Supporting Information

A series of organic hybrid polyoxovanadate clusters incorporating tris(hydroxymethyl)methane derivatives

Li Huang, Congrui Ouyang, Xing Liu, Jian Zhou,* Hua-hong Zou,* Hua Yuan,* and Dou Wen

Table S1 The bond valence sum of V atoms for **1-8**.

1					
Bonds		ν	**Bonds**		ν
V1 – O1	1.9988(18)	0.559	V2－O1	1.9719(19)	0.602
V1－O2$^{\#1}$	2.3186(18)	0.236	V2－O2	2.3394(18)	0.223
V1－O5$^{\#1}$	1.9667(19)	0.610	V2－O2$^{\#1}$	2.0013(18)	0.556
V1－O6	1.604(2)	1.626	V2－O4	1.5895(19)	1.690
V1－O7	1.9871(19)	0.577	V2－O5	1.9764(19)	0.589
V1－O8	1.9986(19)	0.559	V2－N1	2.121(2)	0.401
	sum	4.169		sum	4.068
2					
Bonds		ν	**Bonds**		ν
V1－O1$^{\#1}$	2.0030(15)	0.553	V2－O1$^{\#1}$	2.2880(15)	0.256
V1－O2	1.9613(16)	0.619	V2－O2	1.9903(16)	0.572
V1－O4	1.5962(17)	1.661	V2－O3	1.6005(18)	1.642
V1－O6	2.0009(16)	0.556	V2－O4$^{\#1}$	1.9809(17)	0.587
V1－O1	2.3067(16)	0.243	V2－O6	2.0036(17)	0.552
V1－N1	2.1208(19)	0.402	V2－O8	1.9997(19)	0.558
	sum	4.036		sum	4.169
3a					
Bonds		ν	**Bonds**		ν
V1－O1	2.302(3)	0.246	V3－O10	2.301(3)	0.247
V1－O1$^{\#1}$	2.014(3)	0.537	V3－O10$^{\#1}$	2.010(3)	0.543
V1－O2	1.959(4)	0.623	V3－O9	1.967(4)	0.609
V1－N1	2.123(4)	0.400	V3－O15	1.609(3)	1.604
V1－O4	1.601(4)	1.640	V3－O16	2.000(4)	0.557
V1－O5	2.008(4)	0.545	V3－N2	2.125(4)	0.398
	sum	3.992		sum	3.960
V2－O1	2.284(4)	0.258	V4－O9	1.997(4)	0.562
V2－O2$^{\#1}$	1.999(3)	0.559	V4－O10$^{\#2}$	2.293(4)	0.252
V2－O5	1.989(4)	0.575	V4－O12	1.594(4)	1.671
V2－O6	1.602(4)	1.635	V4－O13	2.001(4)	0.556
V2－O7	2.003(4)	0.553	V4－O14	2.006(4)	0.548
V2－O8	2.011(4)	0.541	V4－O16$^{\#2}$	1.991(4)	0.571
	sum	4.123		sum	4.163

3b					
Bonds		ν	**Bonds**		ν
V1－O1	2.2652(18)	0.272	V3－O9	1.966(2)	0.611
V1－O1$^{\#1}$	1.9968(18)	0.562	V3－O10$^{\#2}$	1.9893(18)	0.574
V1－O2	1.964(2)	0.614	V3－O10	2.2896(18)	0.255
V1－O4	1.6025(19)	1.633	V3－O12	1.6150(18)	1.579
V1－O8	1.991(2)	0.571	V3－O13	1.990(2)	0.573
V1－N1	2.136(2)	0.386	V3－N2	2.119(2)	0.404
	sum	4.041		sum	3.997
V2－O1	2.327(2)	0.230	V4－O9$^{\#2}$	2.0141(19)	0.537
V2－O2$^{\#1}$	2.0075(19)	0.546	V4－O10	2.321(2)	0.235
V2－O5	1.589(2)	1.694	V4－O13	2.0062(19)	0.548
V2－O6	2.015(2)	0.536	V4－O14	1.588(2)	1.698
V2－O7	2.000(2)	0.558	V4－O15	2.010(2)	0.543
V2－O8	1.997(2)	0.562	V4－O16	1.992(2)	0.569
	sum	4.123		sum	4.131
4					
Bonds		ν	**Bonds**		ν
V1－O1$^{\#1}$	2.301(2)	0.247	V2－O1$^{\#1}$	2.014(2)	0.537
V1－O2	1.998(2)	0.561	V2－O1	2.307(2)	0.243
V1－O4$^{\#1}$	2.005(2)	0.550	V2－O2	1.965(2)	0.613
V1－O7	2.012(2)	0.539	V2－O4	2.012(2)	0.540
V1－O8	2.013(2)	0.538	V2－O6	1.6036(19)	1.628
V1－O9	1.591(2)	1.685	V2－N1	2.125(2)	0.398
		4.122			3.960
5					
Bonds		ν	**Bonds**		ν
V1－O1	1.9608(17)	0.620	V2－O1$^{\#1}$	1.9981(17)	0.561
V1－O2$^{\#1}$	1.9992(17)	0.559	V2－O2	2.3268(18)	0.231
V1－O2	2.2973(16)	0.249	V2－O5	2.0020(18)	0.555
V1－O4	1.6031(16)	1.631	V2－O6	1.9969(19)	0.562
V1－O8	1.9900(18)	0.573	V2－O7	1.595(2)	1.667
V1－N1	2.122(2)	0.401	V2－O8	2.0056(17)	0.549
	sum	4.033		sum	4.124
6					
Bonds		ν	**Bonds**		ν
V1－O1	2.255(2)	0.279	V2－O1$^{\#1}$	1.992(2)	0.570
V1－O9	2.090(3)	0.437	V2－O1	2.389(2)	0.195
V1－O8	2.035(2)	0.507	V2－O7	2.017(3)	0.533
V1－O2$^{\#1}$	2.010(2)	0.543	V2－O5	1.617(2)	1.570
V1－O3$^{\#1}$	1.989(2)	0.575	V2－O2	2.007(2)	0.547
V1－O6	1.607(3)	1.613	V2－O3$^{\#1}$	2.003(2)	0.553
	sum	3.955		sum	3.969

