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Spectroscopic Studies and Vibrational Assignments, Homo-Lumo, UV-VIS, NBO Analysis of Benzonitrile

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Abstract : The Fourier transform infrared and FT-Raman spectra of Benzonitrile have been recorded in region of 4000-400 and 4000-100 cm^{-1} respectively. A complete assignments and analysis of fundamental vibrational modes of the molecule have been carried out. The observed fundamental modes have been compared with harmonic vibrational frequencies computed using ab initio and density functional theory calculations by employing B3LYP functional at 6-311G(d, p) level and HF/6-311G(d, p).UV-Vis spectrum of the compound has been recorded, the natural bond orbital (NBO) electronic properties, such as highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies have been calculated with B3LYP/6-311G(d, p) level. These calculated energies show that charge transfer occurs within molecule. NBO analysis, thermodynamics properties and Mulliken charges of the title molecule are also calculated and interpreted.
Keywords : Benzonitrile, DFT, HF, HOMO-LUMO, UV-VIS, NBO.

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