Supplementary Information (SI) for RSC Advances.

Supplementary

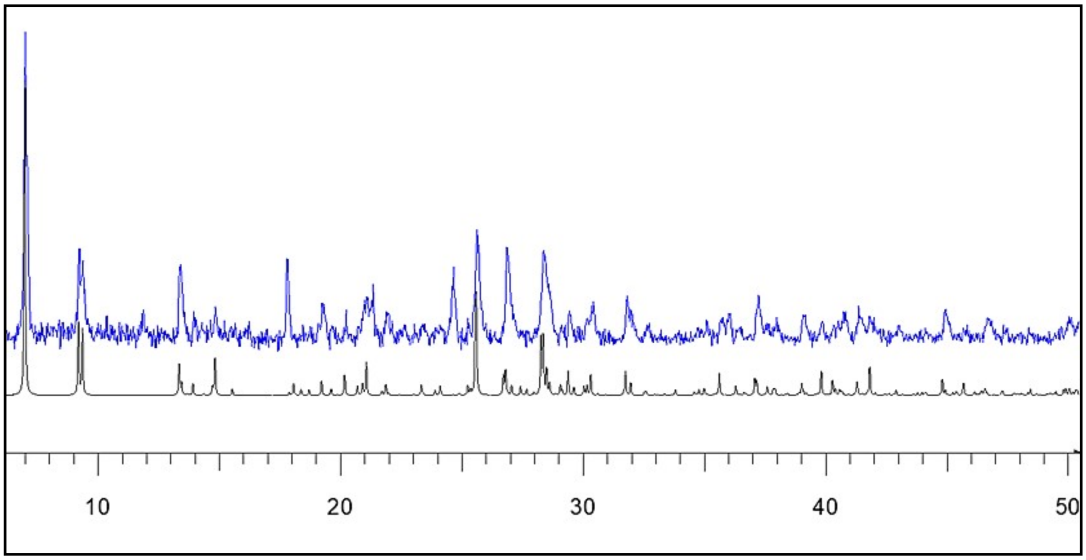


Fig. 1.S: Experimental (blue) vs calculated (black) peaks of PXRD

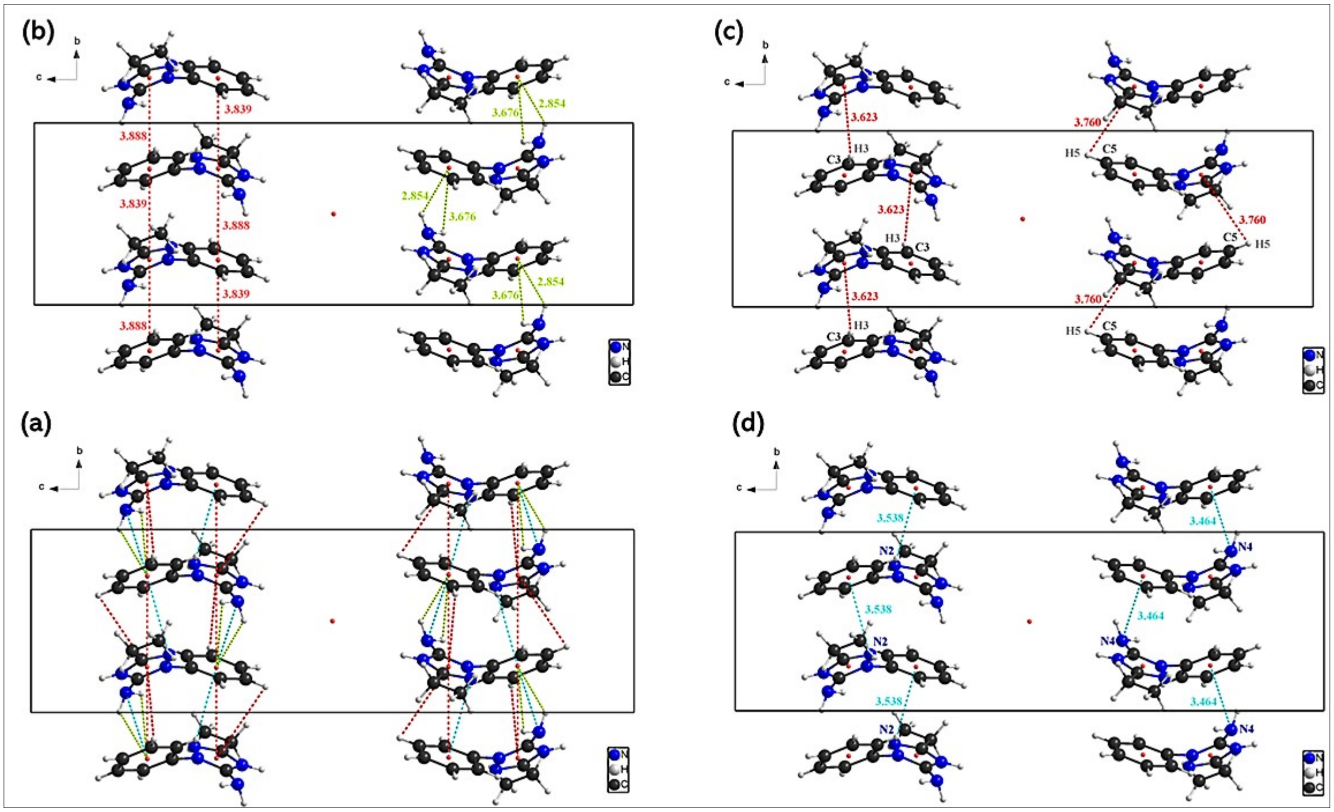


Fig. 2.S: **(a)** all types of π interactions, **(b)** $\pi\cdots\pi$ and N-H$\cdots\pi$ interactions, **(c)** C-H$\cdots\pi$ interactions, **(d)** n$\cdots\pi$ interactions, along the a-axis