7					
Bonds		ν	**Bonds**		ν
V1－O4	1.996(2)	0.565	V4－O4	2.012(2)	0.539
V1－O6	2.004(2)	0.548	V4－O5	2.003(2)	0.553
V1－O10	1.606(3)	1.618	V4－O7	2.006(2)	0.548
V1－O17	2.354(2)	0.214	V4－O8	2.010(2)	0.542
V1－O18	1.995(2)	0.562	V4－O13	1.608(3)	1.609
V1－O19	1.992(2)	0.573	V4－O17	2.282(2)	0.260
	sum	4.081		sum	4.054
V2－O8	2.005(2)	0.550	V5－O1	2.006(2)	0.548
V2－O9	2.005(2)	0.550	V5－O2	1.998(2)	0.561
V2－O15	1.609(3)	1.604	V5－O12	1.609(3)	1.605
V2－O16	1.981(3)	0.587	V5－O16	1.995(3)	0.565
V2－O17	2.331(2)	0.228	V5－O17	2.368(2)	0.206
V2－O19	1.991(2)	0.571	V5－O18	2.007(2)	0.547
	sum	4.092		sum	4.033
V3－O2	2.007(2)	0.547	V6－O1	1.999(2)	0.559
V3－O3	2.008(3)	0.546	V6－O3	1.996(2)	0.564
V3－O7	2.012(2)	0.540	V6－O5	2.009(2)	0.544
V3－O9	2.006(2)	0.549	V6－O6	2.017(2)	0.533
V3－O11	1.606(3)	1.618	V6－O14	1.611(3)	1.596
V3－O17	2.293(2)	0.253	V6－O17	2.233(2)	0.297
	sum	4.052		sum	4.094
8					
Bonds		ν	**Bonds**		ν
V1－O5	2.040(4)	0.5001	V5－O1	1.982(5)	0.586
V1－O7	2.028(5)	0.517	V5－O2	2.020(5)	0.528
V1－O11	2.011(5)	0.541	V5－O5	2.053(5)	0.483
V1－O12	2.005(5)	0.550	V5－O7	2.055(5)	0.481
V1－O18	1.594(5)	1.671	V5－O19	1.602(5)	1.635
V1－O23	2.304(4)	0.245	V5－O21	2.196(4)	0.328
	sum	4.026		sum	4.042
V2－O4	1.940(5)	0.656	V6－O4	2.003(5)	0.552
V2－O5	2.315(4)	0.238	V6－O10	1.994(5)	0.566
V2－O21	1.955(4)	0.629	V6－O11	1.997(5)	0.561
V2－O22	1.657(4)	1.401	V6－O14	2.053(7)	0.482
V2－O23	1.973(4)	0.600	V6－O15	1.591(5)	1.682
V2－N2	2.111(6)	0.413	V6－O23	2.297(4)	0.249
	sum	3.946		sum	4.094
V3－O1	2.331(6)	0.228	V7－O8	1.970(5)	0.604
V3－O2	2.075(4)	0.455	V7－O10	1.975(5)	0.596
V3－O17	1.588(6)	1.696	V7－O12	1.996(5)	0.563
V3－O21	1.947(4)	0.644	V7－O13	2.017(6)	0.532

V3—O22$^{\#3}$	2.011(4)	0.541	V7—O16	1.595(6)	1.664
V3—N1	2.091(6)	0.435		sum	3.958
	sum	3.999			
V4—O7	2.394(5)	0.192			
V4—O8	1.966(5)	0.610			
V4—O20	1.599(5)	1.646			
V4—O21	1.970(5)	0.604			
V4—O23	1.986(4)	0.578			
V4—N3	2.132(6)	0.389			
	sum	4.021			

(#1)1-x,1-y,1-z; (#2)1-x,2-y, -z; (#3)1/2-x,1/2-y,1-z

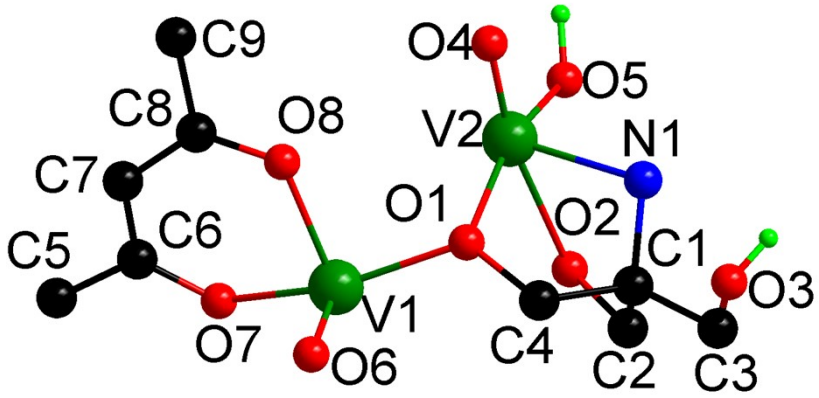


Fig. S1 The asymmetric unit of **1** (H atoms bonded to C and N atoms have been omitted for clarity).

