

Synthesis, crystal structure and luminescence of cadmium(II) and silver(I) coordination polymers based on 1,3-bis(1,2,4-triazol-1-yl)adamantane

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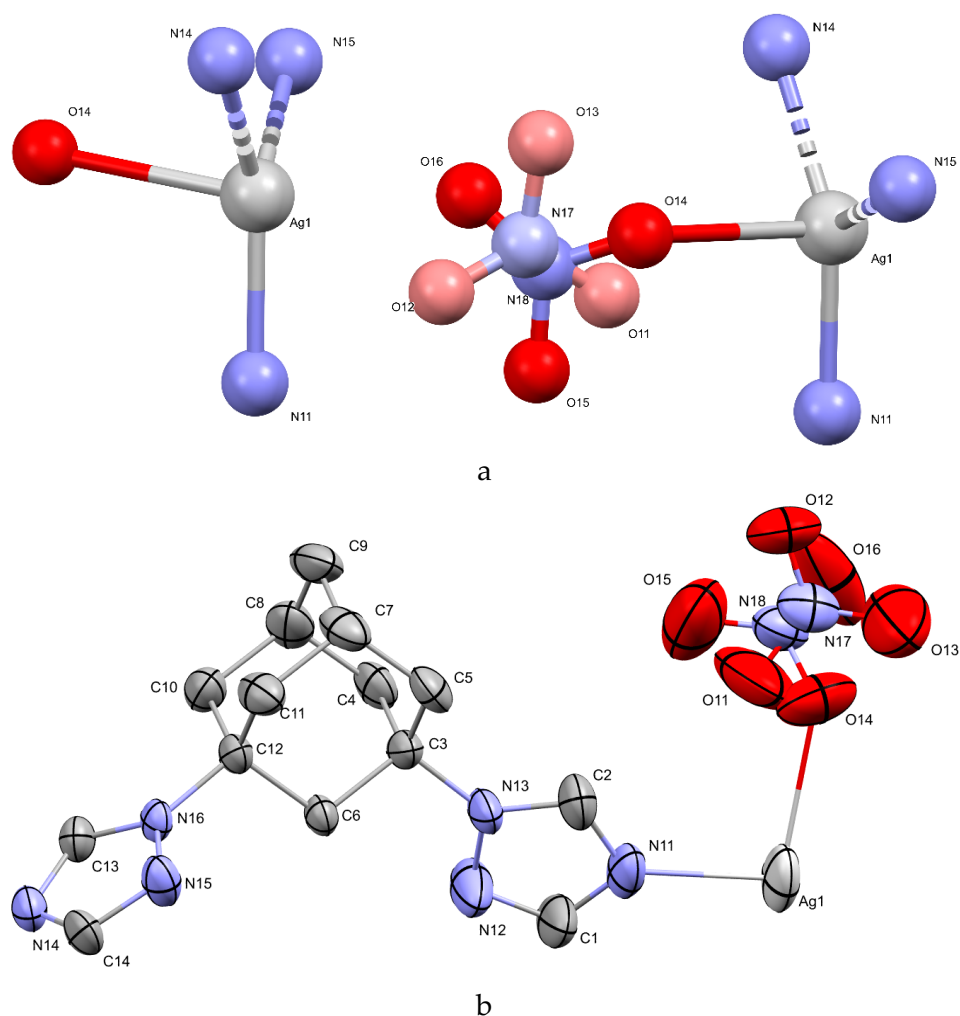


Figure S1. Disorder of nitrate ions in the structure of the coordination polymer 1 (a) and the asymmetric unit of the coordination polymer 1 showing both positions of the nitrate ions (b).

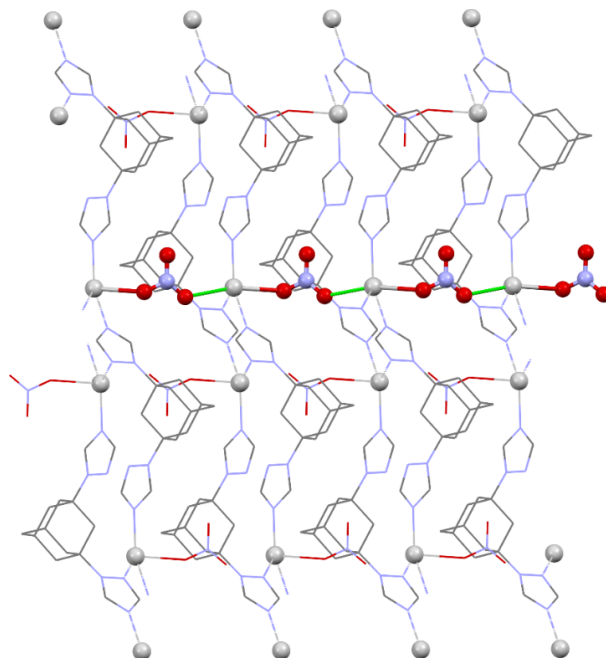


Figure S2. Bridging nitrate ions in the structure of the coordination polymer **1**. View along crystallographic axis *b*. Atom legend: Ag – grey balls; C – dark grey dots; N – blue balls and dots; O – red balls and dots.

