On the Footprints of the Ring Normal Modes in Heterocycles: Pyridine and Derivatives

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Abstract

In the present study, the vibrational frequencies for pyridine, quinoline, 1,8-naphthyridine and 1,10-phenathroline and their corresponding fully fluorinated derivatives were investigated through quantum chemical calculations. In parallel, the electronic structure and the topology of these molecules were analysed in details by means of the Natural Bond Orbital analysis (NBO) and the Bader Atom-In-Molecules (AIM) theory. Among their vibrational normal modes, 7 ring related normal modes (RNMs), defined for pyridine, were found traceable in the heterocyclic pyridinic derivatives and their fluorinated compounds, evidenced by the percentage contribution of the internal coordinates. The shift of the vibrational frequencies from those of pyridine and the disappearance of some RNMs in the derivatives were rationalised from the perspectives of frontier Molecular Orbitals (MOs), maps of Molecular Electrostatic Potential (MEP), NBO and Electron Localization Function (ELF). These RNMs previously identified for pyridine were found out to serve not only as distinctive labels in the characterization of the vibrations of the heterocyclic derivatives of pyridine and corresponding fluorine substitutes, but also useful references to study the potential intermolecular interactions with these compounds involved.

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