



N–H...O versus O–H...O: density functional calculation and first principle molecular dynamics study on a quinoline-2-carboxamide N-oxide.

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Streszczenie

N-oxide-type compounds are the object of current research interest due to the presence of resonance-assisted N–H...O hydrogen bonds. Here, the metric and spectroscopic parameters of N-methyl-quinoline-2-carboxamide 1-oxide were computed on the basis of density functional theory and Car-Parrinello molecular dynamics. Computations were performed in vacuo and in solid state; for both phases additional simulations with Grimme's dispersion correction were carried out. The approaches used were able to reproduce correctly the structural aspects of the studied compound and shed more light on the hydrogen bonding with special focus on bridge proton mobility. Proton transfer phenomena were found not to occur in the investigated compound, and the bridge proton was localized to the donor site. This observation is in agreement with the classical theory of the acidity of donor–acceptor sites. The presence of hydrogen bonding was confirmed using atoms-in-molecules theory. The computational results were compared with available experimental data.

Słowa kluczowe

N-oxide, intramolecular hydrogen bond, density functional theory, atoms in molecules, Car-Parrinello molecular dynamics, Gas and crystalline phase

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