Supporting Information

Hybrid azine–oxamic acid molecular design: synthesis, structure, and supramolecular implications

Ketlyn Wolfart Borth,[a] Letícia dos Santos Leal,[a] Verônica de Carvalho Teixeira,[b] Grazielli da Rocha,[a] Tatiana Renata Gomes Simões.[a*]

[a]*Departamento de Química, Universidade Federal do Paraná, Centro Politécnico, Curitiba-PR,* 81530-900, *Brasil*

[b]*Laboratório Nacional de Luz Síncrotron, Centro Nacional de Pesquisa em Energia e Materiais, Campinas-SP, 13083-100, Brasil*

* Corresponding author: tatiana.renata@ufpr.br (T.R.G.S.)

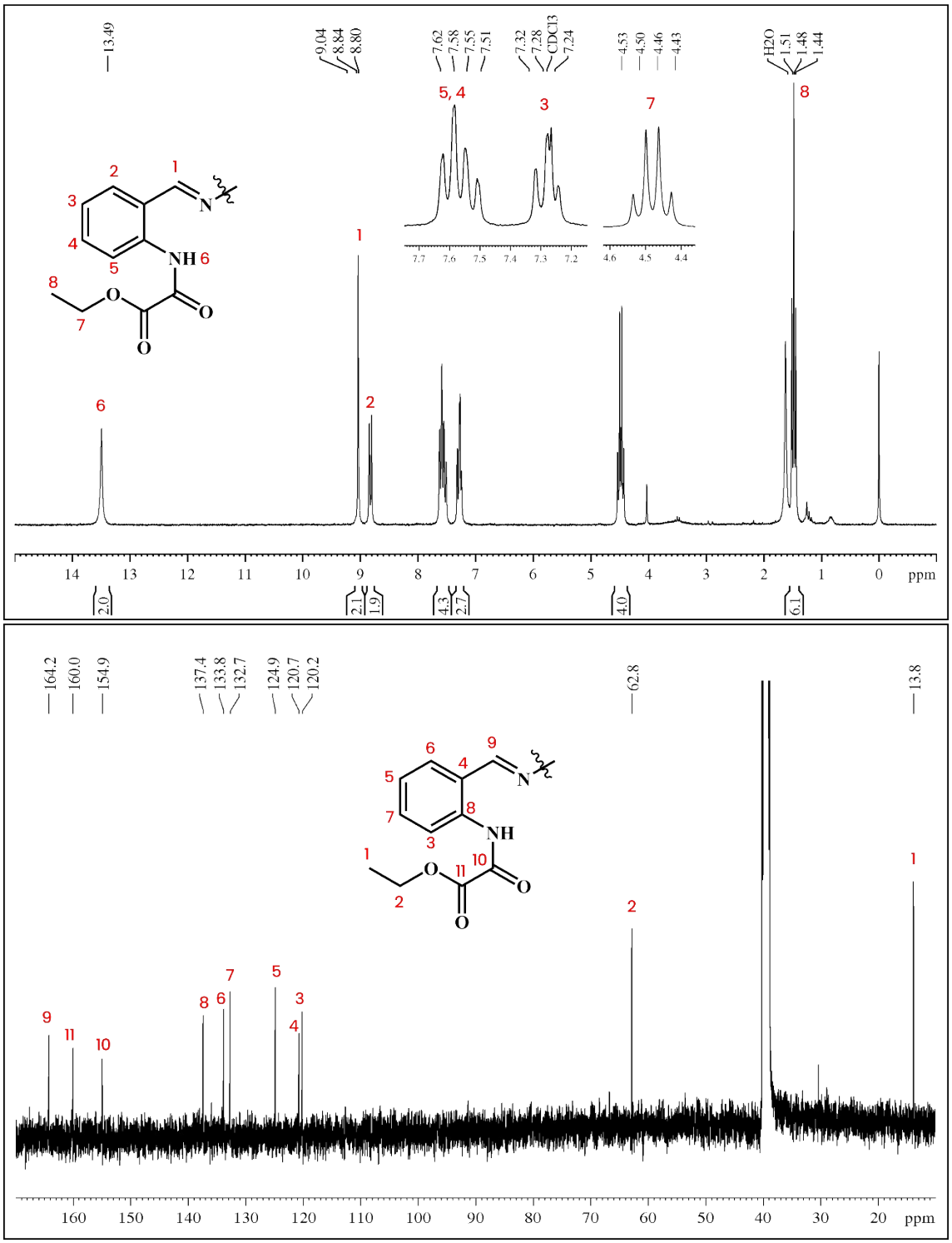


Figure S1. ^{1}H NMR and ^{13}C NMR of NN-Et_2H_4oba.

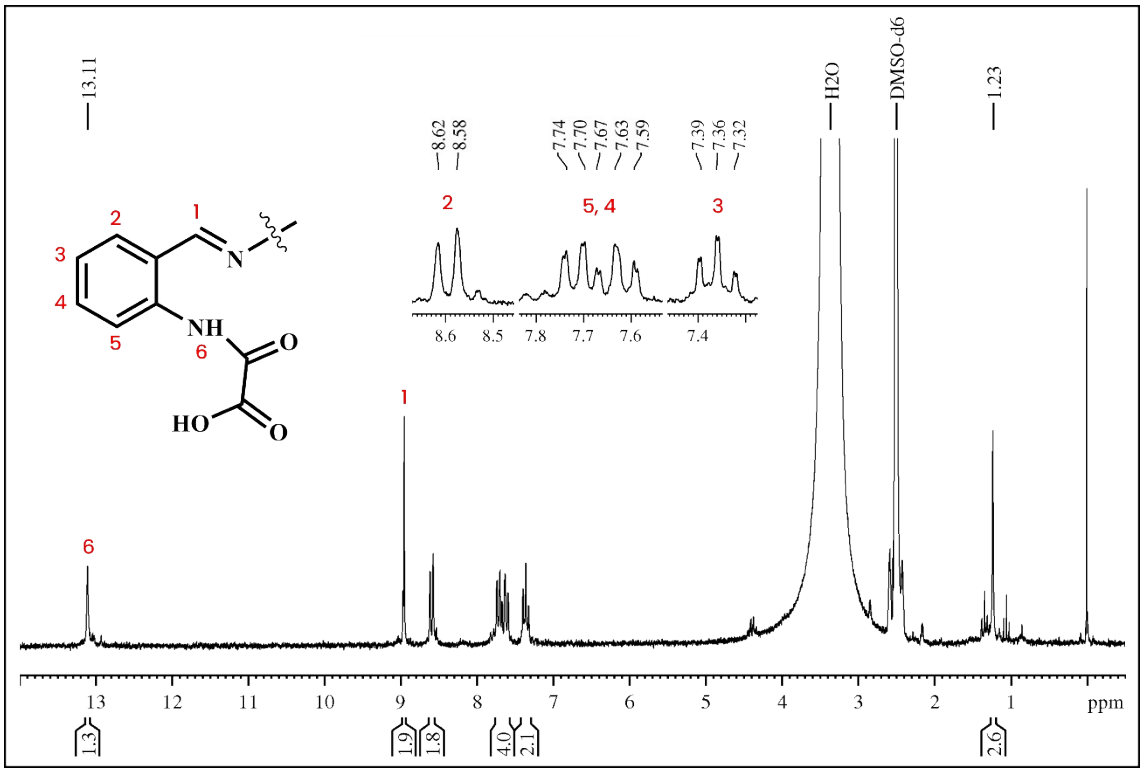


Figure S2. ^{1}H NMR of NN-H_4oba.

