RAMAN AND INFRARED SPECTRA, *AB INITIO* AND DFT CALCULATIONS, AND VIBRATIONAL ASSIGNMENTS FOR 2,3-CYCLOPENTENOPYRIDINE

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Abstract:

Structural properties of 2,3-cyclopentenopyridine (pyrindan) have been investigated using a number of spectroscopic and computational techniques. Raman and infrared spectra of the molecule have been recorded and full vibrational assignments were proposed on the basis of experimental and theoretical results. The vapor-phase Raman spectrum was successfully recorded although the molecule showed very weak Raman peaks barely seen due to the fluorescent effect. It was predicted that the presence of the nitrogen atom in the six-membered ring has almost no effect on the barrier to inversion and puckering frequency (587 cm^{-1} and 139 cm^{-1}, respectively) as proposed from MP2 and DFT calculations as compared to the values previously determined (488 cm^{-1} and 143 cm^{-1}) for the indan molecule.

Keywords: Raman spectra, infrared spectra, 2,3-cyclopentenopyridine.