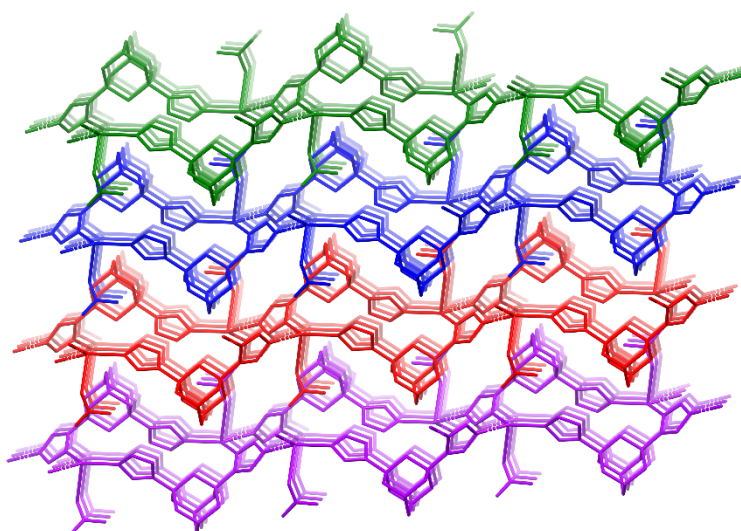


Figure S3. Packing of layers of the coordination polymer **1**. View along crystallographic axis *b*.

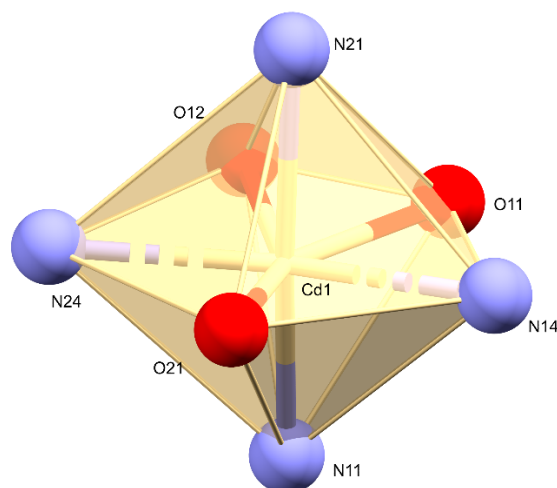


Figure S4. Coordination polyhedron of Cd(II) ion in the coordination polymer **2**.

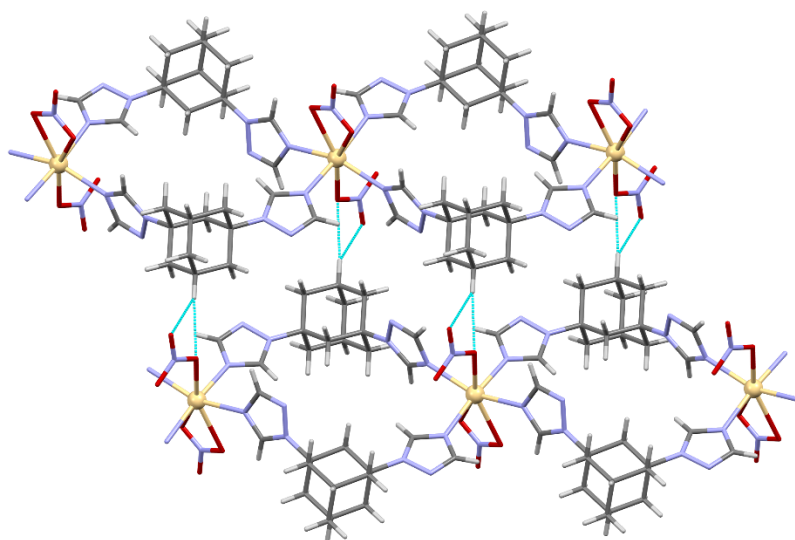


Figure S5. Close CH...O contacts between the chains of the coordination polymer **2**. Atom legend: Cd – yellow balls; C – dark grey dots; N – blue dots; O – red dots; H – white dots.

