

Crystal Engineering with Isosteric Triether and Triamine Linked Aromatic Tri-Carboxylic Acids: Iso-structurality and Synthons interplay in their Co-crystals and Salts with Bis(pyridyl) Derivatives

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Contents

- 1) IR spectra
- 2) XRPD patterns
- 3) pKa of triacids and bipyridyl bases and ΔpK_a values of the complexes Table S1
- 4) Comparison of C-O-C and Interplanar Angles of H₃tcpb and its Complexes Table S2
- 5) C-N-C and Interplanar Angles of H₃btatb in its Complexes Table S3
- 6) ORTEP diagrams of all the structures

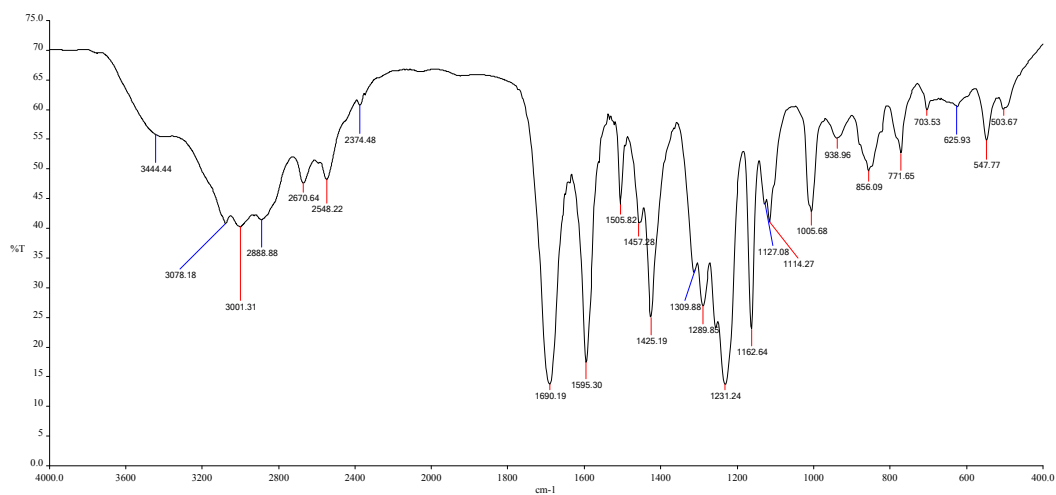


Figure S1: IR spectra of 1

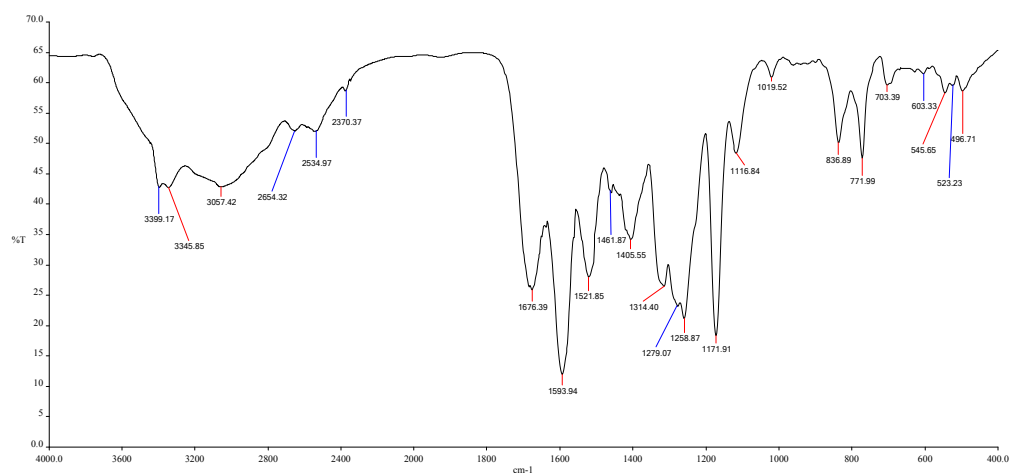


Figure S2: IR spectra of 2

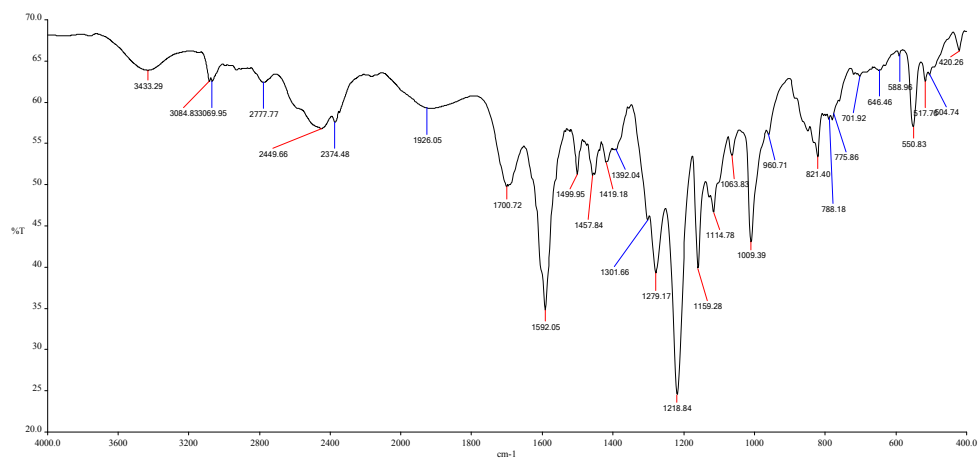


Figure S3: IR spectra of 3

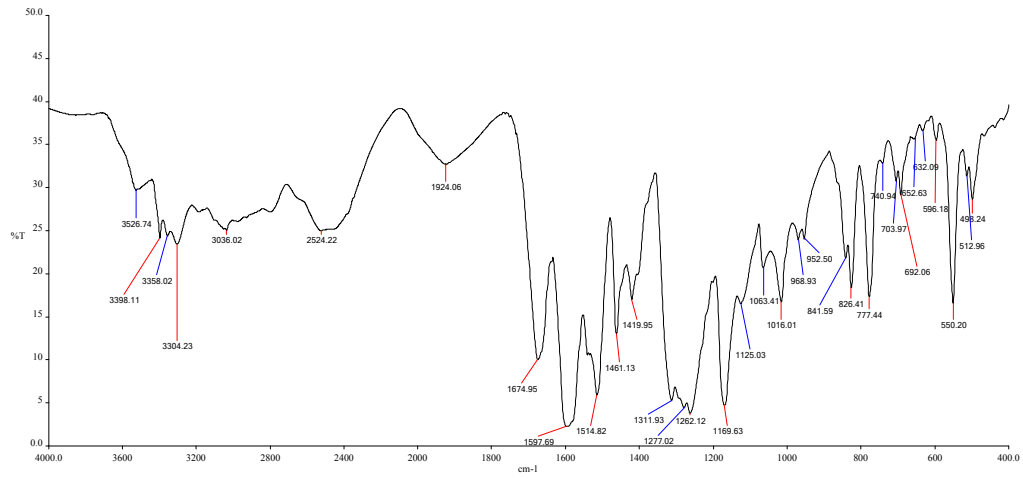


Figure S4: IR spectra of 4

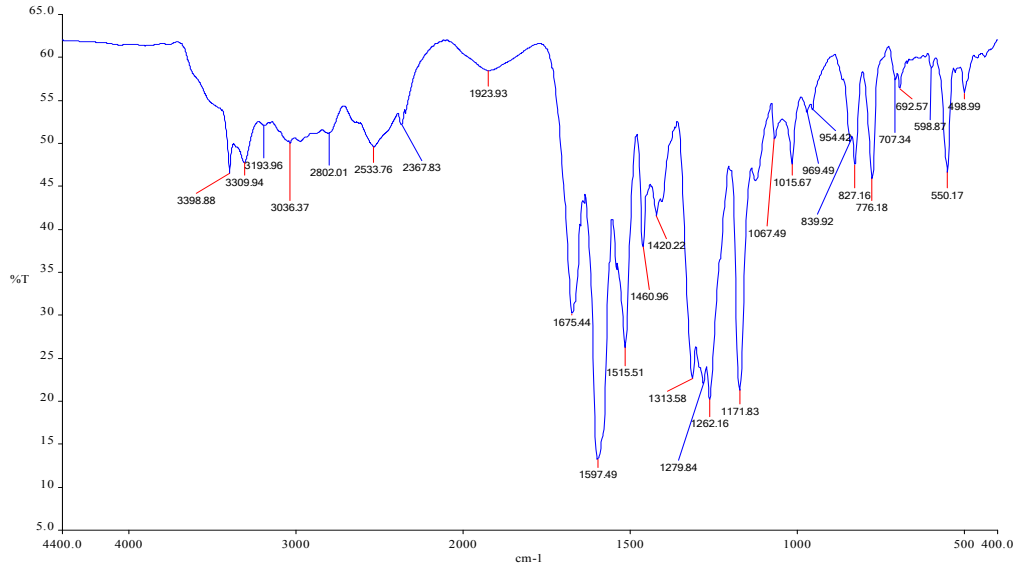


Figure S5: IR spectra of 5

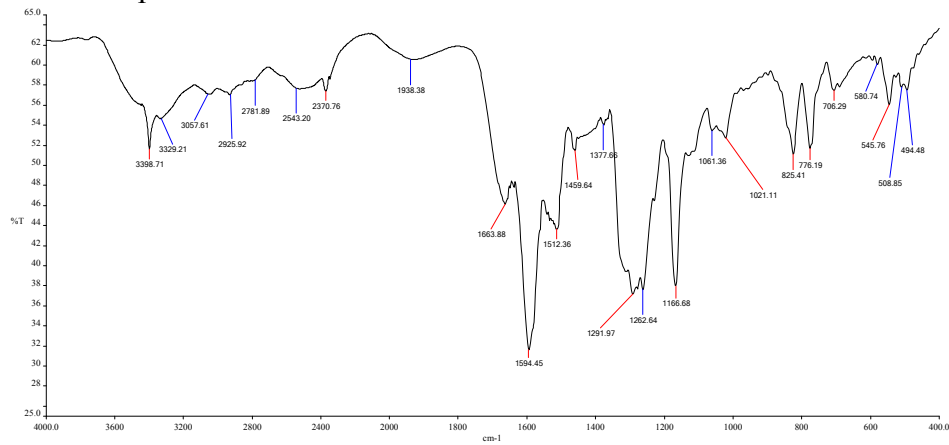


