Molecular Structure, FT-IR, Raman, XRD and Quantum Chemical Studies of 2-Acetyl-5-chlorothiophene

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Thiophene belongs to the class of heterocyclic compounds with a five-membered ring containing one sulfur heteroatom bearing the formula C_4H_4S. Thiophene is also commonly called thiofuran. It is regarded as an aromatic compound due to its extensive substitution reactions obeying $4n+2\pi$ electron rule. Thermochemistry of 2- and 3-acetylthiophenes, calorimetric and computational study has been reported earlier. The 2-acetyl-5-chlorothiophene was used as a starting material for the synthesis chalcones. In the previous publications, NMR studies showed that the acetylthiophenes occur as *O,S-cis* isomer. The structure of 2-acetyl-5-chlorothiophene (ACT) has been characterized by FT-IR, Raman and single-crystal X-ray diffraction techniques. The isomers, optimized geometric parameters, normal mode frequencies and corresponding vibrational assignments of ACT (C_6H_5ClOS) have been examined by the density functional theory, with the Becke-3–Lee–Yang–Parr functional and the 6-311+G(3df,p) basis set. Reliable vibrational assignments have been investigated by the potential energy distribution analysis. ACT crystallizes in monoclinic space group C2/c with the *O,S-cis* isomer. There is a good agreement between the theoretically predicted structural parameters and vibrational frequencies and those obtained experimentally.