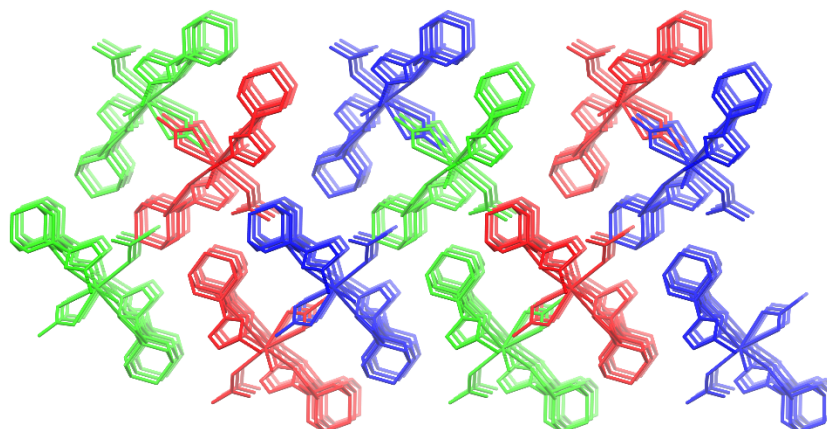


Figure S6. Packing of chains of the coordination polymer **1**. View along crystallographic axis *a*.

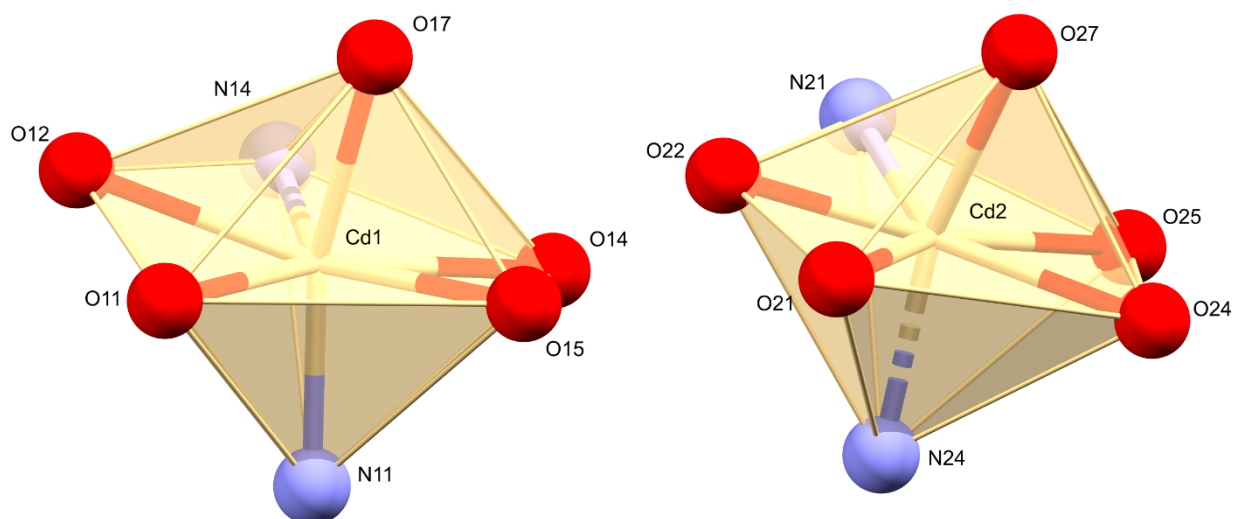


Figure S7. Coordination polyhedra of two crystallographically independent Cd(II) ions in the coordination polymer **3**.

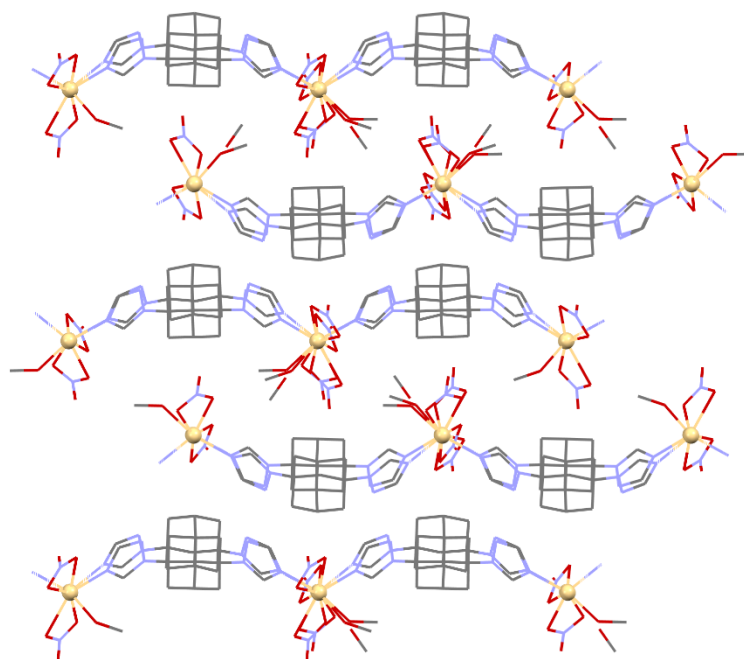


Figure S8. Packing of chains of the coordination polymer **3** into supramolecular layers. View along crystallographic axis *a*. Atom legend: Cd – yellow balls; C – dark grey dots; N – blue dots; O – red dots.

