
55	outpt_integl	output	complete output for radial integral calculations
56	out2ing	intermediate data	data transfer
63	ev_ls.dat	intermediate data	fine structure energy levels
64	ev_ls.dat	output	LS term structure energy levels
65	fv_ls.dat	intermediate data	f-values for transitions between LSJ levels
66	fv_ls.dat	output	f-values for transitions between LS terms
67	ev_nl.dat	output	configuration-average energy levels
68	fv_nl.dat	output	f-values for transition arrays
69	hygen_cfg	input	configuration table for hydrogenic states
71	cfp.tab	input	fractional-parentage-coefficient table
72	tape72_cfp1	intermediate data	data transfer
73	tape73_cfp2	intermediate data	data transfer
74	tape74_cfp3	intermediate data	data transfer

Table 1 (Continued)

Default Unit No.	Default Name (UNIX)	Type	Description
75	ev_lsj.table	output	table for fine structure energy levels
76	ev_ls.table	output	table for LS term structure energy levels
77	fv_lsj.table	output	table for fine structure f-values
78	fv_ls.table	output	table for LS term structure f-values
79	ev_nl.table	output	table for configuration-average energy levels
80	photoionization_x	output	photoionization cross sections
81	config.fff	intermediate data	data transfer
82	wfc_out	intermediate output	continuum wavefunction calculation parameters
83	fv_nl.table	output	table for array f-values
90	ev_final.dat	output	energy level for user specifying structure
91	fv_final.dat	output	f-values for user specifying level structure
92	ev_final.tab	output	energy level table for user specifying level structure
93	fv_final.tab	output	f-value table for user specifying level structure
94	ev_nl.summary	output	configuration-average structure data for use in multiple ionization spectrum calculations
98		SCRATCH	scratch file
99	ev.expdat	input	experimental energy level data

Table 2
Detailed Description for atbase.inp

```

*
* This is the primary input file for ATBASE, an atomic physics calculation code
*
*
$inpdat
*
* (1) switch parameters (on=1, off=0)
*   iswich(1) = 1  energies & f-values
*   iswich(2) = 1  photoionization cross sections
*   iswich(3) = 0  electron impact excitation cross sections
*   iswich(4) = 0  autoionization rate
*   iswich(5) = 0  dielectronic recombination
*
* (2) control parameters for printing
*   itpow = 2      =1,>=3:print SCF iteration information, >=2: print  $\langle r^m \rangle$ 
*   iptvu = 2      >=1: print Coulomb integrals  $F^k, G^k$ 
*                   >=2: print Coulomb interaction energies
*                   >=3: print wavefunction overlap integrals
*                   >=4: print HFS potential (RU, RUEE, etc.)
*                   >=5: print HX potential  $V(nl)$ 
*                   >=6: print relativistic correction to  $V(r)$ 
*   ipteb = 2      >=1: print EE, JJJ, R(JJJ), AZ
*                   >=2: print  $E_k$ , etc.
*   norbpt = -9    <0: do not print wavefunctions
*                   >0: print first two and last NORBPT wavefunctions at 5*i
*                   <=6: print continuum wavefunctions at every mesh point
*                   any: write on tape 2 or 7 the last —NORBPT— wavefunctions
*                   if —NORBPT—=9, write all wavefunctions
*   npr = 0        .ne.0: diagnostic  $V(r)$  and  $P(nl-r)$  are printed during the course of SCF
*   izhxbw = 0     not used
*   iphfwf = 0     not used
*
* (3) control parameters for calculation
*   ihf = 2        =1: skip all RCN calculations of radial integrals if IREL>1, if IREL=0
*                   and TOLEND <1.0e-4, call only ZETA1 to calculate DEr for HF  $E(av)$ 
*                   =2: carry out a HF calculation within RCN
*   irel = 1        =0: normal non-relativistic calculation,
*                   =1: HXR or HFR
*                   =2: including Breit energies
*   ibb = 0         sets the outer boundary of an atom at point IBB, do not use it
*   kutd = -2
*   kut1 = 0
*   maxit = 30     maximum allowable number of SCF iterations

