MOLECULAR AND CRYSTAL STRUCTURE, SPECTROSCOPIC PROPERTIES OF 2-METHYL-4-(3-METHYL-3-PHENYL-CYCLOBUTYL)-THIAZOLE DETERMINED BY THE EXPERIMENTAL METHOD AND A QUANTUM CHEMICAL CALCULATION

© **Ç. Yüksektepe,[1] N. Çalışkan,[2] I. Yılmaz,[3] and A. Çukurovalı[4]**

UDC 548.737:543.422

The structure of the synthesized title compound is characterized by IR, UV-visible spectroscopy, and single crystal X-ray diffraction (XRD). The new compound ($C_{18}H_{23}NS$) crystalizes in the monoclinic $P2_1/c$ space group. In addition to the crystal structure from the X-ray experiment, the molecular geometry, vibrational frequencies, atomic charge distribution, and frontier molecular orbital (FMO) analysis of the title compound in the ground state are calculated by density functional teory (B3LYP) with 6-311G(*d*,*p*) and 6-31G(*d*,*p*) basis sets. The results of the optimized molecular structure are presented and compared with the experimental values. The computed vibrational frequencies are used to determine the types of molecular motions associated with each of the observed experimental bands. To determine the conformational flexibility, the molecular energy profile of (1) is obtained by semi-empirical (AM1) and (PM3) calculations with respect to a selected degree of torsional freedom. Moreover, molecular electrostatic potential (MEP) and thermodynamic parameters of the title compound were calculated by the theoretical methods.

Keywords: *ab initio* calculation, semi-empirical method, B3LYP, conformational analysis, vibrational assignment, X-ray structure determination.