

Supplementary materials

Nickel(II) Coordination Polymers Supported by Bis-pyridyl-bis-amide and Angular Dicarboxylate Ligands: Synthesis, Structures and Iodine Adsorption

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Figure S1. Simulated and experimental PXRD patterns of **1**.

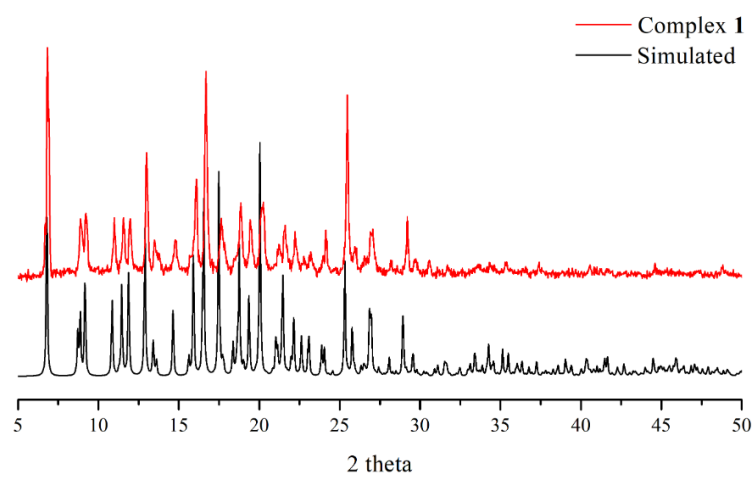


Figure S2. Simulated and experimental PXRD patterns of **2**.

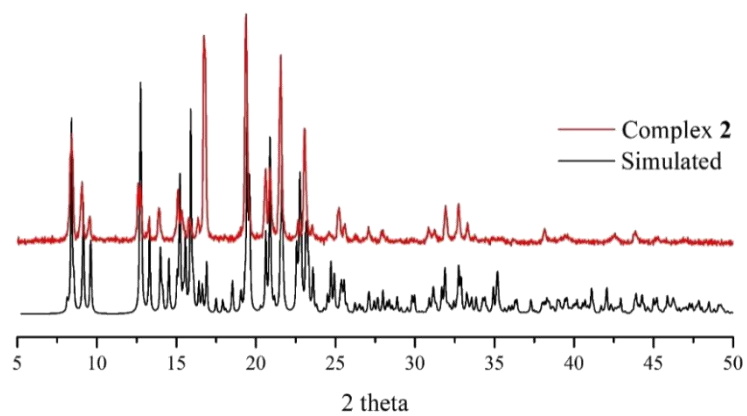


Figure S3. Simulated and experimental PXRD patterns of **3**.

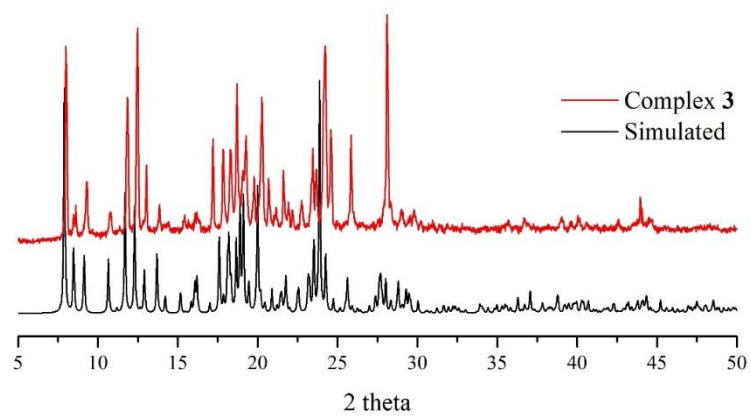


Figure S4. Simulated and experimental PXRD patterns of **4**.

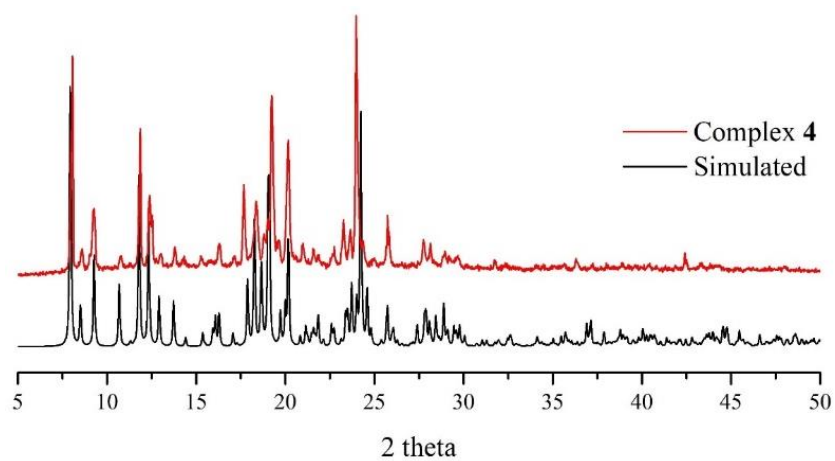


Figure S5. Simulated and experimental PXRD patterns of **5**.

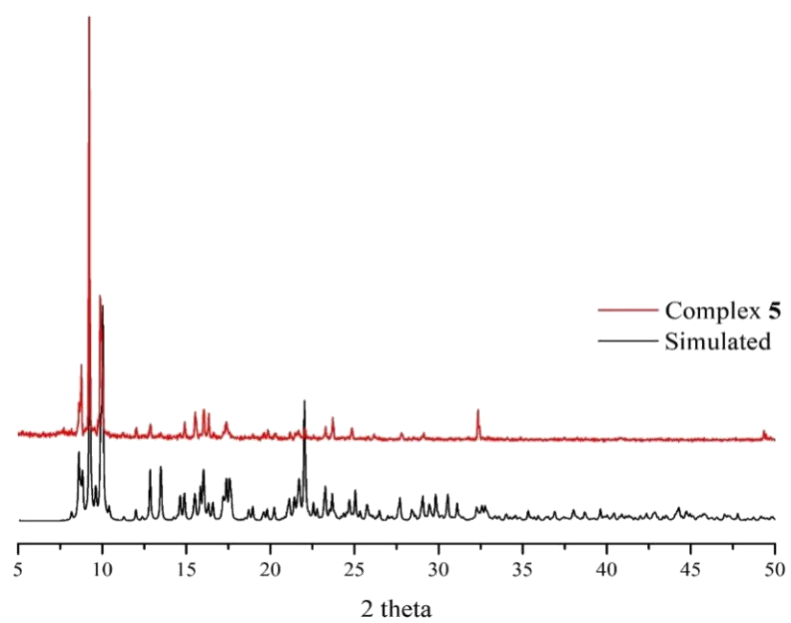


Figure S6. Simulated and experimental PXRD patterns of **6**.

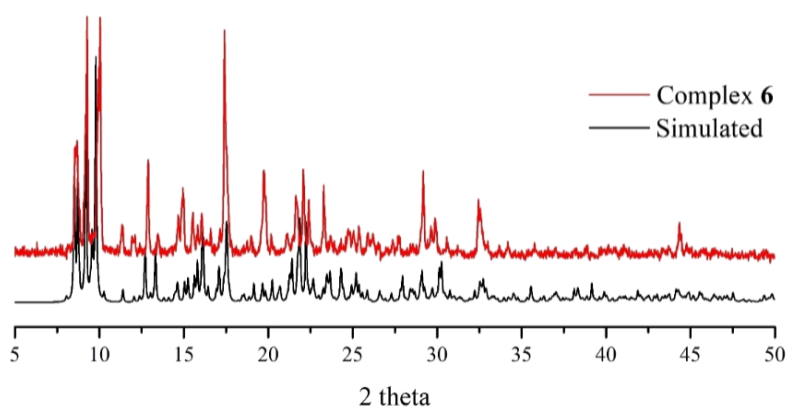


Figure S7. Simulated and experimental PXRD patterns of **7**.

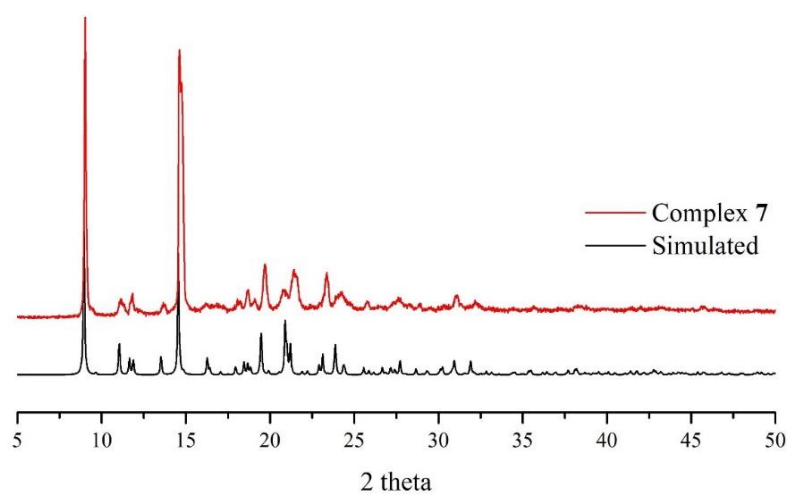


Figure S8. Simulated and experimental PXRD patterns of **8**.

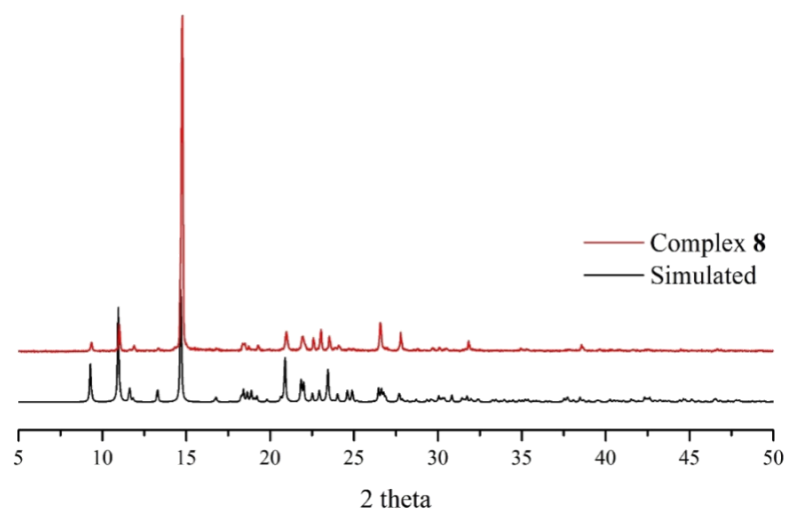


Figure S9. Simulated and experimental PXRD patterns of **9**.