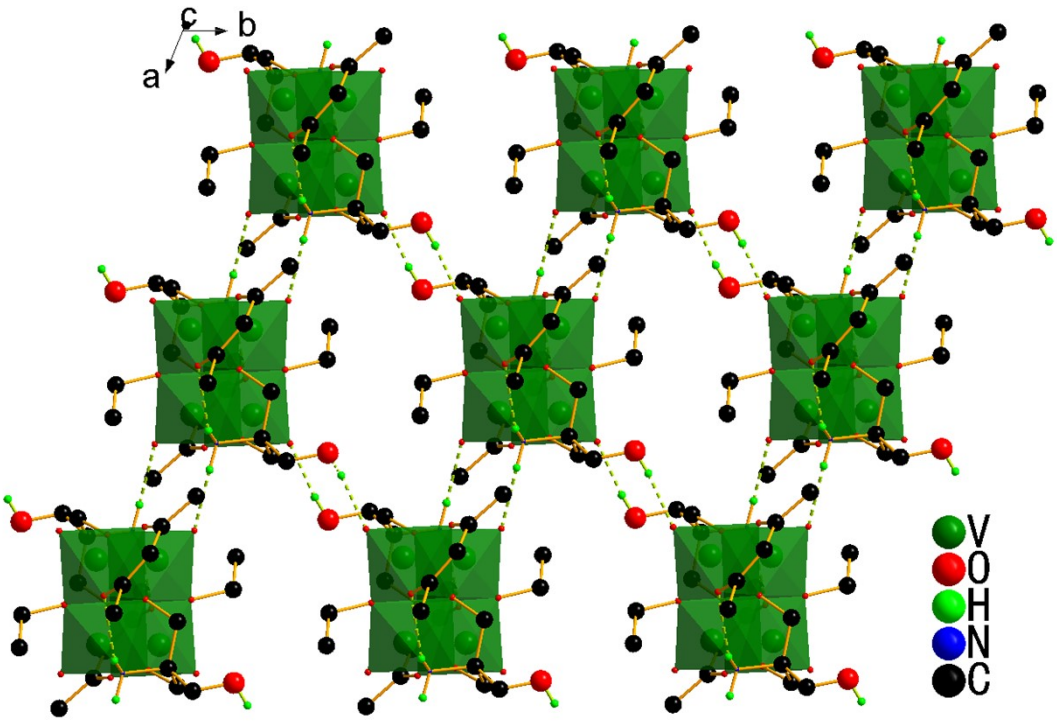


Fig. S2 The 2-D sql layer constructed by N-H···O and O-H···O H-bonds in **3a**. H atoms bonded to C and N atoms are omitted for clarity.

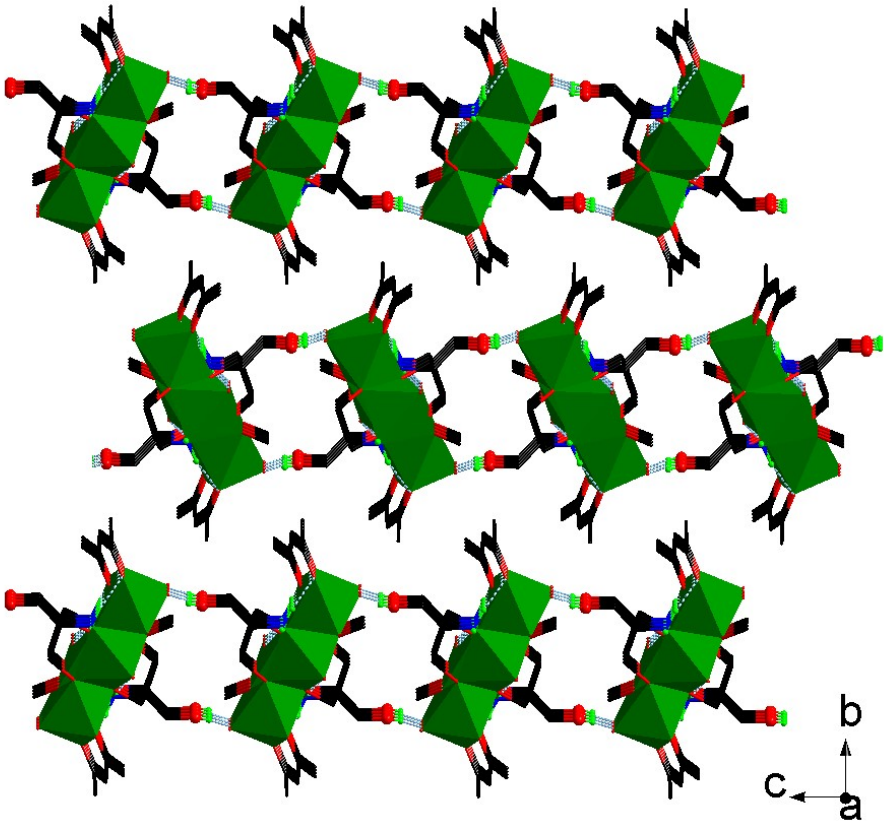


Fig. S3 The packing modes of the tetravanadyl clusters in **2**.

