Electronic Supporting Information

Effects on the magnetic interaction caused by molecular recognition in complexes of 1,2-azole-based oxamate and $[Cu(bpca)]^+$ units

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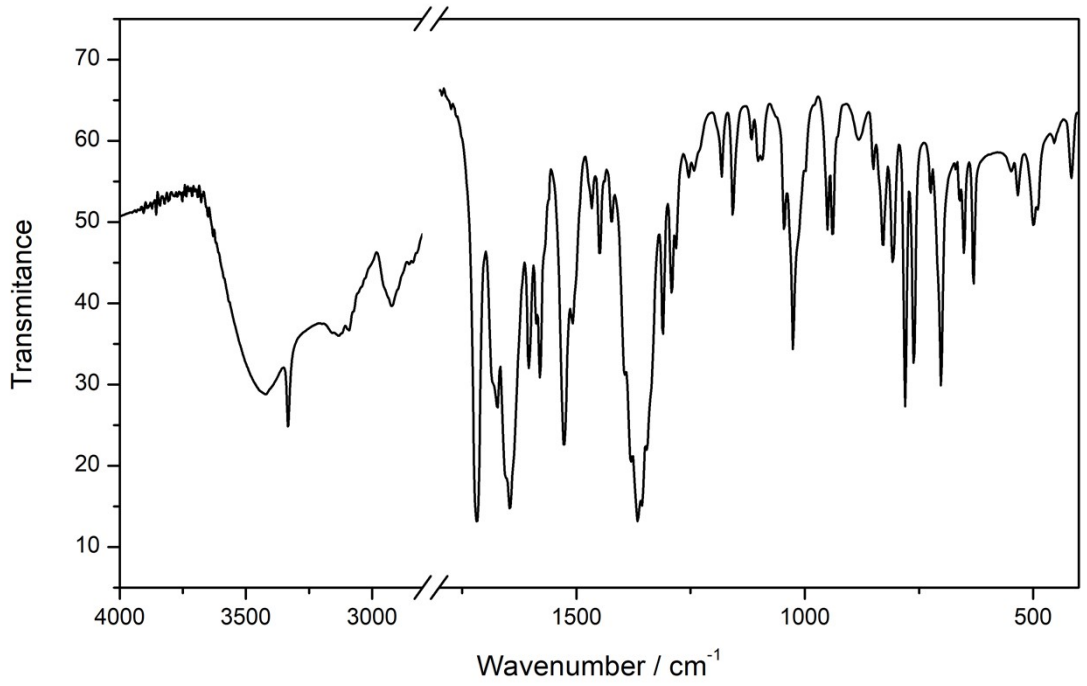


Figure S1. Infrared spectrum for **1** as a KBr disk.

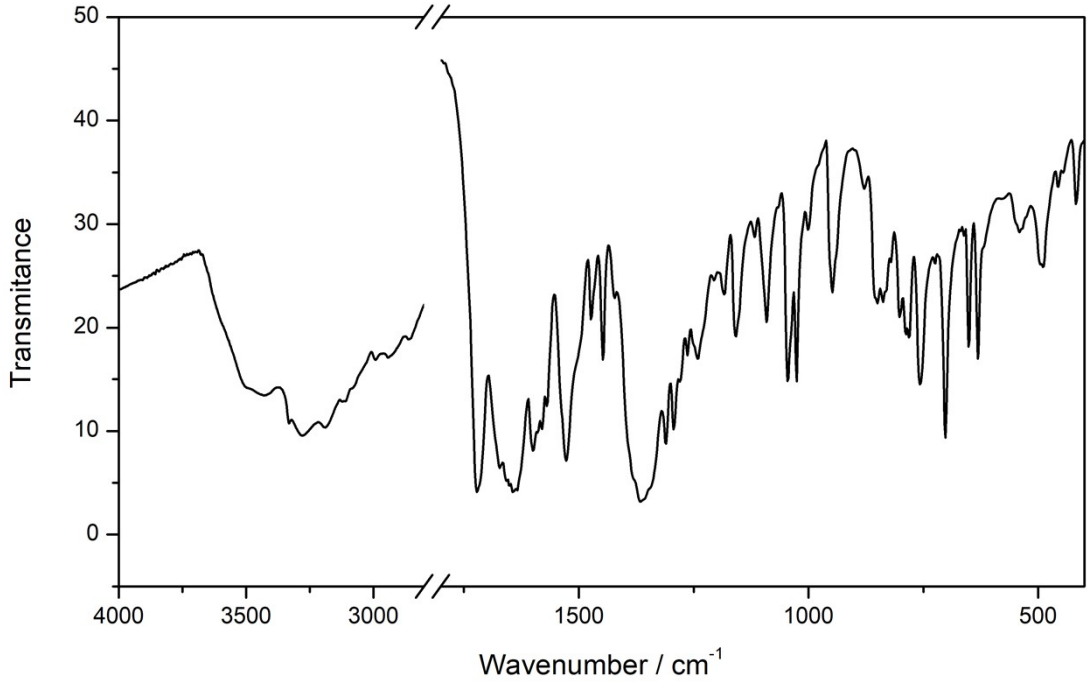


Figure S2. Infrared spectrum for **3** as a KBr disk.