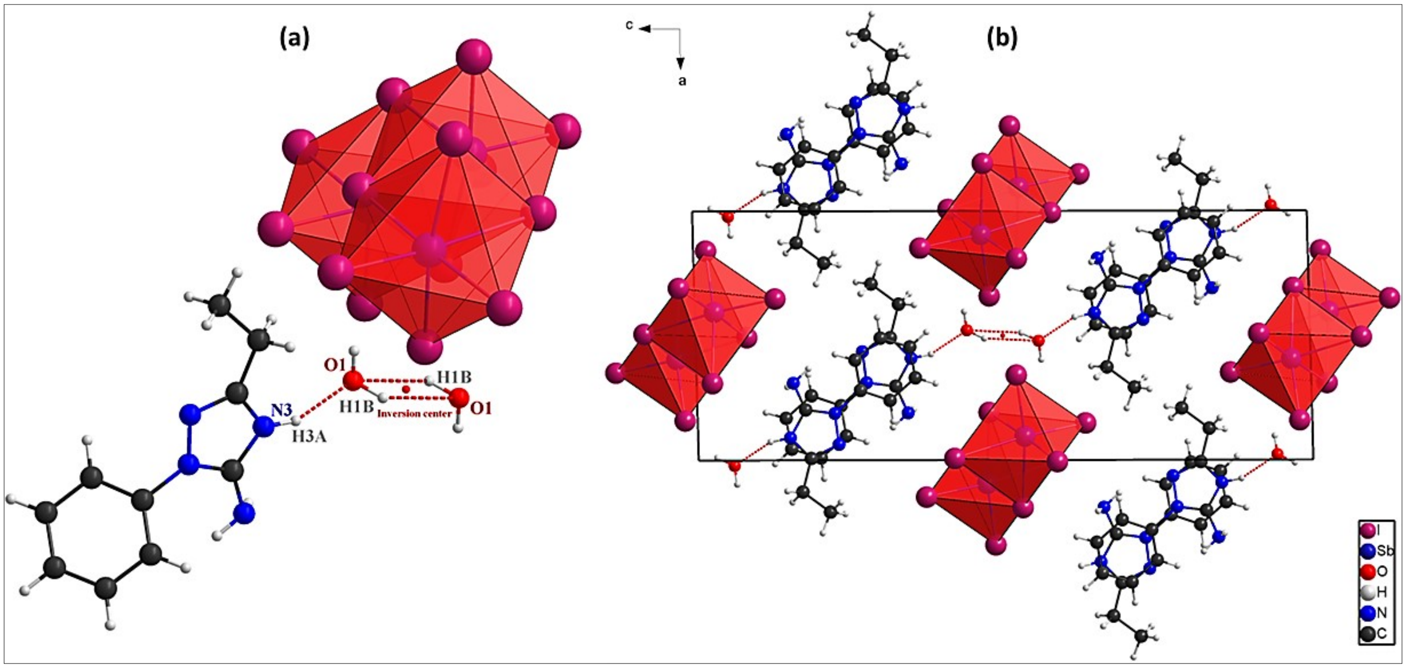


Fig. 3.S: Hydrogen bonding of the titled compound (**(a)** in the formula unit, and **(b)** the unit cell)