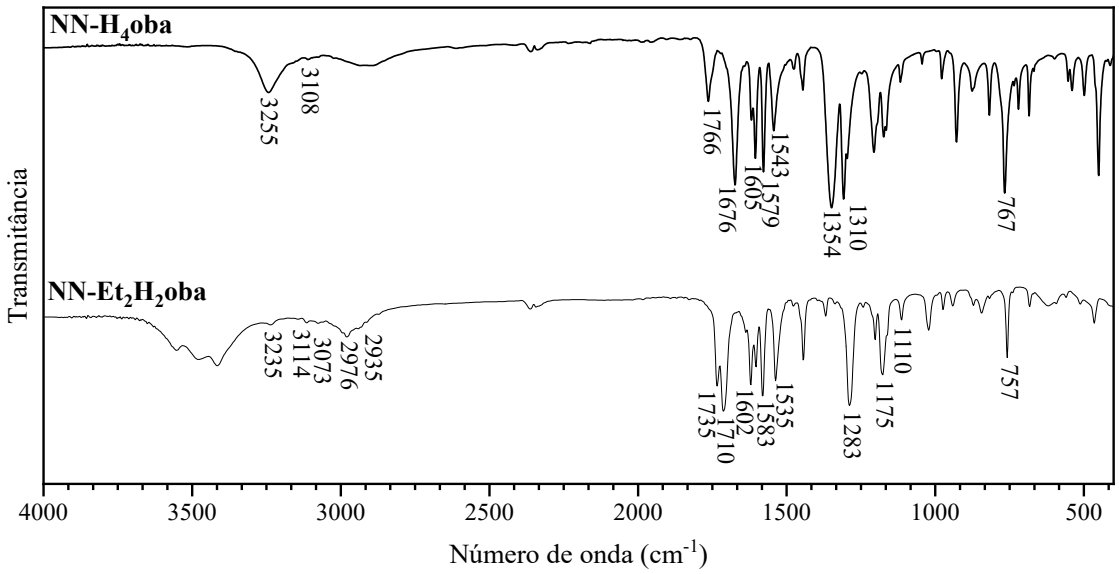


Figure S3. Infrared spectra of NN-Et_2H_4oba and NN-H_4oba.

Table S1. Bond lengths of the azine and oxamate groups in NN-Et_2H_2oba and NN-H_4oba

Bond	Bond lengths (Å)					
	NN-Et_2H_2oba	NN-H_4oba	Compound 1[1]	JDF-OMe[1]	H_2Et_2L[2]	H_3opba[3]
C9–N2	1.2863(19)	1.2853(19)	1.268(4)	1.284(3)		
C20–N4	1.2850(19)					

N2–N2	1.399(2)	1.400(2)	1.402(4)	1.398(2)		
N4–N4	1.398(2)					
C2–N1	1.3496(18)	1.3513(18)			1.346(2)	1.350(8)
C13–N3	1.3558(18)					
C2–O3	1.2144(17)	1.2169(17)			1.218(2)	1.227(8)
C13–O6	1.2147(17)					
C1–O2	1.3236(17)	1.2999(17)			1.334(1)	1.279(7)
C12–O5	1.3286(16)					
C1–O1	1.2057(17)	1.2168(17)			1.199(2)	1.233(8)
C12–O4	1.2008(17)					
C1–C2	1.543(2)	1.5423(19)			1.540(2)	1.534(7)
C12–C13	1.541(2)					