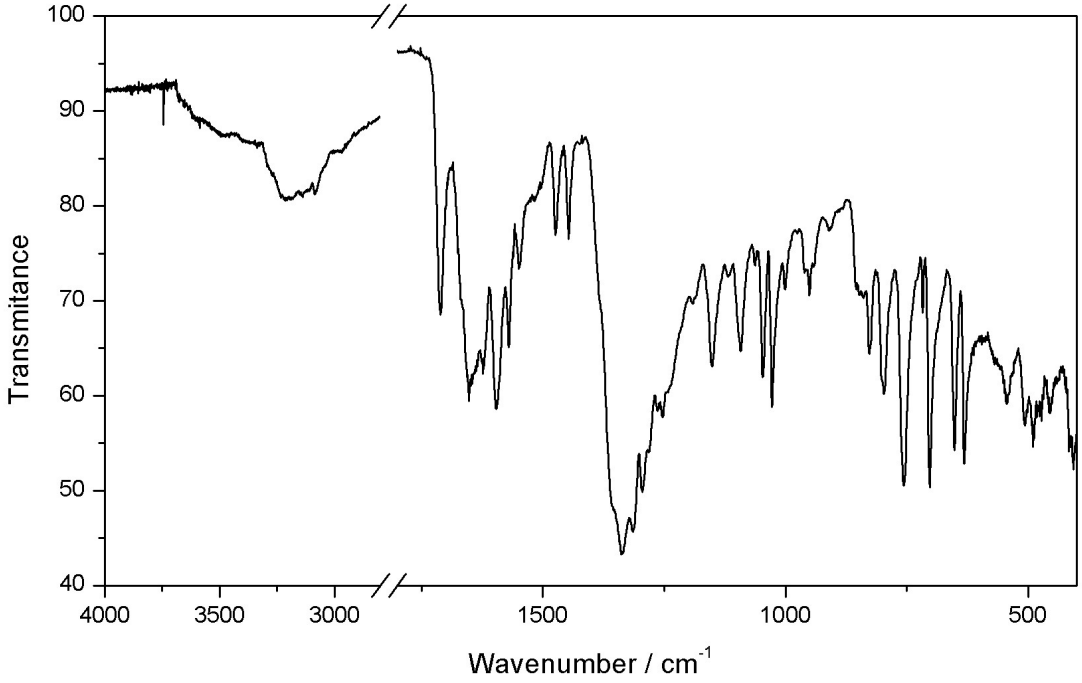


Figure S3. Infrared spectrum for **4** recorded on an ATR equipment.

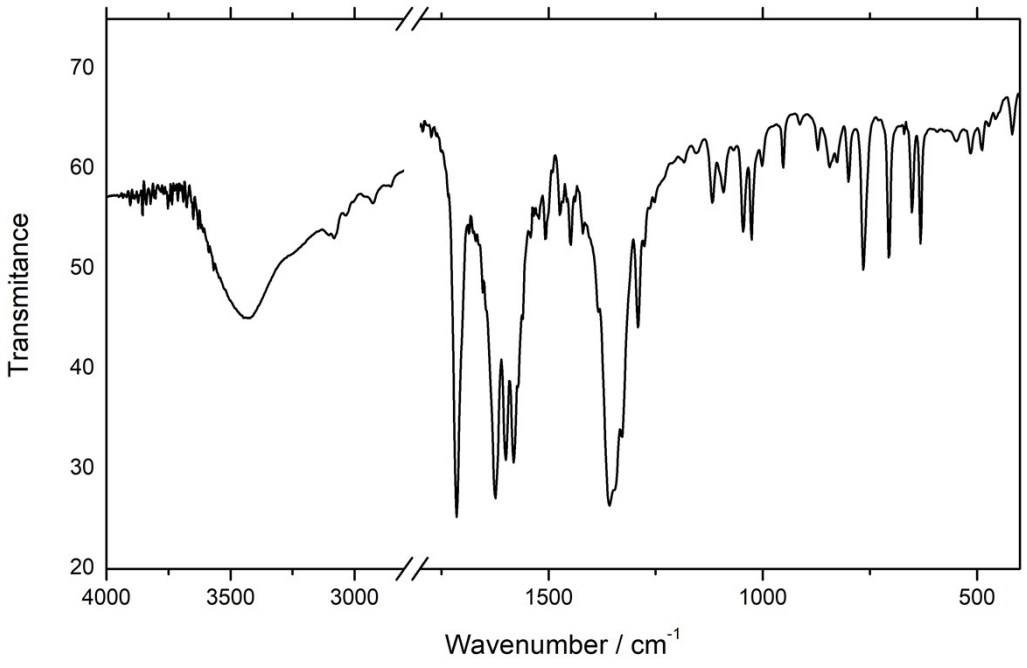


Figure S4. Infrared spectrum of **5** as a KBr disk.

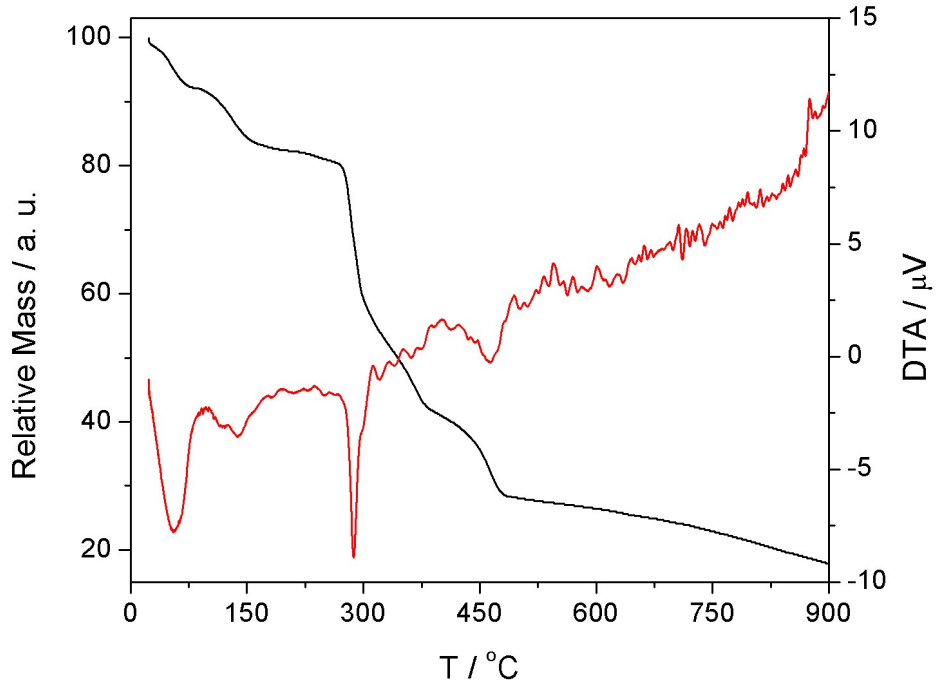


Figure S5. Thermal analysis for **1** under N_2 flow. The black line refers to the mass loss, whereas the red one is the DTA curve.