Figure S6: IR spectra of 6

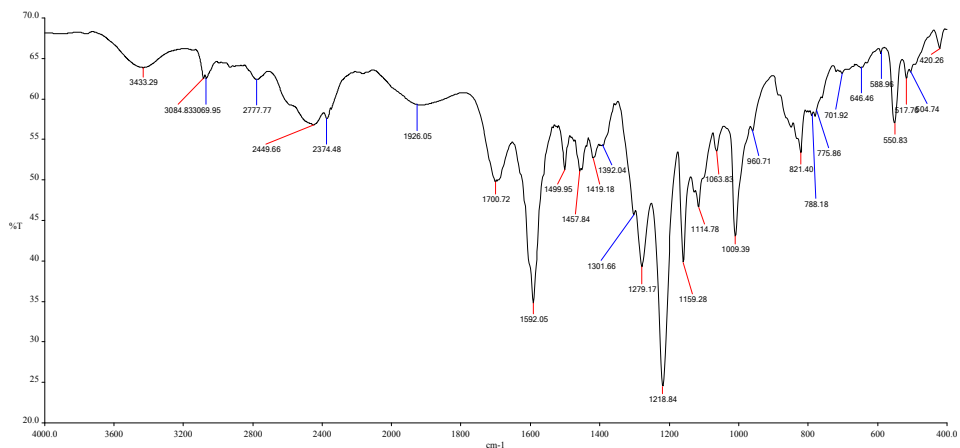


Figure S7: IR spectra of 7

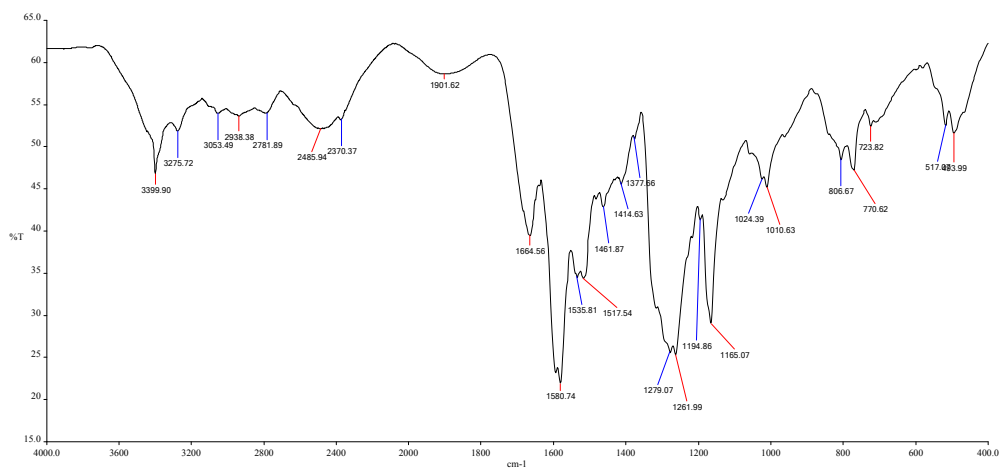


Figure S8: IR spectra of 8

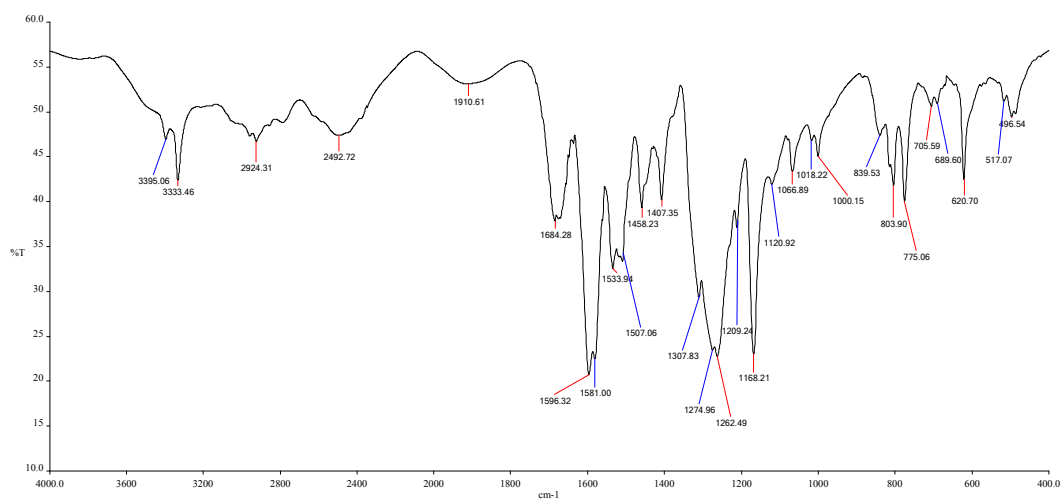


Figure S9: IR spectra of 9

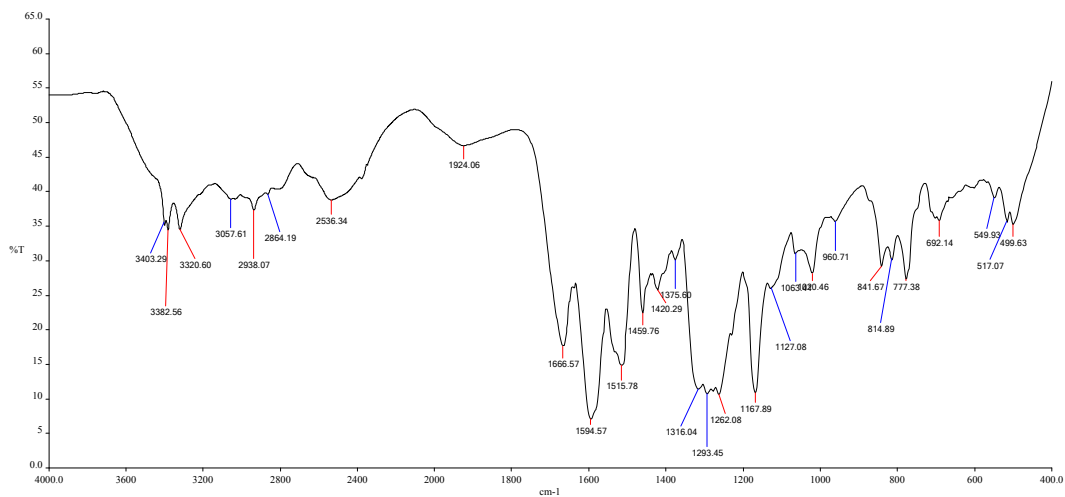


Figure S10: IR spectra of **10**

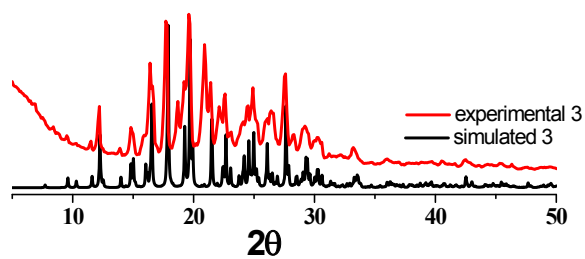


Figure S11: XRPD spectra of **3**

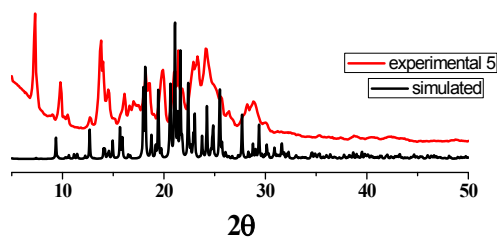


Figure S12: XRPD spectra of **5**

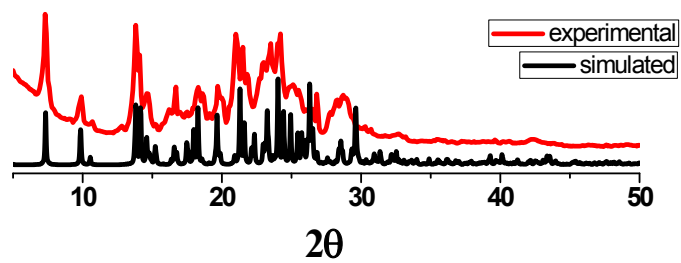