```

Table 2 (Continued)

```

*
  corrf = 1          =0: no correlation; correlation factor
  icrsw = 3          =1: with DEc and DEr for Eav
*                   =2: with DEc without DEr for Eav
*                   =3: with DEc with acrsw*DEr for Eav
*                   =5: without both DEc and DEr for Eav
  acrsw = 0.85       scaling parameter for relativistic correction
  iexpsw = 0         =0: no experimental data is supplied
*                   =1: experimental data is supplied
  ivinti = 0         not used
* * (4) criteria
  tolstb = 1.0
  tolend = 5.0e-8    maximum permissible value pf change in —RU— for ending SCF
  thresh = 1.0e-11  maximum permissible fractional change in the value of eigenvalues
  tolkm2 = 1.0
  exf10 = 0.67       alpha value in X-alpha exchange potential
  exfm1 = 0.65       k1 coefficient in HX potential
  emx = 0            continuum wavefunction parameter
*
* (5) threshold correction for autoionization configuration (Ry)
*
  godeps(1) = 0.0
$end
*
*
* The following are the control parameters for radial integrals calculations
*
*
$inpcn2
*
  rtid = 'g5inp'     RCN2 calls G5INP
  iquad = 0          =1: computes E(2) radial integrals for the first parity config.
*                   =2: ..... second .....
*                   =3: ..... both .....
  imag = 0           =1: computes M(1) radial integrals for the first parity config.
*                   =2: ..... second .....
*                   =3: ..... both .....
  ifttt = 2          =1, readin ifact(i), =2, online calculation
  ifact(1) = 90      scale factors:
  ifact(2) = 99      = 0, 0, 0, 0, 0 → 0.85, 0.95, 0.85, 0.85, 0.85
  ifact(3) = 90      =90,99,90,90,90 → ~10-fold ionized atom with Z ~ 25
  ifact(4) = 90      =80,99,80,80,80 → neutral atoms
  ifact(5) = 90      =92,99,95,95,95 → > 20 ionization stage

```

Table 2 (Continued)

```

*
icon = 2      =1: the RCG-input control and configuration cards are not punched
*            >1: the number of subshells set up on the configuration cards is
*            limited to no more than icon if possible
isli = 2      =0: print all SLI2 output
*            =1: omit restore and most printout
*            =2: omit all but final punched-card image
*            =3: omit all printout
idip = 9      1: do not punch dipole cards
*            =7,8: photoionization calculation
*            >=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 RCG
alf = 0.0
*
ienygd = 1    =0: print full energy matrix
*            =1: do not print matrix
*            =2: print first nevmax rows and columns
*            >9: print first 11*ienygd rows and columns
ispecc = 8    =1,3,5,7, print lines sorted by levels of first parity
*            =2,3,6,7, print lines sorted by levels of second parity
*            =4 to 8, print lines sorted by wavelength
*
fvmin = 1.0e-5 minimum gf-value below which will not be printed out
*
igen = 4      >=5 do PWBA calculation
*
nck(1) = 0
nck(2) = 0
*
nck(k)—if non-zero, then in all spectrum-line lists (and PWBA calculations),
*
only those lines are included that involve levels belonging to the first
*
NCK(k) configuration. For electric-dipole-allowed transitions, K=1,2
*
represents first and second parity; for non-parity-change transitions,
*
K=1,2 represents the upper and lower level, respectively.
*
(default is 50, except NCK(1) = 1 for PWBA calculations
*
for spectrum calculations, set =0).
*
ldmin = 1     Plane-wave-Born calculations for allowed transitions —li-lf—=odd
ldmax = 1     Plane-wave-Born calculations for allowed transitions —li+lf—=odd
lqmin = 0     Plane-wave-Born calculations for forbidden transitions —li-lf—=even
lqmax = 0     Plane-wave-Born calculations for forbidden transitions —li+lf—=even
*
$end

```

Table 2 (Continued)

```
*
*
* ***** optional input for dielectronic recombination calculations
*
*
$dielinp
  eionry = 0.0  is the ionization energy (in Ry) from the ground
*              level of the recombined ion to the center of gravity
*              of the ground configuration of the recombining ion;
  nptkev = 5    number of temperature points of interest (<6)
*
  tkev(1)=0.01  temperature point (in keV)
  tkev(2)=0.02
  tkev(3)=0.03
  tkev(4)=0.04
  tkev(5)=0.05
*
  emina = 0.    minimum kinetic above the bottom of a continuum.
  aedge = 0.    only those levels with  $E_j > aedge$  can autoionize
*              in the unit of 1000cm-1 reference to the same
*              Emin
$end
* _____ FINISH INPUT _____ *
```

Table 3
Detailed Description for config.inp

CASE 1: configuration table for radiative data calculations (energy levels, oscillator strengths, and photoionization cross sections)

- (1) atomic nuclear charge Z.

