



NOTE

Thermal, UV and FTIR Spectroscopic Studies of Mercury Cinnamate

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A single crystal of mercury cinnamate was grown by slow evaporation of methanol solution at room temperature. The effect of mercury on the electronic structure of cinnamic acid was studied. In this research many miscellaneous analytical methods were used: infrared (FT-IR), UV and TG-DTA. The spectroscopic studies lead to conclusions containing the distribution of the electronic charge in molecule, the delocalization of *p*-electrons and the reactivity of metal complexes.

Key Words: Solution growth, Mercury cinnamate single crystal, TG-DTA, UV, FTIR.

Cinnamic acid, a derivative of phenyl alanine, composes a relatively large family of organic isomers¹⁻⁴. In nature, cinnamic acid derivatives are important metabolic building blocks in the production of lignin's for higher plants. Cinnamic acid possesses antibacterial, antifungal and parasite fighting abilities¹⁻⁴. Derivatives of cinnamic acid are an important pharmaceutical for high blood pressure and stroke prevention and possess antitumour activity. In wine, cinnamic acid derivatives and flavonoids in creating pigments and tannin agents that give each vintage its characteristic bouquet and colour. Cinnamic acid extensively studied not only due to its important biological activity, but also because of its specific structure. It would be interesting to compare the electronic structures of cinnamic acid with mercury cinnamate.

The metal compound was prepared by digesting appropriate weighed amount of cinnamic acid in methanol of mercuric chloride in stoichiometric ratio of 1:1. Then methanol was evaporated in a dryer. The results of elementary analysis are as follows; for mercury cinnamate C (%) = 64, H (%) = 5. The IR spectra were recorded with Bruker IFS spectrometer within the range of 4000-400 cm⁻¹. Samples in the solid state were measured in KBr matrix pellets which were obtained with hydraulic press under 739MPa. The UV absorption spectra were recorded using double beam UV spectrometer in the spectral range 100-400 nm. The thermogravimetric and differential thermal analyses were carried out using a Netzsch STA 409C thermal analyzer in the nitrogen atmosphere. The sample was heated between 30 and 800 °C at a heating rate of 10 °C per min.

In FTIR spectrum the region of -OH stretching vibrations, there is an intense band occur at 3456 cm⁻¹ in mercury cinnamate and broad bands in the range 2359-2529 cm⁻¹ assigned to the -OH stretching vibrations of acid dimers. In this range there are as well as the bands of the -CH stretching vibrations. In the infrared spectra of mercury cinnamate there are splitting bands assigned to the stretching vibrations of the C=O group (*i.e.* 1892, 1671 and 1629, 1809 cm⁻¹). This indicates the existence of different types of molecular packing and cinnamic acid with the intermolecular packing and associates cinnamic acid with intermolecular hydrogen bonds C=O...H-O. Replacement of the carboxylic group hydrogen with a metal ion causes a break down of the intermolecular hydrogen bonding and the characteristic changes in the IR spectra of acid appeared. The disappearance of bands which originate from stretching $\nu(\text{OH})$ vibration and appearance of bands of the unsymmetric and symmetric vibration of the carboxylate anion $\nu_{\text{as}}(\text{COO}^-)$ shifted towards wave numbers along the series (cinnamic acid → mercury cinnamate) in IR spectra. This indicates the formation of mercury cinnamate.

In mercury cinnamate, the π - π^* absorption band shifted to lower wavelength compared to cinnamic acid. This is because of the formation of coordinate bond between metal with cinnamic acid, thus greater energy required for this transition and hence the absorption shows the blue end of the spectrum.

SHG efficiency: An Nd:YAG laser with modulated radiation of 1064 nm was used as the optical source and directed on the powder sample through a filter. The doubling frequency was confirmed by the green radiation of 532 nm.

Input radiation is 5.35 mj/pulse. Interesting of second harmonic generation gives an indication of NLO efficiency of the material. Nonlinearity is facilitated in the presence of dopant. The dopant has catalytic effect on the NLO properties of cinnamic acid crystals. It is interesting to observe that the SHG efficiency is more pronounced in the presence of mercury dopant in the growth medium. It appears that the attainment of second order effects requiring favourable alignment of the molecule within the crystal structure is well facilitated in the presence of inorganic dopant mercury.

Thermal analysis: The single crystal of mercury cinnamate was subjected to thermogravimetric analysis (TGA) using Netzsch STA 409C thermal analyser in the nitrogen atmosphere. The sample was heated between 30 and 800 °C at a heating rate of 10 °C/min to study the weight loss and thermal stability. The thermogram reveals that the major weight loss took place at temperature of 286.8 °C in mercury cinnamate. Such change was also observed by differential thermal analysis thermogram shown in figure. This indicates that incorporation

of mercury increase the thermal stability ensuring the suitability of material for possible NLO application up to temperature of 286.8 °C.

Conclusion

Optical quality single crystals of mercury cinnamate were grown by slow evaporation technique at room temperature. UV absorption spectrum was recorded to confirm the transparency of the crystals. FTIR analysis was carried out to study the molecular vibration and functional groups of the grown crystals. From the thermal analysis, the crystals were retaining its texture up to 289.8 °C.

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