

*Dedicated to Full Member of the Russian Academy of Sciences
B.A. Trofimov on the 65th Anniversary of His Birth*

Quantum-Chemical Study of Methyl Phenyl Sulfide

Yu. L. Frolov and A. V. Vashchenko

*Favorskii Irkutsk Institute of Chemistry, Siberian Division, Russian Academy of Sciences,
ul. Favorskogo 1, Irkutsk, 664033 Russia
e-mail: yulf@irioch.irk.ru*

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Abstract - Steric and electronic structure of the methyl phenyl sulfide molecule was studied by nonempirical quantum-chemical methods. The calculations were performed by the B3LYP and MP2 procedures with account taken of electronic correlation using extended 6-311++G(3d,p) basis sets. The use of a balanced method and basis set allowed us to avoid discrepancy between the experimental and calculated data reported by other authors. The results confirmed coplanar orientation of the C–S–C fragment and the benzene ring, which follows from most experimental studies.