

## Electronic Supplementary Information

### Crystal structure and Hirshfeld surface analysis of (*Z*)-4-((5-isopropyl-3,8-dimethylazulen-1-yl)methylene)-2-phenyloxazol-5(*4H*)-one<sup>\*\*/\*\*</sup>

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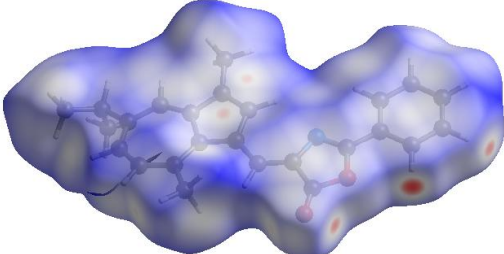
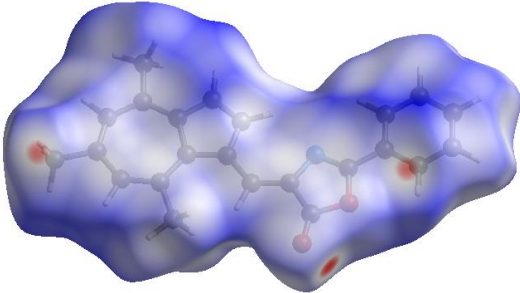
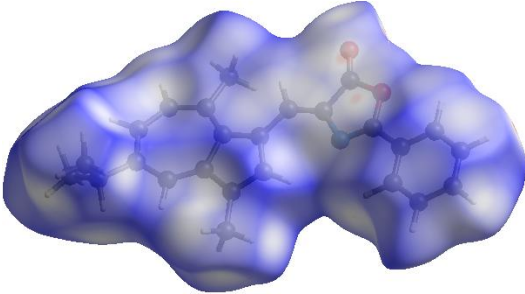
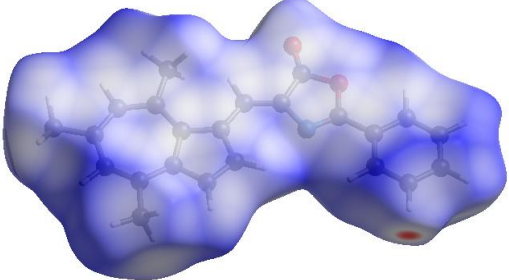
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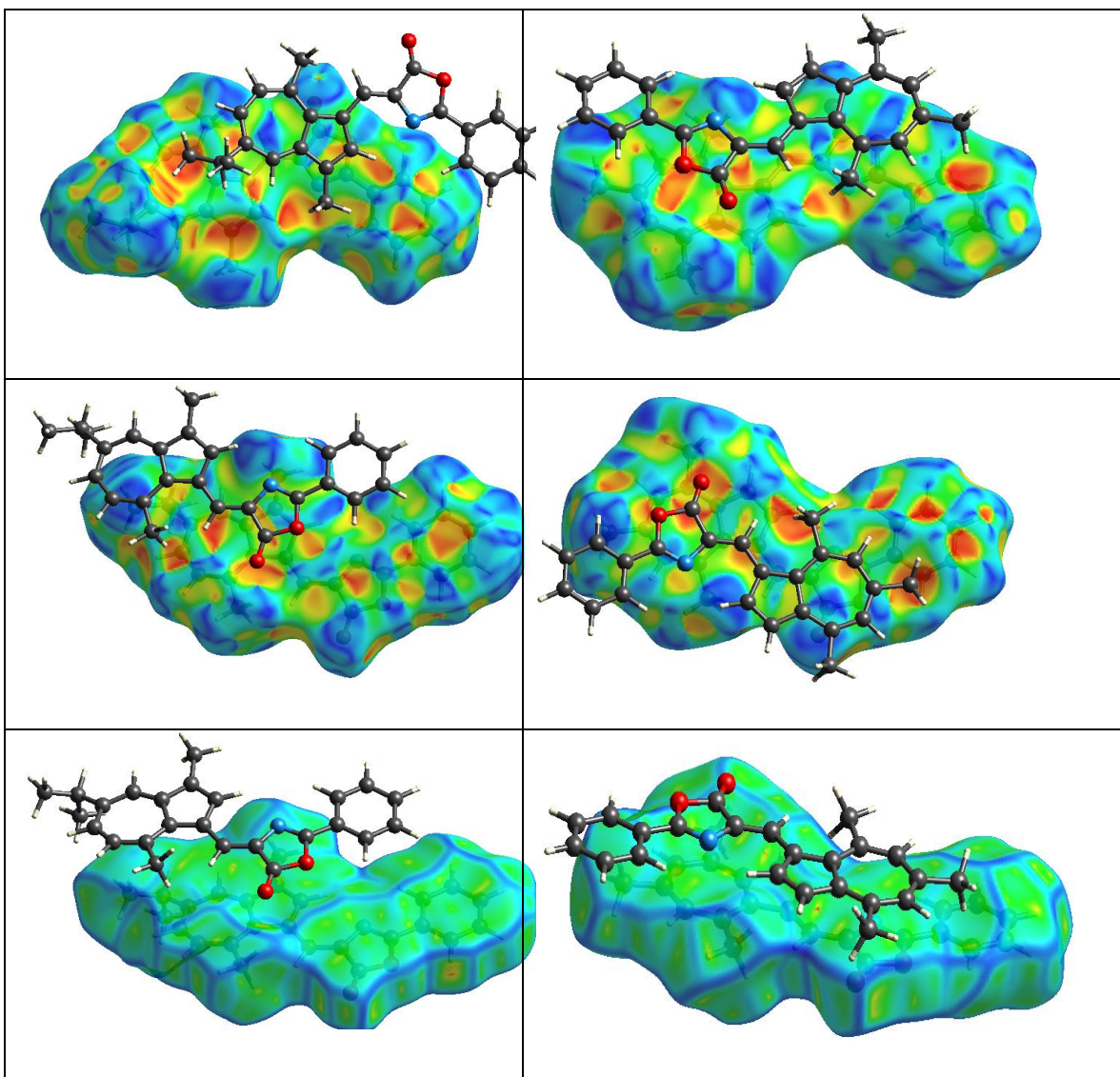
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\*\* This paper is dedicated to the memory of Dr. Liviu Bîrzan.