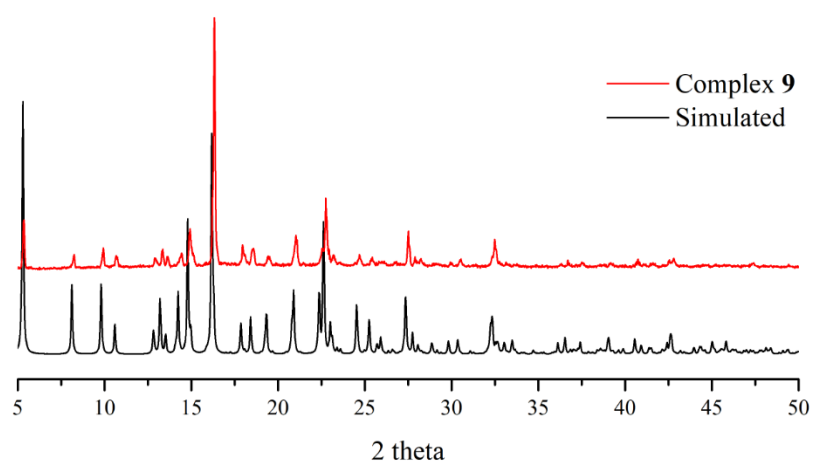


Figure S10. The TGA curve for complex **1**.

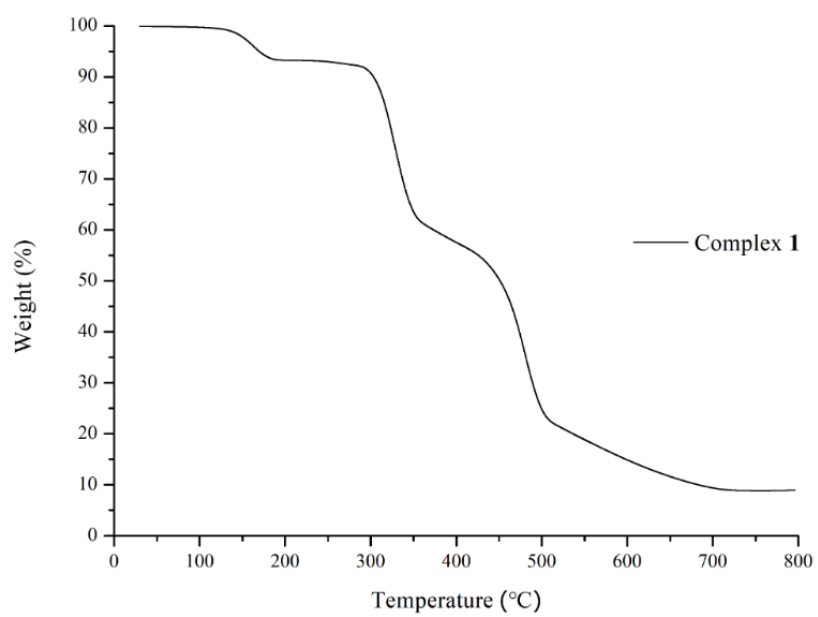


Figure S11. The TGA curve for complex **2**.

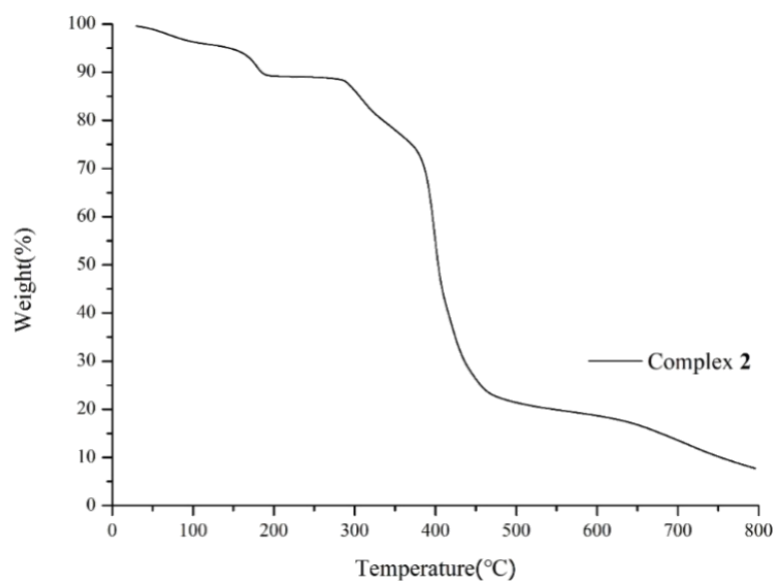


Figure S12. The TGA curve for complex **3**.

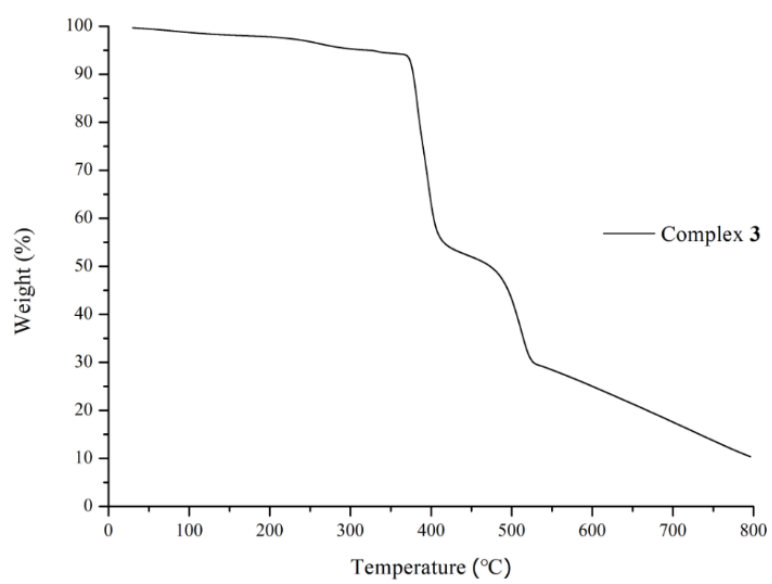


Figure S13. The TGA curve for complex **4**.

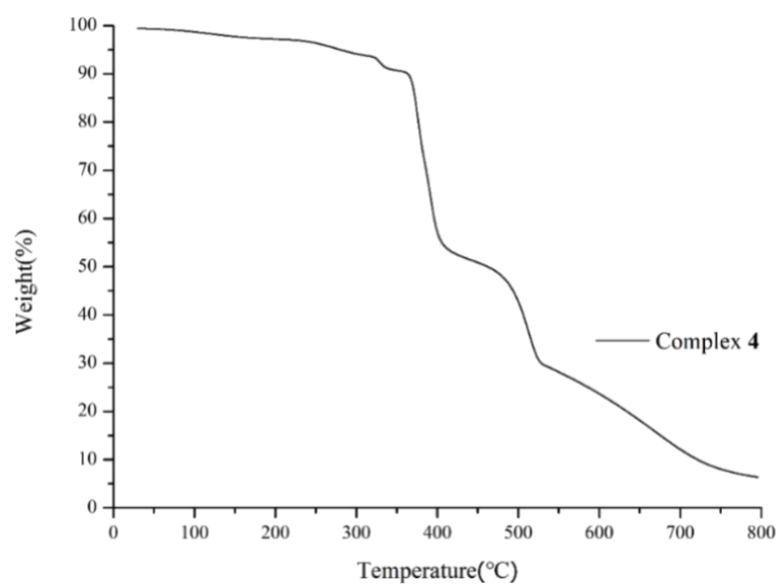


Figure S14. The TGA curve for complex **5**.

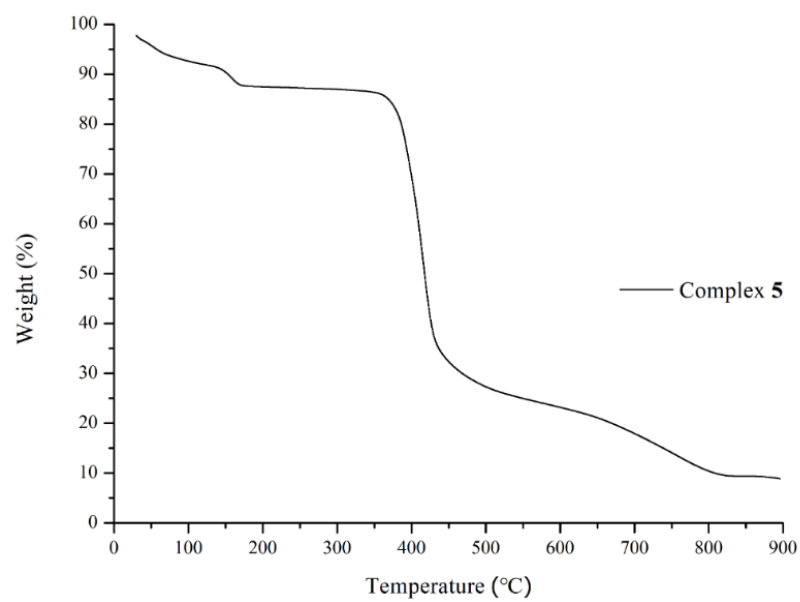


Figure 15. The TGA curve for complex **6**.

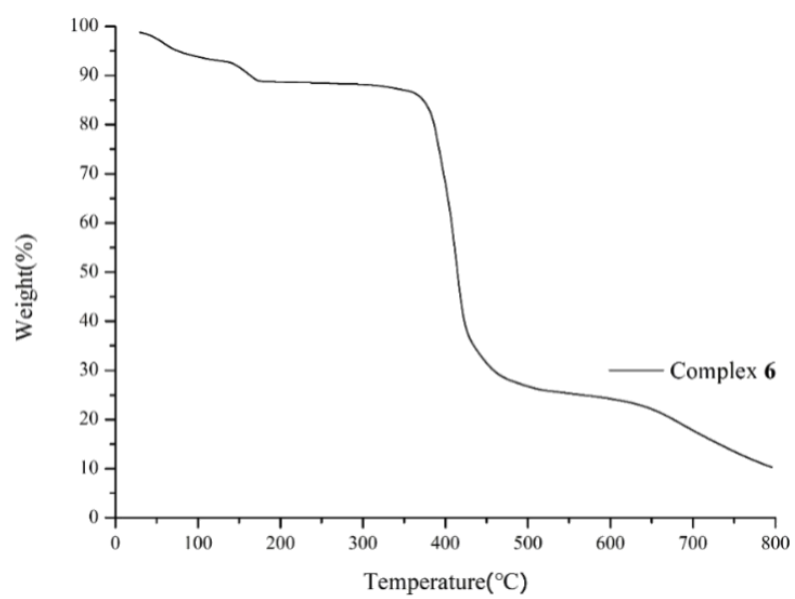


Figure S16. The TGA curve for complex **7**.