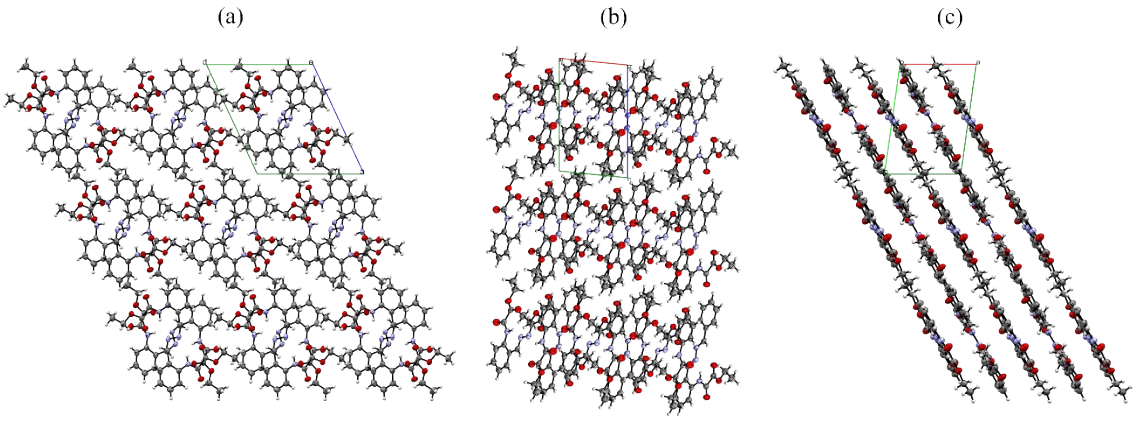


Figure S4. The supramolecular structure of NN-Et_2H_2oba. (a) plane *bc*; (b) plane *ac*; (c) plane *ab*.

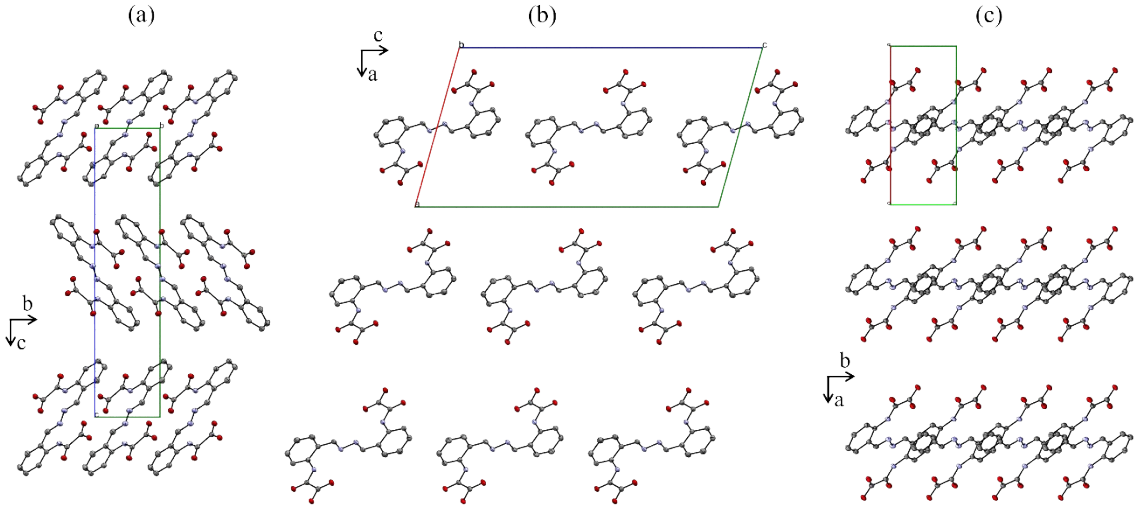


Figure S5. The supramolecular structure of NN-H_4oba. (a) plane *bc*; (b) plane *ac*; (c) plane *ab*.