13 — Al

- (2) charge state of the ion (0 = neutral, Z-1 = hydrogen-like ion).

1 — Al⁺¹

- (3) level structure specifications

The first number:

=1 means that this calculation is for LS term structure and/or fine structure

=3 means that this calculation is only for configuration-average structure.

The second number: principal quantum number (n) of fine structure boundary.

The third number: orbital quantum number (l) of fine structure boundary.

If fine structure is not considered in this calculation, set both of them equal to 0.

1 0 0 — consider LS term structure only

- (4) The number of configurations included in the calculation. 3

- (5) lists of configurations

The first number: parity index. Always set the parity of the ground configuration (or the configuration with the lowest energy) equal to 1. Always list the ground configuration as the first configuration.

The second number: correlation index. =2 means that this configuration is only included for accounting for the correlation effect, but not for structure calculation.

The third number: number of shell of the configuration.

Electronic configuration: 1000*n + 100+l + number of bound electrons.

1	1	4	1002	2002	2106	3002		—	(even parity)	1s ² 2s ² 2p ⁶ 3s ²
0	0	0						—	break	
1	1	5	1002	2002	2106	3001	3201	—	(even parity)	1s ² 2s ² 2p ⁶ 3s ¹ 3d ¹
0	0	0						—	break	
2	1	5	1002	2002	2106	3001	3101	—	(odd parity)	1s ² 2s ² 2p ⁶ 3s ¹ 3p ¹
0	0	0								

- (6) ending indicator (*)

Table 3 (Continued)

CASE 2: configuration table for dielectronic recombination rate coefficient calculation

- (1) atomic nuclear charge Z.

13 — Al

- (2) charge state of the ion (0 = neutral, Z-1 = hydrogen-like ion).

7 — Al⁺⁷

- (3) level structure specifications

The first number:

=1 means that this calculation is for LS term structure and/or fine structure.

=3 means that this calculation is only for configuration-average structure.

The second number: principal quantum number (n) of fine structure boundary.

The third number: orbital quantum number (l) of fine structure boundary.

If fine structure is not considered in this calculation, set both of them equal to 0.

1 0 0 — consider LS term structure only.

- (4) The number of configurations included in the calculation.

3

- (5) lists of configurations

The first number: always set equal to 0

The second number: always set equal to 1

The third number: number of shell of the configuration.

Electronic configuration: 1000*n + 100+l + number of bound electrons.

The configurations must be listed in the following sequence

(a) initial configuration for electron capture;

(b) excited configurations of the ion that the capture atom might autoionize into;

(c) singly excited configurations that the doubly excited configuration might decay to radiatively so as to produce a system stable against autoionization;

(d) autoionizing configuration

0 1 3 1002 2002 2101

0 0 0

0 1 3 1002 2001 2102

0 0 0

0 1 3 1002 2002 2102

0 0 0

0 1 3 1001 2002 2103

0 0 0

- (6) ending indicator (*)

Table 4
Detailed Description for hygen_cfg

4	1002	2002	2102	5001	—	number of shells (4), $1s^2 2s^2 2p^2 5s^1$
1.	0				—	LS term of the core $1s^2 2s^2 2p^2 : (2S + 1 = 1, L = 0)$
4	1002	2002	2102	5001	—	number of shells (4), $1s^2 2s^2 2p^2 5s^1$
1.	2				—	LS term of the core $1s^2 2s^2 2p^2 : (2S + 1 = 1, L = 2)$
4	1002	2002	2102	5001	—	number of shells (4), $1s^2 2s^2 2p^2 5s^1$
3.	1				—	LS term of the core $1s^2 2s^2 2p^2 : (2S + 1 = 3, L = 1)$
4	1002	2002	2102	6001	—	number of shells (4), $1s^2 2s^2 2p^2 6s^1$
1.	0				—	LS term of the core $1s^2 2s^2 2p^2 : (2S + 1 = 1, L = 0)$
4	1002	2002	2102	6001	—	number of shells (4), $1s^2 2s^2 2p^2 6s^1$
1.	2				—	LS term of the core $1s^2 2s^2 2p^2 : (2S + 1 = 1, L = 2)$
4	1002	2002	2102	6001	—	number of shells (4), $1s^2 2s^2 2p^2 6s^1$
3.	1				—	LS term of the core $1s^2 2s^2 2p^2 : (2S + 1 = 3, L = 1)$