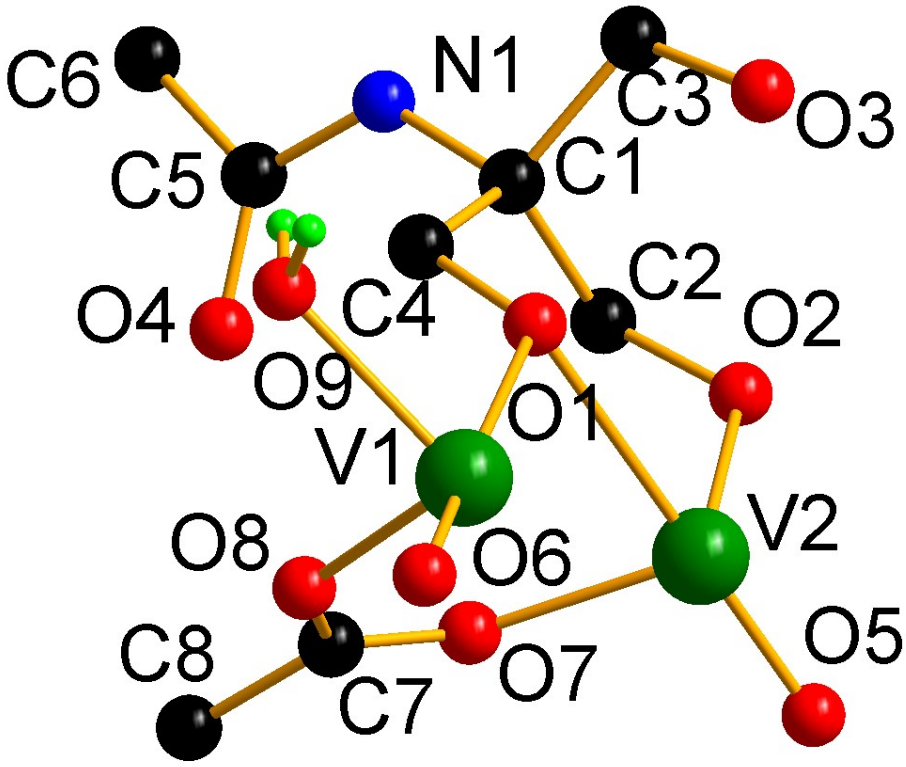


Fig. S4 The asymmetric unit of **6** (H atoms bonded to C and N atoms have been omitted for clarity).

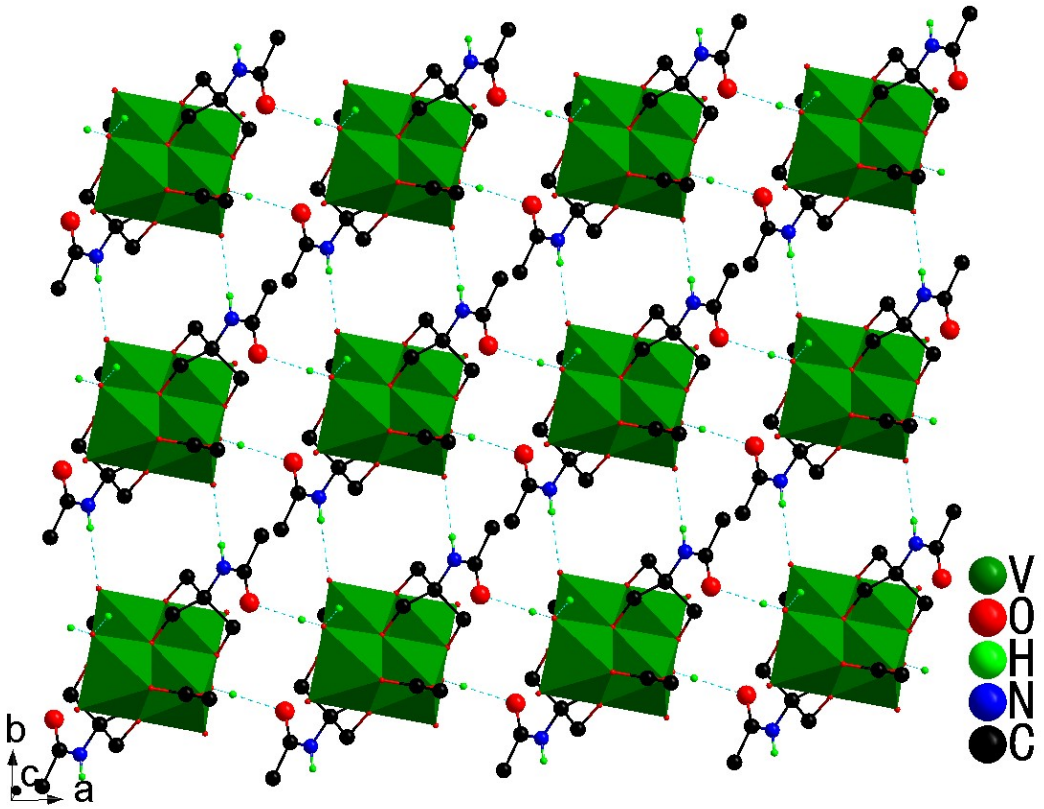


Fig. S5 The 2-D sql layer constructed by N-H···O and O-H···O H-bonds in **6**. H atoms bonded to C and N atoms are omitted for clarity.