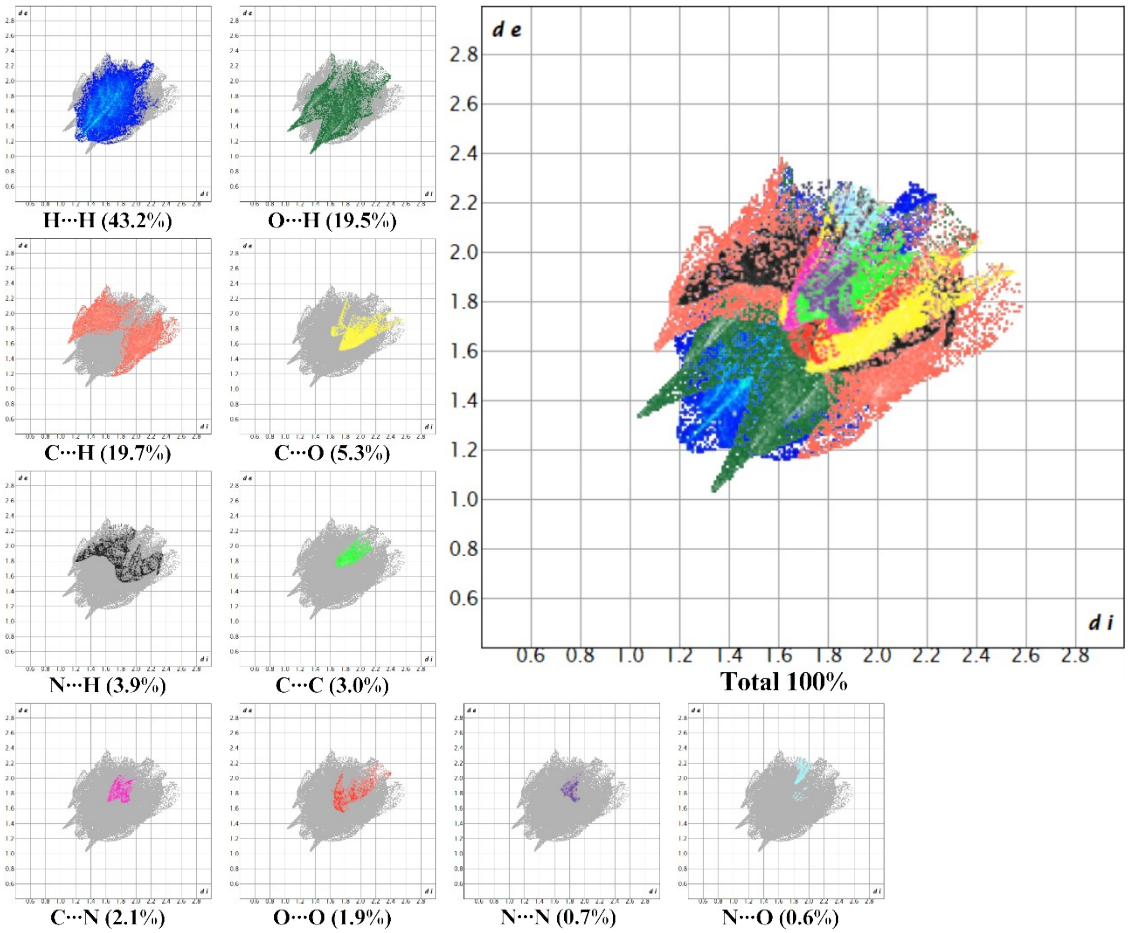


Figure S6. 2D fingerprint plot of NN-Et_2H_2oba.