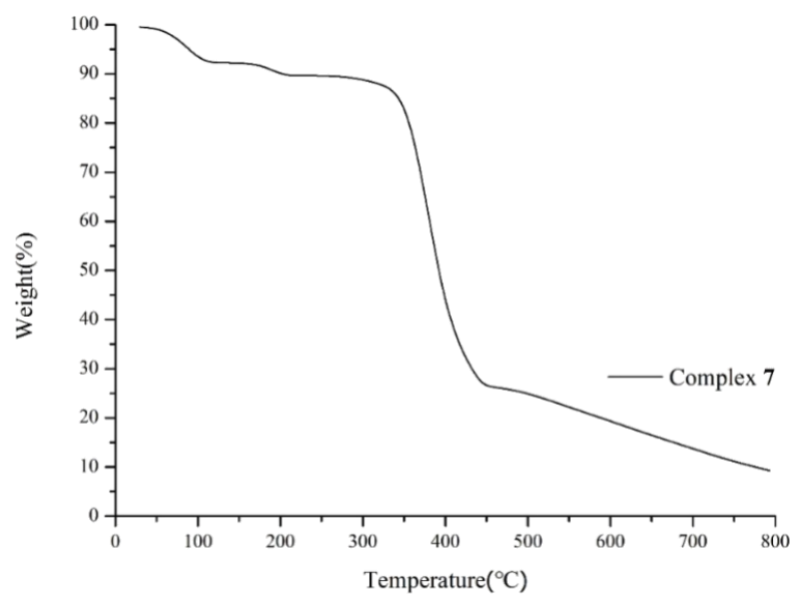


Figure S17. The TGA curve for complex **8**.

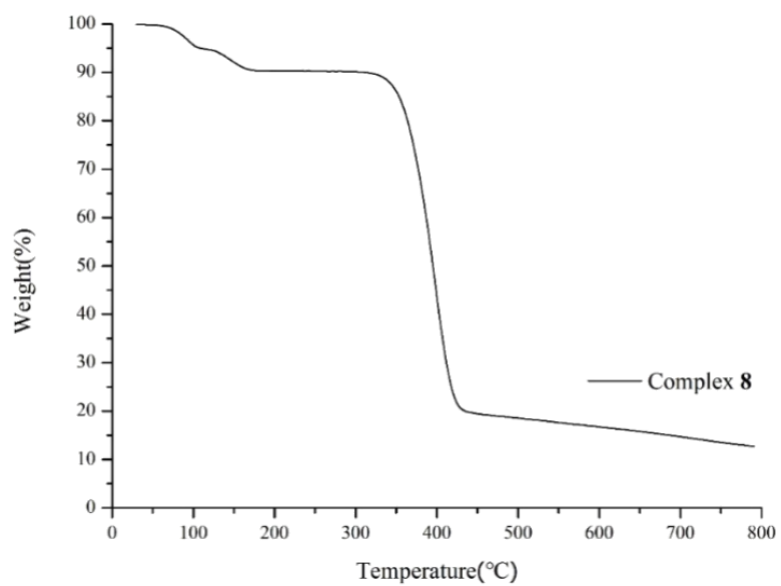


Figure S18. The TGA curve for complex **9**.

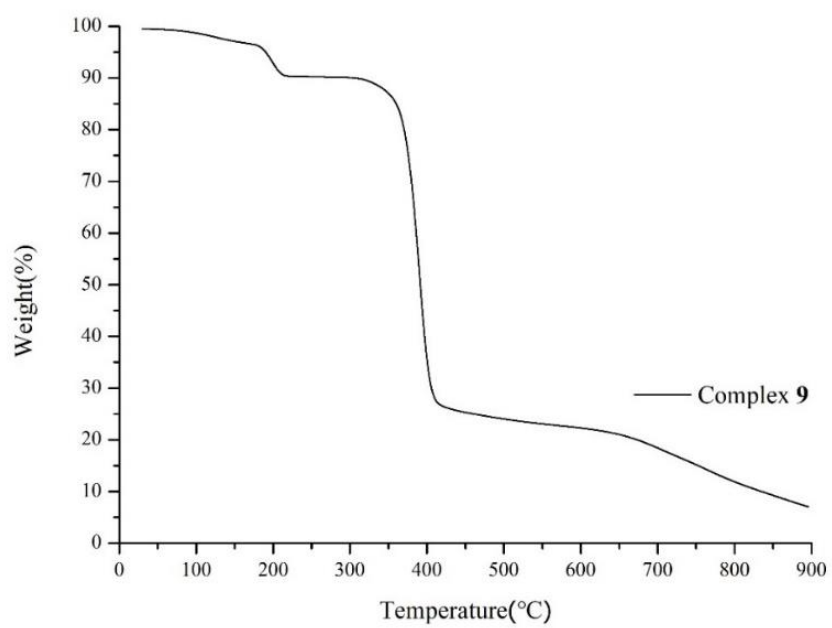


Table S1. Iodine adsorption experiments for complex **7** at 25 °C.

adsorption times (min)	times	initial weight (mg)	final weight (mg)	Iodine content (mg)	Weight change (mg g ⁻¹)	average (mg g ⁻¹)
30	1	35.193	35.201	0.008	0.227	0.208
	2	35.225	35.232	0.007	0.199	
	3	35.227	35.232	0.007	0.199	
60	1	35.192	35.206	0.014	0.398	0.379
	2	35.215	35.228	0.013	0.369	
	3	35.225	35.238	0.013	0.369	
120	1	35.219	35.237	0.018	0.511	0.521
	2	35.216	35.238	0.019	0.540	
	3	35.225	35.243	0.018	0.511	
180	1	35.210	35.290	0.021	0.596	0.587
	2	35.222	35.305	0.020	0.568	
	3	35.228	35.249	0.021	0.596	
360	1	35.227	35.249	0.022	0.625	0.606
	2	35.225	35.246	0.021	0.596	
	3	35.228	35.249	0.021	0.596	

Table S2. Iodine adsorption experiments for complex **7** at 60 °C.

adsorption times (min)	times	initial weight (mg)	final weight (mg)	Iodine content (mg)	Weight change (mg g ⁻¹)	average (mg g ⁻¹)
30	1	35.201	35.215	0.014	0.398	0.379
	2	35.222	35.235	0.013	0.369	
	3	35.221	35.234	0.013	0.369	
60	1	35.180	35.199	0.019	0.540	0.549
	2	35.281	35.301	0.020	0.568	
	3	35.262	35.287	0.019	0.540	
120	1	35.180	35.201	0.021	0.596	0.587
	2	35.281	35.301	0.020	0.568	
	3	35.262	35.289	0.021	0.596	
180	1	35.197	35.219	0.022	0.625	0.606
	2	35.288	35.309	0.021	0.596	
	3	35.268	35.289	0.021	0.596	
360	1	35.240	35.262	0.022	0.625	0.606
	2	35.240	35.261	0.021	0.596	
	3	35.262	35.283	0.021	0.596	

Table S3. Iodine adsorption experiments for complex **8** at 25 °C.

adsorption times (min)	times	initial weight (mg)	final weight (mg)	Iodine content (mg)	Weight change (mg g ⁻¹)	average (mg g ⁻¹)
30	1	38.521	38.522	0.001	0.258	0.258
	2	38.518	38.519	0.001	0.258	
	3	38.512	38.513	0.001	0.258	
60	1	38.517	38.519	0.002	0.519	0.606
	2	38.510	38.512	0.002	0.519	
	3	38.511	38.514	0.003	0.779	
120	1	38.520	38.524	0.004	1.038	0.952
	2	38.515	38.519	0.004	1.038	
	3	38.516	38.519	0.003	0.779	
180	1	38.520	38.525	0.005	1.298	1.298
	2	38.519	38.524	0.005	1.298	
	3	38.518	38.523	0.005	1.298	
360	1	38.520	38.525	0.005	1.298	1.385
	2	38.521	38.527	0.006	1.558	
	3	38.521	38.527	0.006	1.558	

Table S4. Iodine adsorption experiments for complex **8** at 60 °C.

adsorption times (min)	times	initial weight (mg)	final weight (mg)	Iodine content (mg)	Weight change (mg g ⁻¹)	average (mg g ⁻¹)
30	1	38.521	38.523	0.002	0.519	0.606
	2	38.518	38.520	0.002	0.519	
	3	38.512	38.515	0.003	0.779	
60	1	38.517	38.522	0.005	1.298	1.298
	2	38.515	38.520	0.005	1.298	
	3	38.511	38.516	0.005	1.298	
120	1	38.520	38.526	0.006	1.558	1.558
	2	38.515	38.521	0.006	1.558	
	3	38.516	38.522	0.006	1.558	
180	1	38.520	38.526	0.006	1.558	1.558
	2	38.521	38.527	0.006	1.558	
	3	38.522	38.528	0.006	1.558	
360	1	38.520	38.526	0.006	1.558	1.558
	2	38.520	38.526	0.006	1.558	
	3	38.521	38.527	0.006	1.558	

Table S5. Iodine adsorption experiments for complex **9** at 25 °C.

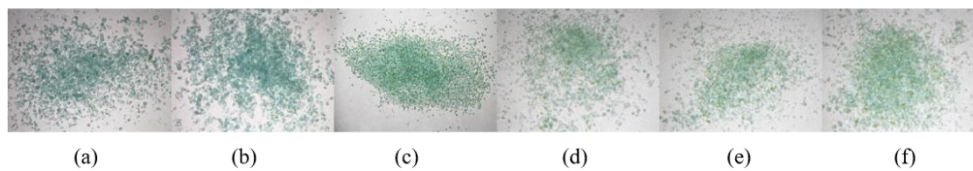
adsorption times (min)	try	initial weight (mg)	final weight (mg)	Iodine content (mg)	Weight change (mg g ⁻¹)	average (mg g ⁻¹)
30	1	29.35	29.98	0.63	21.45	22.73
	2	29.34	30.02	0.68	23.18	
	3	29.30	29.99	0.69	23.55	
60	1	29.36	31.15	1.79	60.97	63.72
	2	29.34	31.33	1.99	67.83	
	3	29.35	31.18	1.83	62.35	
120	1	29.36	32.83	3.47	118.19	118.93
	2	29.37	32.88	3.51	119.51	
	3	29.39	32.89	3.50	119.09	
180	1	29.34	34.08	4.74	161.55	159.75
	2	29.32	34.01	4.68	159.62	
	3	29.35	33.99	4.64	158.09	
360	1	29.36	34.15	4.79	163.15	163.14
	2	29.38	34.18	4.80	163.38	
	3	29.34	34.10	4.78	162.92	

Table S6. Iodine adsorption experiments for complex **9** at 60 °C.

adsorption times (min)	try	initial weight (mg)	finial weight (mg)	Iodine content (mg)	Weight change (mg g ⁻¹)	average (mg g ⁻¹)
30	1	29.36	32.50	3.14	106.94	107.92
	2	29.34	32.47	3.13	106.68	
	3	29.33	32.56	3.23	110.13	
60	1	29.36	33.52	4.16	141.69	140.64
	2	29.37	33.49	4.12	140.28	
	3	29.37	33.58	4.11	139.94	
120	1	29.36	34.15	4.79	163.15	161.30
	2	29.37	34.06	4.69	159.69	
	3	29.37	34.12	4.73	161.05	
180	1	29.39	34.25	4.86	165.36	165.15
	2	29.38	34.26	4.88	166.10	
	3	29.39	34.21	4.82	164.00	
360	1	29.36	34.25	4.89	166.55	166.55
	2	29.38	34.28	4.90	166.78	
	3	29.34	34.20	4.88	166.33	

Figure S19. Color changes of complex **7** heated at 25 and 60 °C: (a) without heating and heated for (b) 30, (c) 60, (d) 120, (e) 180 and (f) 360 minutes.

