f_values

Description:	calculation of f-values for transition between target states based on the asymptotic coefficients in the H.DAT file
Input files:	**H.DAT** or **h.nnn, target**
Output files:	**f_values** or **f_values.nnn**
Call as:	**f_values** [**h**=… **klsp**=…]
	h [H.DAT] – alternative name for input file klsp [1] - partial wave index to choose **h.nnn** file for the process

s_values

Description:	calculation of s-values for transition between target states based on the asymptotic coefficients in the H.DAT file
Input files:	**H.DAT** or **h.nnn, target**
Output files:	**s_values** or **s_values.nnn**
Call as:	**s_values** [**h**=.. **klsp1**=… **klsp2**=… **L1**=… **L2**=...]
	h [H.DAT] - alternative name for H.DAT file
	klsp1[0] -

h [H.DAT]	alternative name for H.DAT file
klsp1[0]	minimum index of partial wave to be considered
klsp2[0]	maximum index of partial wave to be considered
L1[-1]	minimum total orbital moment to be considered
L2[-1]	maximum total orbital moment to be considered

Asymptotic coefficients decomposition

LS coupling

The long-range potential coefficients coupling two channels are

$$ACF(i,j,k) = 2a_{ij}^k = 2 < \bar{\Phi}_i(x_1 \dots x_N, \hat{\boldsymbol{r}}_{N+1}\sigma_{N+1}) \,|\, \sum_{n=1}^{N} r_n^k P_k(\cos \hat{\boldsymbol{r}}_N \bullet \hat{\boldsymbol{r}}_{N+1}) \,|\, \bar{\Phi}_j(x_1 \dots x_N, \hat{\boldsymbol{r}}_{N+1}\sigma_{N+1}) > \quad (1)$$

In tensor notation

$$a_{ij}^k = < \alpha_i L_i S_i l_i s; LM_L SM_S \,|\, \boldsymbol{M}^k \bullet \boldsymbol{C}^k \,|\, \alpha_j L_j S_j l_j s; LM_L SM_S > \quad (2)$$

where

$$M_q^k = \left(\frac{4\pi}{2k+1}\right)^{1/2} \sum_{n=1}^{N} r_n^k Y_q^k(\hat{\boldsymbol{r}}_n) \quad (3)$$

and

$$C_q^k = \left(\frac{4\pi}{2k+1}\right)^{1/2} Y_q^k(\hat{\boldsymbol{r}}_{N+1}) \ . \quad (4)$$

To evaluate expression (2), we may use the general expression (see, e.g., Cowan 1981, Eq.11.47) for matrix elements of a scalar product when angular momenta j_1, j_2 correspond to different subsystems

$$< j_1 j_2 jm \,|\, P^{(k)}(1) \bullet Q^{(k)}(2) \,|\, j'_1\, j'_2\, j'm' >$$
$$= \delta_{j,j'}\delta_{m,m'}(-1)^{j'_1+j_2+j}\begin{Bmatrix} j_1 & j_2 & j \\ j'_2 & j'_1 & k \end{Bmatrix} < j_1 \| P^{(k)} \| j'_1 >< j_2 \| Q^{(k)} \| j'_2 > \quad (5)$$

Then coefficients (2) are reduced to

$$a_{ij}^k = (-1)^{L_j+l_i+L} < l_i \| C^{(k)} \| l_j > \begin{Bmatrix} L_i & l_i & L \\ l_j & L_j & k \end{Bmatrix} < \alpha_i L_i \| M^{(k)} \| \alpha_j L_j > \quad (6)$$

This expression can be used for determination radiative matrix elements for transitions between target states from the asymptotic coefficients in *LS* coupling case.

jj coupling

$$a_{12}^k = < \alpha_1 J_1 (l_1 s) j_1; JM_J \,|\, \boldsymbol{M}^k \bullet \boldsymbol{C}^k \,|\, \alpha_2 J_2 (l_2 s) j_2; JM_J >$$
$$= (-1)^{J_2+j_1+J} < (l_1 s) j_1 \| C^{(k)} \| (l_2 s) j_2 > \begin{Bmatrix} J_1 & j_1 & J \\ j_2 & J_2 & k \end{Bmatrix} < \alpha_1 J_1 \| M^{(k)} \| \alpha_2 J_2 > \quad (7)$$

Here we can use the uncoupling formula when operator operates only within the first subspace (see Cowam 1981, Eq.11.38):

$$< j_1 j_2 j \| P^{(k)}(1) \| j'_1\, j'_2\, j' > = \delta_{j_2,j'_2}(-1)^{j_1+j_2+j'+k}[j, j']^{1/2}\begin{Bmatrix} j_1 & j_2 & j \\ j' & k & j'_1 \end{Bmatrix} < j_1 \| P^{(k)} \| j'_1 > \quad (8)$$

Then

$$a_{12}^k = (-1)^{J_2+j_1+J+l_1+s+j_2+k}[\mathrm{j}_1, \mathrm{j}_2]^{1/2}\begin{Bmatrix} l_1 & s & j_1 \\ j_2 & k & l_2 \end{Bmatrix} < l_1 \| C^{(k)} \| l_2 > \begin{Bmatrix} J_1 & j_1 & J \\ j_2 & J_2 & k \end{Bmatrix} < \alpha_1 J_1 \| M^{(k)} \| \alpha_2 J_2 >$$
$$(9)$$

jK coupling

$$a_{12}^k = < \alpha_1 (J_1 l_1) K_1, s; JM_J \,|\, \boldsymbol{M}^k \bullet \boldsymbol{C}^k \,|\, \alpha_2 (J_2 l_2) K_2, s; JM_J > \quad (10)$$