Figure S13: XRPD spectra of 6

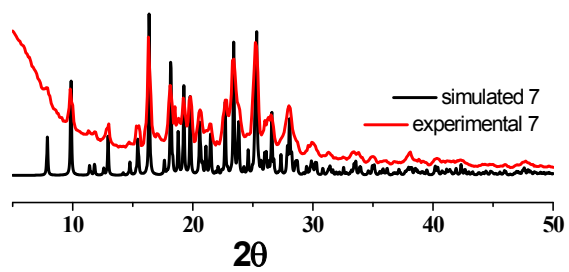


Figure S14: XRPD spectra of 7

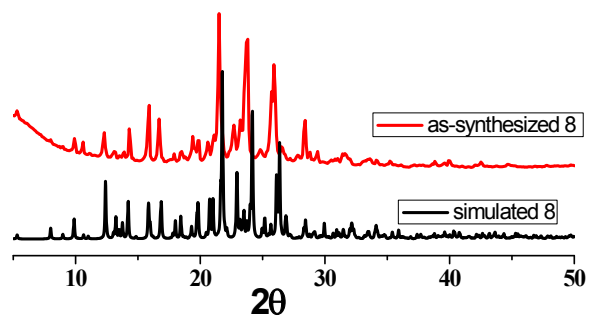


Figure S15: XRPD spectra of 8

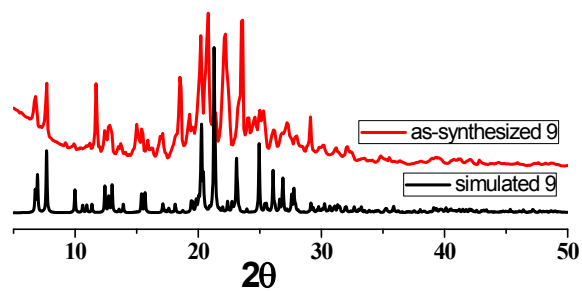


Figure S16: XRPD spectra of 9

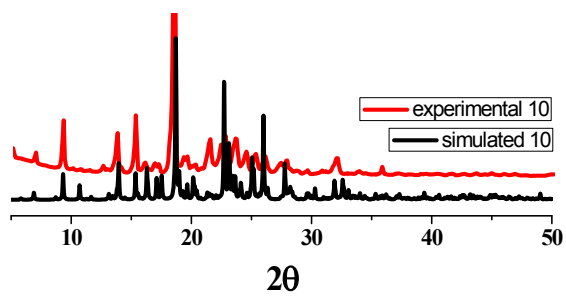


Figure S17: XRPD spectra of 10

Table S1: The pK_a of H₃tcpb, H₃btatb and N-heterocyclic bases and ΔpK_a values of the complexes

Organic acids			Bipy bases	pK _a		Complexes	ΔpK _a =pK _a (NH ⁺)-pK _a (COOH)	Complexes obtained																			
pK _a 1	pK _a 2	pK _a 3		pK _a 1	pK _a 2																						
H ₃ tcpb	3.82	4.30	4.78	bpe	4.99	5.59	3	1.17	salt																		
H ₃ btatb	4.17	4.65	5.13							5	0.82	salt															
				bpea	5.38	5.98	4	1.56	salt																		
							6	1.21	cocrystal																		
								bpys	3.99	4.60	7	0.17	cocrystal														
															bpym	4.38	5.01	8	0.21	cocrystal							
																						bpy	4.44	5.25	9	0.27	cocrystal