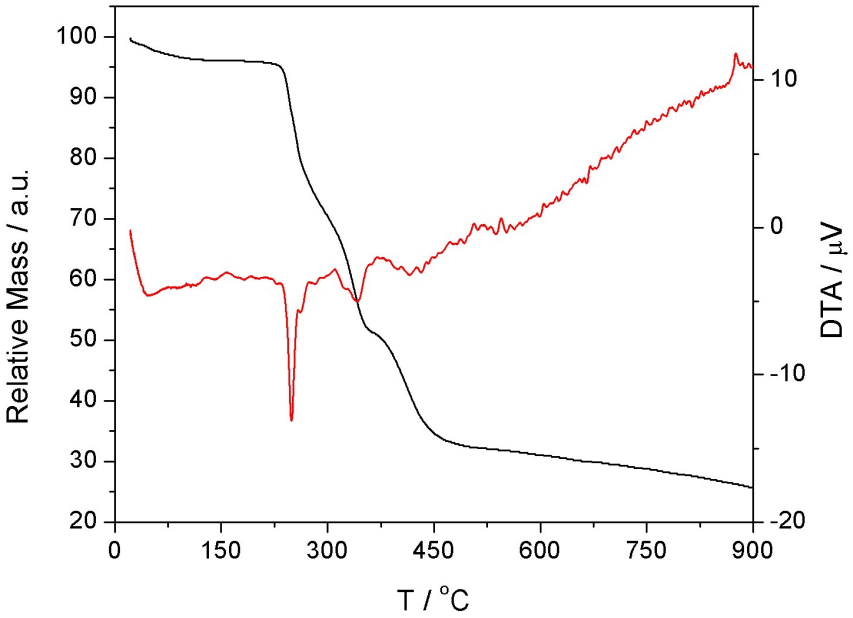


Figure S6. Thermal analysis for **3** under N_2 flow. The black line refers to the mass loss, whereas the red one is the DTA curve.

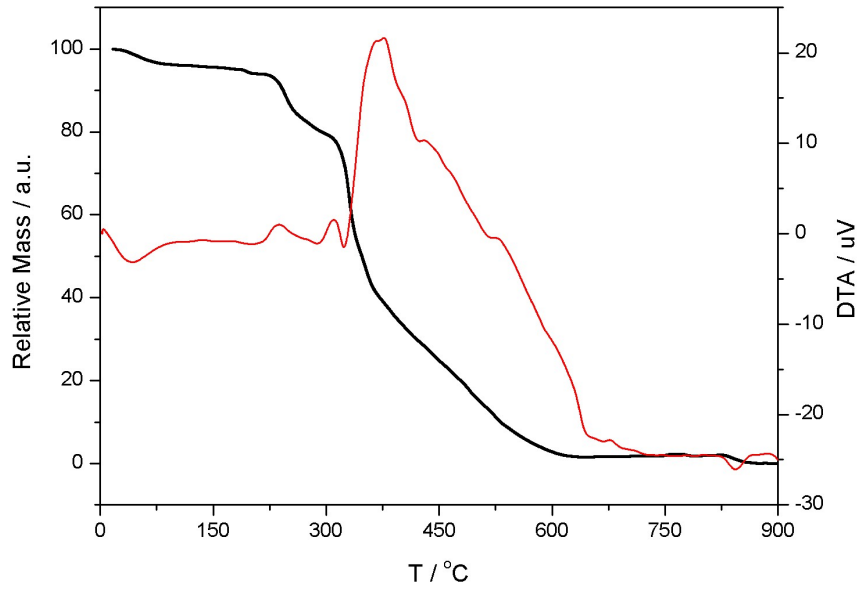


Figure S7. Thermal analysis for **4** under N_2 flow. The black line refers to the mass loss whereas the red one is the DTA curve.

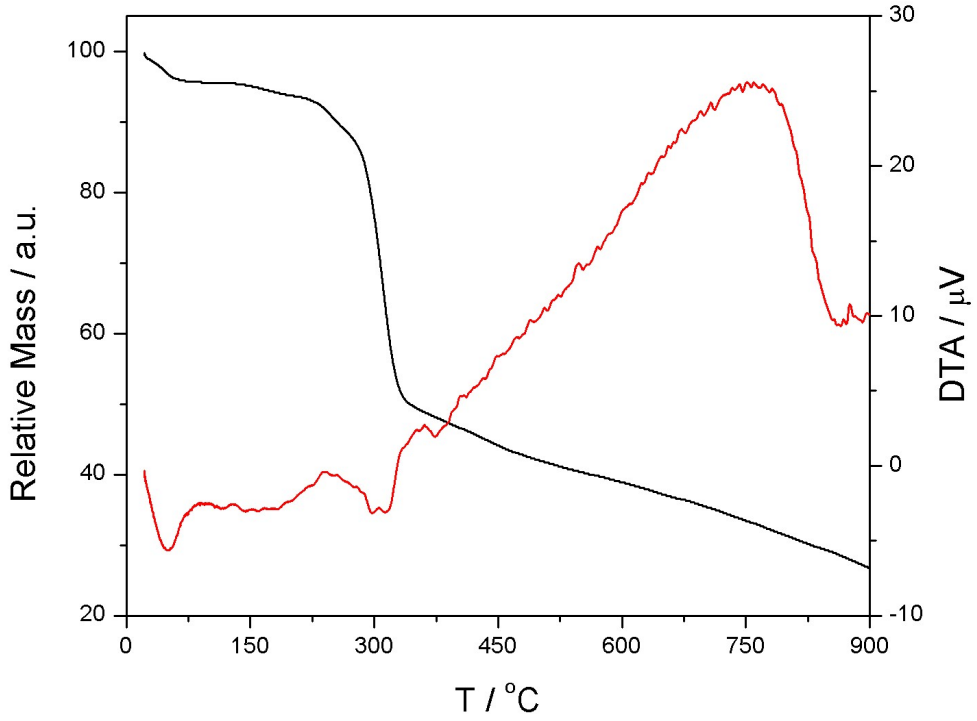


Figure S8. Thermal analysis for **5** under N_2 flow. The black line refers to the mass loss, whereas the red one is the DTA curve.