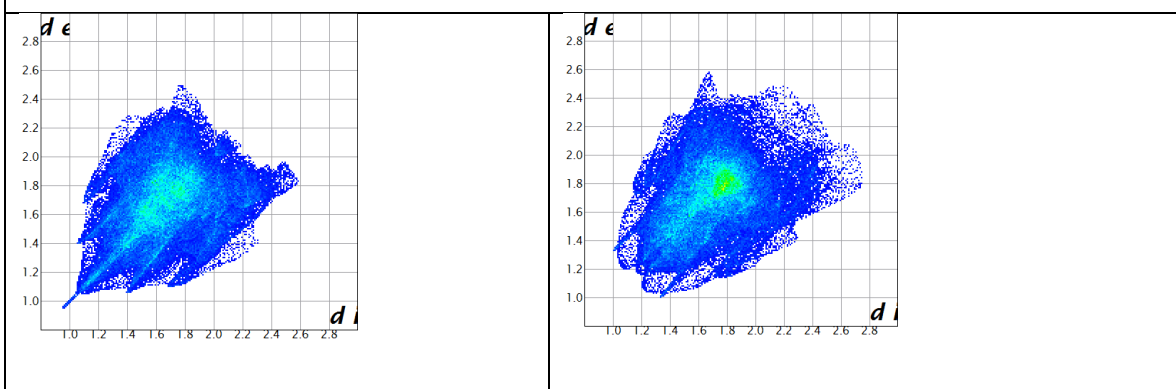
\*\*\* Supplementary information on <https://www.icf.ro/rch/> or <https://revroum.lew.ro/>