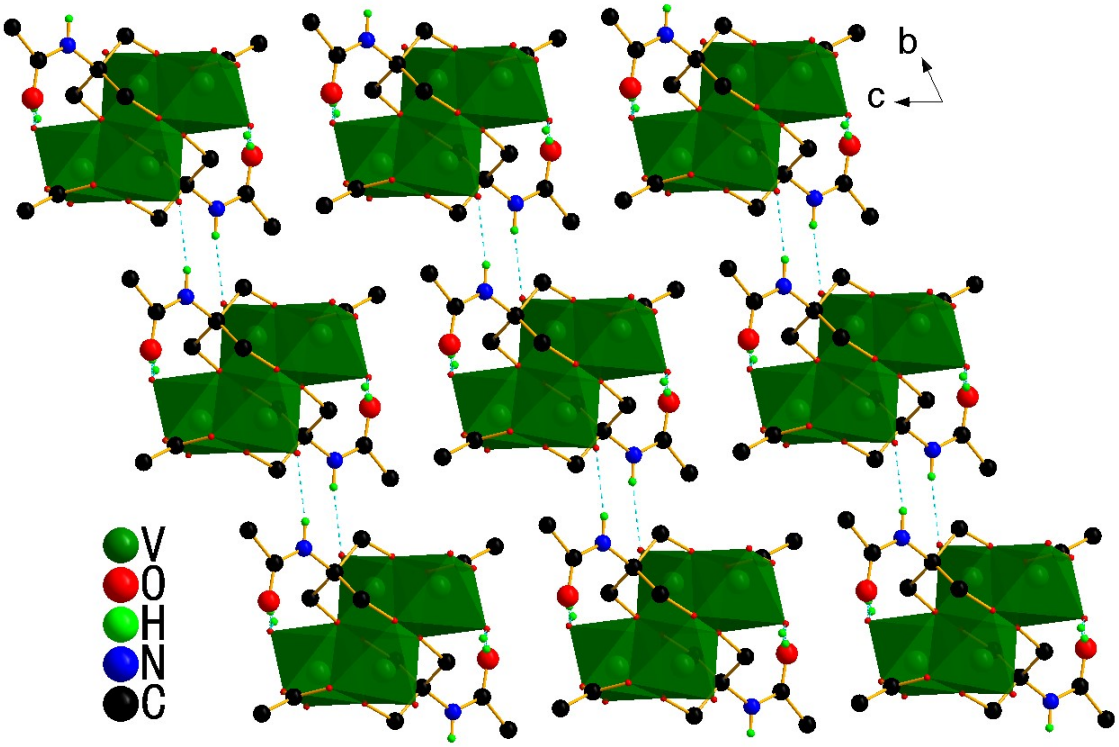


Fig. S6 The layers aligned in a parallel mode in **6**.

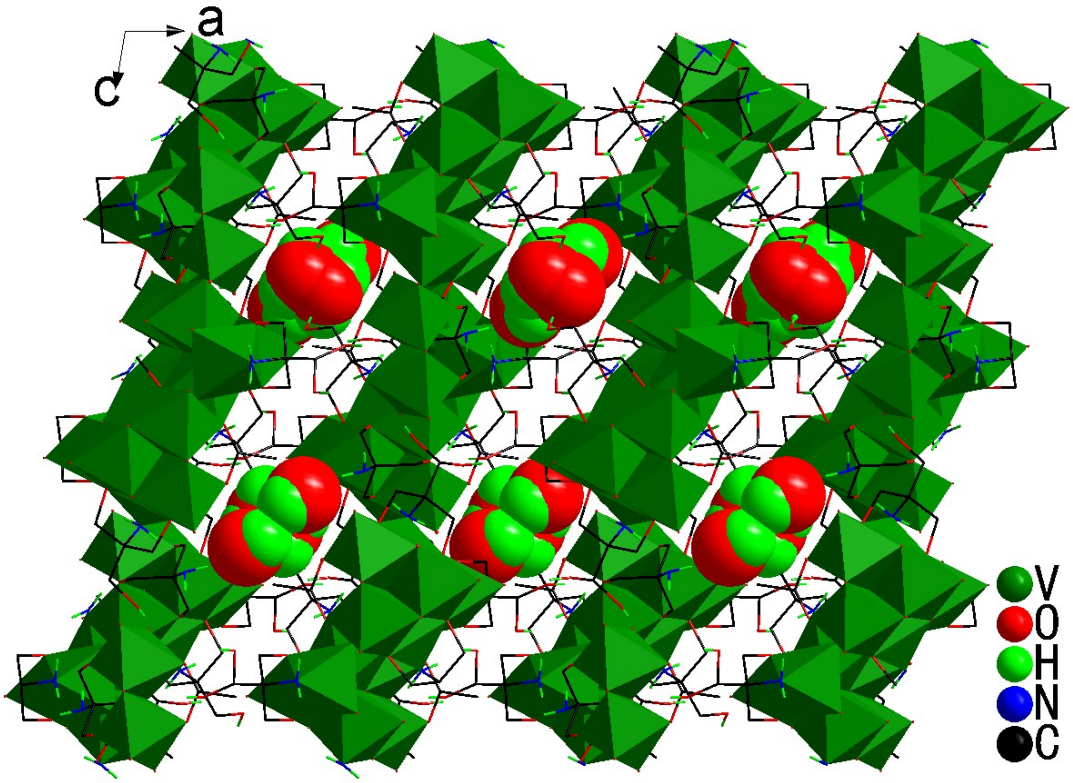


Fig. S7 The 3-D H-bonding network structure in **8**. H atoms bonded to C and N atoms are omitted for clarity.