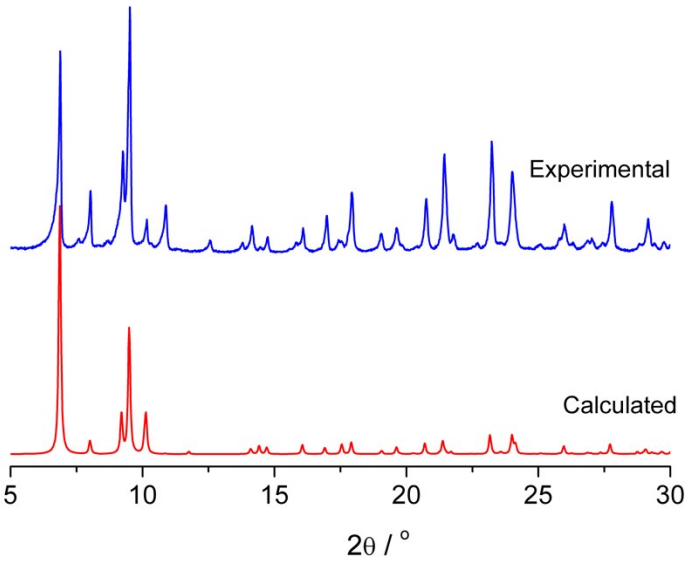


Figure S9. X-ray powder diffraction for **1** and comparison with the calculated pattern from its single crystal structure.

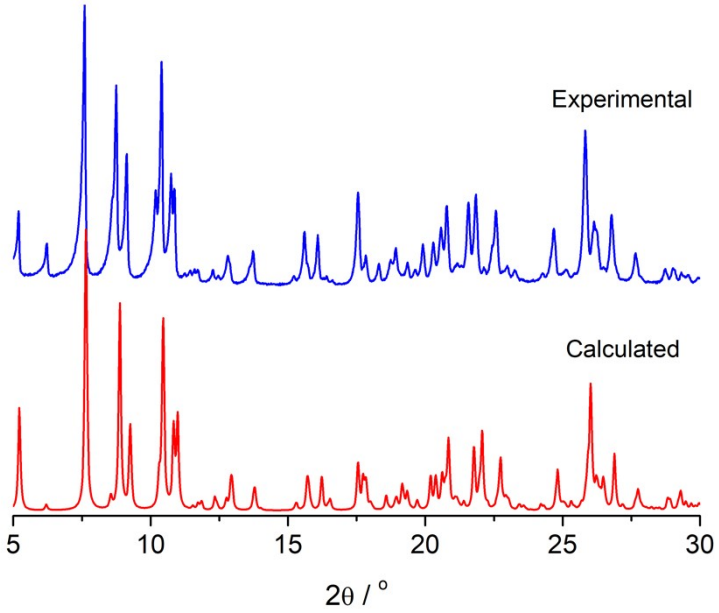


Figure S10. X-ray powder diffraction for **3** and comparison with the calculated pattern from its single crystal structure.

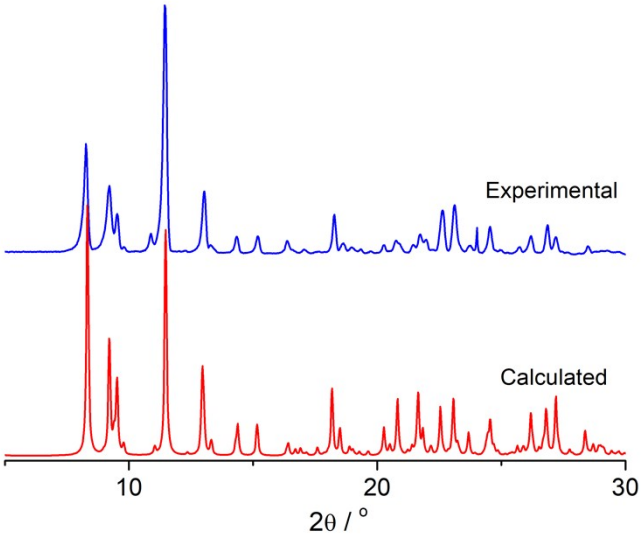
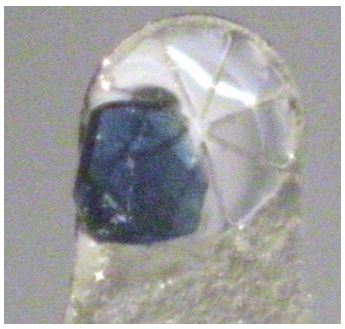
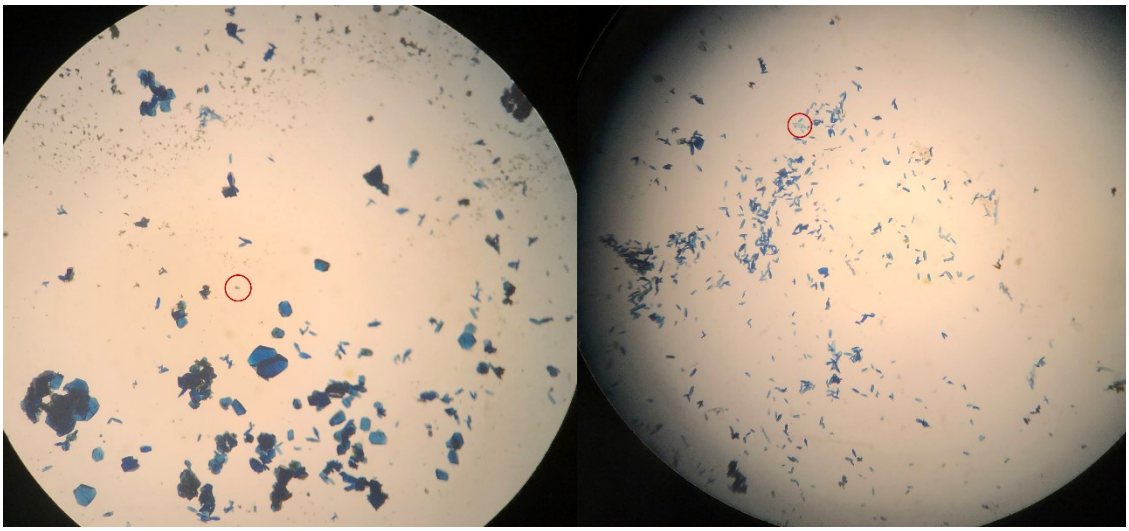


Figure S11. X-ray powder diffraction for **4** and comparison with the calculated pattern from its single crystal structure.

(a)



(b)



(c)

Figure S12 – (a) Single crystal of **1** and (b) single crystal of **4**. (c) Single crystals of **4** and **2** together without separation from their synthesis, showcasing the low yield of **2** (red circles).

