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Raman and FTIR Studies of Azobenzene: Experimental and Theoretical Approach

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Abstract : Photoisomerization has been attracting to researchers due to its wide range of applications in optical switches, polymeric chains, liquid-crystalline systems and bilayer membranes etc. Azobenzene is a photochromic molecule which exhibits a reversible isomerisation process between its trans and cis isomers of different stability. An investigation has been conducted of the effects of temperature on intensity and position of Raman band of N=N, C-N stretching modes of Azobenzene (AZBN). It was found that the N=N stretching mode of Raman band shape shifts to lower frequency region with the increase in temperature. The Raman intensity was also decreased with the increase of temperature. The change in bandwidth with the increase in temperature has been studied. The FTIR spectrum of the molecule is recorded so as to complement the Raman spectra. In order to investigate the possibility of undergoing dimerization and trimerization as well as the stability of this molecule, ab initio calculation for geometry optimization and vibrational wavenumber calculation have been performed. Theoretically calculated values are found in good agreement with the experimental results.

Keywords : azobenzene, temperature, ab-initio, frequency
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