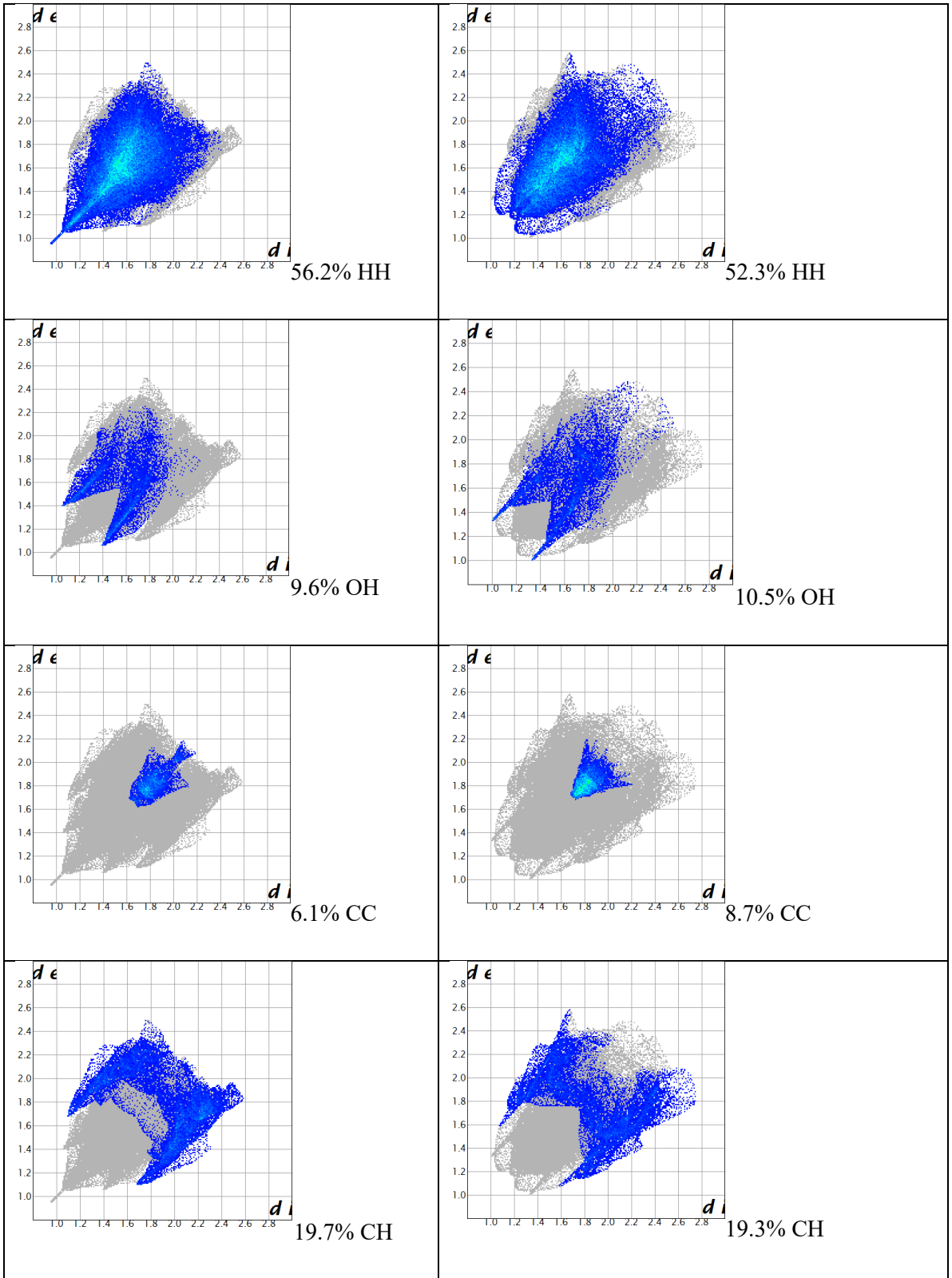
**Table S1.** Comparative data between compound **1** and ZIFSEQ.

