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SUMMARY AND CONCLUSION

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In the present investigation are thoroughly analyzed using quantum chemical calculations of FT-IR, FT-Raman, UV-Vis and NMR spectra of some polyatomic molecules. The complete vibrational assignments of wavenumbers are made on the basis of potential energy distribution(PED). Quantum chemical calculations(QCC) help us to identify the structural and symmetry properties of the chosen compounds. The good agreement between the calculated and observed vibrational wave number revealed the advantages of higher basis set for quantum chemical calculations. The natural bond analysis (NBO) shows inter and intermolecular interactions in the molecular systems studied. The stabilization energy has been calculated from second order perturbation theory. In addition, Mulliken atomic charges, non-linear optical properties and thermodynamic properties were also calculated and discussed elaborately.

The lowering of HOMO-LUMO energy gap shows that charge transfer occurs within the molecules and supports bioactive property of the molecules studied. The UV-Vis absorption spectra were analyzed using solvents in various frequency ranges. The NMR chemical shifts (^{13}C and ^{1}H) were recorded in DMSO solvent. The ^{13}C and ^{1}H NMR spectra were computed by the Gauge Independent Atomic Orbital (GIAO) method.

The calculated results show a good agreement with the experimental values. The methods employed for studying the molecular properties can be used to synthesize new polyatomic molecules and molecular properties of any molecules having similar structures.