First we should uncoupled the J_1 and J_2 by transferring to *jj*-coupling (Cowan 1981, Eq.9.25):

$$< (J_1 l_1) K_1, s; J \,|\, J_1, (l_1 s) j_1; J > = (-1)^{J_1+l_1+s+J}[K_1, j_1]^{1/2}\begin{Bmatrix} J_1 & l_1 & K_1 \\ s & J & j_1 \end{Bmatrix} \quad (11)$$

Then

$$
\begin{aligned}
a_{12}^{k} = & \sum_{j_1,j_2} (-1)^{J_1+l_1+s+J}[K_1, j_1]^{1/2}\begin{Bmatrix} J_1 & l_1 & K_1 \\ s & J & j_1 \end{Bmatrix}(-1)^{J_2+l_2+s+J}[K_2, j_2]^{1/2}\begin{Bmatrix} J_2 & l_2 & K_2 \\ s & J & j_2 \end{Bmatrix} \\
& \times(-1)^{J_2+j_1+J+l_1+s+j_2+k}[\mathrm{j}_1, \mathrm{j}_2]^{1/2}\begin{Bmatrix} l_1 & s & j_1 \\ j_2 & k & l_2 \end{Bmatrix} < l_1 \| C^{(k)} \| l_2 > \begin{Bmatrix} J_1 & j_1 & J \\ j_2 & J_2 & k \end{Bmatrix} < \alpha_1 J_1 \| M^{(k)} \| \alpha_2 J_2 > \\
= & \sum_{j_1,j_2} (-1)^{J_1+2J_2+3J+j_1+j_2+l_2+3s+k}[j_1, j_2]\begin{Bmatrix} J_1 & l_1 & K_1 \\ s & J & j_1 \end{Bmatrix}\begin{Bmatrix} l_1 & k & l_2 \\ j_2 & s & j_1 \end{Bmatrix}\begin{Bmatrix} J_1 & k & J_2 \\ j_2 & J & j_1 \end{Bmatrix} \\
& \times[K_1, K_2]^{1/2}\begin{Bmatrix} J_2 & l_2 & K_2 \\ s & J & j_2 \end{Bmatrix} < l_1 \| C^{(k)} \| l_2 >< \alpha_1 J_1 \| M^{(k)} \| \alpha_2 J_2 >
\end{aligned} \qquad (12)
$$

Now let reduce sum over j_1, using the sum rule (Cowan 1981, Eq. 5.33):

$$
\sum_{x}(-1)^{S+x}[x]\begin{Bmatrix} l_1 & j_2 & l_3 \\ l'_3 & l'_2 & x \end{Bmatrix}\begin{Bmatrix} j_2 & j_3 & j_1 \\ l'_1 & l'_3 & x \end{Bmatrix}\begin{Bmatrix} l_1 & j_3 & l_2 \\ l'_1 & l'_2 & x \end{Bmatrix} = \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}\begin{Bmatrix} l_3 & j_1 & l_2 \\ l'_1 & l'_2 & l'_3 \end{Bmatrix} \qquad (13)
$$

where S = $j_1 + j_2 + j_3 + l_1 + l_2 + l_3 + l'_1 + l'_2 + l'_3$. Then

$$
\begin{aligned}
a_{12}^{k} = & \sum_{j_2} (-1)^{J_1+2J_2+3J+j_2+l_2+3s+k-l_2-l_1-k-J_1-J_2-K_1-j_2-J-s}[j_2]\begin{Bmatrix} l_2 & l_1 & k \\ J_1 & J_2 & K_1 \end{Bmatrix}\begin{Bmatrix} K_1 & l_2 & J_2 \\ j_2 & J & s \end{Bmatrix} \\
& \times[K_1, K_2]^{1/2}\begin{Bmatrix} J_2 & l_2 & K_2 \\ s & J & j_2 \end{Bmatrix} < l_1 \| C^{(k)} \| l_2 >< \alpha_1 J_1 \| M^{(k)} \| \alpha_2 J_2 > \\
= & \sum_{j_2} (-1)^{J_2+2J+2s-l_1-K_1}[j_2]\begin{Bmatrix} J_2 & l_2 & K_1 \\ s & J & j_2 \end{Bmatrix}\begin{Bmatrix} J_2 & l_2 & K_2 \\ s & J & j_2 \end{Bmatrix} \\
& \times[K_1, K_2]^{1/2}\begin{Bmatrix} l_2 & l_1 & k \\ J_1 & J_2 & K_1 \end{Bmatrix} < l_1 \| C^{(k)} \| l_2 >< \alpha_1 J_1 \| M^{(k)} \| \alpha_2 J_2 >
\end{aligned} \qquad (14)
$$

Using the orthogonal relation (Cowan 1981, Eq.5.31)

$$
\sum_{x}[x]\begin{Bmatrix} j_1 & j_2 & a \\ l_1 & l_2 & x \end{Bmatrix}\begin{Bmatrix} j_1 & j_2 & b \\ l_1 & l_2 & x \end{Bmatrix} = \frac{\delta(a,b)}{2a+1} \qquad (15)
$$

finally obtain

$$
a_{12}^{k} = \delta(K_1, K_2)(-1)^{J_2+2J+1-l_1-K_1}\begin{Bmatrix} l_2 & l_1 & k \\ J_1 & J_2 & K_1 \end{Bmatrix} < l_1 \| C^{(k)} \| l_2 >< \alpha_1 J_1 \| M^{(k)} \| \alpha_2 J_2 > \qquad (16)
$$