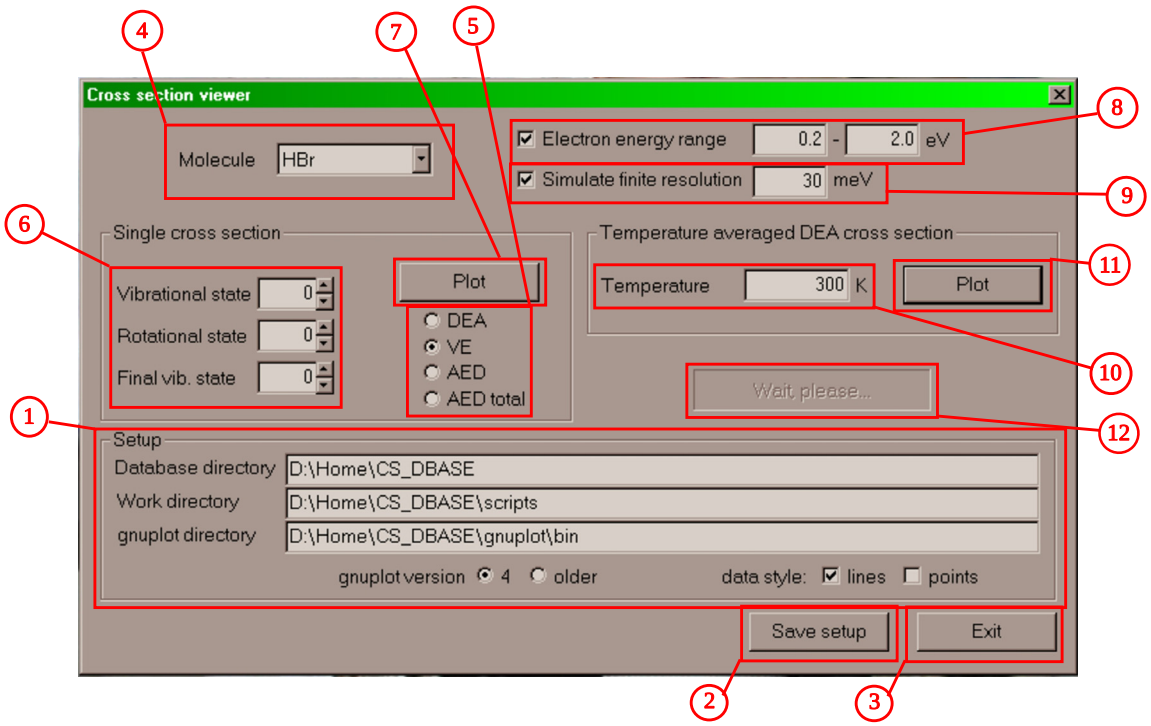
Cross section viewer - Reference

Cross section viewer is an user friendly interface for viewing and basic processing of the data from the cross section database **CS_DBASE**. It plots cross sections for the dissociative electron attachment (DEA), vibrational excitation (VE) and partial and total cross sections of the associative electron detachment (AED). In addition, it can be used to calculate temperature averaged DEA cross sections or to simulate finite energy resolution on the data from the database. **Cross section viewer** also produces scripts for **gnuplot** with absolute paths to the data files, so that figures can be produced without manual search for particular data files.



- **Installation and basic setup**

  The application requires no special installation. When run for the first time the configuration file *CSview.ini* is saved to your user profile directory (typically *C:\Documents and Settings\user\CSview*), containing typical setup of the application.

  In the *Setup* section 1 of the dialog box you can change the database directory and work directory (gnuplot scripts and data files with temperature averaged cross sections will be saved here). Gnuplot directory field has to point at the location of *wgnuplot.exe*. You can also select whether the data will be plotted

with lines or points (or both). All changes made in the section 1 take effect immediately, but you have to click the button *Save setup* 2 to save the information to the *CSview.ini*.

- **Cross section plotting**

  First select molecule from the list 4, then select process 5. In section 6 select particular channel you are interested in (some fields can be inactive depending on the selected process). Then click the button *Plot* 7. Gnuplot is called and figure appears on the screen. Click any button in the *gnuplot pause* window to close the figure window.

  Energy range of the figures is determined by the data in plotted file. Different range can be set in the fields 8.

  When the *Plot* button 7 is clicked gnuplot script is generated and saved in the work directory. It contains full path to the data file and can be used later to produce postscript figure for instance. The file name format is clear from the following examples:

  - *HBr_DA01J03.plt* for the process of DEA to the HBr molecule, initially in the first excited vibrational state ($\nu = 1$) with angular momentum $J = 3$.
  - *HBr_VE00-02J03.plt* for the VE of the HBr molecule from ground to second excited vibrational state, $J = 3$.
  - *HBr_AD01J3.plt* for the process of AED, HBr molecule in the final state $\nu = 1$ and $J = 3$.
  - *HBr_ADTotal.plt* for the total integral cross section of the AED.

- **Temperature averaged DEA cross sections**

  Select molecule from the list 4 and set desired temperature 10. Then click the *Plot* button 11. The data have to be calculated (unless you have plotted the same figure before and the data file is already stored in the *data* subfolder of the work directory). Notification 12 is visible while the program is working. Calculated data are stored in the work directory (for example *HBr_T0300K.dat* for the cross section of the DEA process to the HBr molecule at 300K) and then the figure appears on the screen. Gnuplot script with full path to the data file is stored in the work directory (*HBr_T0300K.plt*).

- **Simulation of the finite energy resolution**

  For better comparison of the theoretical data with experiments it is possible to simulate finite energy resolution of the theoretical data, both in single channels and temperature averaged cross sections. Check *Simulate finite resolution* and set the resolution in meV 9. The theoretical data will be convoluted with the gaussian function with the given half-width after the *Plot* button is clicked. New data file as well as the gnuplot script are stored in the work directory. The file name format is the same as before, only the string *FWHM###* is added, where *###* is the half-width in meV. In the present database the data are calculated on the energy grid with 5 meV step. Therefore the convolution will be evaluated inaccurately if the resolution is set below 10 meV.