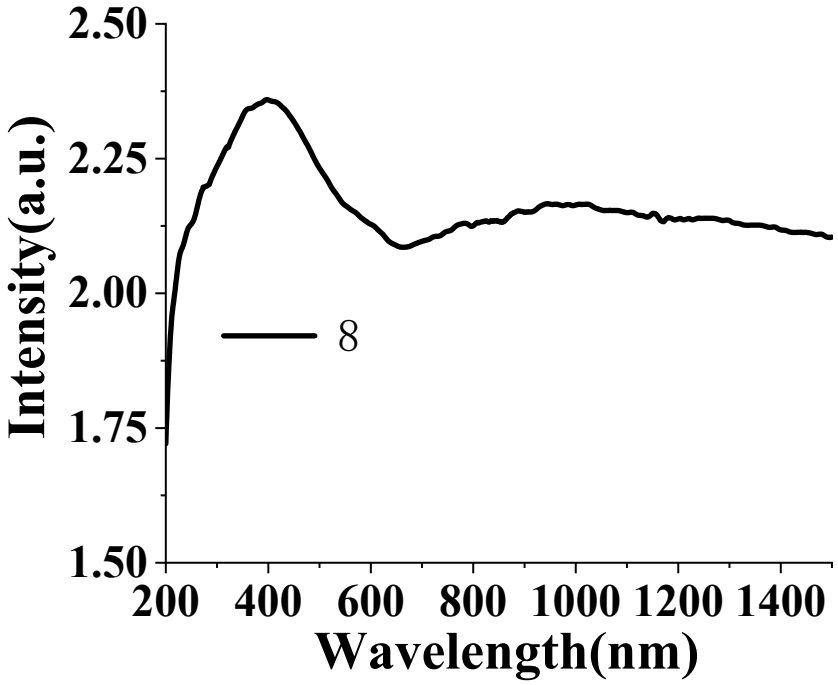
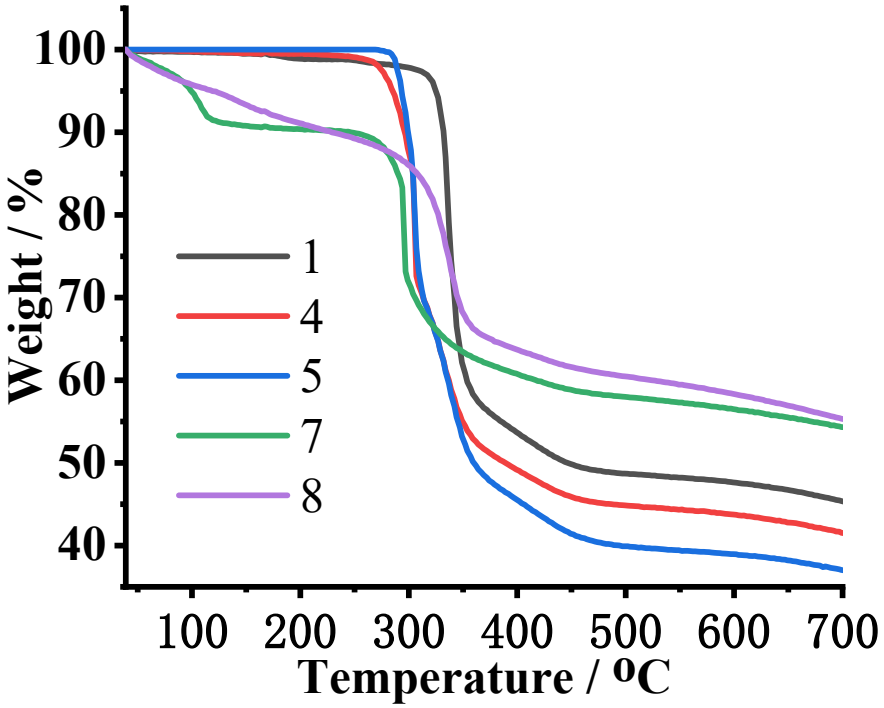


Fig. S8 UV−vis spectrum of **8**.



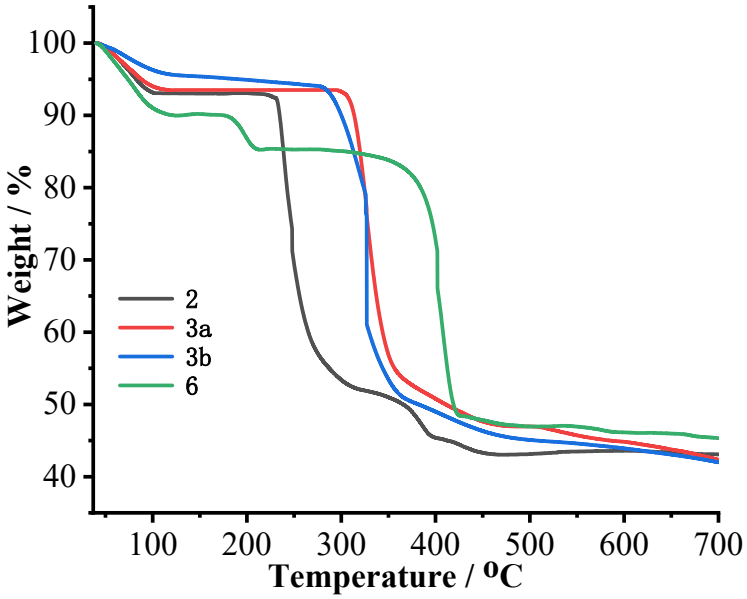


Fig. S9 The thermogravimetric curves of **1-8**.

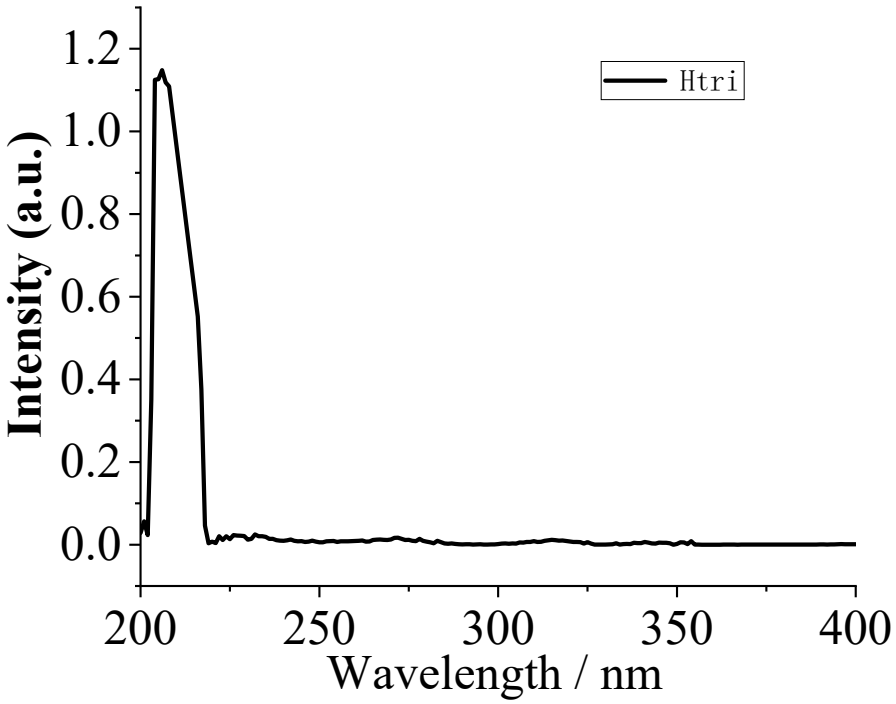


Fig. S10 UV−vis spectrum of Htri.

