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Crystallographic investigation, Hirshfeld surface analysis, NLO characterization and experimental spectral (UV and NMR) studies with DFT probe on(R)-9-(2-hydroxy propyl)adenine

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Abstract

In this study, (R)-9-(2-hydroxy propyl)adenine (HPA) is the molecule of interest for investigation. The XRD from single crystal of HPA has been used to extract its structural features. Since HPA crystallised in a non-centro symmetric space group $P2_12_12_1$, its NLO property was studied and it was found to exhibit very good SHG activity. To explore the intermolecular interactions the generated Hirshfeld surface has been investigated along with 2D-fingerprint plots. The experimental electronic and NMR spectra taken in the UV-visible and radio frequency regions respectively for HPA have been corroborated in correlation with theoretical predictions at Density Function Theory using 6-311++g (d, p) basis set. The experimental XRD geometrical parameters, chemical shifts of ^{13}C and ^{1}H and λ_{max} values of HPA fit satisfactorily with the