

## Rate of Intersystem crossing in organic molecules

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The spin-orbit interaction plays an important part in the photophysics of molecules since it can flip electronic spin polarization to induce an intersystem crossing (ISC) between singlet and triplet states. The spin-orbit coupling determines the ISC rate and consequently the singlet and triplet ratios in any organic materials [1-3]. Incorporation of heavy metal atoms to the molecular system is expected to enhance the spin-orbit interaction and hence the ISC rate, which has been studied theoretically [4-6] and also measured experimentally [7]. Theoretical models have so far been limited to numerical calculations [4-6] or an estimation of the spin-orbit matrix element [8]. In this paper, exciton-spin-orbit-phonon interaction operator suitable for ISC in organic molecules is derived. Using this operator, an expression for ISC rate is derived and calculated for some organic molecules. The effect of incorporation of heavy atoms on the ISC rate is discussed and the results compared with experimental ones.

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