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НАУЧНА ПОСТЕРНА СЕСИЯ
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ТЕОРЕТИЧНО ИЗСЛЕДВАНЕ НА СТРУКТУРАТА НА БЕНЗОХИДРАЗИДИ И КАРБОХИДРАЗИДИ

THEORETICAL STUDY OF THE STRUCTURE OF BENZOHYDRAZIDES AND CARBOHYDRAZIDES

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Theoretical investigation of the structure and possible tautomerism of benzohydrazides and carbohydrazides was carried out by calculations at HF, DFT and MP2 levels of theory. Theoretically all hydrazides (four compounds) can exist in two tautomeric forms in different conformations. The relative stabilities of the tautomers and conformers of the hydrazides were calculated in gas phase and in solvent DMSO using the PCM method. The *ab initio* calculations predict that the hydrazides exist as keto form in gas phase.



X = CH

N'-[(E)-(4-chloro-2-oxo-2H-chromen-3-yl)methylidene]benzohydrazide

X = N

N'-[(E)-(4-chloro-2-oxo-2H-chromen-3-yl)methylidene]pyridine-4-carbohydrazide



X = CH

N'-[(E)-(2-methyl-2H-chromen-3-yl)methylidene]benzohydrazide

X = N

N'-[(E)-(2-methyl-2H-chromen-3-yl)methylidene]pyridine-4-carbohydrazide

Key words: carbohydrazides, benzohydrazides, *ab initio*, DFT, PCM, tautomerism

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