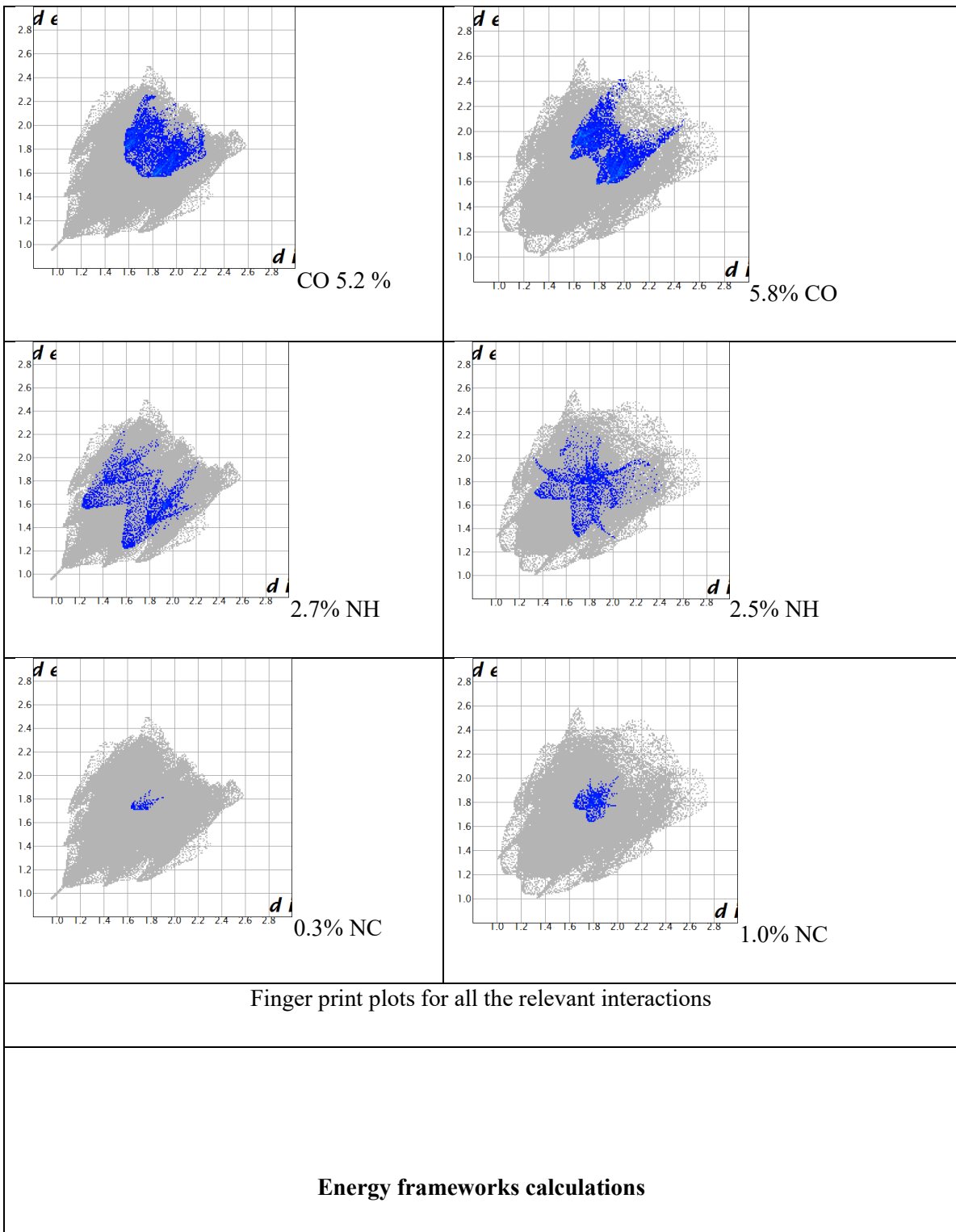
Compound 1	CCDC Ref. ZIFSEQ
	
	
Hirshfeld surface in $d_{\text{norm}}$ mode	



Hirshfeld surface in shpindex and curvedness mode highlighting the  $\pi \cdots \pi$  interactions



