Structural characterization of derivatives of 4-methylcoumarin : theoretical and experimental studies.

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The quantum chemical conformational analysis was performed for 4-methylcoumarin derivatives substituted with the hydroxy, acetyl and/or alkoxy groups. Their crystal structures were determined by a single crystal X-ray crystallography. The structural data in the solid were compared with the results of the quantum chemical analysis in the gas phase. The results indicated that the coumarin system is nearly planar and several conformers differing in the orientation of the methoxy and acetyl groups are observed. The stereochemistry of the lowest energy rotamers in the gas phase is retained in solid state; intermolecular forces are to weak for inducing conformational changes. In the crystals of studied 4-methylcoumarin derivatives the π···π stacking of benzopyran systems is a very characteristic and persistent feature of the molecular association. The extend of the π···π overlapping depends on substituents.

Słowa kluczowe

Coumarin derivatives, DFT calculation, crystal structure, π···π Interactions

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