

The *photo_tab* utility

Description:	produces the tables for channel or total cross sections and asymmetry parameters
Input files:	bsr_phot.nnn , target
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**.

The **photo_tab** utility has a set of different options for output:

- 1 - total cross sections
- 2 - channel cross sections
- 3 - ionic-state cross sections
- 4 - beta-parameters
- 5 - dipole matrix elements for given channel
- 6 - delete points (provide **delete_list**)
- 7 - check archives
- 8 - clean archives (provide **energy_list**)
- 9 - dipole matrix elements for range of channels
- 10 - eigenphases and its derivatives

The **bsr_phot** utility is working interactively. It first outputs the list of available options and as to choose one. Then the program may ask additional parameters and the file name for output. It includes, e.g., the list of partial waves included into consideration, the range of channels or ionic target states of interest. The most of options are clear and self-explained. The program allows to clean the **bsr_phot.nnn** (which can be very big) from not needed energy points indicated in the **delete_list** file. The special interest is the calculation of anisotropy parameter and eigenphases and its derivatives. The related formula are discussed below.

Anisotropy parameters

An anisotropy parameter β defines the angular distribution of photoelectrons. For example, for linearly polarized incident radiation the angular distribution of photoelectrons is given by

$$\frac{d\sigma}{d\hat{k}} = \frac{\sigma}{4\pi} [1 + \beta P_2(\cos \theta)] , \quad (11.11)$$

where θ is the angle of the ejected electron relative to the axis of polarization, while for unpolarized radiation it takes the form

$$\frac{d\sigma}{d\hat{k}} = \frac{\sigma}{4\pi} \left[1 - \frac{\beta}{2} P_2(\cos \theta) \right], \quad (11.12)$$

where θ is the angle of the ejected electron relative to the incident radiation beam. The computation of parameters depends on the coupling scheme and define by following formulas (presented by A. Grum-Grimailo and E. Grizlova, private communication)

LS-case:

$$\beta = \frac{\sqrt{30}(-1)^{L_f+L_0}}{\sum_j |(\Psi_j^- \| D \| \Phi_0)|^2} \sum_{jj'} (-1)^{L-L'} i^{l-l'} e^{-i\sigma_l+i\sigma_{l'}} [(2l+1)(2l'+1)(2L+1)(2L'+1)]^{1/2} \\ \times \begin{pmatrix} l & l' & 2 \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} L & L' & 2 \\ l' & l & L_f \end{Bmatrix} \begin{Bmatrix} L & L' & 2 \\ 1 & 1 & L_0 \end{Bmatrix} (\Phi_0 \| D \| \Psi_{j'}^-)(\Phi_0 \| D \| \Psi_j^-)^* \quad (11.13)$$

JK-case:

$$\beta = \frac{\sqrt{30}(-1)^{J_f+J_0-\frac{1}{2}}}{\sum_j |(\Psi_j^- \| D \| \Phi_0)|^2} \sum_{jj'} i^{l-l'} e^{-i\sigma_l+i\sigma_{l'}} [(2l+1)(2l'+1)(2K+1)(2K'+1)(2J+1)(2J'+1)]^{1/2} \\ \times \begin{pmatrix} l & l' & 2 \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} K & K' & 2 \\ l' & l & J_f \end{Bmatrix} \begin{Bmatrix} K & K' & 2 \\ J' & J & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} J & J' & 2 \\ 1 & 1 & J_0 \end{Bmatrix} (\Phi_0 \| D \| \Psi_{j'}^-)(\Phi_0 \| D \| \Psi_j^-)^* \quad (11.14)$$

JJ-case:

$$\beta = \frac{\sqrt{30}(-1)^{J_f-J_0-\frac{1}{2}}}{\sum_j |(\Psi_j^- \| D \| \Phi_0)|^2} \sum_{jj'} (-1)^{J-J'} i^{l-l'} e^{-i\sigma_l+i\sigma_{l'}} [(2l+1)(2l'+1)(2j+1)(2j'+1)(2J+1)(2J'+1)]^{1/2} \\ \times \begin{pmatrix} l & l' & 2 \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} j & j' & 2 \\ l' & l & J_f \end{Bmatrix} \begin{Bmatrix} j & j' & 2 \\ J' & J & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} J & J' & 2 \\ 1 & 1 & J_0 \end{Bmatrix} (\Phi_0 \| D \| \Psi_{j'}^-)(\Phi_0 \| D \| \Psi_j^-)^* \quad (11.15)$$

Note the order of initial and final states in the D -matrix elements. The change of these orders may introduce of additional phase factors.