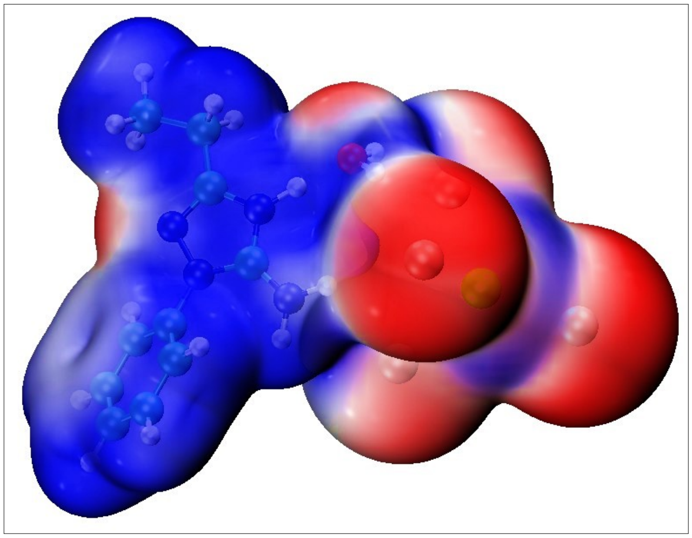


Fig. 4.S: Molecular Electrostatic Potential Analysis of the Target Compound

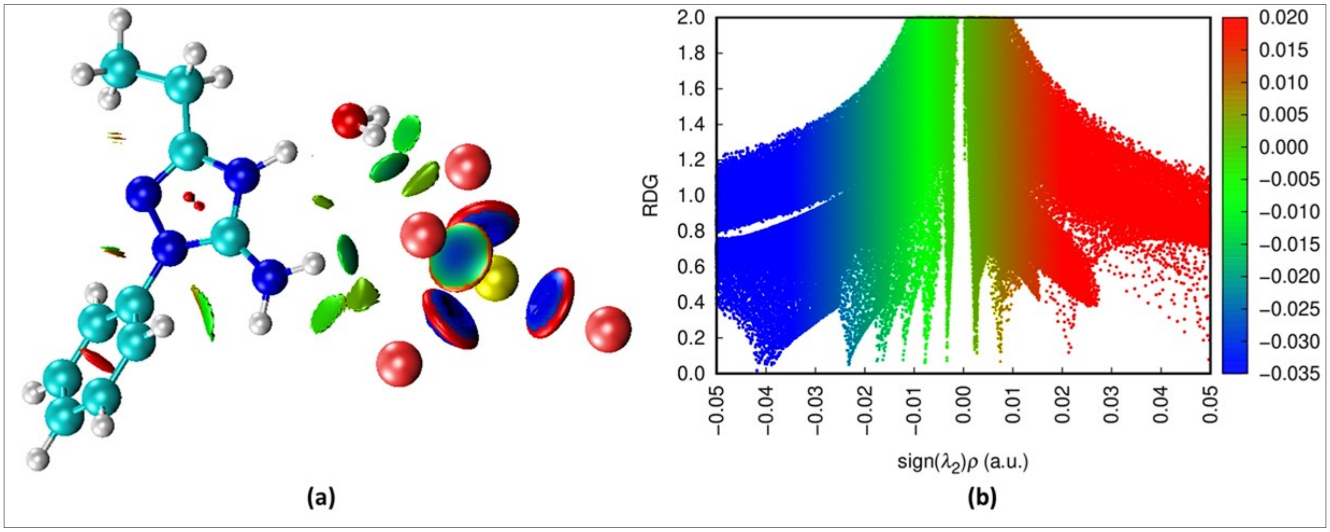