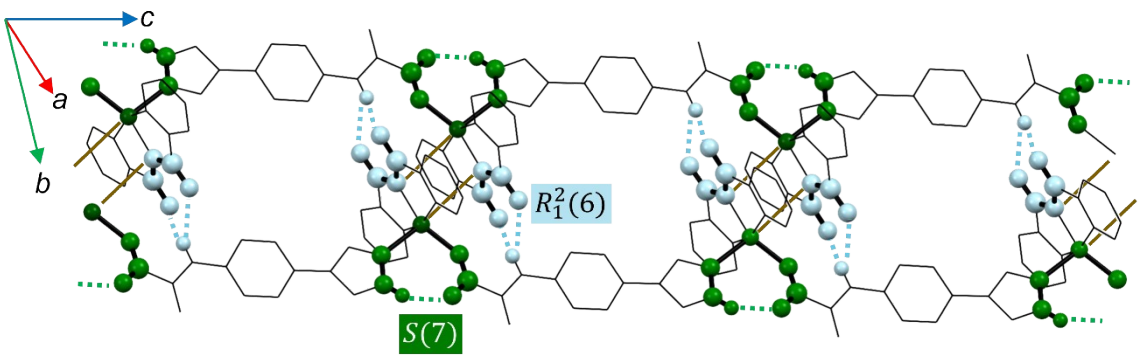


Figure S13. Crystal packing of **1** focusing on the double strain interchain hydrogen bonds.

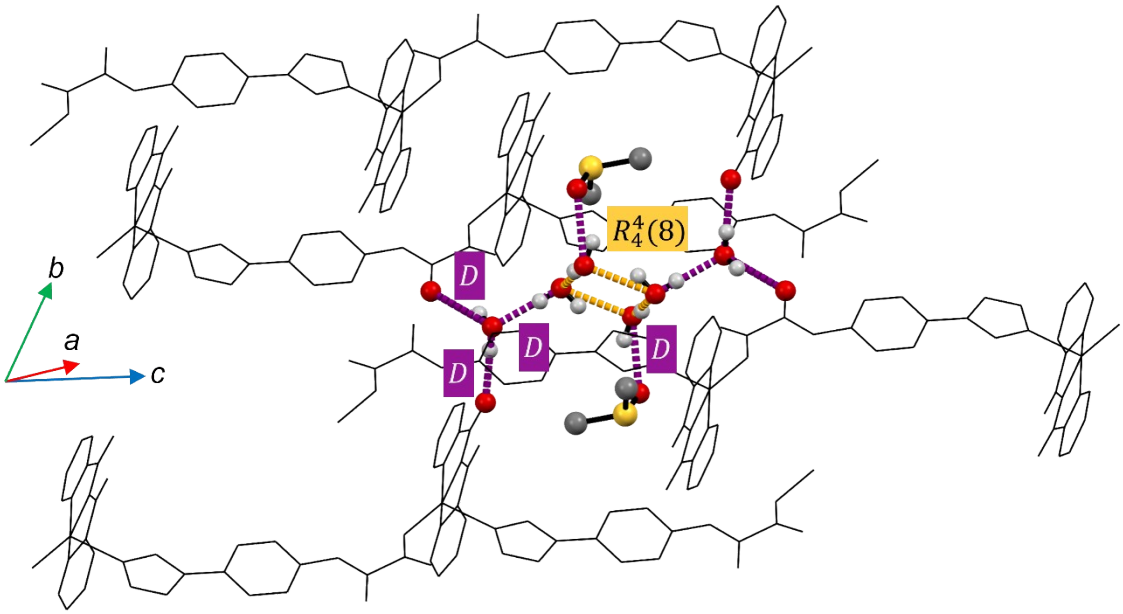


Figure S14. Crystal packing of **2** focusing on the hydrogen bond net between the coordination polymers and the crystallization solvent molecules.

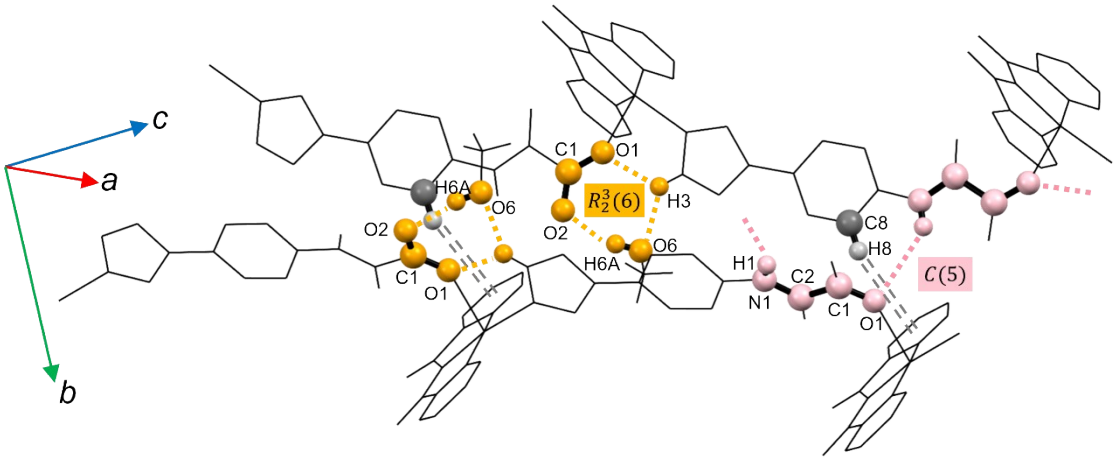


Figure S15. Crystal packing of **2** focusing on the different interchain hydrogen bonds and C–H···π interactions.

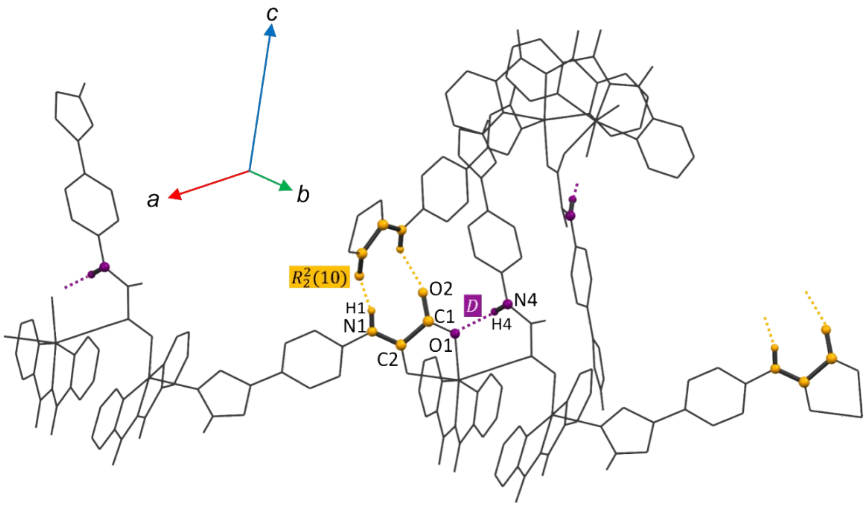


Figure S16. Crystal packing of **3** focusing on the interchain hydrogen bonds.