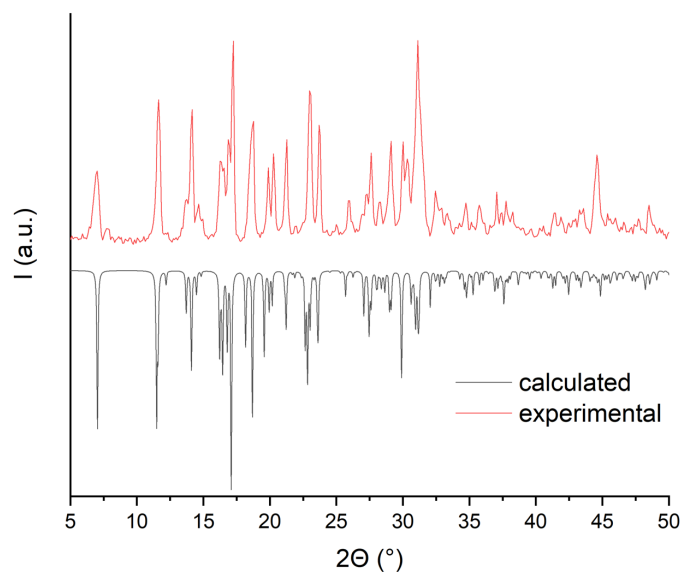


Figure S9. Powder X-ray diffraction plots for the coordination polymer 1.

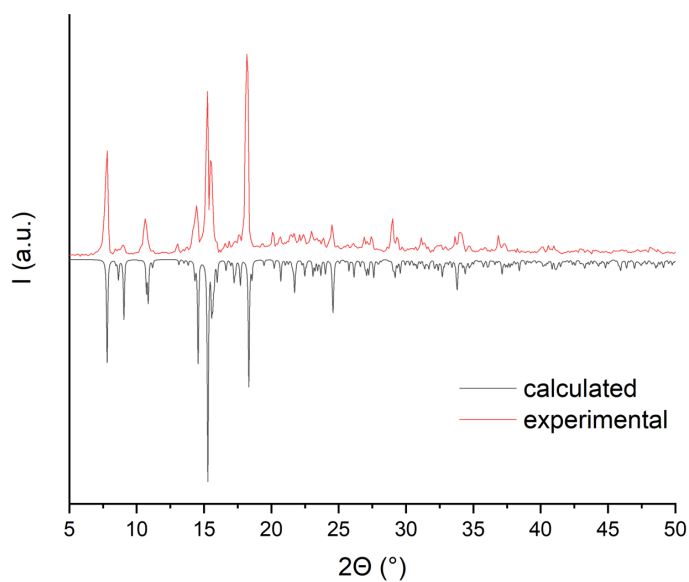


Figure S10. Powder X-ray diffraction plots for the coordination polymer 2.

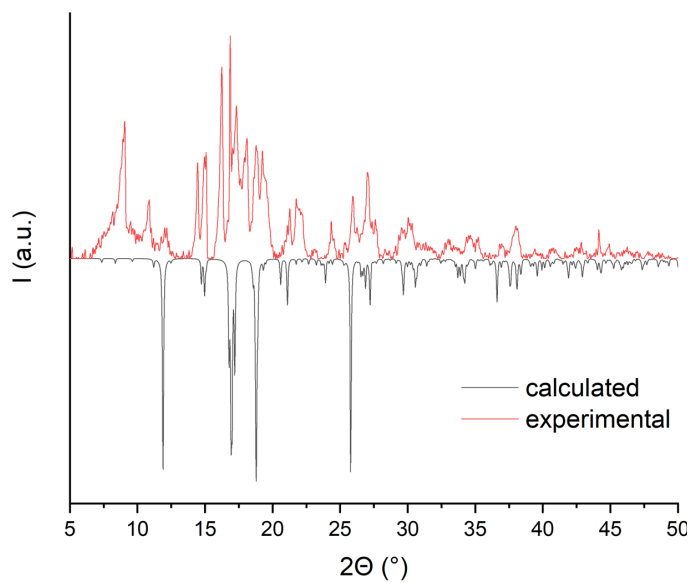


Figure S11. Powder X-ray diffraction plots for the coordination polymer 3.

