In the recent years, various studies has been done in the Diphenyl carbazide (DPC) due to its industrial importance. DPC was a perfect absorber of chromium from the industrial effluents. In the present study, complete vibrational analysis of the title compound has been extensively carried out. To carry out a detailed vibrational spectroscopic analysis of title compound, FT-IR and FT-RAMAN spectra of DPC have been recorded in the condensed phase. Density Functional Theory calculations in the B3LYP/6-31G* level have been carried out to determine the optimized geometry and vibrational frequencies. The calculated optical geometry were in good agreement with the experimentally found XRD data as reported earlier. In order to obtain a close agreement between theoretical and observed frequencies and hence to perform a reliable assignment, the theoretical DFT force field was transformed from cartesian to local symmetry co-ordinates and then scaled empirically using SQM methodology. The SQM treatment resulted in a R.M.S. deviation of 14.2 cm⁻¹. For visual comparison, the observed and calculated spectra are presented on a common frequency scale. The NBO analysis shows that charge in electron density (ED) in the σ* and π* antibonding orbitals and second order delocalization energies E(2) confirms the occurrence of intramolecular charge transfer (ICT) within the molecule. The calculated Homo and Lumo energies show that charge transfer occurs within the molecule. The results obtained from the vibrational, NBO and Homo–Lumo analysis has been properly tabulated (Ref: Ragavendran V, Muthunatesan S. Molecular Structure and vibrational spectroscopic (FT-IR, FT-Raman) analysis of Diphenyl Carbazide by DFT calculations. Indian Journal of Science, 2015, 14(42), 84-97).
ANALYSIS

CHEMISTRY

Host–guest interaction of 2-hydroxy-1-naphthoic acid: β-cyclodextrin inclusion complex
Ragi TR, Parameswari M, Sivakumar K

Inclusion complex of 2-hydroxy -1-naphthoic acid (2H1NA) with β-Cyclodextrin (β-CD) has been investigated by UV spectroscopy and fluorescence techniques. The red shift in λmax and enhanced absorption in β-CD medium confirm that the 2H1NA is inserted in the β-CD cavity. The formation of this complex has been confirmed by Benesi-Hildebrand Plot obtained from the results of UV and fluorescence studies. The stability constant K1:1 and the 1:1 stoichiometric of complexation were determined. The thermodynamic parameter (ΔG) of inclusion process was determined. The inclusion complex formation in solid state was confirmed by IR spectroscopy. The conclusions derived were supported using molecular modeling studies.

Indian Journal of Science, 2015, 14(42), 63-70

CHEMISTRY

Growth and characterization of pure and metal doped KDP crystals in gel medium
Usharani Pisipaty, Dhanabalan O, Abirami S

Optically good quality pure and metal doped KDP crystals have been grown by microbial free gel growth method at room temperature and their characterization have been studied. Gel method is a very simple method and can be utilized to synthesize crystals which are having low solubility. The presences of functional groups of crystals are qualitatively analyzed from FTIR spectra. X-ray diffraction study has been carried out in order to see the effect of dopant on the structural parameters of KDP. The powder X-ray diffraction analysis revealed the tetragonal structure of KDP and doped divalent metal ion. Single crystal XRD revealed the lattice parameter values. Thermal properties like decomposition temperature and weight loss have been reported from the TGA and DTA analysis. The quality, colour and transparency of grown crystals have been confirmed using UV-Vis-spectra. The second harmonic generation (SHG) was measured by using Kurtz powder technique. The relative second harmonic generation (SHG) efficiency of metal doped crystals was higher than the pure KDP crystals. The dielectric behavior of pure and metal doped crystals has been studied in the frequency range from 100Hz to 100 KHz. SEM study was performed to indicate the influence of dopants on surface morphology of KDP crystals.

Indian Journal of Science, 2015, 14(42), 71-83

PHYSICS

Molecular Structure and vibrational spectroscopic (FT-IT, FT-Raman) analysis of Diphenyl Carbazide by DFT calculations
Ragavendran V, Muthunatesan S

In the recent years, various studies has been done in the Diphenyl carbazide (DPC) due to its industrial importance. DPC was a perfect absorber of chromium from the industrial effluents. In the present study, complete vibrational analysis of the title compound has been extensively carried out. To carry out a detailed vibrational spectroscopic analysis of title compound, FT-IR and FT-RAMAN spectra of DPC have been recorded in the condensed phase. Density Functional Theory calculations in the B3LYP/6-31G* level have been carried out to determine the optimized geometry and vibrational frequencies. The calculated optical geometry were in good agreement with the experimentally found XRD data as reported earlier. In order to obtain a close agreement between theoretical and observed frequencies and hence to perform a reliable assignment, the theoretical DFT force field was transformed from cartesian to local symmetry co-ordinates and then scaled empirically using SQM methodology. The SQM treatment resulted in a R.M.S. deviation of 14.2 cm⁻¹. For visual comparison, the observed and calculated spectra are presented on a common frequency scale. The NBO analysis shows that charge in electron density (ED) in the σ* and π* antibonding orbitals and second order delocalization energies E(2) confirms the occurrence of intramolecular charge transfer (ICT) within the molecule. The calculated Homo and Lumo energies show that charge transfer occurs within the molecule. The results obtained from the vibrational, NBO and Homo–Lumo analysis has been properly tabulated.

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