Table 5
Detailed Explanation of ev.expdat

```

*
* ***** experimental energy levels of He I *****
*                               (in the unit of 1/cm)
*
* (1) total number of levels
14
*
* (2) level index, # of shells, electronic configuration
* (3) 2Sp+1, Lp, 2S+1, L, J, E(LSJ)
*
1 1 1002
1 0 1 0 0.0 0.00
*
2 2 1001 2001
2 0 1 0 0.0 166271.70
*
3 2 1001 3001
2 0 1 0 0.0 184859.06
*
4 2 1001 4001
2 0 1 0 0.0 190934.50
*
5 2 1001 5001
2 0 1 0 0.0 193657.78
*
6 2 1001 2101
2 0 1 1 1.0 171129.148

```

Table 5 (Continued)

*
7 2 1001 3101
2 0 1 1 1.0 186203.62
*
8 2 1001 4101
2 0 1 1 1.0 191486.95
*
9 2 1001 5101
2 0 1 1 1.0 193936.75
*
10 2 1001 3201
2 0 1 2 2.0 186099.22
*
11 2 1001 4201
2 0 1 2 2.0 191440.71
*
12 2 1001 5201
2 0 1 2 2.0 193912.54
*
13 2 1001 4301
2 0 1 3 3.0 191447.24
*
14 2 1001 5301
2 0 1 3 3.0 193914.31
*
*
* end

Table 6
Kinetic Energy Mesh of the Ejected Electron for
Photoionization Cross Section Calculation

1.000E-02	1.778E-02	3.162E-02	5.623E-02	1.000E-01	1.166E-01	1.359E-01	1.585E-01	1.848E-01	2.154E-01
2.512E-01	2.929E-01	3.415E-01	3.981E-01	4.642E-01	5.412E-01	6.310E-01	7.356E-01	8.577E-01	1.000E+00
1.166E+00	1.359E+00	1.585E+00	1.848E+00	2.154E+00	2.512E+00	2.929E+00	3.415E+00	3.981E+00	4.642E+00
5.412E+00	6.310E+00	7.356E+00	8.577E+00	1.000E+01	1.259E+01	1.585E+01	1.995E+01	2.512E+01	3.162E+01
3.981E+01	5.012E+01	6.310E+01	7.943E+01	1.000E+02	1.380E+02	1.904E+02	2.627E+02	3.624E+02	5.000E+02

This dimensionless kinetic energy mesh is used universally for all photoionization cross section calculations. The corresponding photon energy mesh is determined from the following relations:

$$h\nu(i) = I_{nl}(1 + e_k(i)) \text{ if } I_{nl} \leq 2$$

$$h\nu(i) = I_{nl}(1 + e_k(i)/2) \text{ if } I_{nl} > 2$$

where, I_{nl} is binding energy of the nl subshell, $e_k(i)$ is the i th mesh point value in above table.

Table 7
Input/Output Files in STATES

Default Unit No.	Default Name (UNIX)	Type	Description
1	config.inp	output	electronic configuration table for ATBASE input
2	hygen_cfg	output	configuration table for hydrogenic states
11	CONFIG.TAB	input	electronic configuration table of thermal levels for some important atomic systems
12	AUTOST.TAB	input	electronic configuration table of K_{α} levels for some important atomic systems

Table 8
Input/Output Files in ATTABLE

Default Unit No.	Default Name (UNIX)	Type	Description
1	attable.inp	input	namelist input file for ATTABLE
2	levels.inp	input	level index for the atomic model
3	atomic.dat	output	atomic model data table
4	pixfit.dat	output	photoionization cross sections
11 – 10+N*	#.lev	input	atomic structure data output from ATBASE calculations
10+N+1 – 10+2*N	#.fda	input	oscillator strengths
10+2*N+1 – 10+3*N	#.pda	input	photoionization cross sections
10+3*N+1 – 10+4*N	#.streng	input	collision strengths

* Note: Here N is the total number of ions included in the calculation. For example, if one only includes the first 20 ionization states of Au ($Au^{+0} - Au^{+19}$) in the calculation, then N = 20, unit 11 for 79.lev, unit 12 for 78.lev, unit 30 for 59.lev, unit 31 for 79.fda, unit 51 for 79.pda, unit 71 for 79.streng, etc.

