Theoretical DFT, FT-IR and NMR studies of 2-methoxy-6-(5-H/Me/NO_2-1*H*-benzimidazol-2-yl)-phenols

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Benzimidazolyl-phenol ligands known to be strong chelating agents are potential N,O donors and they react easily with the metal ions to give stable chelate complexes. Various transition metal chelate complexes of benzimidazolyl-phenol type ligands were reported[1,2].

In this study, theoretical DFT, FT-IR and NMR spectral studies of 2-methoxy-6-(5-H/Me/NO_2-1*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 -800.47, -840.05 and -999.97 a.u. for **I**, **II**, **III**, respectively. Dipole moment value of the compounds **I**, **II** and **III** are 4.42, 4.22 and 7.56 Debye, respectively. Also, charge distribution of the compounds was determined (Fig. 1).

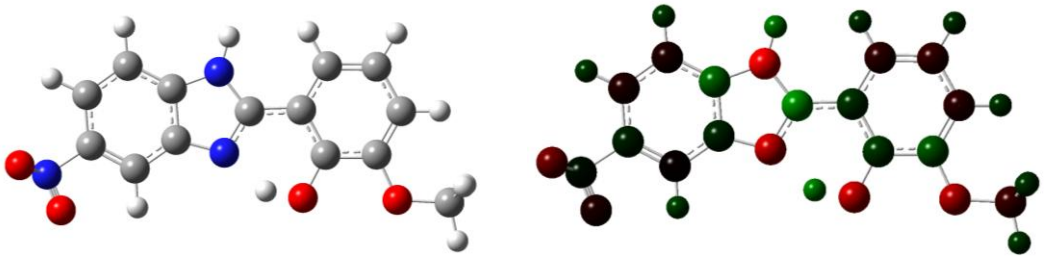

Fig. 1. Geometric optimization (left) and charge distribution (right) of **III**

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