Table S2: Comparison of C-O-C and Interplanar Angles of H₃tcpb and its Complexes

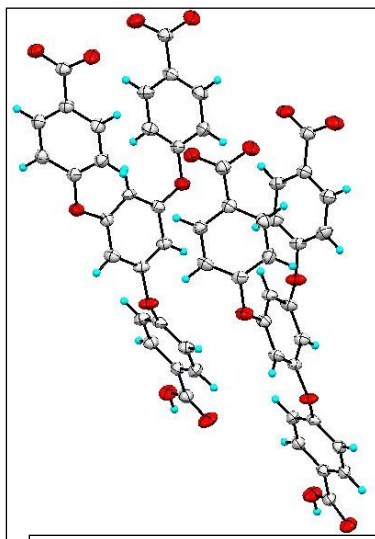
	1	3	4	7
C-O-C(Å)	119.33°, 117.53°, 121.25°; 116.10°, 116.85°, 125.15°	118.21°, 120.36°, 121.00°	116.27°, 118.58°, 120.09°	120.24°, 119.07°, 119.77°
Interplanar angles(°)*	62.67°, 69.88°, 81.53°; 74.11°, 77.46°, 56.87°	62.57°, 56.85°, 68.37°	66.76°, 64.29°, 80.01°	76.50°, 64.13°, 71.13°

Table S3: Comparison of C-N-C and Interplanar Angles of H₃btatb and its Complexes

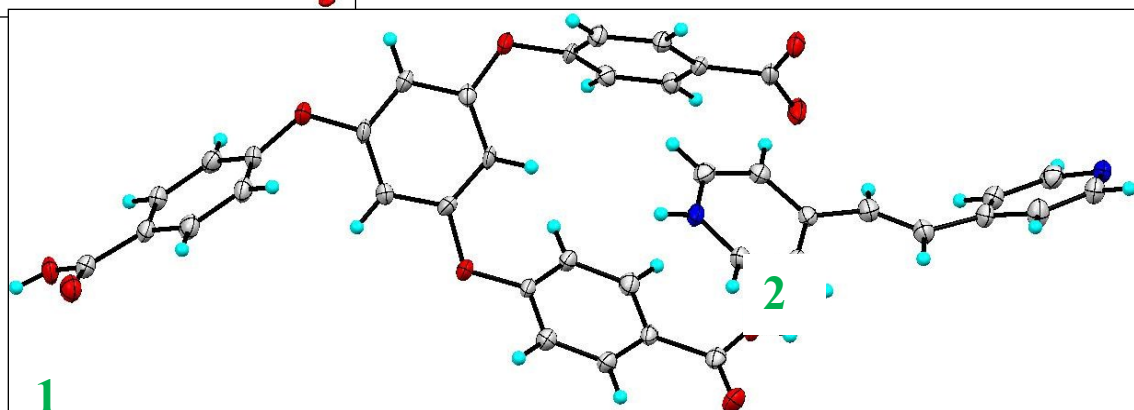
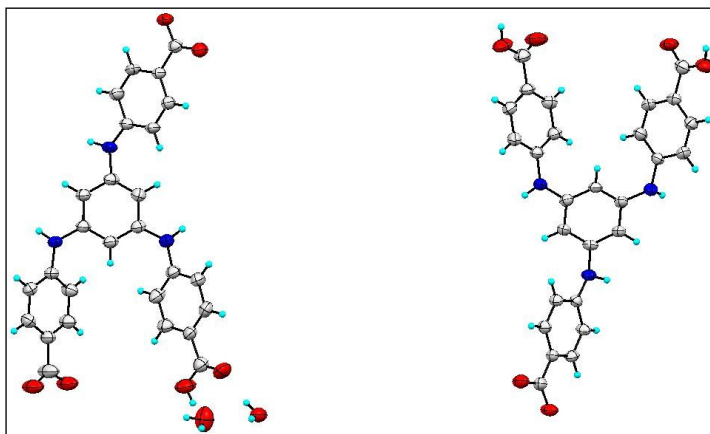
	2	5	6	8	9	10
C-N-C(Å)	124.67°, 129.38°, 129.87°; 125.93°, 126.17°, 126.41°	124.92°, 127.87°, 128.56°	124.86°, 126.04°, 128.38°	127.27°, 128.13°, 132.18°	126.36°, 126.45°, 126.61°	123.95°, 127.28°, 131.87°
Interplanar angles(°)	47.12°, 44.12°, 49.24°; 37.85°, 47.26°, 33.81°	48.94°, 53.05°, 45.89°	46.03°, 52.80°, 46.47°	44.47°, 42.47°, 22.56°	42.62°, 43.02°, 64.57°	45.70°, 51.13°, 27.45°

