GAS ELECTRON DIFFRACTION AND QUANTUM CHEMICAL STUDIES OF THE MOLECULAR STRUCTURE OF 2-NITROBENZENESULFONIC ACID

© **V. M. Petrov,[1] N. I. Giricheva,[1] G. V. Girichev,[2] V. N. Petrova,[2] S. N. Ivanov,[1] and A. V. Bardina[1]**

UDC 539.27:547.541:544.12:544.14

A combined gas electron diffraction and quantum chemical (B3LYP/6-311+G**, B3LYP/cc-pVTZ) study of the molecular structure of 2-nitrobenzenesulfonic acid (2-NBSA) is performed. Quantum chemical calculations show that the 2-NBSA molecule has five conformers, and the Gibbs energy of one of them is lower by more than 4.5 kcal/mol than the energy of the other conformers. It is found experimentally that the saturated vapor of 2-NBSA at $T = 394(5)$ K contains only the low-energy conformer that has an intramolecular hydrogen bond between the H atom of the hydroxyl group and one of the O atoms of the NO_2 group. The C–C–S–O(H) torsion angle determining the position of the S–O(H) bond is –72(7)°, while the NO_2 group is substantially turned relative to the benzene ring plane (C1–C2–N–O = 40(5)°). The following experimental values of the internuclear distances are obtained for this conformer (Å): r_{h1}(C–H)$_{av}$ = 1.07(2), r_{h1}(C–C)$_{av}$ = 1.401(4), r_{h1}(C–S) = 1.767(6), r_{h1}(S=O)$_{av}$ = 1.412(4), r_{h1}(S–O) = 1.560(6), r_{h1}(N–O)$_{av}$ = 1.217(5), r_{h1}(C–N) = 1.461(8), r_{h1}(O–H) = 0.99(3).

Keywords: 2-nitrobenzenesulfonic acid, conformer, molecular structure, gas electron diffraction, quantum chemistry, mass-spectrometry.