

Zero-order Diabatic Potentials Defined in VCH-FIT

Potentials are defined by the frequency, ω , and a set of “expansion coefficients”, $k_1, k_2, \dots$

Harmonic	$\frac{1}{2}\omega Q^2$
General harmonic	$\frac{1}{2}\omega^2 Q^2 + k_1 Q + \frac{1}{2}k_2 Q^2 + \frac{1}{24}k_3 Q^4$
General quadratic	$k_1 Q + \frac{1}{2}k_2 Q^2$
Quartic	$\frac{1}{2}\omega^2 Q^2 + k_1 Q + \frac{1}{2}k_2 Q^2 + \frac{1}{24}k_3 Q^4$
General quartic	$k_1 Q + \frac{1}{2}k_2 Q^2 + \frac{1}{24}k_3 Q^4$
General aquartic	$k_1 Q + \frac{1}{2}k_2 Q^2 + \frac{1}{6}k_3 Q^3 + +\frac{1}{24}k_4 Q^4$
Morse	$D_0 [\exp(\alpha(Q - Q_0) - 1)]^2 + E_0$ with $D_0 = k_1$ $\alpha = \sqrt{\frac{\omega+k_2}{2D_0}}$ $Q_0 = k_3$ $E_0 = -D_0 [\exp(\alpha Q_0 - 1)]^2$
Anti-Morse	$D_0 [\exp(-\alpha(Q - Q_0) - 1)]^2 + E_0$ with $D_0 = k_1$ $\alpha = \sqrt{\frac{\omega+k_2}{2D_0}}$ $Q_0 = k_3$ $E_0 = -D_0 [\exp(\alpha Q_0 - 1)]^2$

Exp	$E_{\infty} [\exp(-\alpha Q) - 1]$ with $E_{\infty} = k_1$ $\alpha = k_2$
Avoided_crossing	$\frac{1}{2} \left\{ \nu_b + \nu_d - \sqrt{(\nu_b - \nu_d)^2 + 4\lambda^2} \right\}$ with $\nu_b = D_b [1 - \exp(-\alpha_b(Q - Q_{0b}))]^2$ $\nu_d = A \exp(-\alpha_d(Q - Q_{0d})) + D_d$ $D_b = k_1$ $\alpha_b = k_2$ $Q_{0b} = k_3$ $A = k_4$ $\alpha_d = k_5$ $Q_{0d} = k_6$ $D_d = k_7$ $\lambda = k_8$
General_morse	$D_0 [1 - \exp(-\alpha(Q - Q_0))]^2 + E_0$ with $E_0 = -D_0 [1 - \exp(\alpha Q_0)]^2$ $D_0 = k_1$ $\alpha = k_2$ $Q_0 = k_3$
Morse_lorentzian	$D_0 [1 - \exp(-\alpha(Q - Q_0))]^2 + E_0 + \left[\frac{\delta}{1 + (Q - \epsilon)^2 / \phi} \right]$ with $D_0 = k_1$ $\alpha = k_2$ $Q_0 = k_3$ $E_0 = k_4$ $\delta = k_5$ $\epsilon = k_6$ $\phi = k_7$

Morse_gaussian	$D_0 [1 - \exp(-\alpha(Q - Q_0))]^2 + E_0 + \delta \exp(-\epsilon(Q - \phi)^2) \text{ with}$ $D_0 = k_1$ $\alpha = k_2$ $Q_0 = k_3$ $E_0 = k_4$ $\delta = k_5$ $\epsilon = k_6$ $\phi = k_7$
Avoided_crossing2	$\frac{1}{2} \left\{ \nu_b + \nu_d - \sqrt{(\nu_b - \nu_d)^2 + 4 [\alpha \tanh(\beta Q)]^2} \right\} \text{ with}$ $\nu_b = D_b [1 - \exp(-\alpha_b(Q - Q_{0b}))]^2$ $\nu_d = A \exp(-\alpha_d(Q - Q_{0d})) + D_d$ $D_b = k_1$ $\alpha_b = k_2$ $Q_{0b} = k_3$ $A = k_4$ $\alpha_d = k_5$ $Q_{0d} = k_6$ $D_d = k_7$ $\alpha = k_8$ $\beta = k_9$
Avoided_crossing_quartic	$\frac{1}{2} \left\{ \nu_l + \nu_u - \sqrt{(\nu_l - \nu_u)^2 + 4(\lambda Q)^2} \right\} \text{ with}$ $\nu_l = \frac{1}{2}\omega^2 Q^2 + \frac{1}{2}\gamma_l Q^2 + \frac{1}{24}\epsilon_l Q^4$ $\nu_u = \frac{1}{2}\omega^2 Q^2 + \frac{1}{2}\gamma_u Q^2 + \frac{1}{24}\epsilon_u Q^4 + \Delta E$ $\gamma_l = k_1$ $\epsilon_l = k_2$ $\gamma_u = k_3$ $\epsilon_u = k_4$ $\lambda = k_5$ $\Delta E = k_6$

