**Crystal Structure, spectroscopic characterization and computational investigations of organic cytosine single crystal for nonlinear optical applications**

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**Abstract**

Organic nonlinear optical single crystal of cytosine was grown by slow evaporation technique at room temperature. The crystal structure of grown cytosine was confirmed by Single Crystal X-ray diffraction analysis and it revealed that cytosine crystallized in monoclinic crystal system with noncentrosymmetric space group. The experimental parameters were compared with theoretical values by DFT method. The NBO analysis interprets all the possible inter and intra molecular interactions present in the crystal structure for stabilization. The diverse inter contacts existing within the crystal were visualized through 3D Hirshfeld surface analysis and 2D fingerprint plot ensures the percentage of interactions takes place in cytosine molecule. FT-IR spectral analysis was used to recognize the various functional groups present in cytosine. The UV-Visible spectrum of cytosine crystal exhibits good optical transmittance in the entire visible region. The emission behavior was analysed by fluorescence spectral analysis. The nonlinear optical behavior was confirmed by Kurtz and Perry powder technique.

Keywords: DFT, NBO, FT-IR, UV, Fluorescence, nlo