Methyl Phenyl Sulfide: Quantum-Chemical Investigation

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Abstract - Steric structure of methyl phenyl sulfide molecule was studied using a scope of quantum-chemical methods: semiempirical MINDO/3, MNDO, AM1 and PM3; one-determinant Hartree–Fock approximation with basic sets STO–3G, STO–3G*, 3–21G*, D95*, 6–31G*, 6–31G**, 6–31++G**, and 6–311G**; accounting for electron correlation energy in the framework of the Møller–Plesset perturbation theory on the levels MP2, MP3, and MP4(S,D,Q); calculation schemes based on the density functional theory (DFT): Becke LYP, Becke3 LYP, and Becke3 Perdew86. We found that in the MeSPh molecule there is a boundary situation between free rotation around the C_{sp^2}–S bond and restricted rotation with a low barrier and a wide amplitude of fragment motion in a potential well with a flattened bottom.