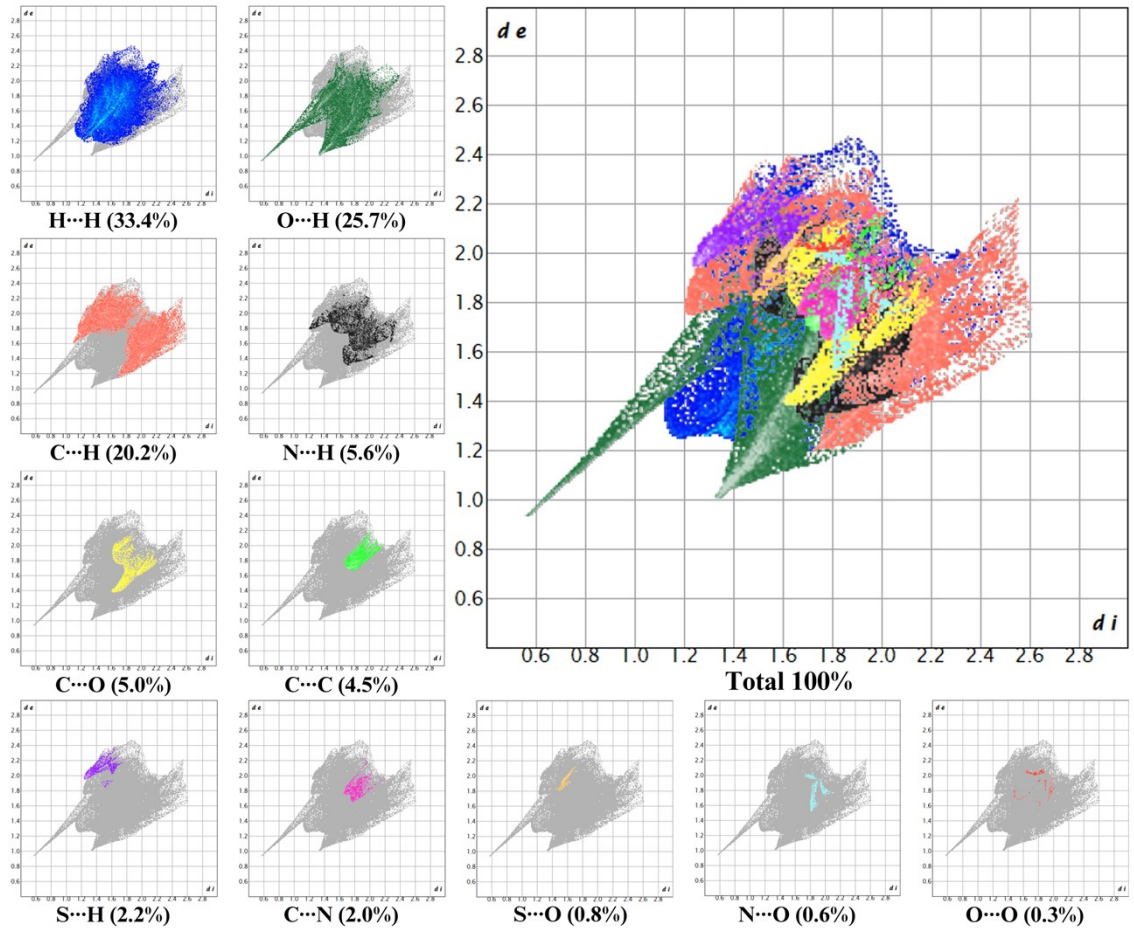
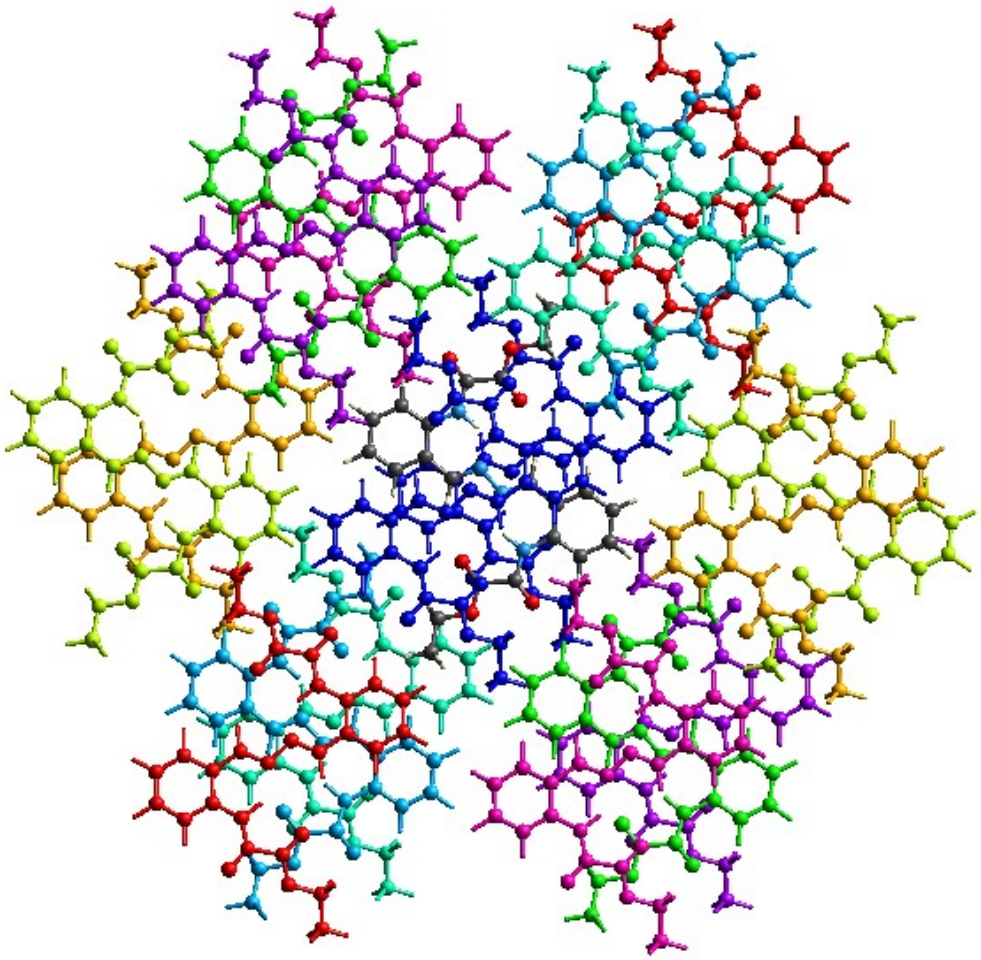