25 °C



60 °C

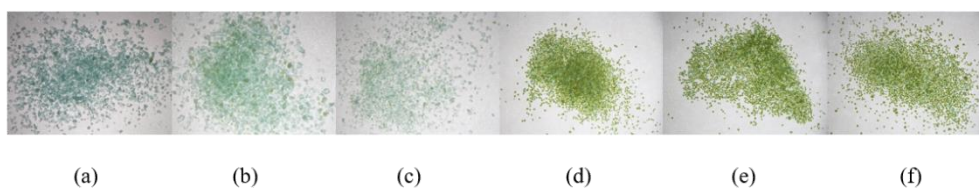
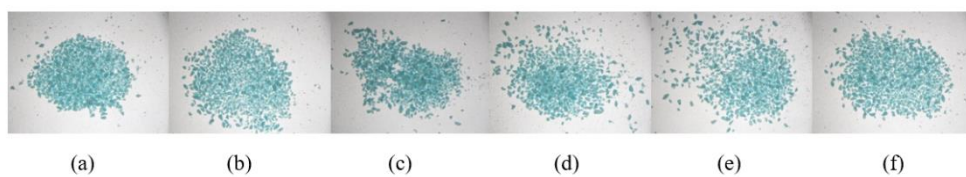


Figure S20. Color changes of complex **8** heated at 25 and 60 °C: (a) without heating and heated for (b) 30, (c) 60, (d) 120, (e) 180 and (f) 360 minutes.

25 °C



60 °C

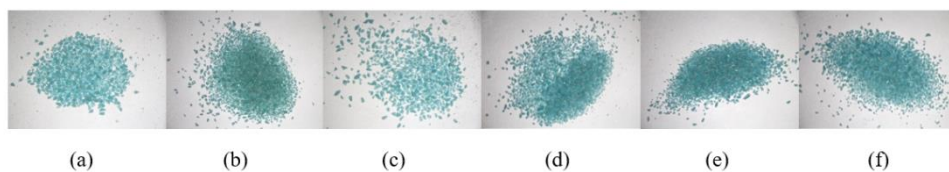


Figure S21. Color changes of complex **9** heated at 25 and 60 °C: (a) without heating and heated for (b) 30, (c) 60, (d) 120, (e) 180 and (f) 360 minutes.

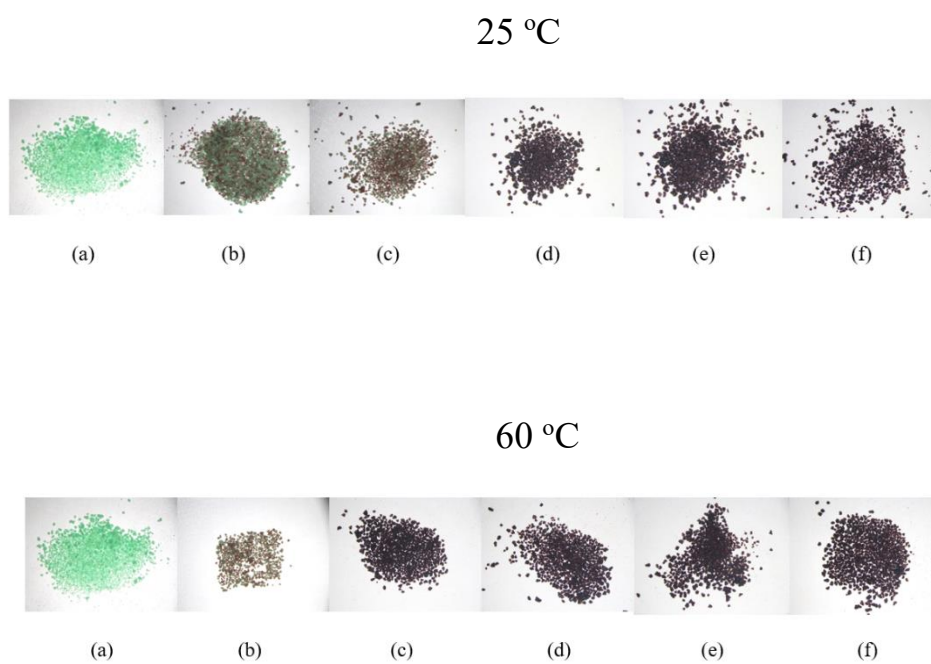
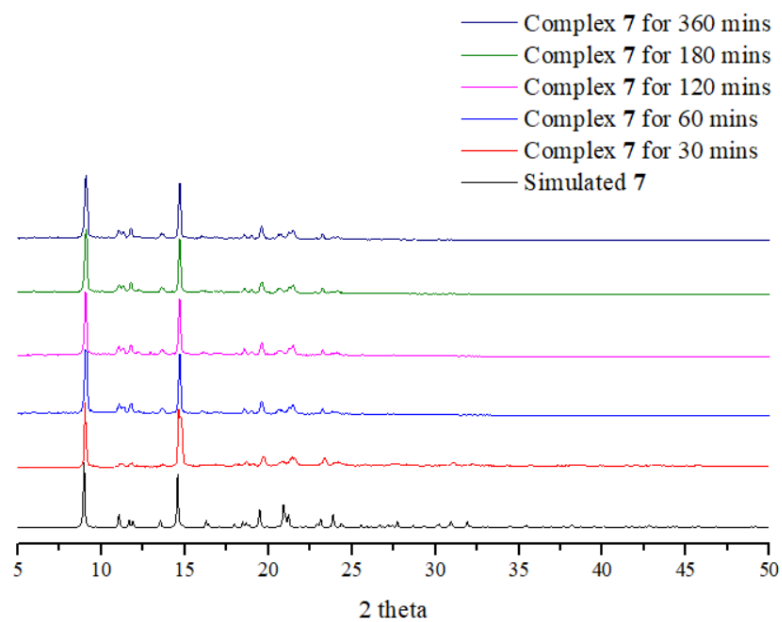
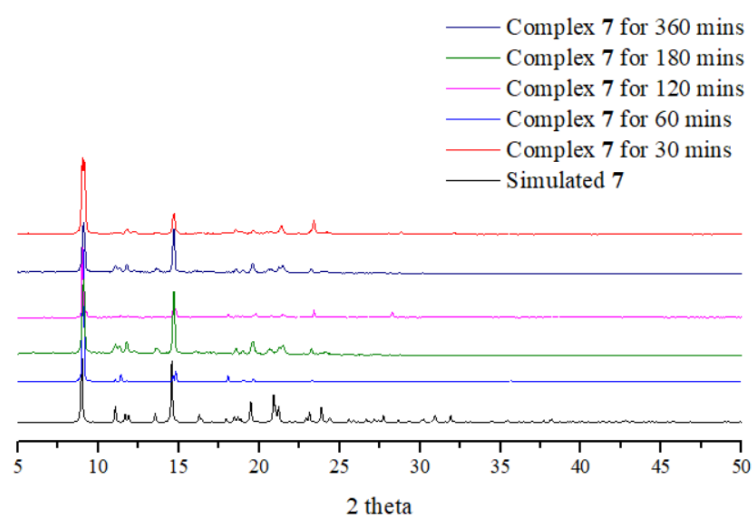


Figure S22. PXRD patterns of complex **7** after heated at (a) 25 and (b) 60 °C for various intervals.

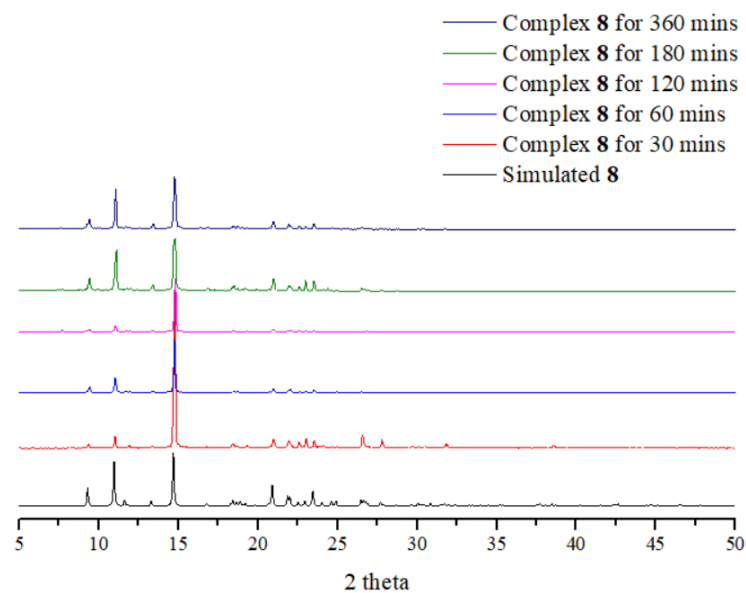


(a)

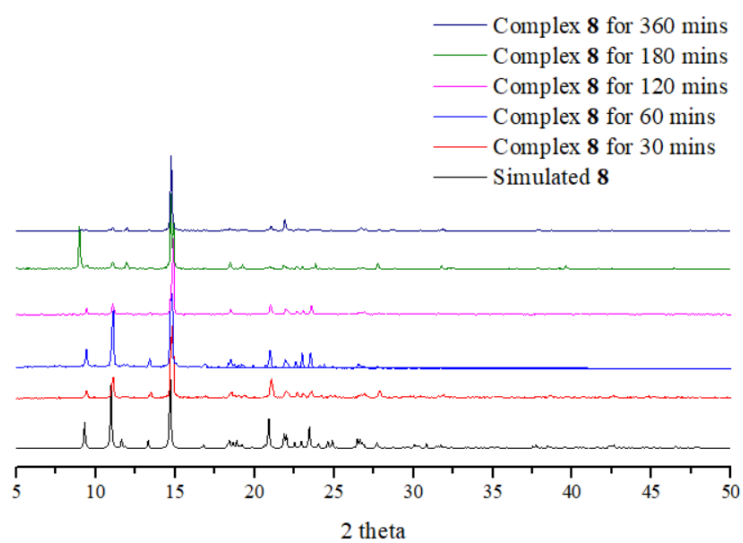


(b)

Figure S23. PXRD patterns of complex **8** after heated at (a) 25 and (b) 60 °C for various intervals.