Table 9
Detailed Description of attable.inp

<code>\$datainput</code>		Name of the namelist
<code>Z</code>	<code>= 2,</code>	Atomic nuclear charge
<code>nzstar</code>	<code>= 3,</code>	Number of ionization states to be included in the calculation. For example, if one wants to include only the first 20 ionization states of Au (Au^{+0} - Au^{+19}) in the calculation, set <code>nzstar = 20</code> .
<code>te0</code>	<code>= 0.5,</code>	Minimum plasma temperature in the table (eV)
<code>dlogte</code>	<code>= 0.2699,</code>	Logarithmic increment in plasma temperature
<code>ntemp</code>	<code>= 10,</code>	Number of plasma temperature mesh points
<code>de0</code>	<code>= 1.0e8,</code>	Minimum electron density in the table (cm^{-3})
<code>def</code>	<code>= 1.0e16,</code>	Maximum electron density in the table (cm^{-3})
<code>nden</code>	<code>= 4</code>	Number of electron density mesh points
<code>\$end</code>		end of namelist file

Table 10
Detailed Description of levels.inp

This file should be consistent with the parameter `NZSTAR` in `attable.inp`. There must be `NZSTAR` pair numbers in this file, each specifying the ion and the number of levels of the ion.

The first column: charge state of the ion `#`

The second column: number of levels for the ion `#`. This number can be found by checking the level index in data file `#.lev`.

<code>0</code>	<code>25</code>	— <code>0</code> : neutral atom; <code>25</code> : 25 levels are considered for the neutral atom
<code>1</code>	<code>10</code>	— <code>1</code> : first ionization state; <code>10</code> : 10 levels are considered for this ion
<code>2</code>	<code>17</code>	— <code>2</code> : second ionization state; <code>17</code> : 17 levels are considered for this ion
<code>:</code>	<code>:</code>	<code>:</code>
<code>:</code>	<code>:</code>	<code>:</code>
<code>nzstar-1</code>	<code>1</code>	— The last ionization state to be considered.

Table 11
DWBORN Data Files

Default Unit No.	Default Name (UNIX)	Type	Description
1	dwnorn.inp	input	namelist input file for dwborn
2		scratch	scratch file
3	dwborn.sts	input	atomic state input file
4	debug.out	output	debugging output file
7	eaout.rate	output	rate coefficients and average collision strength for electron impact excitation
8	eaout.read	output	cross sections and collision strengths
9	eaout.plot	output	cross sections and collision strengths output for plotting x – incident electron energy y1 – cross section y2 – collision strength
10	streng.dat	output	collision strength in the format accepted by ATTABLE
11		scratch	scratch file
12		scratch	scratch file
13		scratch	scratch file
14		scratch	scratch file
15		scratch	scratch file

Table 12
Detailed Explanation of dwborn.inp

```

*
* *****
*
*                               DWBORN.INP
*   This is an input file for computer code DWBORN. DWBORN is a code for computing
*   electron impact excitation cross sections with distorted-wave Born method.
*
$bornin
*
*   ..... target ion information .....
*
*   element='Al',      ! target ion ID
*   z = 13,            ! nuclear charge
*   nee =3,            ! total number of bound electrons
*
*   ..... incident electron energy .....
*
*   units=1,          ! energy units: 1=2Ry, 2=eV
*   ekmin = 0.001,    ! minimum energy
*   ekmax = 100,      ! maximum energy
*   kepoit = 15,      ! number of grid points in energy mesh
*                     ! if kepoit=25, default Gaussian nodes
*
*   ..... control switches .....
*
*   contrl(1)=2,      ! =1: Born approximation (no exchange)
*                     ! =2: distorted wave approximation (with exchange)
*   contrl(2)=1,      ! =1: output in energy unit
*                     ! =2: output in threshold unit E/DE
*
*   contrl(3)=2,      ! =1: on-line calculate Hartree-Fock wavefunctions
*                     ! =2: read in wavefunctions from supplied data file
*
*   lspdf=6,          ! number of partial waves to be included
*   seedbg=0,         ! debug output (0=no, 1=yes )
*
*   ..... temperature range for maxwellian average .....
*
*   temin = 10,       ! minimum temperature (eV)
*   temax = 500,      ! maximum temperature (eV)
*
$ end