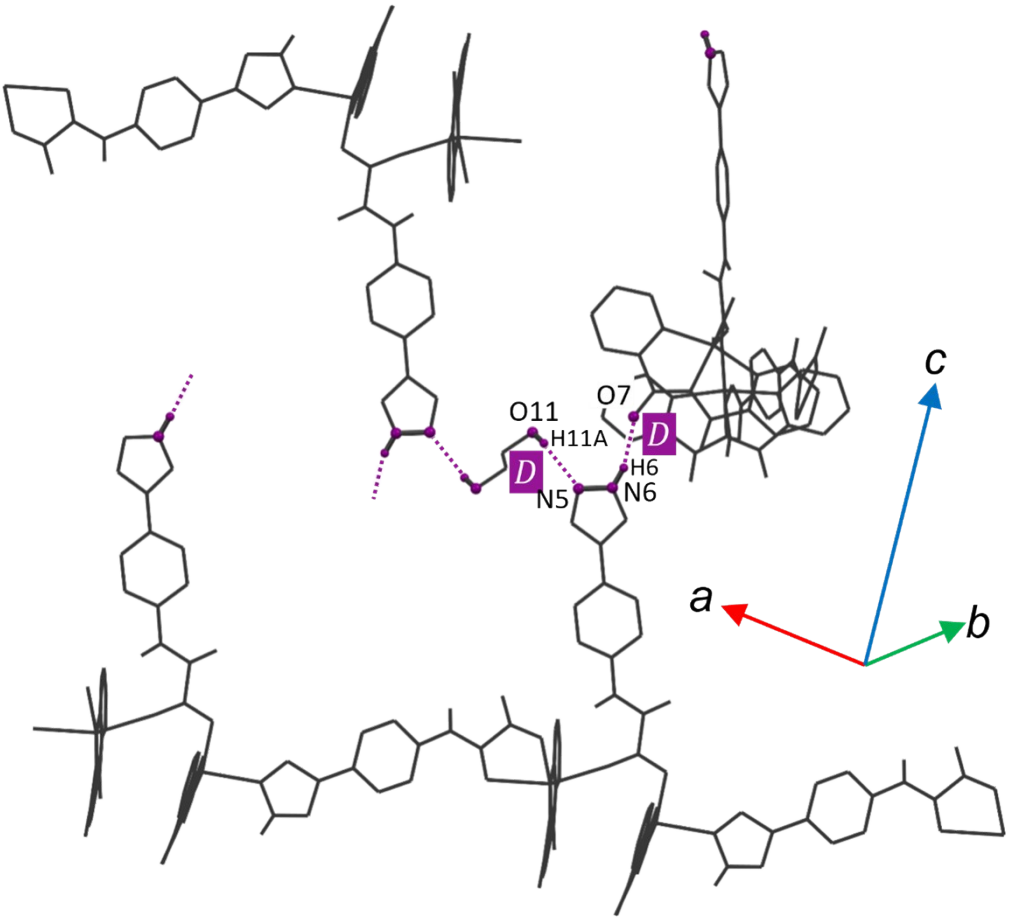


Figure S17. Crystal packing of **3** focusing on the interactions involving the coordination polymers and the solvent molecules.

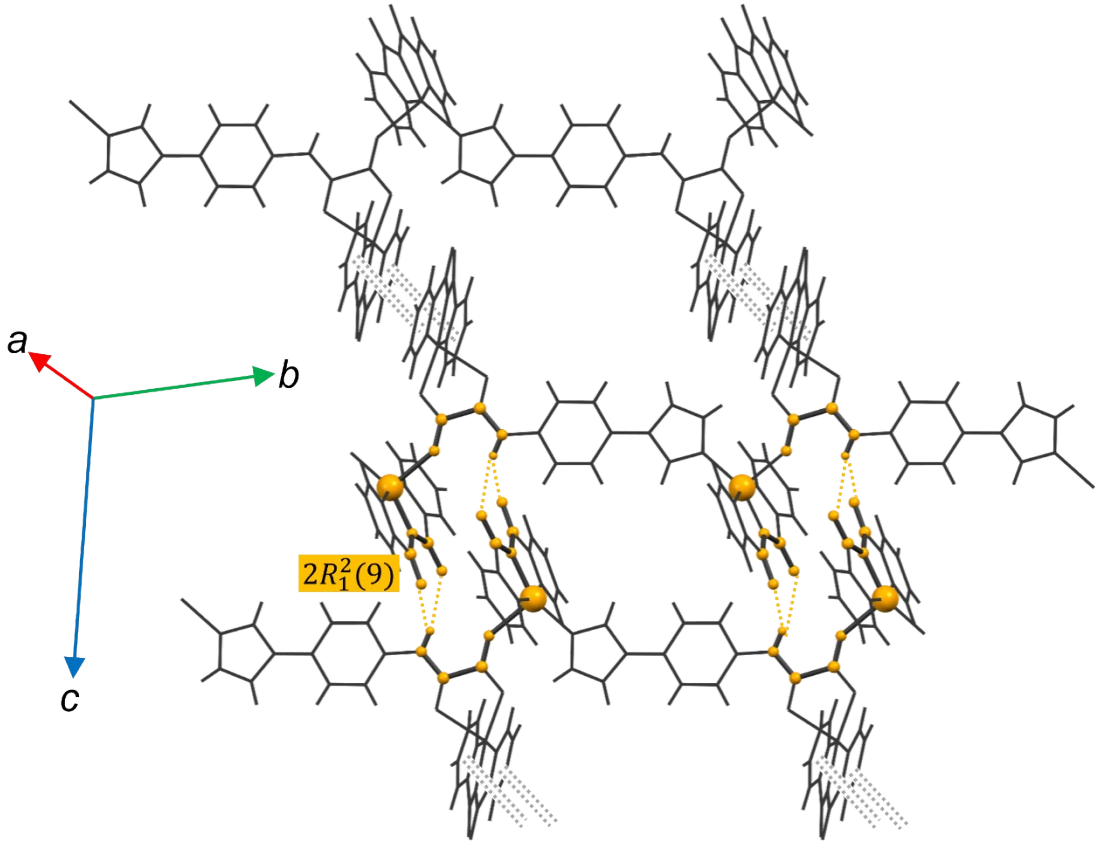


Figure S18. Crystal packing of **4** featuring the interchain hydrogen bonds and π-π stacking.

