N-oxide derivatives: Car–Parrinello molecular dynamics and electron localization function study on intramolecular hydrogen bonds.

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Streszczenie

First-principle molecular dynamics simulations (CPMD) and electron localization function (ELF) topological analysis were performed for two *N*-oxides, 2-[(*N*,*N*-dimethylamino-*N*-oxy)methyl]-4,6-dimethylphenol (**I**) and 5,5′-dibromo-3-[(diethylamino)methyl]-2,2′-biphenol *N*-oxide (**II**). Special attention was paid to hydrogen bond dynamics and spectroscopic features. Simulations were carried out *in vacuo* and in the crystalline phase. It was found that for compound **I** proton transfer phenomena do not occur spontaneously. An opposite situation was noticed for one of the two intramolecular hydrogen bonds of compound **II**. The influence of the neighboring molecules (including microsolvation) and the crystal field on the hydrogen bond properties cannot be neglected. Hydrogen bond spectroscopic signatures were quite well reproduced by power spectra of atomic velocity. Metric and spectroscopic theoretical findings were compared with experimental data available, especially in a view of the fact that experimental X-ray diffraction and FT-IR data of compound **II** indicate strong delocalization of the *N*-oxide bridge proton. ELF analysis showed that for compound **II** the *N*-oxide bridge belongs to the topological category of strong hydrogen bonds with the separate ELF basin for the bridged hydrogen atom.

Adres publiczny

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https://www.acs.org/content/acs/en.html