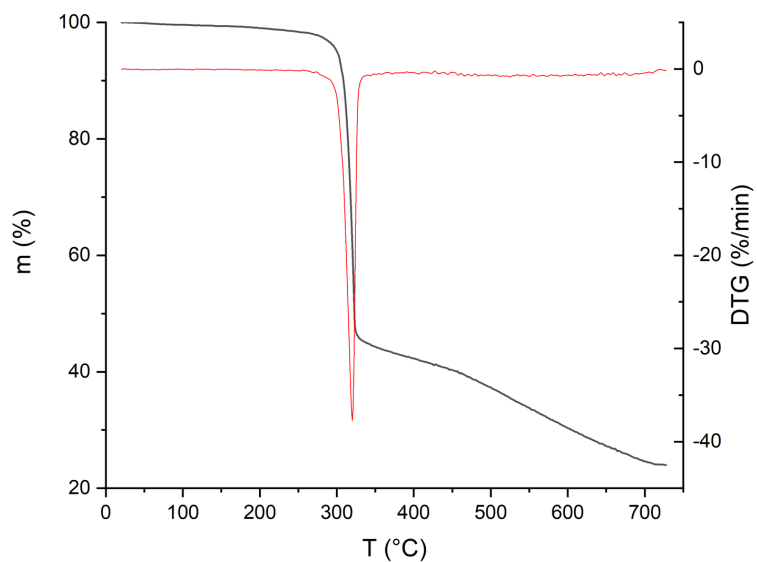


Figure S12. TG and DTA curves for the coordination polymer 1.

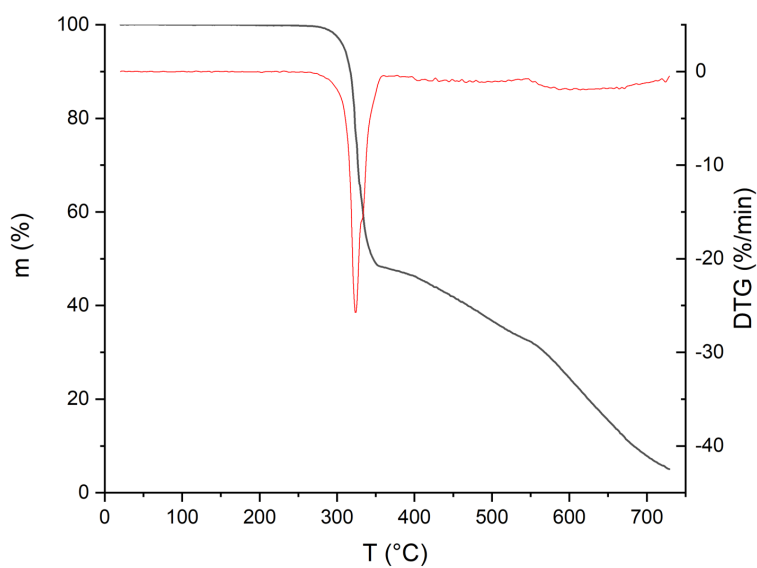


Figure S13. TG and DTA curves for the coordination polymer 2.

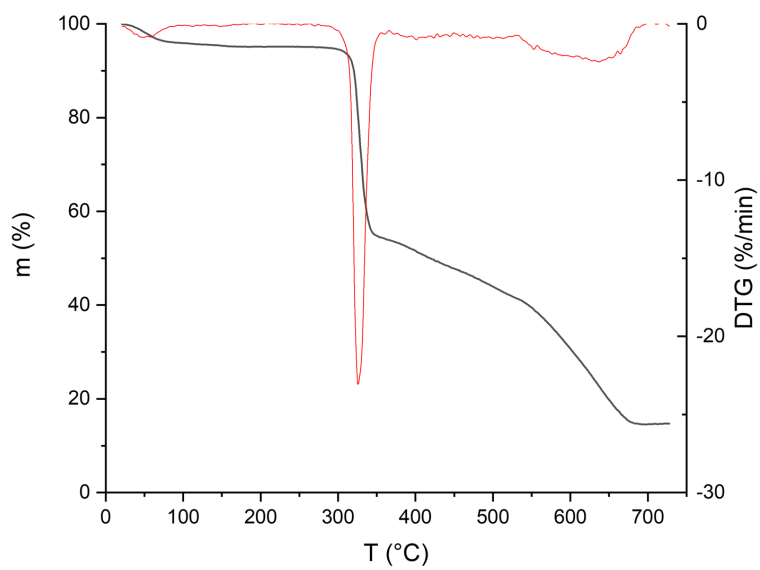


Figure S14. TG and DTA curves for the coordination polymer 3.