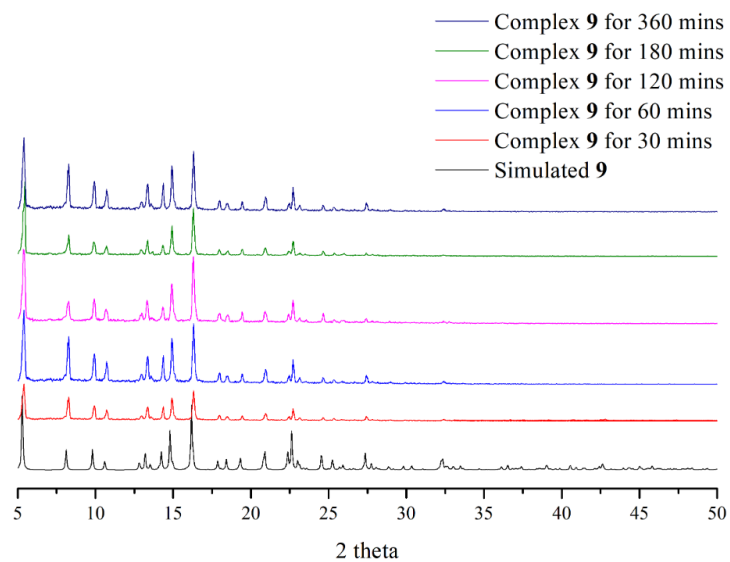


(a)

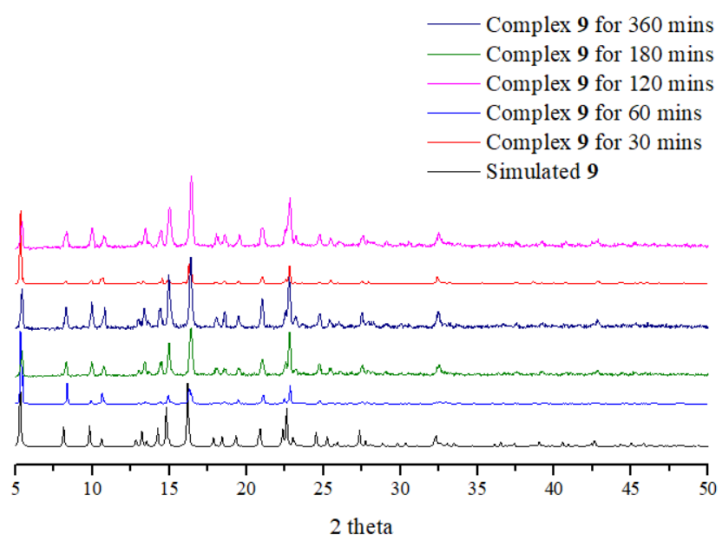


(b)

Figure S24. PXRD patterns of complex **9** after heated at (a) 25 and (b) 60 °C for various intervals.

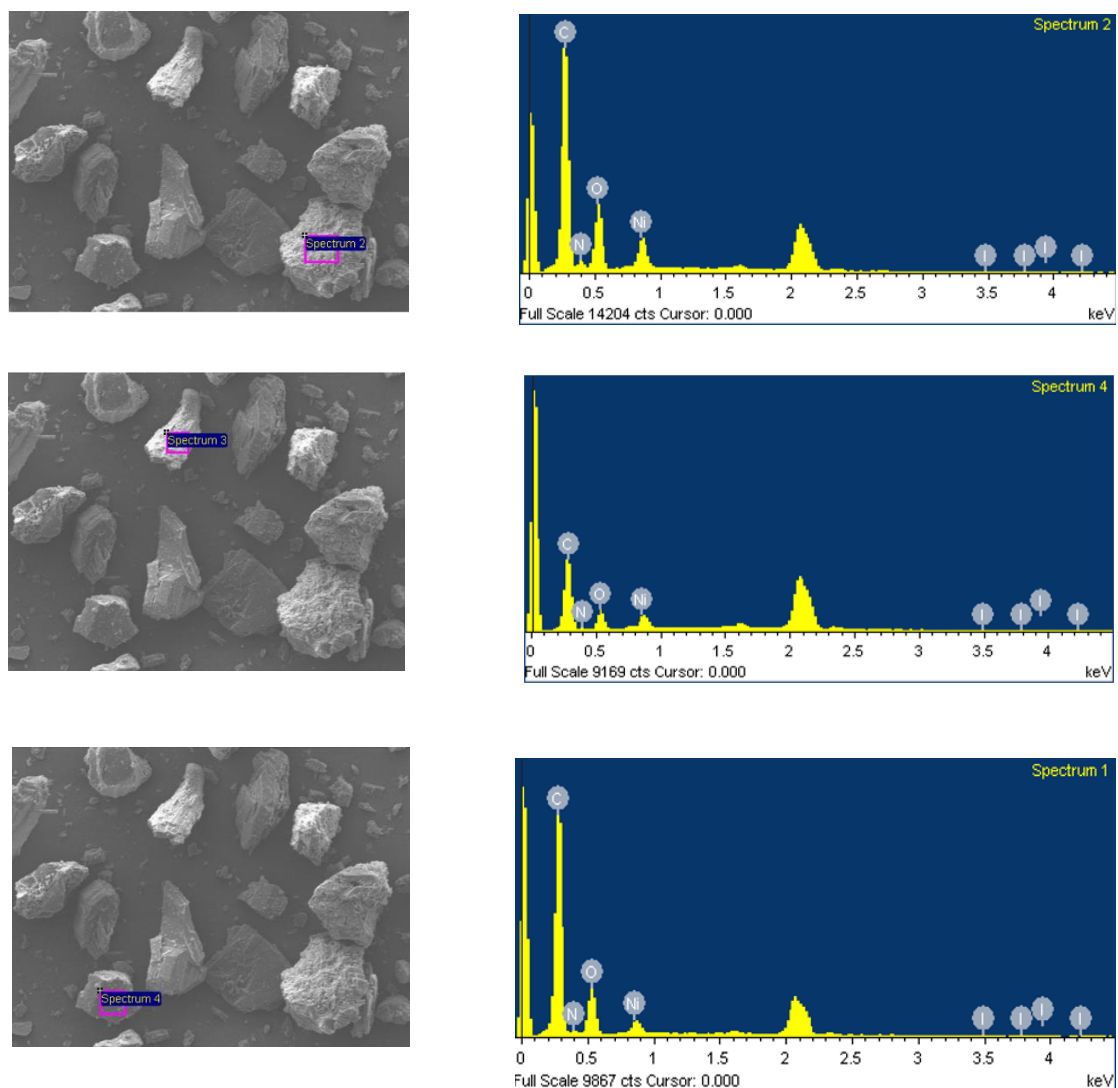


(a)



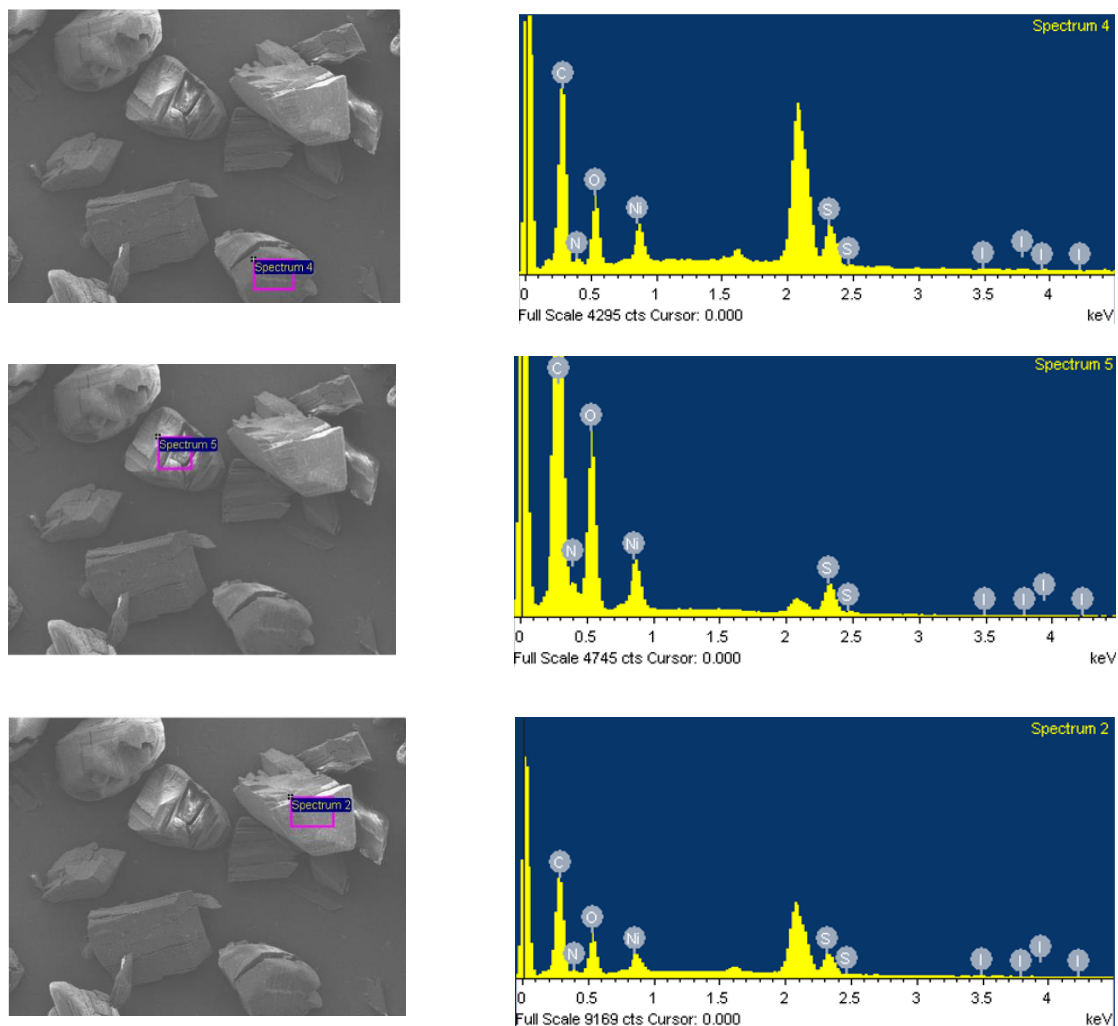
(b)

Figure S25. EDX data for complex **7** at three different regions.



