

Switching Functions Defined in VCHFIT

In the following, $\tau(Q)$ represents a general parameter τ of the vibronic coupling Hamiltonian ($\kappa_\alpha^{(i)}$, $\lambda_\alpha^{(i,j)}$, etc.) that is taken as a function of the coordinate Q *via* the use of a switching function that is in turn parameterised by a number of coefficients k_i . $\tau(Q_0)$ here corresponds to the value of the parameter τ at the reference value of Q .

Function label	Definition
tanh	$\tau(Q) = \tau(Q_0) + \alpha \tanh(\beta Q)$ with $\alpha = k_1$ $\beta = k_2$
dtanh	$\tau(Q) = \tau(Q_0) [1 - \tanh(\alpha Q)]$ with $\alpha = k_1$
cdtanh	$\tau(Q) = \frac{\tau(Q_0)}{2} \left[1 - \tanh\left(\frac{Q-\alpha}{\beta}\right) \right]$ with $\alpha = k_1$ $\beta = k_2$
adtanh	$\tau(Q) = \tau(Q_0) [1 - \tanh(\alpha Q)] + (\beta Q + \gamma Q^2) \exp(-\delta Q)$ with $\alpha = k_1$ $\beta = k_2$ $\gamma = k_1$ $\delta = k_2$