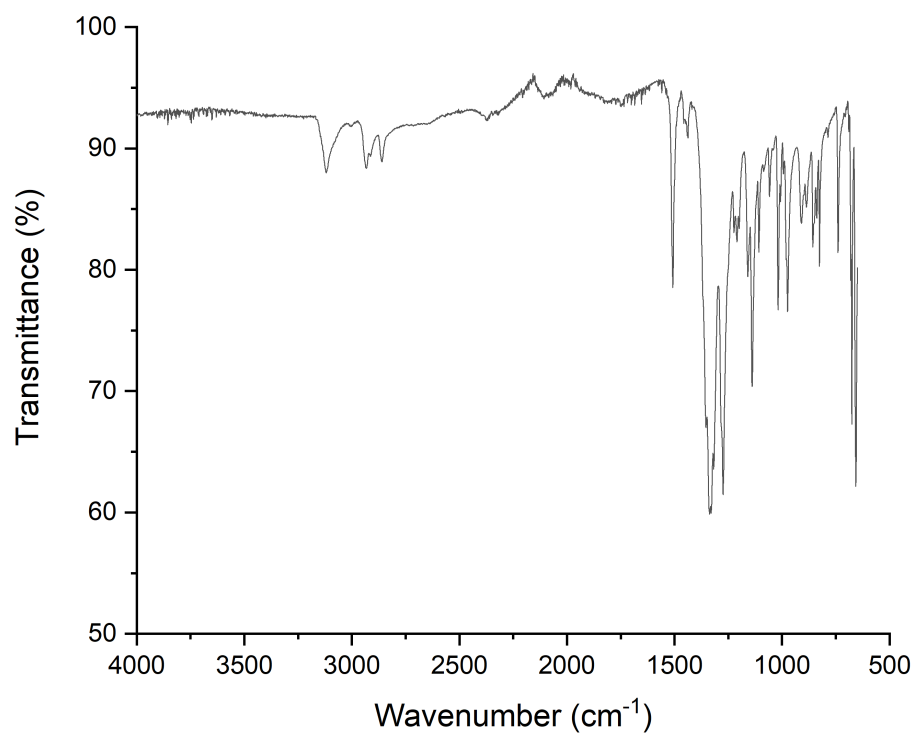


Figure S15. FT-IR spectrum of the coordination polymer **1**.

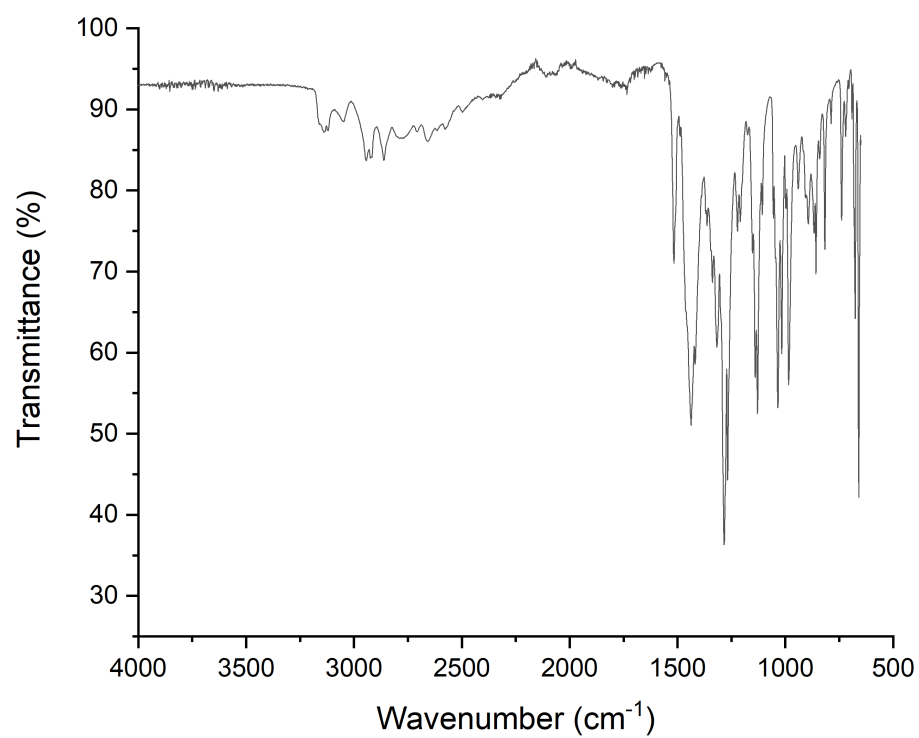


Figure S16. FT-IR spectrum of the coordination polymer **2**.

