

Structural stability, S-O rotational barrier and vibrational analyses of monomeric non-planar halosulfonic acids X-SO₂-OH (X = F, Cl and Br). Badawi, Hassan M..

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Abstract

The structural stability of halosulfonic acids F-SO₂-OH, Cl-SO₂-OH, and Br-SO₂-OH were investigated by DFT-B3LYP/6-311+G** and ab initio MP2/6-311+G** calcns. The potential energy curve for the XSOH internal rotation around S-O bond was consistent with one min. that corresponds to nonlinear structure with XSOH torsional angle of about 80°. The vibrational frequencies were computed at DFT-B3LYP level for the stable nonplanar structure of the three mols. Normal coordinate calcns. were then carried out and the potential energy distributions (PED) were calcd. for the mols. On the basis of PED values and comparison with exptl. data reliable assignments were provided for the normal modes of these acids.