

Diabatic Coupling Functions Defined in VCH-FIT

Each one-mode coupling function $W_{ij}(Q_\alpha)$ is defined with respect to a set of parameters $\{k_n\}$, and is selected using the function labels given below.

Function label	Definition
tanh	$W_{ij}(Q_\alpha) = \Delta \tanh(\rho Q_\alpha)$ with $\Delta = k_1$ $\rho = k_2$
poly_to_tanh	$W_{ij}(Q_\alpha) = \Delta \tanh(\rho Q_\alpha) + (\zeta Q_\alpha + \eta Q_\alpha^2) \exp(-v Q_\alpha)$ with $\Delta = k_1$ $\rho = k_2$ $\zeta = k_3$ $\eta = k_4$ $v = k_5$
tanh2	$W_{ij}(Q_\alpha) = \frac{\Delta}{2} \left[1 - \tanh\left(-\frac{Q_\alpha - \zeta}{\eta}\right) \right]$ with $\Delta = k_1$ $\zeta = k_2$ $\eta = k_3$
cubic	$W_{ij}(Q_\alpha) = \lambda Q_\alpha + \frac{1}{3!} \eta Q_\alpha^3$ with $\lambda = k_1$ $\eta = k_2$