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Structural property investgations of 1-[2-(2-methoxyphenyl)ethyl]piperidinium chloride: an experimental and computational study.

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Streszczenie

A phenethyl containing piperidinium compound was synthesized and the results of an X-ray crystallographic and computational analysis of this compound are reported. The compound, 1-[2-(2-methoxyphenyl)ethyl]piperidinium chloride, contains a C-H···O contact, which stabilizes the experimentally found conformation. Additionally, an ionic bond between N-H···Cl atoms is present as shown by the crystallographic measurements. The presence of these two contacts prompted us to perform further theoretical studies. The first part of the computational investigations was carried out on the basis of the Car-Parrinello molecular dynamics (CPMD) in the solid-state using experimental parameters and conditions as a starting point of the simulation. The time evolution of the interatomic distances of the atoms involved in the N-H···Cl interaction was investigated. Vibrational features of the compound were studied by predicted and power spectra. In addition, static models, based on density functional theory (DFT) and second-order Møller-Plesset perturbation calculus, were built to describe the geometric and electronic structure parameters. Finally, the details of the ionic bridge were analyzed using the natural bond orbitals (NBO) approach. The electron density topology was investigated by the atoms in molecules (AIM) theory. In summary, the ionic bridge modifies the spectroscopic properties of the bridge proton. The negative charge of the chloride anion is partially delocalized via the ammonium moiety to the organic subunit.

Słowa kluczowe

AIM, Crystal structure, NBO, Piperidine derivatives, Solid-state Car-Parrinello molecular dynamics

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