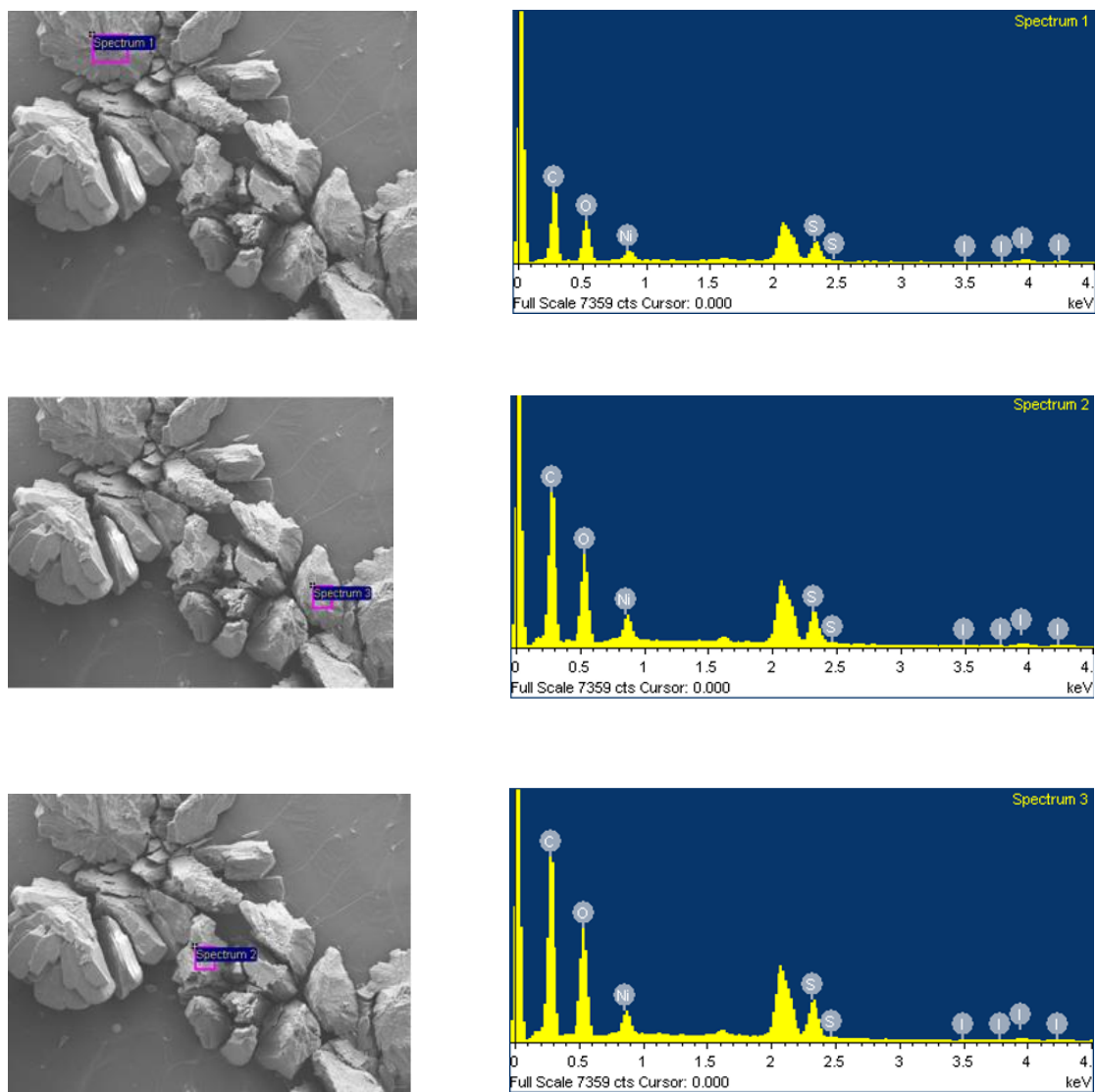
	1st		2nd		3rd	
Element	Weight %	Atomic %	Weight %	Atomic %	Weight %	Atomic %
C K	54.07	64.91	53.37	65.89	63.35	72.98
N K	10.34	10.64	8.40	8.89	4.57	4.50
O K	23.50	21.57	23.23	21.52	23.88	20.61
Ni L	11.62	2.85	14.32	3.62	8.08	1.90
I L	0.46	0.03	0.68	0.08	0.12	0.01
Totals	100.00		100.00		100.00	

Figure S26. EDX data for complex **8** at three different regions.



	1st		2nd		3rd	
Element	Weight %	Atomic %	Weight %	Atomic %	Weight %	Atomic %
C K	61.92	72.47	52.46	66.46	52.73	67.47
N K	3.87	3.79	4.86	5.28	4.56	5.01
O K	22.87	20.09	22.48	21.20	20.77	19.95
S K	4.21	1.85	7.65	3.63	8.38	4.02
Ni L	7.12	1.70	12.54	3.25	13.54	3.27
I L	0.01	0.10	0.01	0.18	0.02	0.28
Totals	100.00		100.00		100.00	

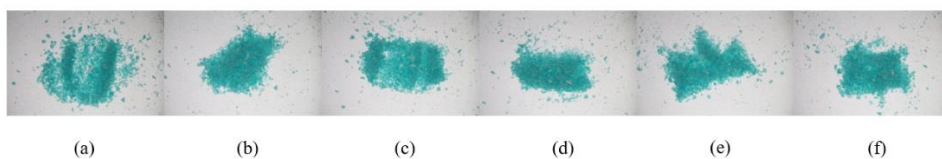
Figure S27. EDX data for complex **9** at three different regions.



	1st		2nd		3rd	
Element	Weight %	Atomic %	Weight %	Atomic %	Weight %	Atomic %
C K	47.33	66.52	49.98	66.61	51.03	66.20
O K	23.33	24.62	25.87	25.88	27.79	27.06
S K	9.21	4.85	7.59	3.79	7.74	3.76
Ni L	8.63	2.48	11.10	3.03	9.30	2.47
I L	11.50	1.53	5.46	0.69	4.14	0.51
Totals	100.00		100.00		100.00	

Figure S28. Color changes of complex **1** heated at 25 and 60 °C: (a) without heating and heated for (b) 30, (c) 60, (d) 120, (e) 180 and (f) 360 minutes.

25 °C



60 °C.

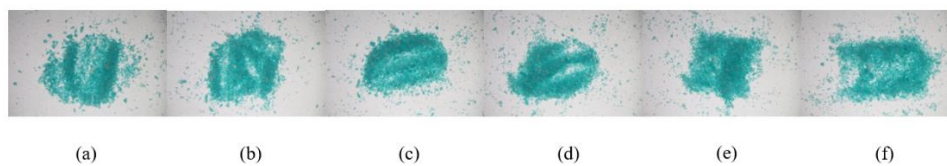
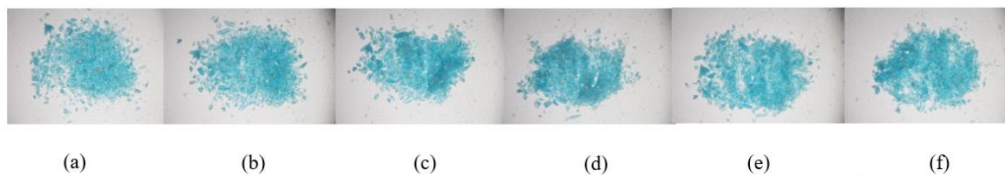


Figure S29. Color changes of complex **2** heated at 25 and 60 °C: (a) without heating and heated for (b) 30, (c) 60, (d) 120, (e) 180 and (f) 360 minutes.

25 °C



60 °C.

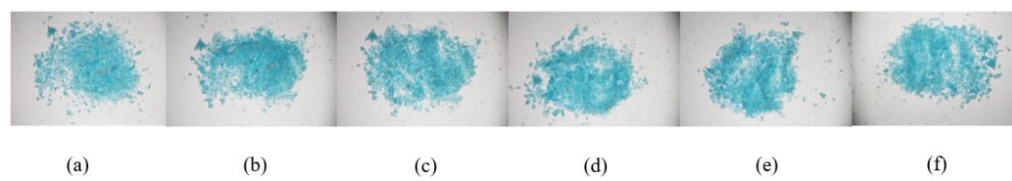


Figure S30. Color changes of complex **3** heated at 25 and 60 °C: (a) without heating and heated for (b) 30, (c) 60, (d) 120, (e) 180 and (f) 360 minutes.

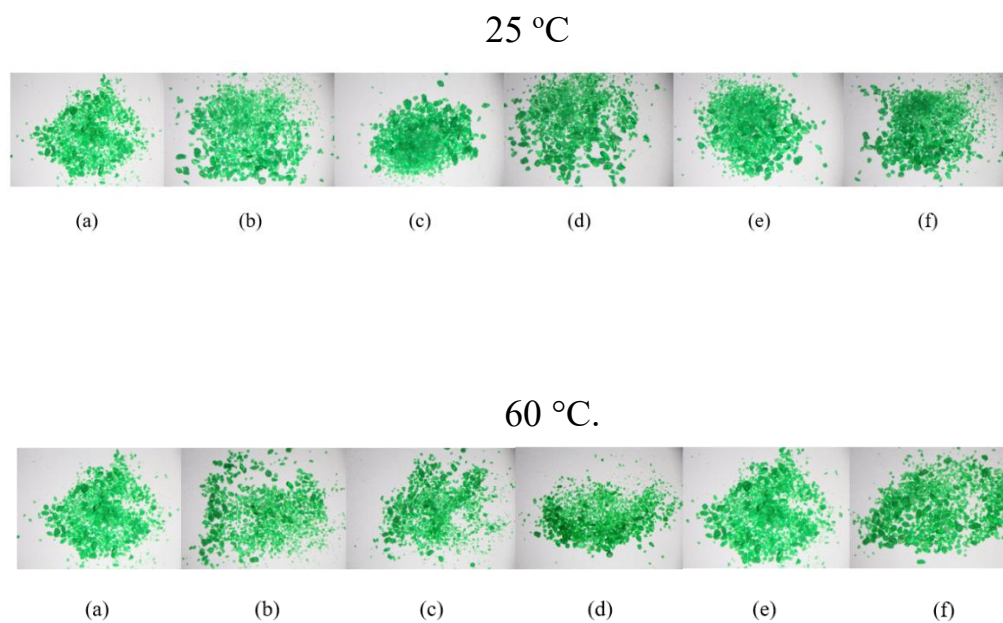
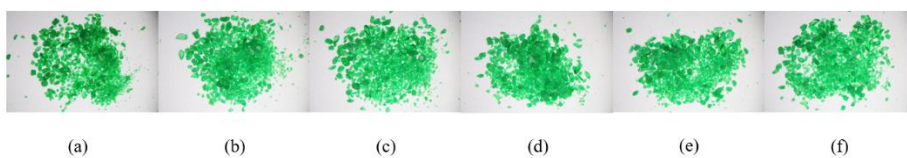


Figure S31. Color changes of complex **4** heated at 25 and 60 °C: (a) without heating and heated for (b) 30, (c) 60, (d) 120, (e) 180 and (f) 360 minutes.