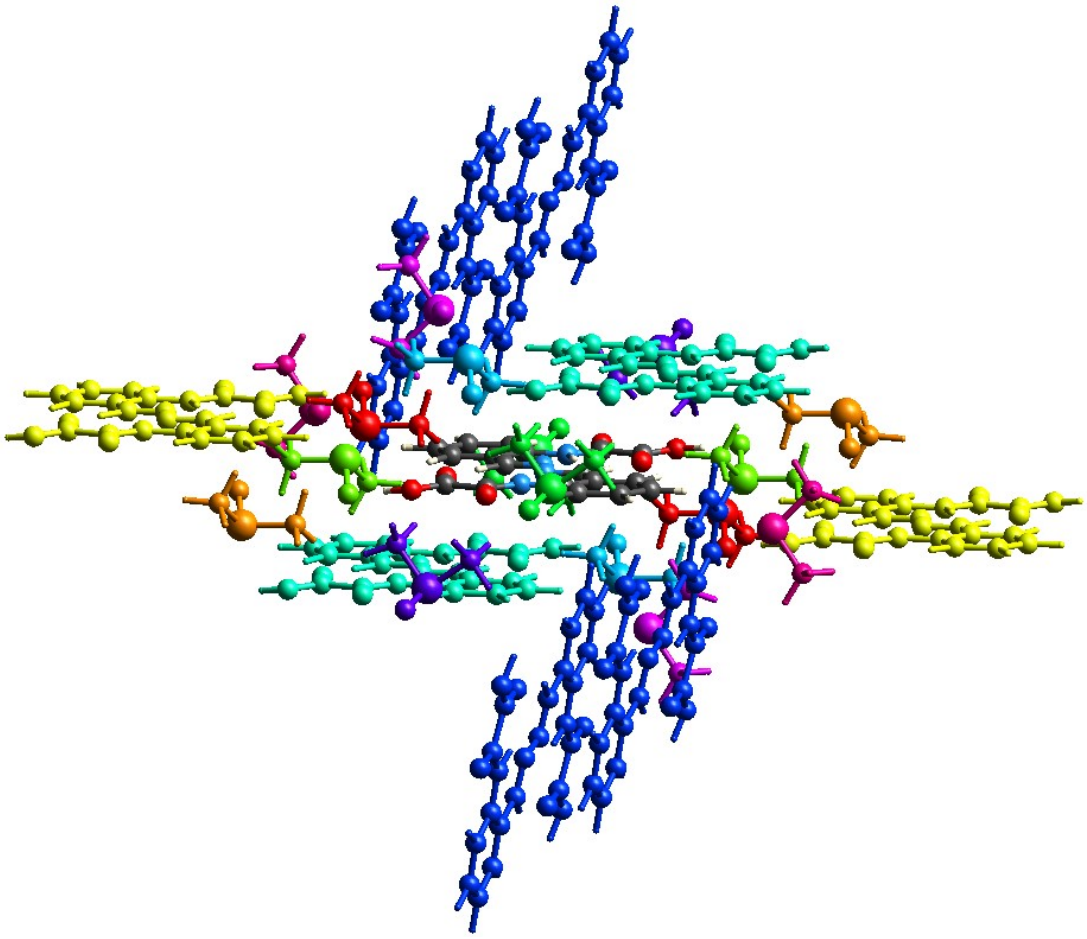