Table S1. Main bond lengths and angles for **1** and **2**.

1				**2**			
Bond length Cu–L/Å		Bond angle L–Cul–L'/º		Bond length Cu–L/Å		Bond angle L–Cul–L'/º	
Cu1–N2	2.207 (3)	N2–Cu1–N4	94.09 (13)	Cu1–N2	1.987 (2)	N2–Cu1–N4	96.42 (10)
Cu1–N4	2.024 (3)	N2–Cu1–N25	98.16 (13)	Cu1–N4	2.018 (2)	N2–Cu1–N5	170.79 (10)
Cu1–N5	1.956 (3)	N2–Cu1–N6	95.31 (13)	Cu1–N5	1.935 (2)	N2–Cu1–N6	99.15 (10)
Cu1–N6	2.036 (3)	N2–Cu1–O1	106.06 (12)	Cu1–N6	1.997 (2)	N2–Cu1–O1	85.45 (9)
Cu1–O1	1.944 (3)	N4–Cu1–N5	81.20 (13)	Cu1–O1	2.267 (2)	N4–Cu1–N5	81.63 (10)
Shortest Cu···Cu distance / Å		N4–Cu1–N6	160.91 (13)	Shortest Cu···Cu distance / Å		N4–Cu1–N6	162.90 (10)
Cu1···Cu1^{vi}	4.366(1)	N4–Cu1–O1	94.27 (12)	Cu1···Cu1^{iii}	5.1663(8)	N4–Cu1–O1	98.55 (10)
Shortest intrachain Cu···Cu distance/Å		N5–Cu1–N6	81.05 (13)	Shortest intrachain Cu···Cu distance/Å		N5–Cu1–N6	81.87 (10)
Cu1···Cu1^{i}	13.672(5)	N5–Cu1–O1	155.64 (12)	Cu1···Cu1^{i}	13.884(1)	N5–Cu1–O1	103.73 (9)
		N6–Cu1–O1	99.02 (13)			N6–Cu1–O1	89.72 (10)

Symmetry codes. **1**: (i) = *x*, *y*, 1+*z*; (vi) = 2–*x*, 2–*y*, –*z*. **2**: (i) = –1+*x*, *y*, –1+*z*; (iii) = 1–*x*, –*y*, –*z*.

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Table S2. Main bond lengths and angles for **3** and **4**.

3				**4**			
Bond length Cu–L/Å		Bond angle L–Cul–L'/º		Bond length Cu–L/Å		Bond angle L–Cul–L'/º	
Cu1–N7	2.020 (4)	N7–Cu1–N8	82.03 (17)	Cu1–N4	2.013 (4)	N4–Cu1–N5	81.51 (15)
Cu1–N8	1.939 (4)	N7–Cu1–N9	163.68 (17)	Cu1–N5	1.934 (3)	N4–Cu1–N6	162.31 (14)
Cu1–N9	2.002 (4)	N7–Cu1– O1	95.28 (14)	Cu1–N6	2.017 (4)	N4–Cu1–O1	98.07 (14)
Cu1–O1	1.973 (3)	N7–Cu1–O3	93.86 (13)	Cu1–O1	1.983 (3)	N4–Cu1–O3	94.56 (13)
Cu1–O3	2.399 (3)	N7–Cu1–O4	92.31 (15)	Cu1–O3	2.277 (2)	N5–Cu1–N6	81.93 (14)
Cu1–O4	2.370 (3)	N8–Cu1–N9	82.20 (18)	Cu2–N7	2.001 (3)	N5–Cu1–O1	171.09 (12)
Cu2–N2	2.241 (3)	N8–Cu1–O1	170.97 (14)	Cu2–N8	1.943 (3)	N5–Cu1–O3	111.37 (12)
Cu2–N10	2.017 (4)	N8–Cu1–O3	94.98 (13)	Cu2–N9	2.009 (3)	N6–Cu1– O1	97.32 (13)
Cu2–N11	1.943 (3)	N8–Cu1–O4	110.01 (14)	Cu2–O2	2.272 (2)	N6–Cu1–O3	97.24 (13)
Cu2–N12	2.024 (4)	N9–Cu1– O1	100.94 (16)			O1–Cu1–O3	77.54 (9)
Cu2–O5	1.963 (3)	N9–Cu1–O3	91.67 (13)			N2–Cu2–N8	97.80 (14)
Shortest Cu···Cu distance/Å		N9–Cu1–O4	89.15 (15)	Shortest Cu···Cu distance/Å		N2–Cu2–N8	156.41 (13)
Cu1···Cu2	4.624(1)	O1–Cu1–O3	76.54 (11)	Cu1···Cu1^{vii}	4.8757(7)	N2–Cu2–N9	97.72 (14)
Intrachain Cu···Cu distance/Å		O1–Cu1–O4	78.64 (12)	Intrachain Cu···Cu distance/Å		N2–Cu2–O2	99.04 (11)
Cu1···Cu1^{v}	17.450(1)	O3–Cu1–O4	154.86 (11)	Cu1···Cu2	5.7391(7)	N7–Cu2–N8	81.73 (13)
Cu1···Cu2^{v}	13.375(1)	N2–Cu2–N10	97.92 (14)	Cu1···Cu1^{i}	13.719(2)	N7–Cu2–N9	163.29 (13)
Cu2···Cu2^{v}	17.450(1)	N2–Cu2–N11	103.09 (14)	Cu2···Cu2^{i}	13.719(2)	N7–Cu2–O2	92.38 (12)
		N2–Cu2–N12	95.64 (14)	Cu1···Cu2^{i}	13.030(2)	N8–Cu2–O2	104.55 (11)

N2–Cu2–O5	88.46 (13)	Cu2···Cu1^{i}	16.508(2)	N8–Cu2–N9	81.58 (13)
N10–Cu2–N11	81.64 (15)			N9–Cu2–O2	91.26 (12)
N10–Cu2–N12	160.42 (15)				
N10–Cu2–O5	96.06 (18)				
N11–Cu2–N12	81.57 (15)				
N11–Cu2–O5	168.41 (14)				
N12–Cu2–O5	98.36 (17)				

Symmetry code: (v) = –1+*x*, 1+*y*, *z* (**3**); (i) = –1+*x*, 1+*y*, *z* and (vii) = 2–*x*, 1–*y*, 1–*z* (**4**).

