GAS-PHASE ELECTRON DIFFRACTION AND QUANTUM CHEMICAL STUDY OF THE STRUCTURE OF THE 4-NITROBENZENE SULFONYL CHLORIDE MOLECULE

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A combined gas-phase electron diffraction and quantum chemical (B3LYP/6-311+G**, B3LYP/cc-pVTZ, MP2/6-31G*, and MP2/cc-pVTZ) study of the structure of the 4-nitrobenzene sulfonyl chloride molecule is performed. It is found that at a temperature of 391(3) K only one conformer with C_s symmetry is present in the gas phase. The following experimental values of structural parameters are obtained: $r_{h1}(C–H)_{av}$ = 1.086(6) Å, $r_{h1}(C–C)_{av}$ = 1.395(3) Å, $r_{h1}(C1–S)$ = 1.773(4) Å, $r_{h1}(S=O)$ = 1.423(3) Å, $r_{h1}(S–Cl)$ = 2.048(4) Å, $r_{h1}(N–O)$ = 1.224(3) Å, $r_{h1}(N–C4)$ = 1.477(3) Å, ∠(C1–S=O) = 109.0(4)°, ∠(Cl–S–O) = 106.7(2)°, ∠C1–S–Cl = 100.2(13)°, ∠O=S=O = 122.9(11)°, ∠O=N=O = 123.6(5)°. The C2–C1–S–Cl torsion angle that characterizes the position of the S–Cl bond relative to the benzene ring plane is 89(4)°. The NO_2 group lies in the benzene ring plane. Internal rotation barriers calculated by B3LYP/6-311+G** and MP2/6-31G* methods are: V_1 = 4.7 kcal/mol and 5.3 kcal/mol for the sulfonyl chloride group; V_2 = 4.9 kcal/mol and 6.0 kcal/mol for the nitro group.

Keywords: 4-nitrobenzene sulfonyl chloride, conformer, molecular structure, internal rotation, potential functions, gas-phase electron diffraction, quantum chemistry, mass-spectrometry.