Fig. 5.S: (a) NCI and **(b)** RDG Visualization of the Target Compound

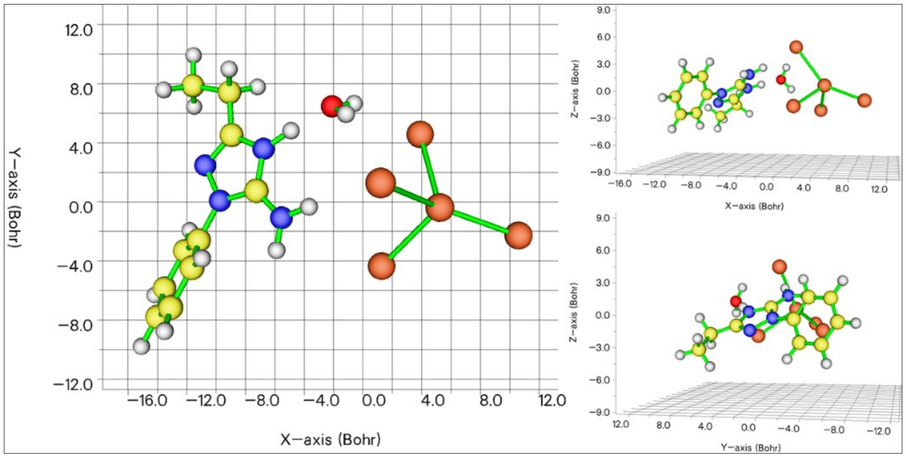


Fig. 6.S: Visualization in (XY), (XZ), and (YZ) planes