ORTEP diagrams of all the structures

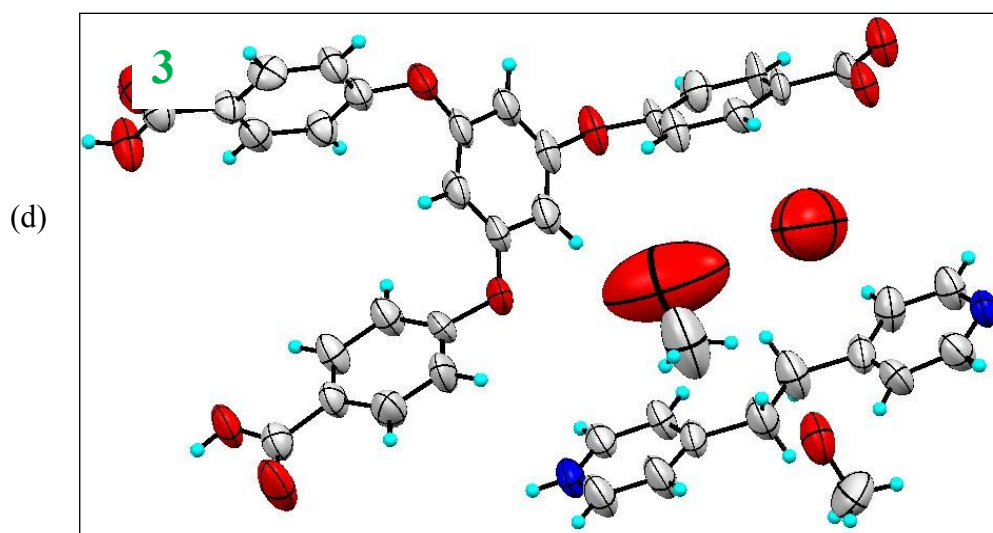
(a)



(b)

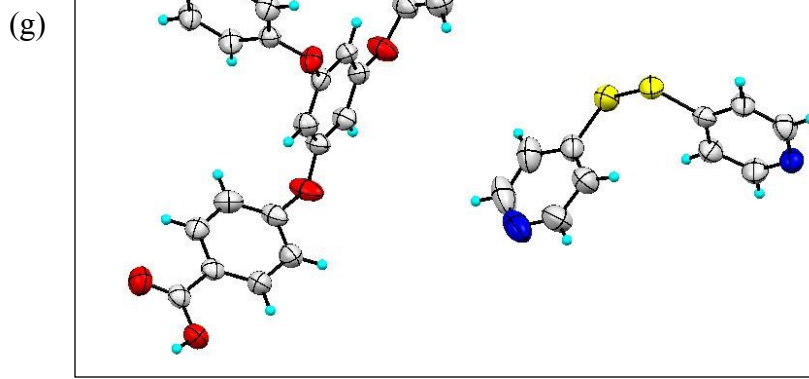
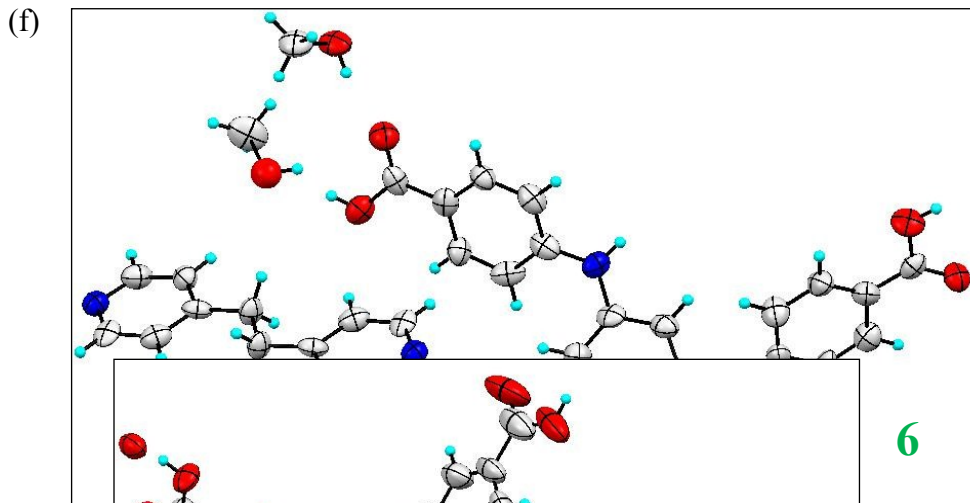
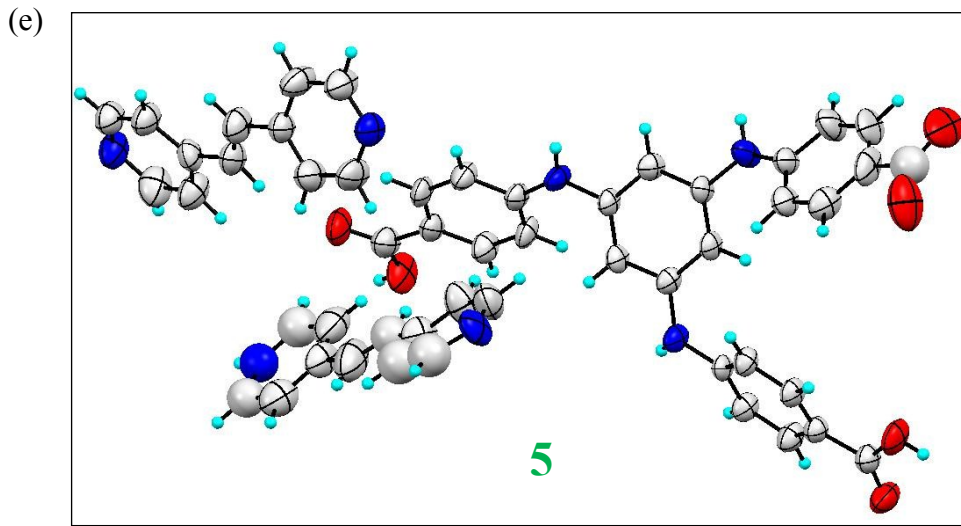