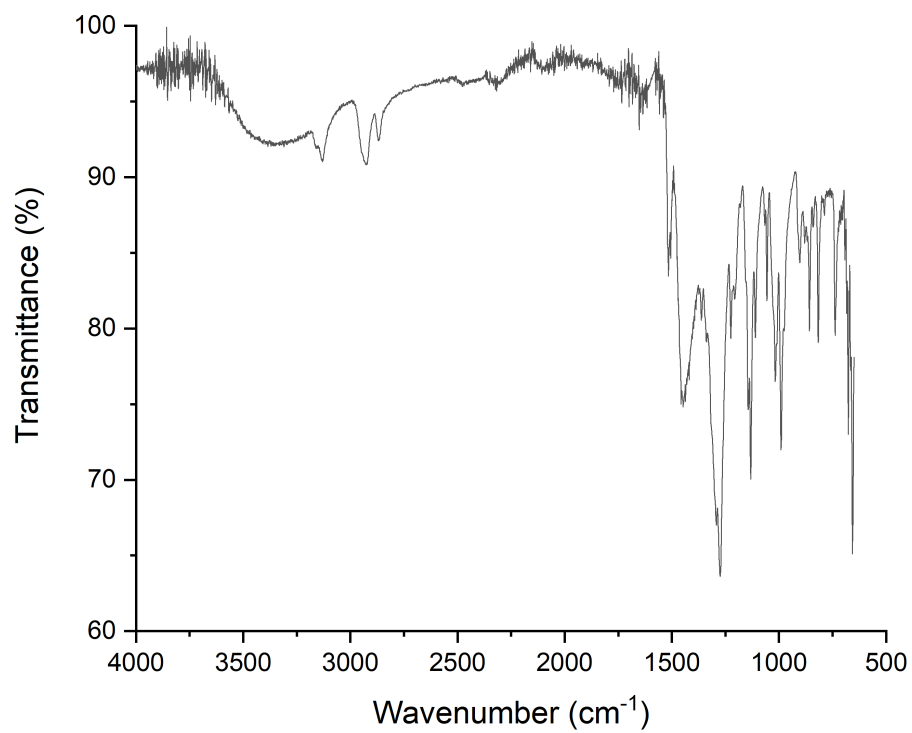


Figure S17. FT-IR spectrum of the coordination polymer **3**.

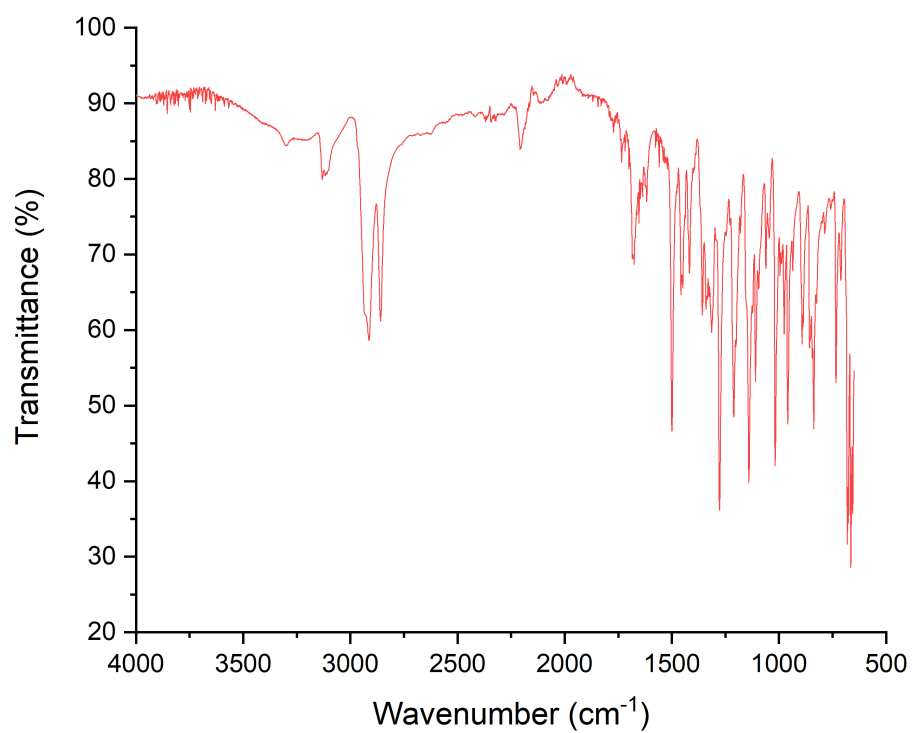


Figure S18. FT-IR spectrum of the ligand **L**.

Table S1. Interatomic distances, angles and geometrical criteria for nitrate coordination in compounds **1-3**.

