MODELING AND COMPARATIVE ANALYSIS OF BENZENAMINE CONFORMATIONS

Abulyaissova L.K.
Buketov Karaganda University
abu.lyazzat@gmail.com

Schiff bases are of interest for many areas of chemistry, physics (liquid crystals and nonlinear optics) and biochemistry. Benzenamine $C_2H_5OC_6H_4CHNC_6H_4C_4H_9$ is one of compounds having a nematic phase and widely used in experimental studies. The structure and properties of benzeneamine are studied experimentally and theoretically.

In the solid state of benzenamine, the triclinic space group P-1 is realized with two molecules in a unit cell (one crystallographically independent molecule) [1]. The molecule has a deviation from the intrinsic symmetry inherent in an isolated molecule, namely the *gt* (gosh-trans -) - configuration of the terminal butyl substituent.

In this work, the possible conformations of the amine are modelled. Comparative analysis of the structural, energetical, and spectral properties of gas-phase and crystal structures has been carried out using quantum-chemical calculations by the B3LYP functional supplemented with 6-31G(d) and cc-pVTZ basis sets [2].

Comparing the conformational forms, the most energetically stable conformation is one with complete *p, π*- and *π, π*-conjugation. Deviations from the intrinsic symmetry of the isolated molecule lead to destabilization of the other structures. The realization of an energetically unfavorable conformation in a crystal is explained by intermolecular forces and molecular packing. The latters also determine the geometric features of the crystalline conformation.

The assignment of the bands in the experimental spectrum [3] is carried out. The vibrational frequencies and intensities of the absorption bands of the infrared spectra of the calculated conformations are compared. The theoretical frequencies are in qualitative agreement with the experimental data in the literature.

References

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