13. Additional programs-utilities

In addition to the programs that were described separately, a number of short utility programs are available that assist in the processing and managing of the data.

B O U N D _ B S W

Description:	converts the close-coupling *B*-spline expansions to the *c*- and *bsw*-files
Input files:	**bound.nnn, bound_bsw.inp**
Output files:	*c*- and *bsw*-files for given states
Call:	**bound_bsw < bound_bsw.inp**

The results of the bound-state *B*-spline calculations are recorded in the **bound.nnn** files in the form of the corresponding close-coupling expansions (7.3). They are similar to the *l*- or *j*-files in the MCHF complex, and contain descriptions of all states for a given total term. The BOUND_BSW utility collects the information for a given bound state indicated in the file **bound_bsw.inp**, and records it as pair **name.c** and **name.bsw**. These files can be used as input target files for the BSR scattering calculations.

B O U N D _ T A B

Description:	produces the total list of resulting bound states
Input files:	**bound.nnn**
Output files:	**bound.tab**
Call:	**bound_tab**

This rogram sorts the energy levels in different **bound.nnn** files and prints them in atomic units, eV or cm^{-1}, relative to the lowest state. The user can define the range of partial waves and the energy range to restrict the output.

B S W _ W

Description:	converts the *bsw*-file to the *w*-file
Input files:	**name.bsw**
Output files:	**name.w**
Call:	**bsw_w name.bsw**

C F I L E

Description:	extracts the given state from *l*- or *j*-file in separate *c*-files
Input files:	**name.l or name.j**
Output files:	**result.c**
Call:	**cfile** `name.l(j) nn 2J result.c eps_c`

In the BSR complex, each target state is described by a pair **name.c** and **name.bsw**. The CI program from the MCHF complex produces the results in the *l*(*j*)-files as a list of states. The CFILE utility allows one to extract the expansion coefficients for a given state and create the corresponding *c*-file. The user should indicate in the command line the name of the input *l*- or *j*-file, the pointer for the given state, `nn`, the value of 2*J* if it is a *j*-file, the name for the output c-file, and the tolerance for the expansion coefficients, eps_c.

P H O T O _ T A B

Description:	produces the tables for channel or total cross sections and asymmetry parameters
Input files:	**bsr_phot.nnn**
Output files:	indicated by user
Call:	**photo_tab** with interactive response

This utility serves for processing the data recorded during photoionization calculations with program BSR_PHOT. The program BSR_PHOT can be run for different energy intervals and different partial waves separately. The results are accumulated in files **bsr_phot.nnn**. Then final tables for channel or total cross sections and asymmetry parameters may be generated with utility **photo_tab**. More details are given in the description of the BSR_PHOT program.

S L A T E R _ W

Description:	transfers Slater-type orbitals to MCHF format
Input files:	**name.slw**
Output files:	**name.w**
Call:	**slater_w name.slw**

The Slater orbitals are supposed to be given as in the RMATRX1 code, i.e.,

$$P_{nl}(r) = \sum_{j=1}^{NCO} C(j) * r^{IRAD(j)} * e^{-ZE(j)*r} \ .$$

The formatted file name.slw contains the Slater-type orbital parameters in the form:

1. `Z, atom, term` – nuclear charge, and optional identification for atom and term
2. `nwf` – number of radial wave functions
3. `n,l,k` – quantum numbers for given orbital
4. `NCO`
5. `IRAD(1:NCO)`
6. `ZE(1:NCO)`
7. `C(1:NCO)`

   Repeat records 3-7 `nwf` times

S U M _ H H

Description:	merges the set of **h.nnn** files to the final H.DAT
Input files:	**h.nnn**
Output files:	**h.dat**
Call:	**sum_hh** `klsp1 klsp2`

W _ B S W

Description:	converts the *w*-file to the bsw-file format
Input files:	**name.w**
Output files:	**name.bsw**
Call:	**bsw_w name.w**