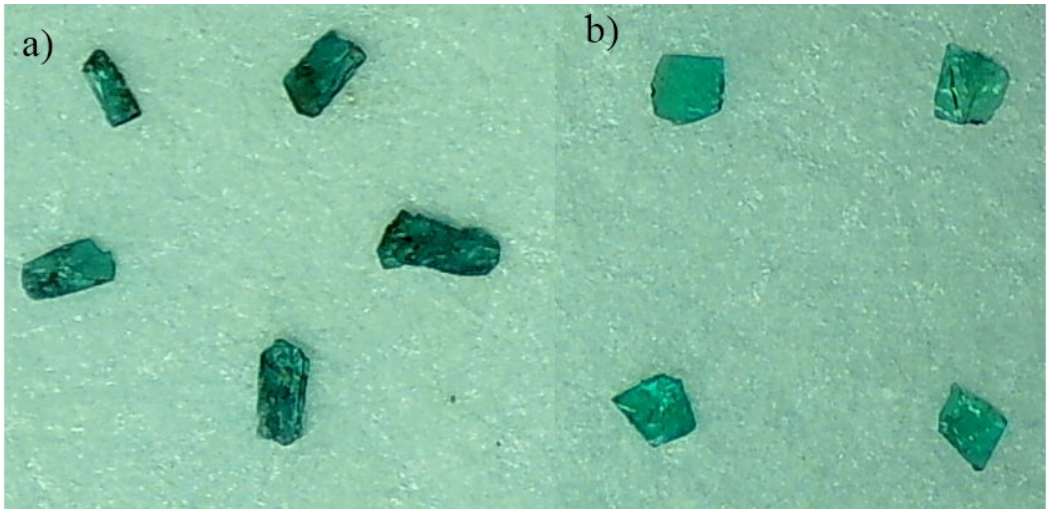
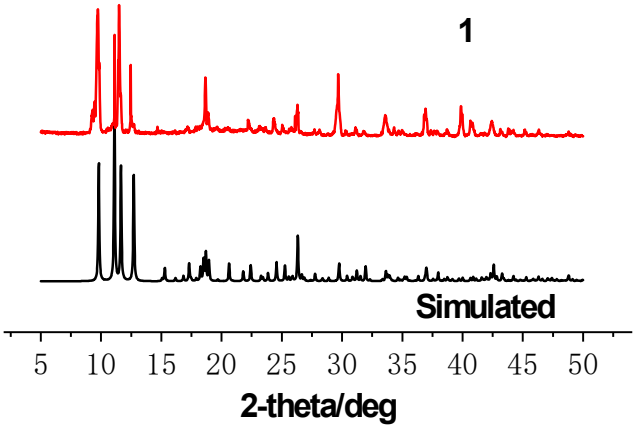
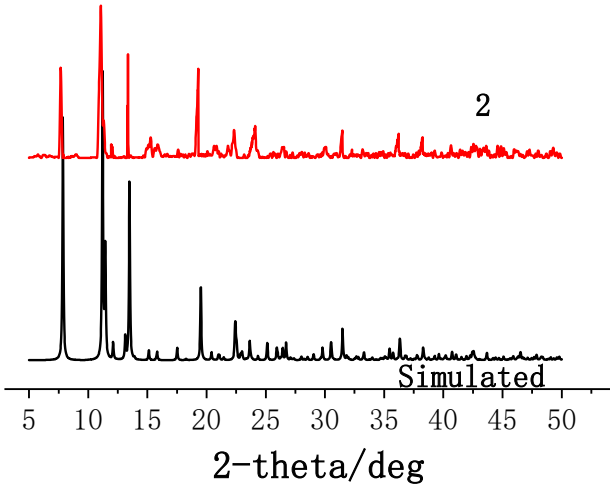
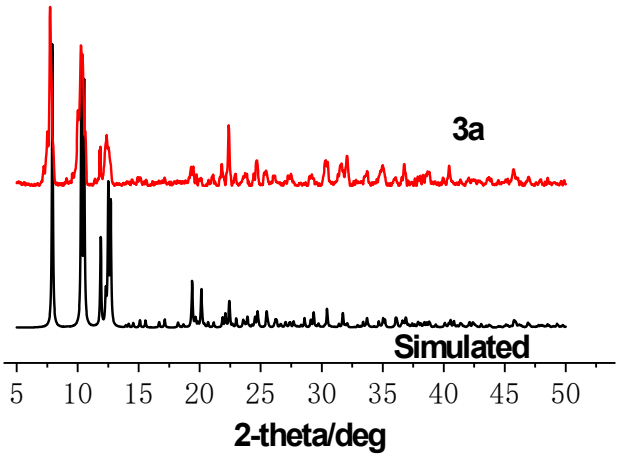


Fig. S11 Single crystal photo maps of **3a** and **3b**, showing different crystal shapes.