Figure S7. 2D fingerprint plot of NN-H_4oba.



	N	Symop	R	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	2		15.31	-2.0	-0.3	-5.8	0.0	-7.4
	2		13.58	0.8	-0.2	-7.2	0.0	-5.6
	2	x, y, z	14.56	0.5	-0.2	-3.4	0.0	-2.6
	2	x, y, z	13.23	-13.5	-7.0	-20.6	0.0	-37.4
	2		11.98	-5.4	-1.1	-25.2	15.2	-19.1
	2	x, y, z	13.24	-3.4	-1.4	-28.6	0.0	-29.6
	2		3.71	-27.4	-6.4	-134.9	75.4	-104.6
	2		13.59	2.2	-0.5	-11.4	0.0	-8.0
	2		13.90	-5.3	-1.8	-15.9	0.0	-20.8

Figure S8. Chemical environments around NN-Et_2H_2oba
($E_{tot} = k_{ele}E_{ele} + k_{pol}E_{pol} + k_{dis}E_{dis} + k_{rep}E_{rep}$ - scale factors: k_{ele}: 1.057; k_{pol}: 0.740; k_{dis}: 0.871; k_{rep}: 0.618).



	N	Symop	R	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0		8.66	-13.5	-2.4	-10.4	11.0	-18.3
	0		10.61	-1.5	-0.7	2.1	0.3	-3.8
	0	x, y, z	14.29	-0.8	-0.2	-1.0	0.0	-2.0
	0		6.57	-110.2	-24.8	-19.1	143.3	-62.8
	0		9.16	0.0	nan	0.0	0.0	nan
	0	x, y, z	5.30	-7.6	-2.9	-79.1	34.2	-57.9
	0		4.96	-12.0	-5.7	-27.7	26.2	-24.8
	0	-x, y +½, -z+½	12.47	-0.6	-0.4	-11.3	0.0	-10.8
	0		9.02	-7.6	-2.9	-79.1	34.2	-58.0
	0		6.48	2.5	-0.4	-11.3	0.0	-7.5
	0		8.53	-0.6	-0.4	-11.3	0.0	10.8

Figure S9. Chemical environments around NN-H_4oba
($E_{tot} = k_{ele}E_{ele} + k_{pol}E_{pol} + k_{dis}E_{dis} + k_{rep}E_{rep}$ - scale factors: k_{ele}: 1.057; k_{pol}: 0.740; k_{dis}: 0.871; k_{rep}: 0.618).

References

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