

Summary

The thesis aims to systematically extend recent observations indicating that the molecular conformation and certain vibrational modes of polysubstituted benzenes vary strongly when their environment varies. The molecules retained for the study are benzenes with methyl substituents plus halogens or nitro groups.

X-ray diffraction or inelastic neutron scattering in various environments will establish the precise molecular conformation: pure crystal, molecules in cages or halotriazine channels.

Intermolecular interactions within these compounds have been studied through the Hirshfeld surface.

A particular review will be devoted to examining the evolution of 'restricted rotation' modes and tunneling transitions of methyl groups.

At the same time, theoretical calculations will be carried out using the density functional theory to determine the molecular conformations, the normal modes of vibration, as well as the distribution of potential energy.

The results of quantum mechanics calculations carried out by (DFT) with the functional MPW1PW91 and the basis Lanl2DZ, led to similar results in the angles and bond lengths compared to the experiment.

The theoretical calculations of spectroscopy allowed the identification of the various modes of vibration of the isolated molecules, they will be confronted with the experimental spectra IR and Raman.

Keywords: Halogenotriazine channels, X-ray diffraction, inelastic neutron scattering, quantum mechanics, IR, Raman.