(c)



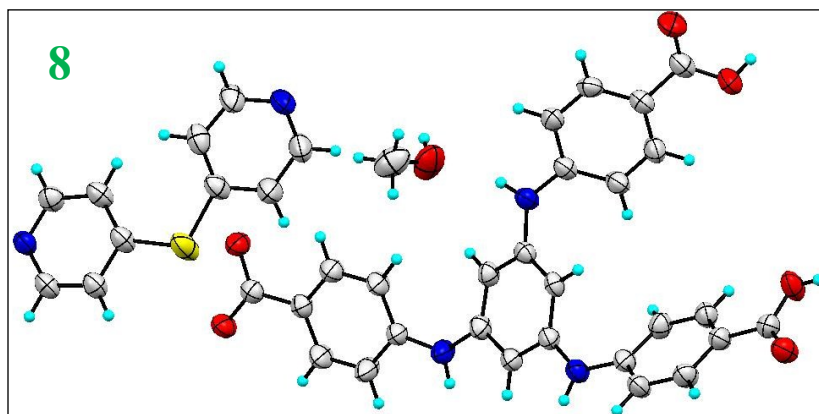
(d)

4

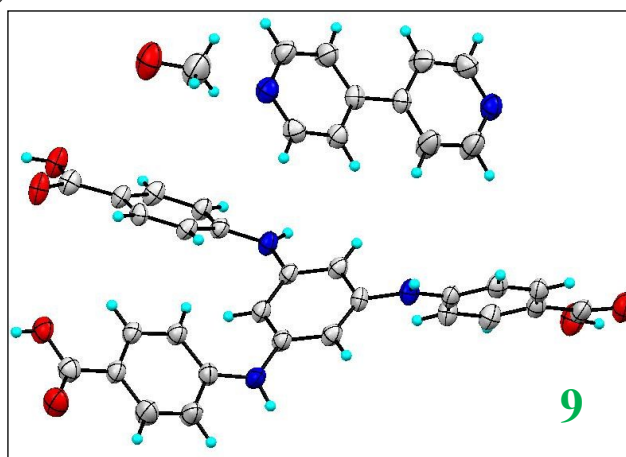


7

(h)



(i)



(j)

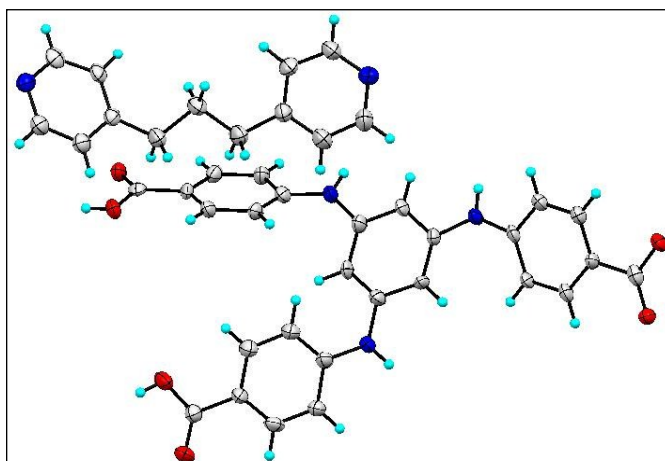


Figure S18. Illustrations of ORTEP diagrams of structures: (a) H₃tcpb and (b) H₃btatb; (c)-(j) complexes **3** to **10**.