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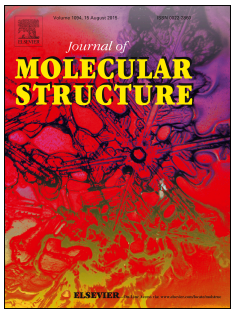

Structural, computational and Hirshfeld surface analysis of a proton transfer crystal, amino (2-(propan-2-ylidene) hydrazinyl) methaniminium picrate

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Abstract

Single crystals of amino (2-(propan-2-ylidene) hydrazinyl) methaniminium picrate (APHMP) were grown and crystallized at room temperature by slow evaporation- solution growth technique. The structure of the APHMP was confirmed by single crystal X-ray diffraction analysis and various spectroscopic techniques like FT-IR, ^{1}H and ^{13}C NMR. The optical quality of the crystal was evaluated through UV-vis absorption, UV-vis-NIR transmittance, photoluminescence. The compound was thermally stable up to 203 $^{\circ}C$. The molecular structure was optimized using B3LYP method using 6-311G(d,p) basis set. The energy gap between HOMO and LUMO in APHMP is 3.46 eV.

Key words:

Crystal structure; Hirshfeld surface analysis; Density Functional Theory

Highlights

- Single crystals were grown by slow evaporation-solution growth technique
- Structural analysis was done by single crystal X-ray diffraction analysis
- Thermal stability was investigated by TG/DTA
- HOMO -LUMO gap was found to be 3.46 eV