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Structural, spectroscopic, antimictobial activity and DFT studies on 4-methyl-N-(4-methylphenylsulfonyl)-N-phenylbenzenesulfonamide*

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This study reports the structural characterization of a disulfonimide derivative, 4-methyl-N-(4-methylphenylsulfonyl)-N-phenylbenzenesulfonamide (MPBSA), using spectroscopic and quantum chemical methods. The molecule was characterized with FT-IR, ^{1}H ^{13}C-NMR and UV-Vis spectroscopies. Quantum chemical calculations of molecular geometry, vibrational wavenumbers and gauge including atomic orbital (GIAO) ^{1}H and ^{13}C-NMR chemical shifts of the compound were carried out by using density functional method (DFT) at B3LYP/6–311++G(d,p) level of theory. Electronic absorption spectra of the compound have been computed using the time-dependent density functional theory (TD-DFT) method at the same level. A satisfactory consistency between the experimental and theoretical findings was obtained. The antimicrobial activity screening of the compound was performed on some bacteria and fungus species using microdilution method. The results showed that the title molecule have noteworthy antibacterial and antifungal activities.

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