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** [**klsp =…**]

This program sorts the energies of states recorded 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. The end of the file contains the parameters used by program. The range of partial waves is defined by **klsp1**, **klsp2**, and **klsp3**, as the initial, final and step for partial wave. **Emin**, **Emax** restrict the energy region under consideration (zero values mean no restrictions). Nuclear charge **Z** and **AWT** (if they are not zero) are used to define conversation factor from atomic units (Ry, au) to other units (eV, cm-1). **E0** defines the reference points to calculate excitation or bound energies. If reference point is not defined by user, the program chooses the energy of the first target state as the reference points. All above parameters can be redefined by corresponding command-line arguments (as parameter=value), or user can change these parameters directly in the **bound_tab** file and re-run the program.

```
klsp  sol   label     L  S  P     E_Ry        E_eV       E_cm       E_au

   1   1   4s_4s_1S   0  1  1   -0.217888   -5.92898   -47820.4   -676.80847440
   4   1   4s_4p_3P   1  3 -1   -0.147927   -4.02526   -32465.9   -676.73851340
   3   1   4s_4p_1P   1  1 -1   -0.109965   -2.99226   -24134.2   -676.70055090
   8   1   4s_3d_3D   2  3  1   -0.105841   -2.88004   -23229.1   -676.69642660
   7   1   4s_3d_1D   2  1  1   -0.102908   -2.80023   -22585.4   -676.69349370
   2   1   4s_5s_3S   0  3  1   -0.078572   -2.13803   -17244.4   -676.66915820
   1   2   4s_5s_1S   0  1  1   -0.070551   -1.91976   -15483.9   -676.66113670
  12   1   3d_4p_3F   3  3 -1   -0.059778   -1.62664   -13119.7   -676.65036440
   4   2   4s_5p_3P   1  3 -1   -0.056834   -1.54651   -12473.5   -676.64741990
.....................................................................................
   5   9   3d_kd_1P   1  1  1    0.081296    2.21216    17842.3   -676.50928960
   5  10   4p_6p_1P   1  1  1    0.083449    2.27072    18314.6   -676.50713740
*

Z    =  20.000
AWT  =   0.000

E0   =   -676.59058592
Emax =      0.00000000

klsp1 =   1
klsp2 =  14
klsp3 =   1

au_eV=        27.211055
au_cm=    219471.99

nstate =  218
```

Figure 1. Example of the **bound_tab** file.