Compound 1				
d ₁ (Ag1–O14), Å	2.640	d ₂ –d ₁ , Å	1.204 > 0.6	unidentate
d ₂ (Ag1–O15), Å	3.844	A ₁ –A ₂ , °	61.46 > 28	
d ₃ (Ag1–N18), Å	3.508	d ₃ –d ₂ , Å	-0.336 < 0.1	
A ₁ (Ag1–O14–N18), °	126.56	A ₃ , °	123.92 < 162	
A ₂ (Ag1–O15–N18), °	65.10			
A ₃ (Ag1–N18–O16), °	123.92			
d ₁ (Ag1–O11), Å	2.852	d ₂ –d ₁ , Å	1.105 > 0.6	unidentate
d ₂ (Ag1–O13), Å	3.957	A ₁ –A ₂ , °	59.85 > 28	
d ₃ (Ag1–N17), Å	3.827	d ₃ –d ₂ , Å	-0.13 < 0.1	
A ₁ (Ag1–O11–N17), °	134.77	A ₃ , °	155.06 < 162	
A ₂ (Ag1–O13–N17), °	74.92			
A ₃ (Ag1–N17–O12), °	155.06			
Compound 2				
d ₁ (Cd1–O12), Å	2.524	d ₂ –d ₁ , Å	0.103 < 0.3	bidentate
d ₂ (Cd1–O11), Å	2.627	A ₁ –A ₂ , °	4.87 < 14	
d ₃ (Cd1–N3), Å	2.967	d ₃ –d ₂ , Å	0.34 > 0.2	
A ₁ (Cd1–O12–N3), °	97.89	A ₃ , °	171.84 > 168	
A ₂ (Cd1–O11–N3), °	93.02			
A ₃ (Cd1–N3–O13), °	171.84			
d ₁ (Cd1–O21), Å	2.388	d ₂ –d ₁ , Å	0.860 > 0.6	unidentate
d ₂ (Cd1–O22), Å	3.248	A ₁ –A ₂ , °	41.97 > 28	
d ₃ (Cd1–N4), Å	3.220	d ₃ –d ₂ , Å	-0.028 < 0.1	
A ₁ (Cd1–O21–N4), °	119.67	A ₃ , °	156.73 < 162	
A ₂ (Cd1–O22–N4), °	77.70			
A ₃ (Cd1–N4–O23), °	156.73			
Compound 3				
d ₁ (Cd1–O11), Å	2.385	d ₂ –d ₁ , Å	0.217 < 0.3	bidentate
d ₂ (Cd1–O12), Å	2.602	A ₁ –A ₂ , °	11.50 < 14	
d ₃ (Cd1–N51), Å	2.917	d ₃ –d ₂ , Å	0.315 > 0.2	
A ₁ (Cd1–O11–N51), °	103.03	A ₃ , °	175.74 > 168	
A ₂ (Cd1–O12–N51), °	91.53			
A ₃ (Cd1–N51–O13), °	175.74			
d ₁ (Cd1–O15), Å	2.448	d ₂ –d ₁ , Å	0.052 < 0.3	bidentate
d ₂ (Cd1–O14), Å	2.500	A ₁ –A ₂ , °	-2 < 14	
d ₃ (Cd1–N52), Å	2.861	d ₃ –d ₂ , Å	0.361 > 0.2	
A ₁ (Cd1–O14–N52), °	93.97	A ₃ , °	176.72 > 168	
A ₂ (Cd1–O15–N52), °	95.97			
A ₃ (Cd1–N52–O16), °	176.72			
d ₁ (Cd2–O22), Å	2.330	d ₂ –d ₁ , Å	0.178 < 0.3	bidentate
d ₂ (Cd2–O21), Å	2.508	A ₁ –A ₂ , °	7.99 < 14	
d ₃ (Cd2–N72), Å	2.828	d ₃ –d ₂ , Å	0.320 > 0.2	
A ₁ (Cd2–O22–N72), °	100.23	A ₃ , °	172.38 > 168	
A ₂ (Cd2–O21–N72), °	92.24			
A ₃ (Cd2–N72–O23), °	172.38			
d ₁ (Cd2–O25), Å	2.401	d ₂ –d ₁ , Å	0.035 < 0.3	bidentate
d ₂ (Cd2–O24), Å	2.436	A ₁ –A ₂ , °	0.95 < 14	
d ₃ (Cd2–N71), Å	2.823	d ₃ –d ₂ , Å	0.387 > 0.2	
A ₁ (Cd2–O25–N71), °	96.00	A ₃ , °	173.48 > 168	
A ₂ (Cd2–O24–N71), °	95.05			
A ₃ (Cd2–N71–O26), °	173.48			

Table S2. Continuous shape measures criteria for seven-coordinated cadmium centers in compounds **2** and **3**.

Compound	S(PBPY)	S(COC)	S(CTPR)
Cd1 in 2	1.279	7.553	5.924
Cd1 in 3	3.927	7.726	6.245
Cd2 in 3	2.570	8.910	7.211