25 °C



60 °C.

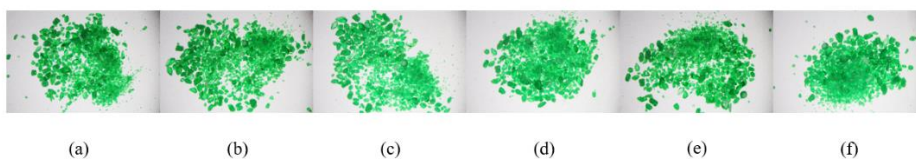
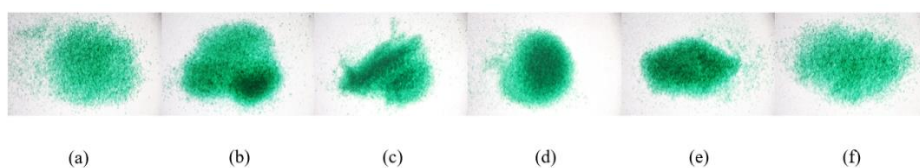


Figure S32. Color changes of complex **5** heated at 25 and 60 °C: (a) without heating and heated for (b) 30, (c) 60, (d) 120, (e) 180 and (f) 360 minutes.

25 °C



60 °C.

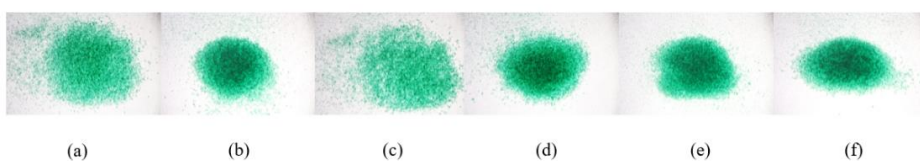
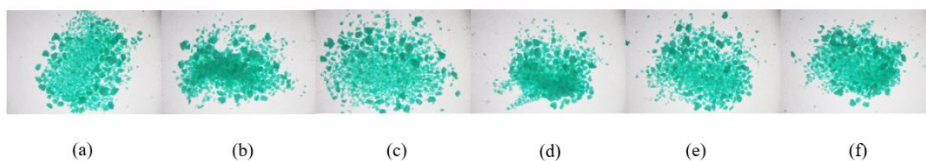


Figure S33. Color changes of complex **6** heated at 25 and 60 °C: (a) without heating and heated for (b) 30, (c) 60, (d) 120, (e) 180 and (f) 360 minutes.

25 °C



60 °C.

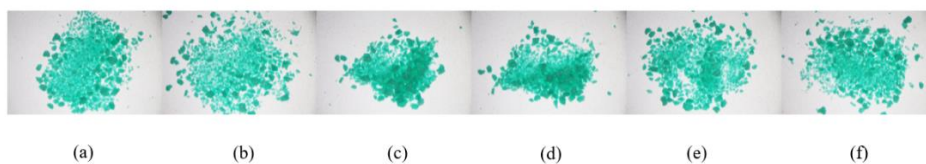
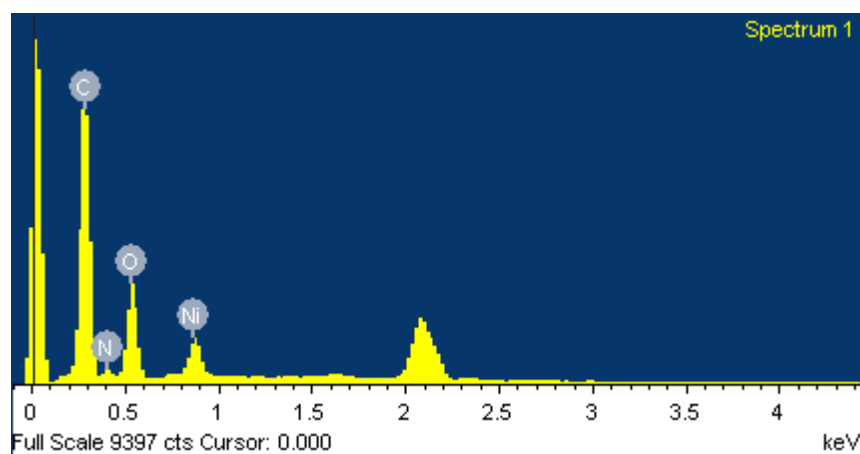
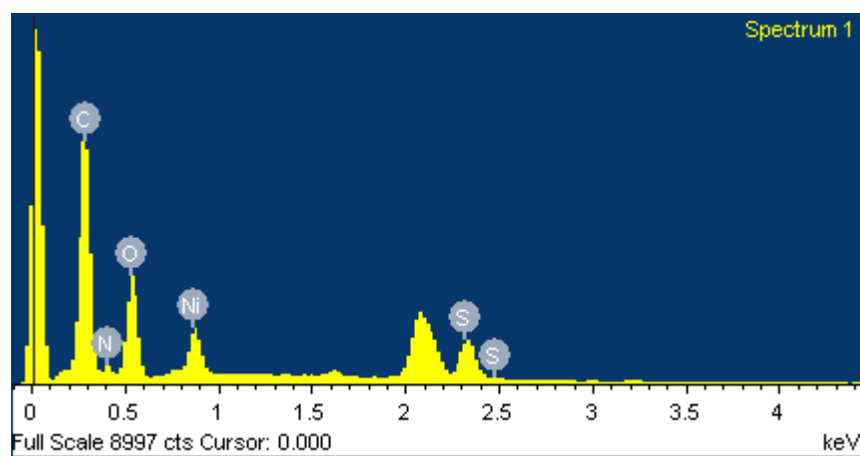


Figure S34. EDX data for iodine-adsorbed complex **1**.



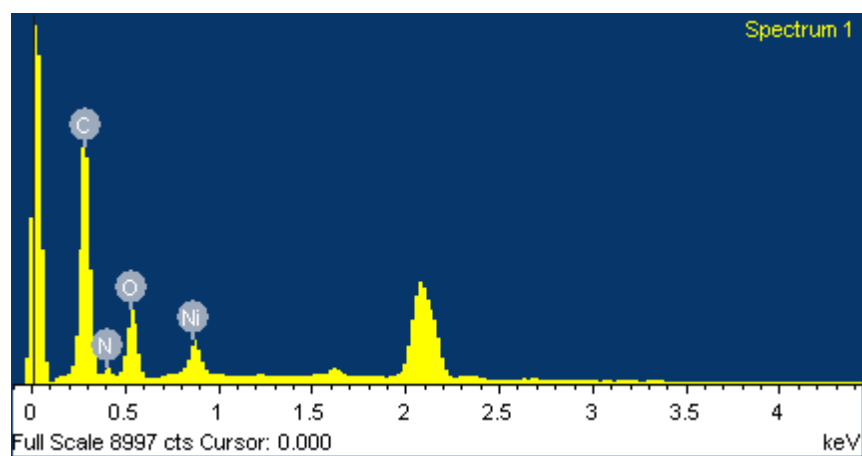
Element	Weight%	Atomic%
C K	52.41	64.68
N K	7.19	7.60
O K	25.99	24.08
Ni L	14.41	3.64
Totals	100.00	

Figure S35. EDX data for iodine-adsorbed complex **2**.



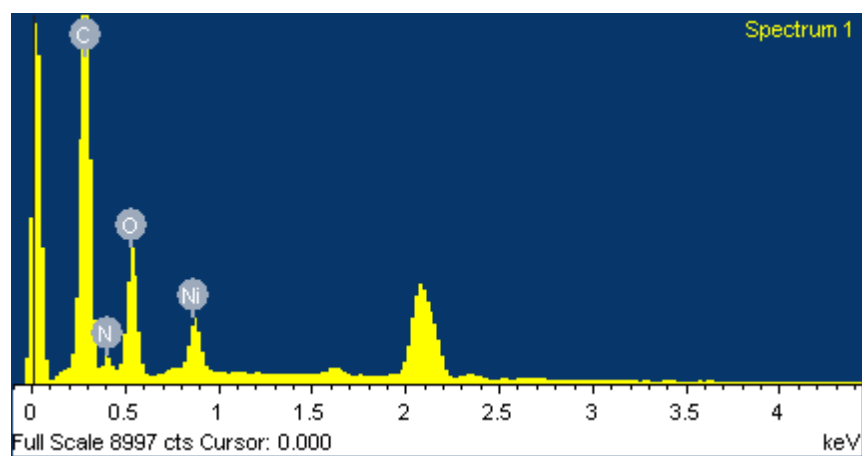
Element	Weight%	Atomic%
C K	49.88	63.50
N K	7.35	8.03
O K	23.04	22.02
S K	6.09	2.90
Ni L	13.64	3.55
Totals	100.00	

Figure S36. EDX data for iodine-adsorbed complex **3**.



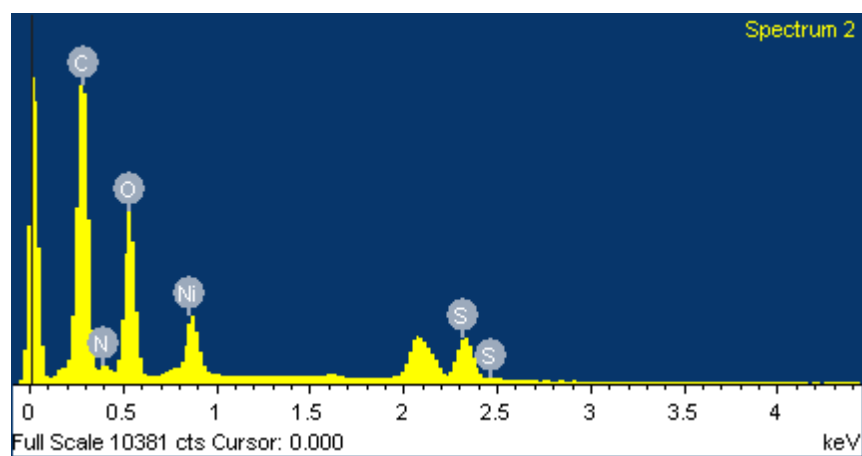
Element	Weight%	Atomic%
C K	52.28	64.75
N K	9.29	9.86
O K	23.14	21.51
Ni L	15.30	3.88
Totals	100.00	

Figure S37. EDX data for iodine-adsorbed complex **4**.



