Summary and Conclusion
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Spectroscopic studies and theoretical calculations have been performed on some polyatomic molecules. The molecules employed for investigations are 3-amino-2-bromopyridine, 4-amino-2-bromopyridine, 5-bromo-2-pyridinecarbonitrile, 9-fluorenone-2-carboxylicacid, O-Bromobenzoyl chloride, and 1, 5-dimethoxynapthalene. FT-IR, FT-Raman, UV, and NMR spectra have been obtained for the investigated molecules. Theoretical calculations were undertaken at the ab initio, HF and density functional theory (DFT)/B3LYP method with 6-311G (2df, 2p) basis sets. The aforementioned calculations allowed the vibrational, electronic and NMR spectra to be computed at the optimized molecular geometry and the results were compared with the experimental findings. The molecular geometry of investigated compounds have been provided with the computed bond lengths, bond angles and torsional angles, as well as the calculated vibrational wave numbers. Normal coordinate analysis was also done which yielded the calculated vibrational spectra which are in good agreement with the experimental spectra.

Molecular properties of investigated molecules such as HOMO-LUMO energy gap, dipole moment as well as non linear optical activity have been calculated. It was found that the low HOMO-LUMO energy gap and large hyperpolarizability value provide the evidence for the intra molecular charge transfer interactions of investigated compounds. Natural bond orbital (NBO)
analysis explains the charge delocalization and stability of the investigated molecules.

The FT-IR and FT-Raman spectra have been recorded and a detailed vibrational assignment is presented for 5-bromo-2-pyridine carbonitrile for the first time based on the potential energy distribution (PED). Optimized geometrical parameters of this compound are in agreement with the crystal structure data obtained from XRD studies. The NMR results indicated that the observed chemical shifts depend not only the structure of the molecule being studied but also on the solvent used. The NBO analysis revealed that the strongest stabilization to the system. The Molecular Electrostatic Potential (MEP) studies of investigated compounds could be used to ascertain the reactive sites. We hope our results will be of assistance in the quest of the experimental and theoretical evidence for the investigated compounds in reaction intermediates, non linear optical and photoelectric materials. And, will also be helpful for the design and synthesis of new materials.