Theoretical DFT, FT-IR and NMR studies of 2-methoxy-6-(5-F/Cl/Br-1*H*-benzimidazol-2-yl)-phenols

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2-(1*H*-benzimidazol-2-yl)phenol and its derivatives are known to be chelating agents and biologically active compounds. For example, some benzimidazolyl-phenol type ligands and their Fe(III), Cu(II) and Zn(II) complexes showed broad spectrum of antimicrobial activity that were either more active or equipotent the references[1,2].

In this study, theoretical DFT, FT-IR and NMR spectral studies of 2-methoxy-6-(5-F/Cl/Br-1*H*-benzimidazol-2-yl)-phenols (**I-III**) were performed. The optimized molecular geometry, dipole moment and total energy were calculated using Hartree-Fock and density functional method (B3LYP) with 6-31G(d,p) basis set. The vibrational wavenumbers and the infrared intensities were calculated scaled quantum mechanics (SQM) methodology by using Parallel Quantum Solutions (PQS) program. According to the calculations, the compounds are nearly planar (Fig. 1). The global minimum energy values of the compounds are -899.68, -1260.04 and -3371.44 a.u. for **I**, **II**, **III**, respectively. Dipole moment value of the compounds **I**, **II** and **III** are 5.01, 6.07 and 5.06 Debye, respectively. Also, charge distribution of the compounds was determined (Fig. 1).

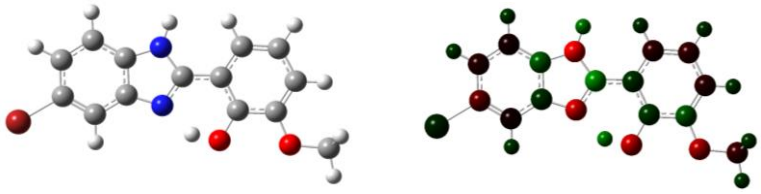

Fig. 1. Geometric optimization (left) and charge distribution (right) of **III**

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[2] Tavman, A., Boz, I., Birteksoz, A. S., Cinarli, A., *J. Coord. Chem.*, 63:1398-1410, 2010.