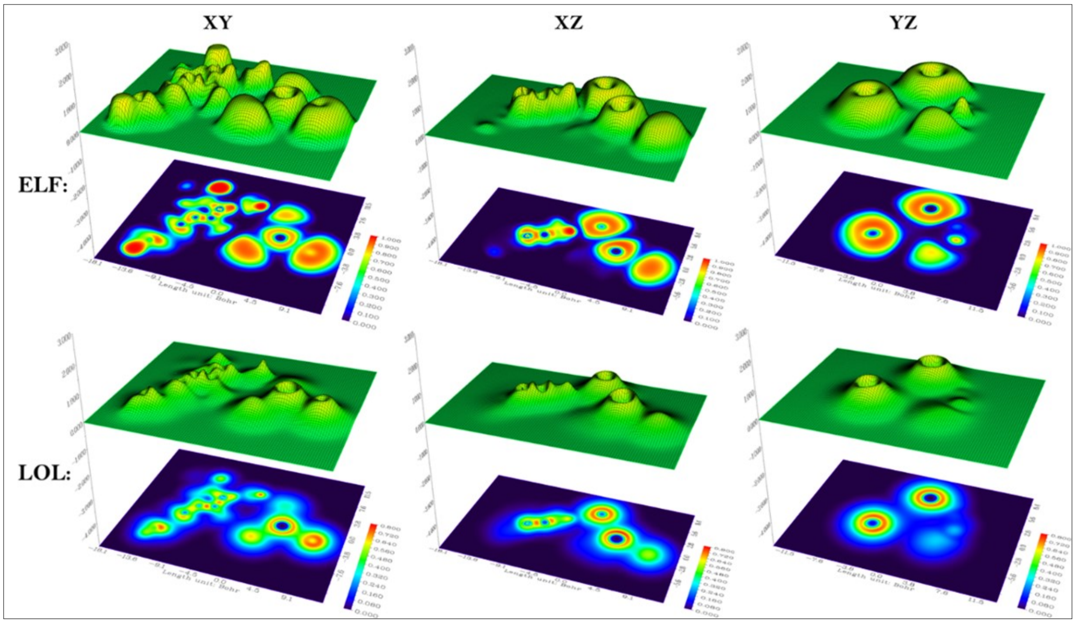


Fig. 7.S: Electron Localization Function (ELF) and LOL analyses

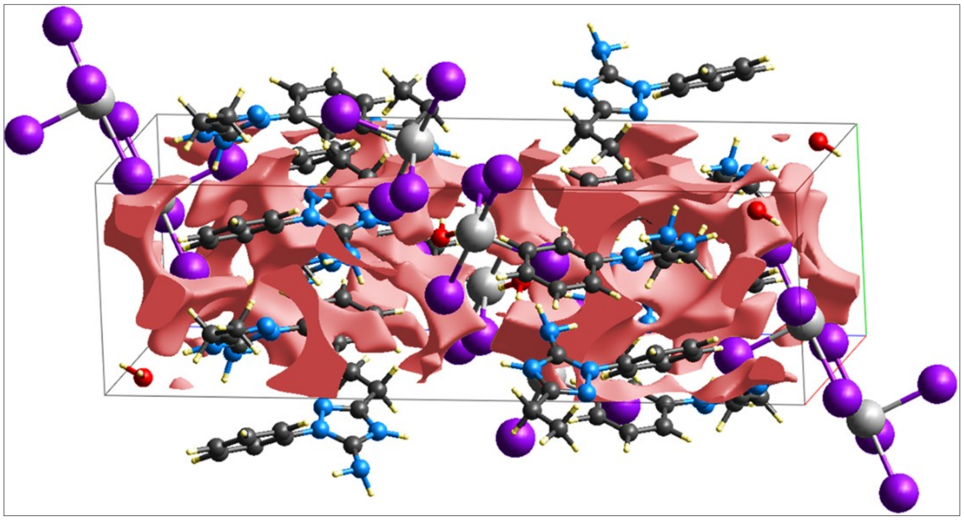
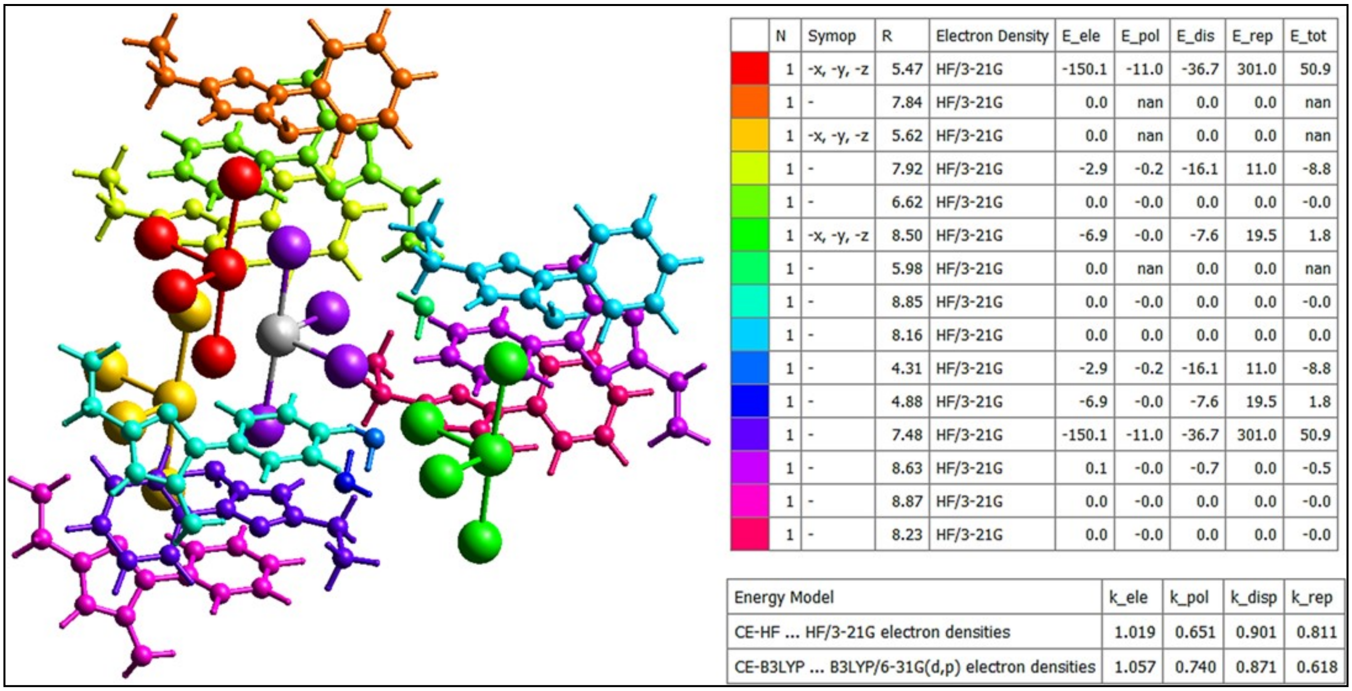


