REFLECTION OF CONFORMATIONAL PROPERTIES OF A FREE MOLECULE OF NONMESOGEN 4-PHENYLAZOBENZOIC ACID IN CRYSTAL STRUCTURES

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Introduction

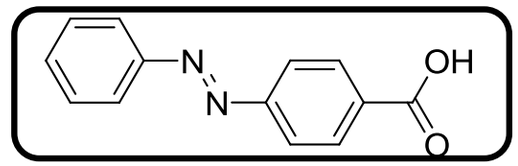
The principles of supramolecular chemistry are successfully applied in the creation of new hydrogen bonded mesomorphic complexes with mesogen and nonmesogen complementary compounds. The structure of nonmesogen 4-phenylazobenzoic acid (4-PABA) allows its use as a monofunctional component of potentially mesogen hydrogen bonded complexes.

Purpose of the work

Quantum-chemical study of the conformational properties of a free 4-PABA molecule, comparison of the obtained data with structures stabilized in the crystal.

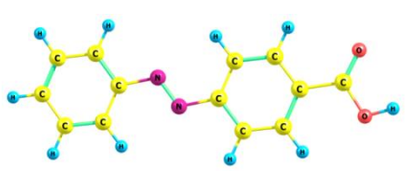
Method

Quantum chemical calculations **(study of conformational properties)**
Gaussian09 (DFT/B3LYP/cc-pVTZ)

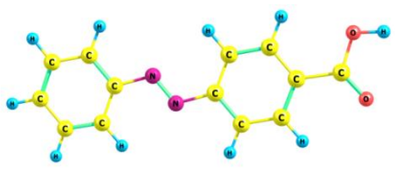


(4-phenylazo)benzoic acid (4-PABA)

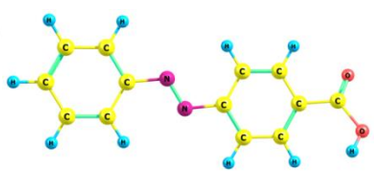
trans



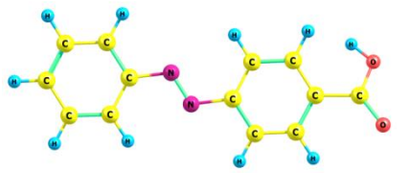
Conformer-1
ΔE=0 (kcal/mol)



Conformer-2
ΔE=0.01 (kcal/mol)

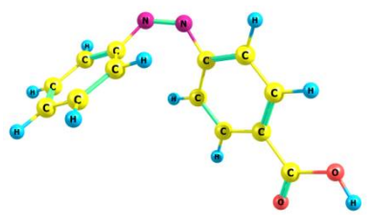


Conformer-3
ΔE=6.42 (kcal/mol)

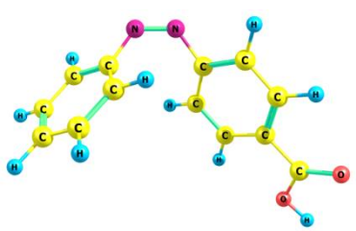


Conformer-4
ΔE=6.41 (kcal/mol)

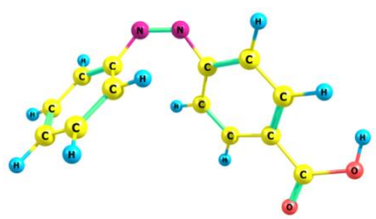
cis



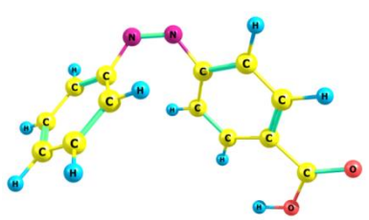
Conformer-5
ΔE=14.91 (kcal/mol)



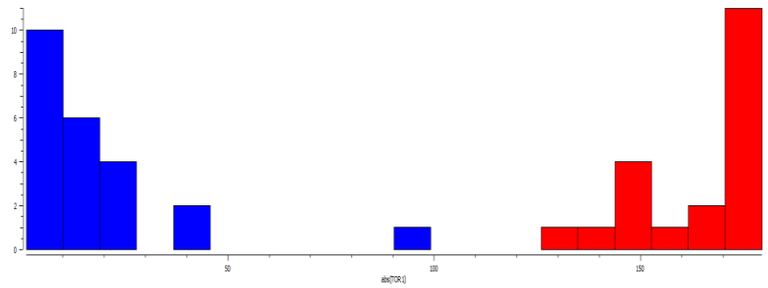
Conformer-6
ΔE=14.91 (kcal/mol)



Conformer-7
ΔE=21.50 (kcal/mol)



Conformer-8
ΔE=21.54 (kcal/mol)



Histogram of the distribution of the angle N=N...C=O in the substituted 4-PABA from the CCDC (43 objects)

Conclusions

Using the DFT method, it was determined that the 4-PABA molecule has 8 conformers, among which the conditional "cis“ and "trans " conformers can be distinguished. The relative energy of the "cis" conformers is significantly higher (15-22 kcal/mol) than the energy of the "trans" conformers. The most energetically advantageous are the "trans" conformers 1 and 2, which differ from each other in the position of the carboxyl group relative to the plane of the molecule. The torsion angle N=N...C=O in conformer 1 takes the value 0°, and in conformer 2-180°. This torsion angle is selected as a search criterion in the Cambridge database. It was determined that the crystal contains structures close to conformer 1 (53.5%) and conformer 2 (46.5%). No " Cis " conformers were detected. Thus, the calculated data adequately describe the conformational properties of the molecules. Modeling of H-complexes can be based on using the structure of a more favorable conformer.

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