

## Spectroscopic Investigation of the Vibrational Spectra of the Benzoxazine

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Vibrational spectrum of the benzoxazine molecule has been systematically investigated by combined approach of infrared spectrum, *ab initio* and density functional theory (DFT) calculations. Infrared spectrum of the benzoxazine molecule in KBr pellet has been recorded in the wavenumber region 400-4000 cm<sup>-1</sup>. Optimized geometries, harmonic vibrational wavenumbers and the intensities of the vibrational bands have been calculated at the RHF/6-311++g\*\* and B3LYP/6-311++g\*\* levels. Some appropriate scale factors have also been considered to scale the calculated frequencies. The scaled values have been compared with experimental frequencies observed in infrared spectrum. The molecule benzoxazine consists of 16 atoms and thus it possesses 42 normal modes of vibrations. Each vibrational frequency has been assigned to their corresponding normal mode with the help of band intensities and vector displacements. The vibrational frequencies and infrared intensities so obtained have been discussed.