Table S3. Main bond lengths and angles for **5**

5			
Bond length Cu–L/Å		Bond angle L–Cul–L'/º	
Cu1–N6	2.015 (3)	N7–Cu1–N6	82.65 (13)
Cu1–N7	1.928 (3)	N6–Cu1–N8	164.54 (14)
Cu1–N8	2.003 (3)	N6–Cu1–O2	95.54 (12)
Cu1–O2	1.959 (3)	N6–Cu1–O3	93.01 (12)
Cu1–O3	2.238 (3)	N7–Cu1–N8	82.84 (13)
Cu2–N1	1.971 (3)	N7–Cu1–O2	169.54 (14)
Cu2–N3	2.020 (3)	N7–Cu1–O3	111.40 (12)
Cu2–N4	1.929 (3)	N8–Cu1–O2	97.78 (12)
Cu2–N5	2.011 (4)	N8–Cu1–O3	97.20 (12)
Cu2–O1	2.225 (3)	O2–Cu1–O3	78.94 (10)
Intramolecular Cu---Cu distance/Å		N1–Cu2–N3	98.77 (13)
Cu1···Cu2	5.456(9)	N1–Cu2–N4	170.19 (15)
Shortest intramolecular Cu---Cu distance/Å		N1–Cu2–N5	95.43 (13)
Cu2···Cu1^{i}	3.7987(9)	N1–Cu2–O1	80.39 (12)
		N3–Cu2–N4	82.50 (14)
		N3–Cu2–N5	164.88 (14)
		N3–Cu2–O1	92.80 (13)
		N4–Cu2–N5	82.63 (14)
		N4–Cu2–O1	109.31 (13)
		N5–Cu2–O1	94.69 (13)

Symmetry code: (i) = 1–*x*, 2–*y*, 1–*z*.

Table S4. Hydrogen bonds for **1**.

D–H···*A*	*D*–H/Å	H···*A*/Å	*D*···*A*/Å	*D*–H···*A*/ º
N3–H3···O2	0.86	2.04	2.785 (4)	144
N3–H3···O7	0.86	2.56	3.162 (6)	128
N1–H1···O5^{iii}	0.86	2.30	3.068 (4)	149
O7–H7*A*···O6	0.90 (1)	1.97 (1)	2.865 (5)	177 (4)
O7–H7*B*···O8^{iv}	0.90 (1)	2.03 (3)	2.799 (6)	143 (5)
O6–H6*A*···O5^{v}	0.90 (1)	1.92 (1)	2.807 (4)	168 (4)
O6–H6*B*···O3	0.90 (1)	2.06 (3)	2.882 (4)	152 (5)
O8–H8*A*···O9*A*^{a}	0.90 (1)	2.03 (5)	2.797 (9)	143 (6)
O8–H8$^{A\cdots O9B}$b	0.90 (1)	2.49 (2)	3.389 (17)	175 (7)
O8–H8*B*···O7^{vi}	0.90 (1)	1.93 (2)	2.824 (7)	170 (7)

Symmetry code: (iii) -*x*+2, -*y*+2, -*z*; (iv) *x*-1, *y*, *z*; (v) *x*, *y*-1, *z*; (vi) -*x*+2, -*y*+1, -*z*+1.

Table S5. Hydrogen bonds for **2**.

D–H···*A*	*D*–H/Å	H···*A*/Å	*D*···*A*/Å	*D*–H···*A*/º
N3–H3···O6	0.86	2.20	2.883 (4)	136
N3–H3···O1	0.86	2.16	2.729 (3)	124
O7–H7*B*···O5	0.82	2.12	2.839 (4)	147
O6–H6*A*···O2	0.82	1.96	2.749 (4)	161

Table S6. Hydrogen bonds for **3**.

D–H···*A*	*D*–H/Å	H···*A*/Å	*D*···*A*/Å	*D*–H···*A*/º
N6–H6*A*···O7^{iv}	0.88	1.97	2.796 (5)	156
N3–H6···O9^{v}	0.88	2.27	2.865 (5)	125
N3–H6···O10^{v}	0.88	2.00	2.800 (5)	150
N4–H10···O1	0.88	2.34	3.213 (5)	172

Symmetry code: (iv) *x*, -*y*+2, *z*+1/2; (v) -*x*, -*y*+2, -*z*.

Table S7. Hydrogen bond for **4**.

D–H···*A*	*D*–H/Å	H···*A*/Å	*D*···*A*/Å	*D*–H···*A*/º
N3–H3···O1^{i}	0.86	2.04	2.851 (4)	156
N1–H1···O5^{v}	0.86	2.53	3.311 (4)	152
N1–H1···O4^{v}	0.86	2.51	3.127 (4)	130
O12–H12*A*···O6^{vi}	0.82	1.97	2.778 (6)	168
O10–H10···O4^{v}	0.82	2.06	2.874 (6)	174

Symmetry code: (i) *x*-1, *y*+1, *z*; (v) -*x*+1, -*y*+1, -*z*+2; (vi) -*x*+2, -*y*+1, -*z*+1.

Table S8. SHAPE calculations for metal atoms

Compound	Atom	Coordination Number	Deviation from Shapes[a]			
			TBPY-5	SPY-5	OC-6	TPR-6
1	Cu1	5	8.212	7.917		
2	Cu1	5	12.715	8.942		
3	Cu1	5			47.871	49.086
	Cu2	6	19.773	18.618		
4	Cu1	5	11.338	8.056		
	Cu2	5	8.535	7.432		
5	Cu1	5	13.664	8.581		
	Cu2	5	13.940	8.968		

[a]Code associations: TBPY-5 = Trigonal bipyramid (D_{3h}), SPY-5 = Spherical square pyramid (C_{4v}), OC-6 = Octahedron (O_h) and TPR-6 = Trigonal prism (D_{3h}).