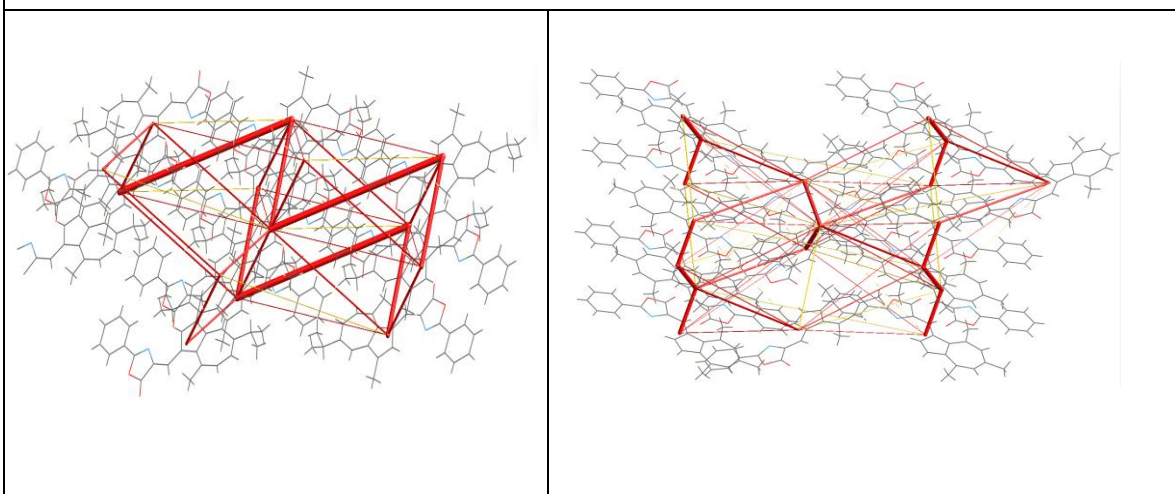




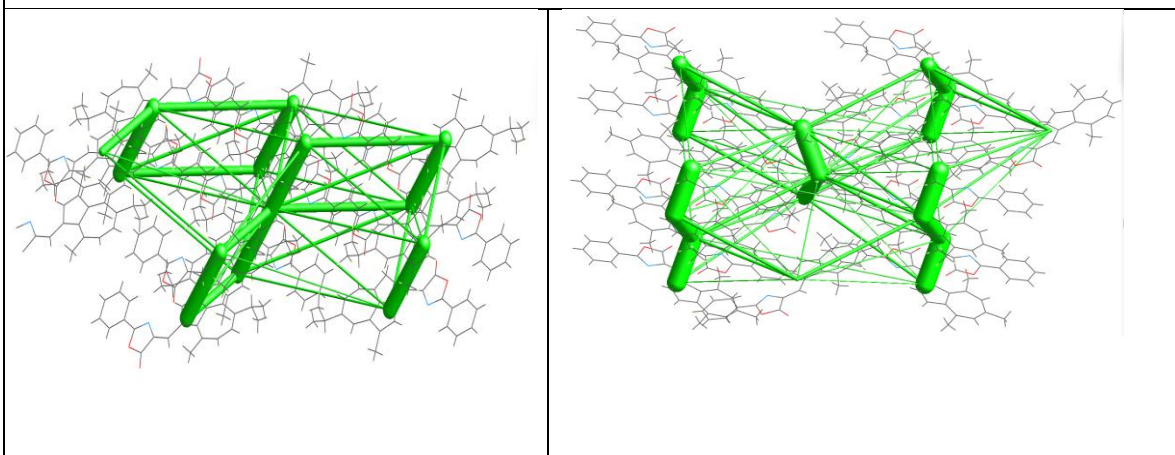
N	Symp	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
1	x, y, z	13.75	HF/3-21G	-8.5	-0.9	-12.5	0.0	-20.6
0	-x, -y, -z	10.08	HF/3-21G	4.1	-3.8	-48.3	18.5	-26.9
0	-x, -y, -z	10.33	HF/3-21G	-4.2	-1.0	-9.8	1.0	-13.0
1	-x, -y, -z	9.37	HF/3-21G	-25.8	-9.2	-21.1	12.0	-41.6
1	x, y, z	5.54	HF/3-21G	-13.5	-7.5	-95.4	43.4	-69.5
0	-x, -y, -z	7.96	HF/3-21G	-9.6	-3.3	-49.8	27.9	-34.2
1	x, y, z	16.23	HF/3-21G	-3.8	-0.9	-12.0	0.0	-15.4
0	-x, -y, -z	13.69	HF/3-21G	-30.8	-7.0	-19.3	0.0	-53.4
0	-x, -y, -z	11.47	HF/3-21G	0.7	-1.0	-17.8	5.7	-11.3
1	-x, -y, -z	16.45	HF/3-21G	3.9	-0.6	-8.1	0.0	-3.6

N	Symp	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
1	-x, -y, -z	4.68	HF/3-21G	-24.8	-8.3	-103.0	51.3	-81.9
1	x+1/2, -y+1/2, z+1/2	10.09	HF/3-21G	-10.9	-4.2	-16.6	8.6	-21.8
1	x+1/2, -y+1/2, z+1/2	14.23	HF/3-21G	-2.9	-0.3	-1.6	0.0	-4.6
1	x+1/2, -y+1/2, z+1/2	13.44	HF/3-21G	3.7	-1.3	-8.7	0.0	-4.9
1	x+1/2, -y+1/2, z+1/2	11.12	HF/3-21G	1.4	-0.6	-6.1	0.4	-4.1
2	-x+1/2, y+1/2, -z+1/2	11.30	HF/3-21G	-5.8	-1.8	-23.3	8.5	-21.2
2	-x+1/2, y+1/2, -z+1/2	12.04	HF/3-21G	-2.9	-4.7	-15.5	0.0	-20.0
0	-x, -y, -z	16.98	HF/3-21G	3.2	-0.5	-7.3	0.0	-3.6
0	-x, -y, -z	3.71	HF/3-21G	-21.3	-9.0	-121.9	55.0	-92.8
0	-x+1/2, y+1/2, -z+1/2	12.15	HF/3-21G	-3.7	-0.4	-6.5	0.0	-9.8
0	-x, -y, -z	12.75	HF/3-21G	5.9	-0.5	-7.2	0.0	-0.7

