GAS ELECTRON DIFFRACTION AND QUANTUM CHEMICAL STUDY OF THE STRUCTURE OF A 2-NITROBENZENESULFONYL CHLORIDE MOLECULE

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

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A combined gas electron diffraction and quantum chemical (B3LYP/6-311+G**, B3LYP/cc-pVTZ, B3LYP/cc-pVTZ, midix (Cl), and MP2/cc-pVTZ) study of the structure of a 2-NO_2–C_6H_4–SO_2Cl molecule is performed. It is found experimentally that at a temperature of 345(5) K the gas phase contains two conformers of the C_1 symmetry. Conformer I with a nearly perpendicular arrangement of the S–Cl bond with respect to the benzene ring plane (the C(NO_2)–C–S–Cl torsion angle is 84(3)°) is contained predominantly (69(12)%). In conformer II, the S–Cl bond is located near the benzene ring plane (the C(NO_2)–C–S–Cl angle is 172(3)°). The following experimental internuclear distances (Å) are obtained for conformer I: r_{h1}(C–H) = 1.064(15), r_{h1}(C–C)$_{av}$ = 1.397(3), r_{h1}(C–S) = 1.761(6), r_{h1}(S–O)$_{av}$ = 1.426(4), r_{h1}(S–Cl) = 2.043(5), r_{h1}(N–O)$_{av}$ = 1.222(4), r_{h1}(C–N) = 1.485(16). In both conformers, the NO_2 group is turned by more than 30° relative to the benzene ring plane.

Keywords: 2-nitrobenzenesulfonyl chloride, conformer, molecular structure, internal rotation, potential functions, gas electron diffraction, quantum chemical calculations, mass spectrometry.