2
Simulated
5 10 15 20 25 30 35 40 45 50
2-theta/deg


3a
Simulated
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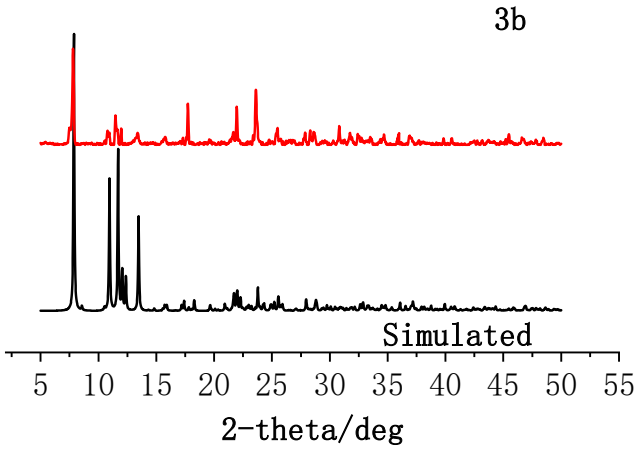
2-theta/deg


3b
Simulated
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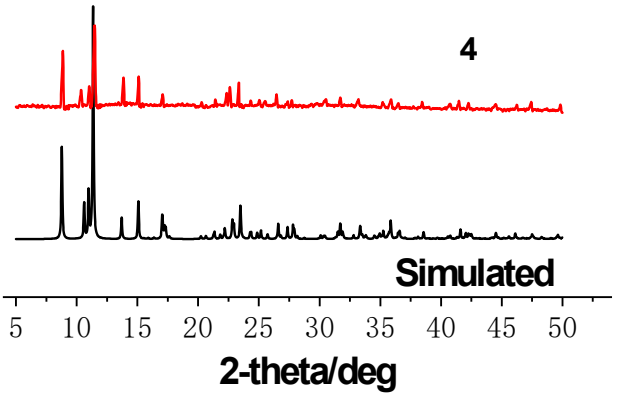
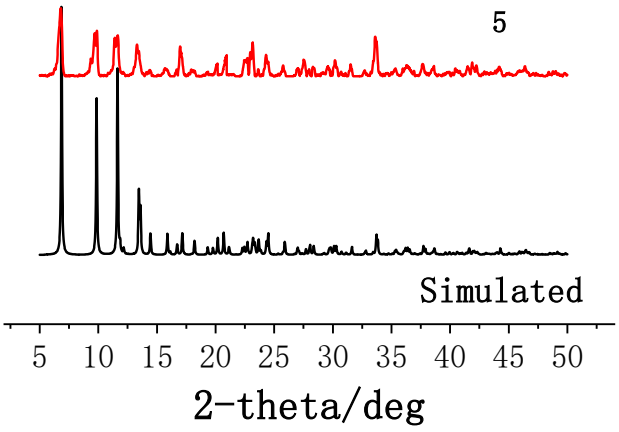
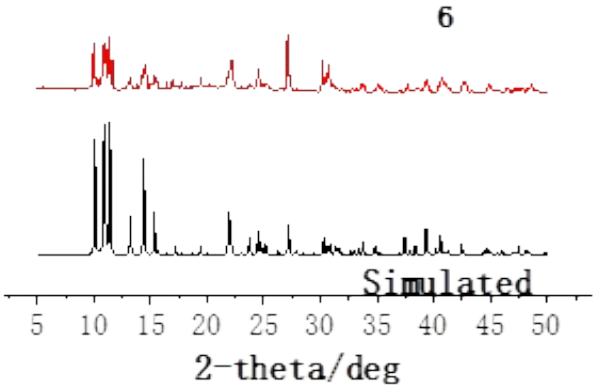
2-theta/deg


4
Simulated
5 10 15 20 25 30 35 40 45 50
2-theta/deg


5
Simulated
5 10 15 20 25 30 35 40 45 50
2-theta/deg


6
Simulated
5 10 15 20 25 30 35 40 45 50
2-theta/deg

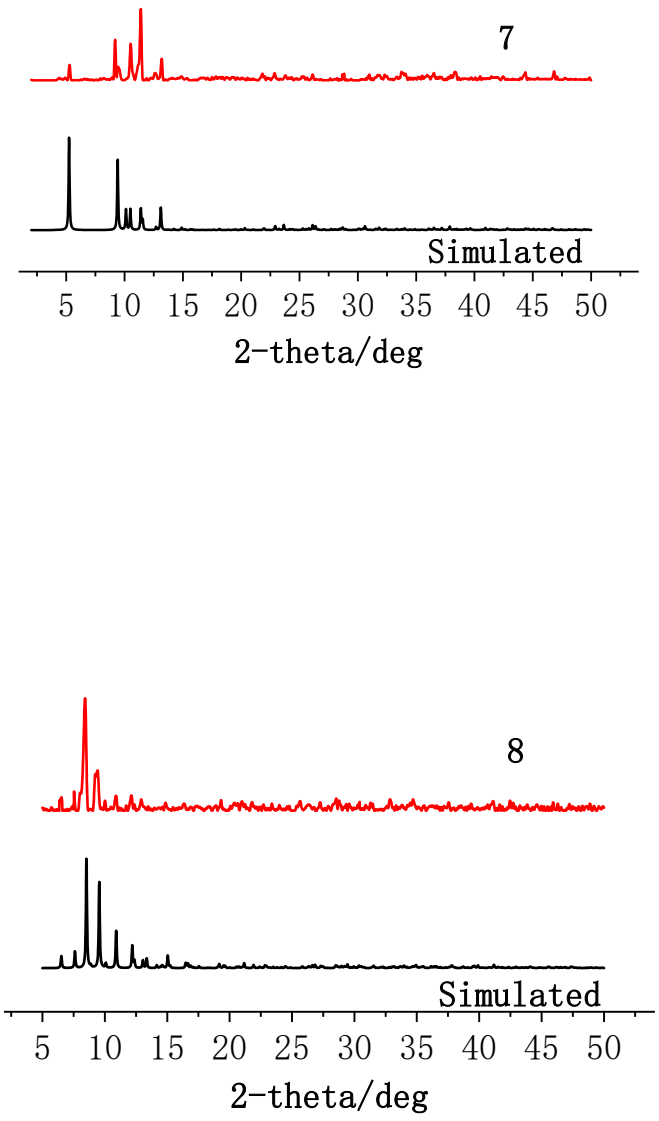


Fig. S12 Simulated and experimental powder XRD patterns of all compounds.