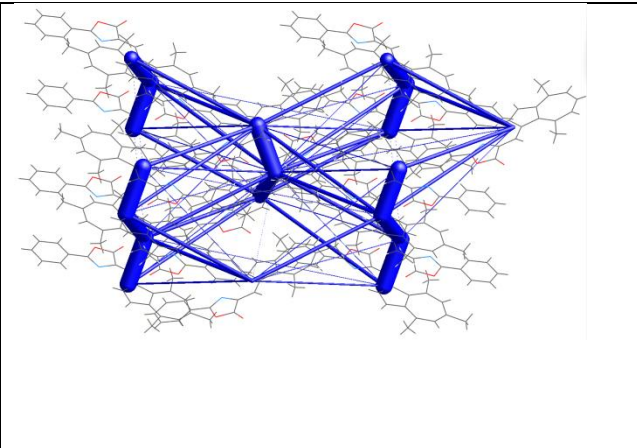
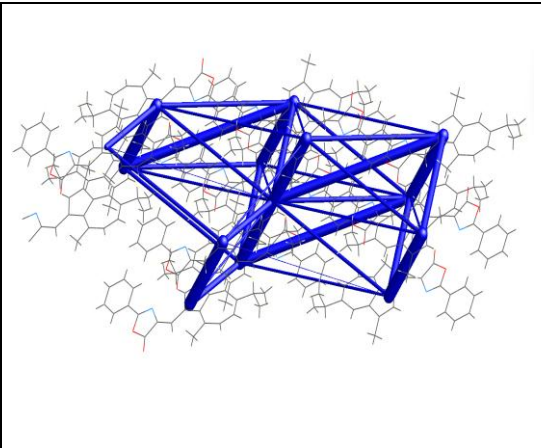
Relevant dimer energies within the crystals (kJ)



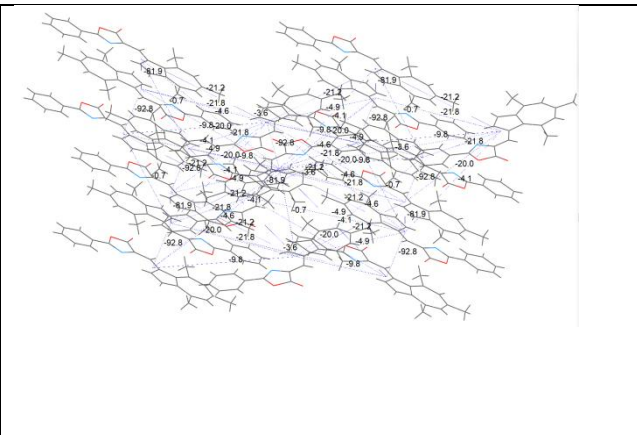
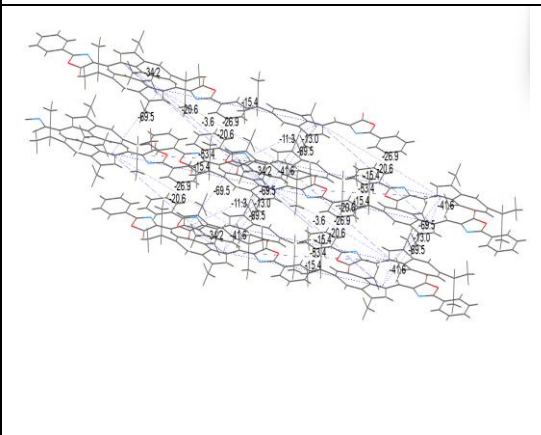
Electrostatic Energy Framework



Dispersion Energy Framework



Total energy Framework



Selected values for dimer energies within the crystal network (kJ)