```

Table 13
Detailed Explanation of dwborn.sts

3		Number of levels to be considered
1 2 1001 2002		level index; number of shell; electronic configuration 1: the first level; 2: two shells; $1s^1 2s^2$
2 0 2		coupling sequence, always input number of shell, 0, number of shell
1 1 2 0 1 1 .5 -1.20397751E+02		left to right LS coupling scheme 0 1 2 0 1 2 J value; energy of the level E. If only considering LS term structure, set J = -1 if energy is not known, set E=0, program will do calculation to determine E.
2 3 100 2001 2101 3 0 3 1 1 2 1 1 2 1 3 2 0 1 2 0 1 3 0 3 4 .5 -1.20195938E+02		The second level
3 3 1001 2001 2101 3 0 3 1 1 2 1 1 2 1 3 2 0 1 2 0 1 3 0 3 4 1.5 -1.20185051E+02		The third level

Table 14
MICPSSR Data Files

Default Unit No.	Default Name (UNIX)	Type	Description
1	mi_cpssr.inp	input	namelist input file
2		SCRATCH	scratch file
3	Xsection.tab	output	a readable data table for ion impact ionization cross sections
6	debug.out	output	debugging output file
13	Xsection.dat	output	data table for ion impact ionization cross sections in the format accepted by BEAMTAB.

Table 15
Detailed Description of mi_cpssr.inp

```

* ****
*
*          NAMELIST INPUT FILE
*
*          FOR
*
*          ION IMPACT IONIZATION CROSS SECTION CALCULATION
*
*          direct ionization,
*          electron capture,
*          multiple ionization
*          (plane-wave-Born model + CPSSR)
* ****
* &inputii
*
* . . . . . (1) target atom information
*
* element='Al',          ! target ion ID
* z = 13,                ! target nuclear charge
* nee = 4,               ! number of bound electrons
* mass = 27,             ! target atomic weight
*
* . . . . . (2) target state (electron configuration)
*          default setup for OI, AII, CII, ArI, and AuI
*
* ideft = 0,             ! =1 using default configuration for neutral atom
* shelln = 3,            ! number of subshells of the configuration
* nle(1) = 1002, 2001,   ! 1s2, 2s2
* nle(3) = 2101, 3002,   ! 2p6, 3s2
* nle(5) = 3101, 3205,   ! 3p6, 3d10 . . .
* nle(7) = 4002, 4106,   !
* nle(9) = 4210, 4314,   ! 1000*n + 100*l + e
* nle(11)= 5002, 5106,   !
* nle(13)= 5210, 6001,   !
*
* . . . . . (3) ionized shell information (up to 5 subshells)
*
* nid(1)=1,2,2          ! principal quantum # (n) of the ionized shell
* lid(1)=0,0,1          ! orbital quantum # (l) of the ionized shell
* vj(1) =-1,-1,-1,     ! j value of the ionized shell (for ls coupling
*                          ! set vj=-1)

```

Table 15 (Continued)

```
*
* . . . . . (4) incident ion information
*
*   massint = 7,    ! atomic weight
*   zinct = 3,     ! nuclear charge of the projectile
*   qinct = 3,     ! net charge of the projectile
*
* . . . . . (5) beam energy
*
*   units=2,       ! unit of energy (1=2Ry, 2=eV)
*   ekmin=9.0e6,   ! minimum beam energy
*   ekmax=5.0e6,   ! maximum beam energy
*
*
* . . . . . (6) calculation parameter
*
*   lspdf =4,      ! # of partial wave included (suggested value=4)
*   kepoit=1,     ! energy mesh point used for the calculation
*   seedbg=0,     ! debug switch: 1=on, 0=off
*
*
* . . . . . (7) control switches
*
*   contrl(1)=1,   ! contrl(1): binding & polarization effects (0=no,1=yes)
*   contrl(2)=1,   ! contrl(2): Coulomb deflection effect (0=no,1=yes)
*   contrl(3)=1,   ! contrl(3): relativistic corrections (0=no,1=yes)
*   contrl(4)=1,   ! contrl(4): calculate multiple ionization X (0=no,1=yes)
*   contrl(5)=1,   ! contrl(5): calculate electron capture X (0=no,1=yes)
&end
```