Fig. 8.S: Presence of a Crystal Void in the Compound



	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
🟥	1	-x, -y, -z	5.47	HF/3-21G	-150.1	-11.0	-36.7	301.0	50.9
🟧	1	-	7.84	HF/3-21G	0.0	nan	0.0	0.0	nan
🟨	1	-x, -y, -z	5.62	HF/3-21G	0.0	nan	0.0	0.0	nan
🟨	1	-	7.92	HF/3-21G	-2.9	-0.2	-16.1	11.0	-8.8
🟩	1	-	6.62	HF/3-21G	0.0	-0.0	0.0	0.0	-0.0
🟩	1	-x, -y, -z	8.50	HF/3-21G	-6.9	-0.0	-7.6	19.5	1.8
🟩	1	-	5.98	HF/3-21G	0.0	nan	0.0	0.0	nan
🟦	1	-	8.85	HF/3-21G	0.0	-0.0	0.0	0.0	-0.0
🟦	1	-	8.16	HF/3-21G	0.0	0.0	0.0	0.0	0.0
🟦	1	-	4.31	HF/3-21G	-2.9	-0.2	-16.1	11.0	-8.8
🟦	1	-	4.88	HF/3-21G	-6.9	-0.0	-7.6	19.5	1.8
🟪	1	-	7.48	HF/3-21G	-150.1	-11.0	-36.7	301.0	50.9
🟪	1	-	8.63	HF/3-21G	0.1	-0.0	-0.7	0.0	-0.5
🟪	1	-	8.87	HF/3-21G	0.0	-0.0	0.0	0.0	-0.0
🟥	1	-	8.23	HF/3-21G	0.0	-0.0	0.0	0.0	-0.0

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

Fig. 9.S: Energy Framework Analysis of Intermolecular Interactions

Table 1.S: The attributions of calculated and observed frequencies of the vibration modes of the compound

IR (cm^{-1})	Raman (cm^{-1})	Calc. wavenumbers (cm^{-1})	Assignement
3556	-	3576	$\upsilon_{as}(NH_2)$
3427	-	3426	$\upsilon_s(H_2O)$
3362	-	3268	$\upsilon_s(NH_2)$
3129	-	3129	$\upsilon_{as}(C-H)$
3052	-	3056	$\upsilon_s(C-H) + \upsilon_{as}(CH_3)$
2965	-	2966	$\upsilon_s(CH_3) + \upsilon_{as}(CH_2)$
1800-2800	-	2539	$\upsilon(N-H....O)$
1668	-	1633	$\delta(H-O-H) + \delta(NH_2)$
1582	-	1565	$\upsilon(C=C) + \delta(CH_2)$
1491	-	1462	$\omega(CH_3)$
1453	-	1427	$\gamma(CH_3)$
1168	-	1168	$\upsilon(C-C)$
1017	-	1001	$\omega(NH_2)$
941	-	938	$\beta(C-H)$
849	-	870	$\gamma(C-H)$
754	-	714	$\omega(H-O-H)$
668	-	634	$\delta(H-O-H)$
556	-	551	$\rho(C-C-C)$
-	-	293	$\upsilon_{as}(Sb-I)$

-	**159**	**142**	**υ_s(Sb-I)**
-	**108**	**106**	**δ_{as}(I-Sb-I)**
-	**86**	**92**	**δ_s(I-Sb-I)**
-	**60**	**59**	**Lattice mode**

υ_s :*symmetric stretching*, υ_{as} :*asymmetric stretching*, β : *in plane bending*, γ :*out plane bending*, δ :*scissoring*, ρ :*rocking* ,
ω:*wagging*, τ : Twisting