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Computational note on molecular structure and vibrational spectra of 6- and 8-methylquinoline molecules by quantum mechanical methods

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Methyl derivatives of quinoline are raw materials for industrial production of pyridine carboxylic acids and derivatives by aqueous ozonolysis [1]. These products are precursors for agro chemicals and active pharmaceutical ingredients. Interestingly, some methyl quinolines are also present in biological systems such as in the secretion of the skunk [2], whereas others show carcinogenic properties [3–5]. For example, 6-methylquinolines are important on the hepatit metabolism [6]. Many studies have indicated that some of azaarenes, including 8-methylquinolines, are active as tumor initiators on mouse skin [7].The molecular structures of 6MQ and 8MQ in the ground state (in vacuo) are optimized by HF and B3LYP with the 6-31G(d) basis set [8,9].

The molecules of 6MQ and 8MQ consist of 20 atoms, so they have 54 normal vibrational modes. Except 2-chlorolepidine molecule, the molecular structure of lepidine series has not been studied by any diffraction technique, therefore we have taken into account two different symmetries depending on the conformation of the CH_3 groups. Staggered and eclipsed conformers of both molecules belong to C_s point group. Any other rotamer appearing with the torsion around C—CH_3 bonds have no symmetry element other than identity and thus belong to C_1 point group. Our calculated results show that the aromatic ring in studied molecules are distorted from regular hexagon due to electronic effects of substituted quinolines.

If we summarize, the optimized bond lengths and bond angles obtained by B3LYP and BLYP methods by using standard 6-31G(d) basis set show the best agreement with the experimental values. Comparison of the observed fundamental vibrational frequencies of 6MQ and 8MQ, and the results calculated by density functional B3LYP, BLYP and Hartree–Fock methods indicate that B3LYP is superior to the scaled Hartree–Fock approach for molecular vibrational problems.

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.theochem.2006.09.009.

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