Table 16
CKFYED Data Files

Default Unit No.	Default Name (UNIX)	Type	Descriptions
1	yields.inp	input	namelist input file n
2		SCRATCH	scratch file
3	ckf.state	input	autoionizing configurations to be considered
4	Auger.states	intermediate	all autoionizing terms generated by code
5	debug.out	output	debugging output
8	ls.terms	not used	
10		SCRATCH	scratch file
11		SCRATCH	scratch file
12		SCRATCH	scratch file
13		SCRATCH	scratch file
14		SCRATCH	scratch file
90	Auger_CK_fyield.tab	output	readable table for Auger rates, Coster-Kroning rates and fluorescence yields
91	fyield_config.dat	output	configuration averaged fluorescence yields
92	fyield_term.dat	output	term-dependent fluorescence yields

Table 17
Description of yields.inp

```

*
* *****
*
* This is an input file for C-K and fluorescence yield calculation
*
* *****
*
*
&ckfinp
  seedbg = 0,                ! debug output switch (0=no, 1=yes)
* *****
*                               atomic system
* *****
  Z = 13,                    ! atomic nuclear charge
* *****
*                               hole transitions
* *****
  klmno = 1,                ! shell index of the initial hole (K=1,L=2...)
  nih = 1,                  ! principal quantum # of the initial hole
  lih = 0,                  ! orbital quantum # of the initial hole

  nfhole = 2,              ! # of final holes produced by radiative tran.
  nfh(1) = 2,3,            ! principal quantum # of the final hole
  lfh(1) = 1,1,            ! orbital quantum # of the final hole
* *****
*                               jj-coupling configuration
* *****
  jjcog = 0                 ! jj-coupling switch (0=no, 1=yes)

```

Table 17 (Continued)

```
*
* If one is only interested in LS coupling system, ignore the following.
* The following parameters are set particularly for Au system.
*
-----
issr = 22          ! # of shell of the jj-coupling config.
* ... electron configuration
nler(1) = 1002,           ! K shell
nler(2) = 2002,2102,2104, ! L shell
nler(5) = 3002,3102,3104,3204,3206, ! M shell
nler(10)= 4002,4102,4104,4204,4206,4306,4308, ! N shell
nler(17)= 5002,5102,5104,5204,5206, ! O shell
nler(22)= 6001,          ! P shell

* ... binding energies
ebr(1) = 2998.63,
ebr(2) = 540.85, 517.66, 449.37,
ebr(5) = 131.20, 121.44, 105.97, 89.68, 86.31,
ebr(10) = 30.44, 26.11, 22.32, 15.12, 14.39, 4.87, 4.71,
ebr(17) = 5.33, 3.81, 3.15, 0.982, 0.907,
ebr(22) = 0.626,

* ... ratios of degeneracy to the non-relativistic shell
* for example: L1 subshell=1, L2 subshell=0.33, L3 subshell=0.67)
facr(1) = 1,
facr(2) = 1, 0.33, 0.67,
facr(5) = 1, 0.33, 0.67, 0.4, 0.6,
facr(10)= 1, 0.33, 0.67, 0.4, 0.6, 0.43, 0.57,
facr(17)= 1, 0.33, 0.67, 0.4, 0.6,
facr(22)= 1,

* shell index of the initial 'hole'
isidr = 0

* end of the input file

* &end
```

Table 18
Description of ckf.state

```

* *****
* This is an input file for CKF calculations
* This file includes all the autoionizing configurations to be calculated
* *****
*
* (1) number of the configurations to be considered
* 4
* (2) configurations : (# of shells), (1000*n + 100*l + e)
* F-like Al
* 3 1001 2002 2106      ! 3 shells, 1s12s22p6
* 4 1001 2002 2105 3001 ! 4 shells, 1s12s22p53s1
* 4 1001 2002 2105 3101 ! 4 shells, 1s12s22p53p1
* 4 1001 2002 2105 3201 ! 4 shells, 1s12s22p53d1

```

Note: Lines with * in the first column are comment lines.