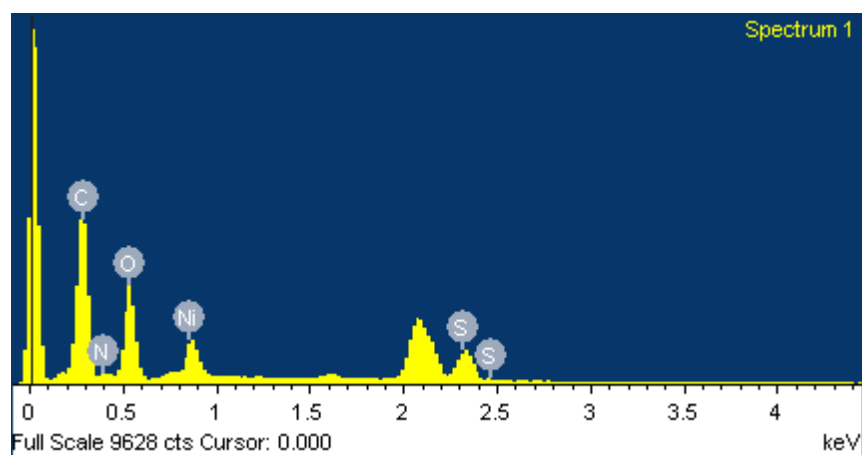
Element	Weight%	Atomic%
C K	52.92	64.62
N K	9.35	9.79
O K	24.25	22.23
Ni L	13.48	3.37
Totals	100.00	

Figure S38. EDX data for iodine-adsorbed complex **5**.



Element	Weight%	Atomic%
C K	47.72	61.13
N K	5.61	6.16
O K	27.67	26.62
S K	5.08	2.44
Ni L	13.92	3.65
Totals	100.00	

Figure S39. EDX data for iodine-adsorbed complex **6**.



Element	Weight%	Atomic%
C K	48.32	62.53
N K	4.28	4.74
O K	26.50	25.75
S K	6.58	3.19
Ni L	14.33	3.79
Totals	100.00	

Figure S40. The N₂ adsorption for complex **7** at 77 K.

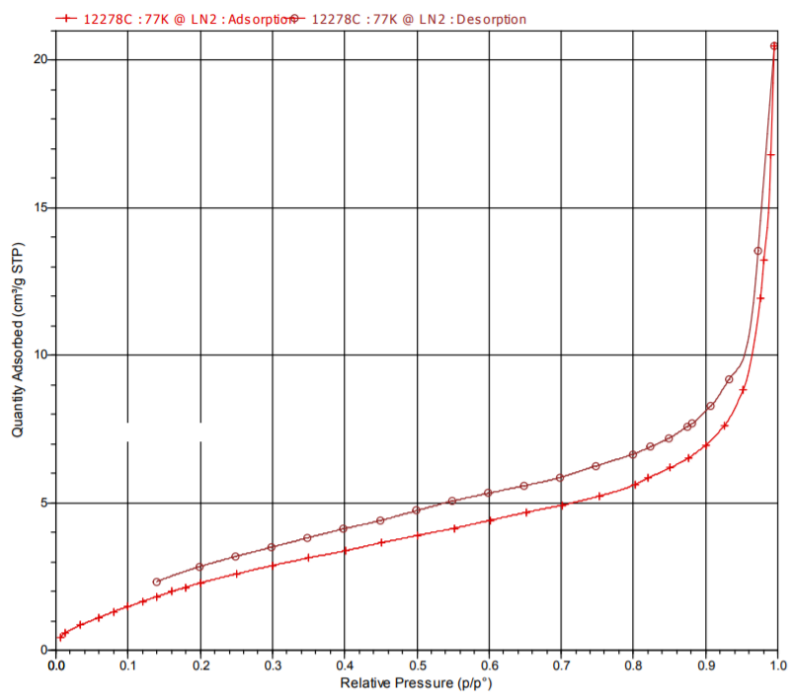


Figure S41. The N₂ adsorption for complex **8** at 77 K.

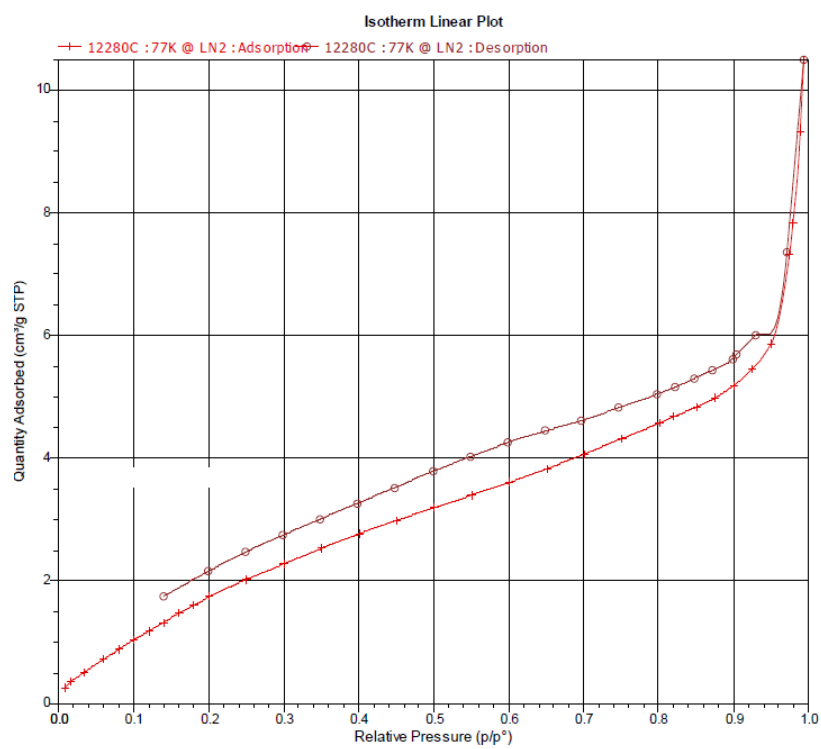
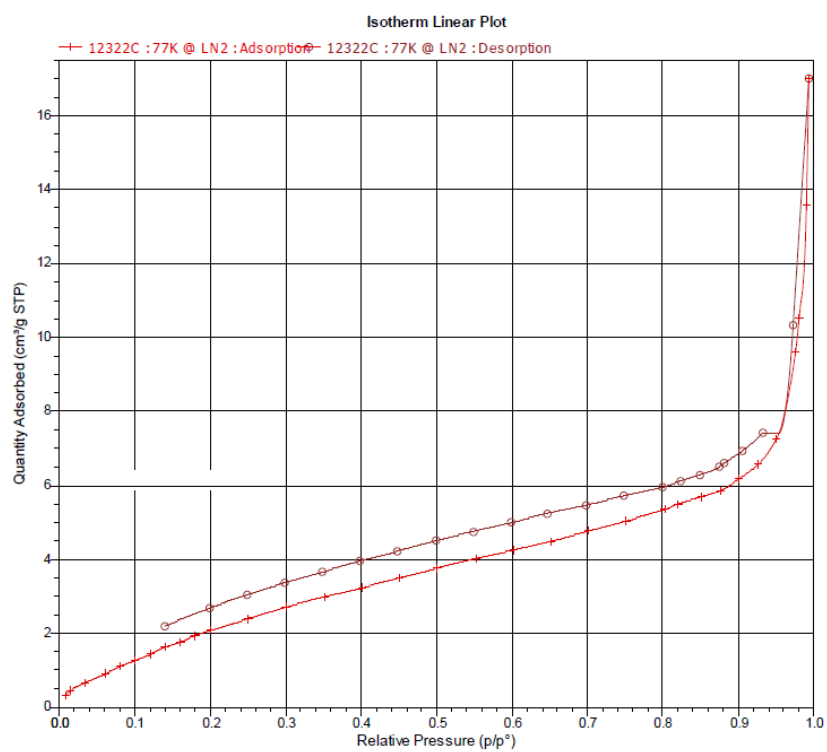
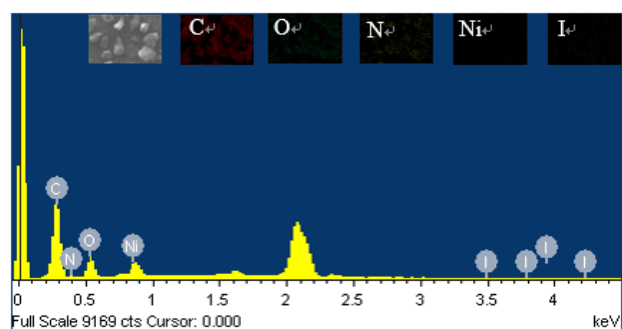
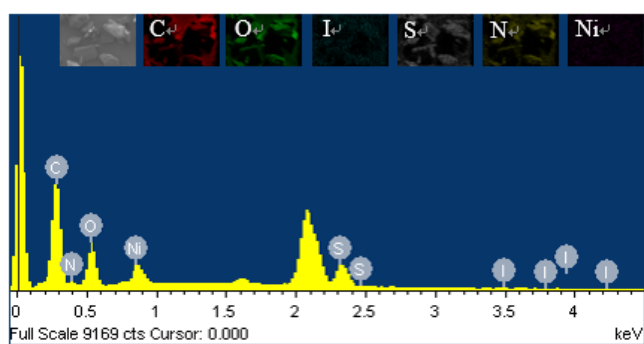


Figure S42. The N₂ adsorption for complex **9** at 77 K.





(a)



(b)

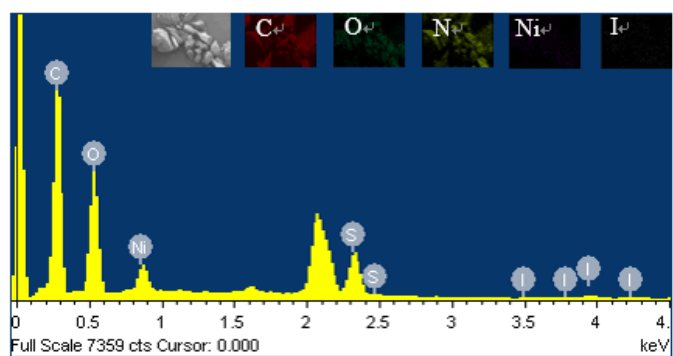


Table S7. Solvent accessible volumes of complexes **1** – **9**.

	Solvent assemble volume %
1	3.2
2	12.6
3	10.4
4	10.2
5	15.2
6	15.6
7	6.9
8	9.3
9	13.7