A computational protocol to calculate intersystem crossing rate constants

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ABSTRACT

We present a computational protocol [1] based on Fermi's Golden Rule, aimed at quantifying the Intersystem Crossing (ISC) rate constants. ISC, crucial in numerous chemical and physical processes, poses challenges due to its intricate nature and mechanisms involving Franck-Condon and HerzbergTeller effects [2]. Our protocol uniquely incorporates these effects, offering a nuanced perspective essential for relatively accurate ISC rate constants calculations in complex molecular systems. Notably, our protocol showcases a remarkable quantitative agreement with experimental findings obtained from Time-Resolved Electron Paramagnetic Resonance (TREPR) experiments[3]. This alignment highlights the protocol's robustness in capturing intricate photophysical properties and provides a comprehensive and reliable approach for evaluating ISC phenomena across diverse contexts.

References

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