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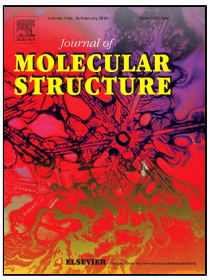

A computational Perspective of Vibrational and Electronic Analysis of potential photosensitizer 2-Chlorothioxanthone

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1. For CTX the HOMO is delocalized over the whole π-conjugated CC backbone and over the C-O, C-S and C-Cl.
2. The HOMO-LUMO topologies exhibit overlap of orbitals in certain regions of conjugated system. This overlap is supposed to be a prerequisite for effective charge transfer.
3. From NBO analysis the orbital intensive overlap between bonding orbitals C1—C2 → antibonding (C1—C6), (C6—C7); C3—C4 → (C5—C6), (C1—C2) and C11—C12 → (C13—C14), (C8—C9) with higher stabilization energies result in intra charge transfer which cause system stabilization.
4. For CTX, vibrations at 516 cm^{-1} is termed as C—Cl stretching and strong bands at 857 and 689 cm^{-1} are located as in plane bending of C—Cl.
5. The vibrations at frequency 857 and 689 cm^{-1} are characterized as in plane bending vibrations of C-S bond while out of plane deformations of C-S are conceived at 91 cm^{-1}.