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Solvent effect on the conformation of benzil.

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The conformation of benzil is investigated by PM3 and density functional theory (B3LYP) combined with the 6-31G(d,p) basis set. The variation of the relative energy with the OC–CO torsion angle indicates only one rather flat minimum, reflecting the flexibility of the benzil molecule. The dipole moment is measured in several organic solvents of various polarity and the IR and Raman spectra investigated in the CO stretching region in the same solvents. The torsional OC–CO angle is evaluated from the dipolar and vibrational data. The results indicate that, in all the solvents, benzil is in a *skewed* conformation, the *cisoid* conformation being slightly favoured when the polarity of the solvent increases. The contribution of electrostatic and specific interactions to the reduction of the torsional angle is discussed.

Słowa kluczowe

Benzil, Conformation, Theoretical calculations, IR and Raman spectra

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