

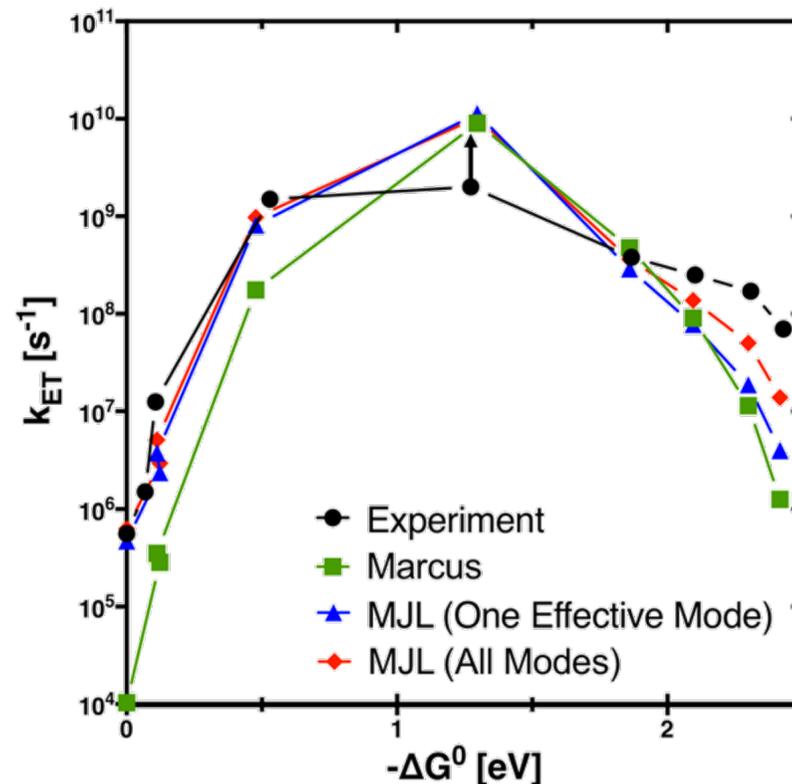
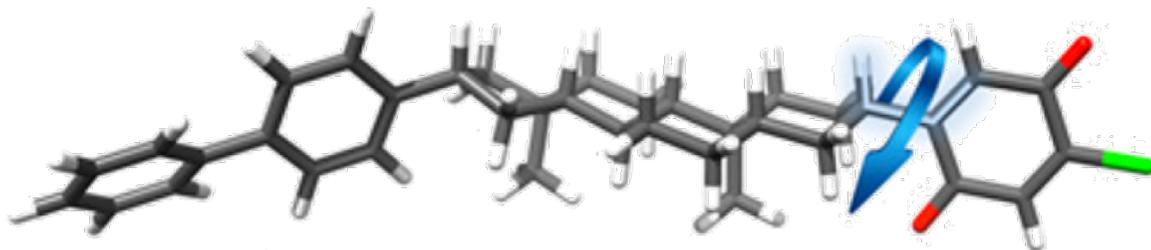


Electron Transfer Assisted by Vibronic Coupling from Multiple Modes



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$$k_{\text{ET,MJL,expl}} = \frac{\pi |H_{\text{AD}}|^2}{\hbar \sqrt{\pi \lambda_S k_B T}} \exp\left(\sum_{i=1}^N -S_i\right) \sum_{v_1=0}^{\infty} \cdots \sum_{v_i=0}^{\infty} \cdots \sum_{v_N=0}^{\infty} \times \left(\prod_{i=1}^N \left(\frac{S_i^{v_i}}{v_i!} \right) \exp\left(-\frac{(\Delta G^0 + \lambda_S + \sum_{i=1}^N \hbar \omega_i v_i)^2}{4 \lambda_S k_B T}\right) \right)$$



- ❑ Multiple configurations sampled with a dihedral scan
- ❑ Rates computed with an implementation of Marcus-Jortner-Levich Theory using a combination of DFT and Monte Carlo methods.
- ❑ All rates predicted are in the same order of magnitude as the experiments
- ❑ Big improvement over Marcus Theory in the inverted region