SUPPORTING INFORMATION

One-Dimensional Oxalato-Bridged Cu(II), Co(II), and Zn(II) Complexes with Purine and Adenine as Terminal Ligands

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Table S1. Hydrogen-bond parameters in compounds **1**–**4**[a]

D–*H*···*A*[b]	*H*···*A*	*D*···*A*	*D*–*H*···*A*
1			
O5w–H1w···N1^{i}	1.98	2.826(4)	170
O5w–H2w···O3^{ii}	2.27	3.017(3)	158
N7–H7···O2^{iii}	2.09	2.793(3)	138
2			
O5w–H1w···N1^{i}	1.99	2.750(2)	178
O5w–H2w···O3^{ii}	2.03	2.836(2)	165
N7–H7···O2^{iii}	2.12	2.802(2)	136
3			
O5w–H1w···N1^{i}	1.89	2.766(3)	170
O5w–H2w···O3^{ii}	1.99	2.824(3)	166
N7–H7···O2^{iii}	2.20	2.805(3)	125
4			
O5w–H···N1^{i}	1.82	2.756(4)	173
O5w–H2w···O3^{ii}	1.93	2.837(3)	165
N7–H7···O2^{iii}	2.15	2.845(4)	137
N6–H6A···O5w^{iv}	2.55	3.261(13)	140
N6–H6B···O1^{v}	2.23	2.903(13)	135

[a] Symmetry: (i) 1/2 + x, 1/2 – y, 1+ z ; (ii) 1– x, – y, 2 – z; (iii) 1/2 + x, 1/2 – y, z; (iv) –1/2 + x, 1/2 – y, 1 – z; (iv) 3/2 – x, 1/2 + y, 1 – z. [b]D = donor; A = acceptor.

Table S2. - stacking parameters in compounds **1**–**4**[a]

Ring···*Ring*[b, c]	*Angle*	*DC*	α	*DZ*	*DXY*	*Dist.*
1						
1–1^{i}	12.7	3.65	23.7	3.34	1.47	3.23–3.76
1–2^{ii}	11.5	3.41	10.3	3.36	0.61	3.17–3.76
2–2^{i}	10.2	3.66	23.5	3.36	1.46	3.17–3.71
2						
1–1^{i}	8.3	3.51	23.4	3.22	1.39	3.26–3.64
1–2^{ii}	7.3	3.39	15.3	3.27	0.89	3.44–4.63
2–2^{i}	6.2	3.49	22.5	3.22	1.34	3.15–3.58
3						
1–1^{i}	8.9	3.53	23.9	3.23	1.43	3.26–3.60
1–2^{ii}	7.6	3.40	14.9	3.29	0.87	3.16–3.53
2–2^{i}	6.3	3.51	23.0	3.23	1.37	3.16–3.53
4						
1–1^{i}	7.3	3.47	21.8	3.22	1.29	3.23–3.52
1–2^{ii}	6.5	3.36	15.8	3.23	0.91	3.15–3.48
2–2^{i}	5.4	3.45	21.7	3.21	1.28	3.15–3.47

[a] Symmetry: (i) – 1/2 + x, 1/2 – y, z; (ii) 1/2 + x, 1/2 – y, z. [b] Ring 1: pentagonal ring; Ring 2: hexagonal ring.

[c] Angle: dihedral angle between the rings (°), DC: distance between the centroids of the rings (Å), α: angle between the perpendicular to the first ring and the DC vector (°), DZ: distance between planes (Å), DXY: lateral displacement (Å), Dist: shortest distances between the non-hydrogen atoms from the two rings (Å).

Table S3. Hydrogen-bond parameters in compounds **5** and **6**[a]

D–H···A[b]	H···A		D···A		D–H···A	
	5	**6**	**5**	**6**	**5**	**6**
O5w–H51w···N1b^{i}	1.99	1.85	2.858(3)	2.869(4)	167	176
O5w–H52w···O4^{ii}	1.99	1.68	2.693(2)	2.691(3)	168	164
N9c–H9c···N3c^{iii}	2.03	1.92	2.885(3)	2.886(4)	177	168
O6w–H61w···N7c	2.17	2.13	3.015(3)	3.006(4)	155	135
N9a–H9a···O1^{ii}	2.38	2.22	3.091(3)	3.089(3)	140	147
O6w–H62w···N3c^{iv}	2.09	1.90	2.819(3)	2.810(4)	170	149
N9b–H9b···O6w	1.94	1.79	2.775(3)	2.774(4)	162	157
N6a–H6aA···N7c^{v}	2.27	2.17	3.123(3)	3.123(4)	175	172
N6a–H6aB···N1c^{vi}	2.06	1.99	2.884(3)	2.888(4)	161	160
N6b–H6bA···O3^{ii}	2.33	2.27	3.137(3)	3.143(4)	157	155
N6b–H6bB···O3^{vii}	2.23	2.06	3.062(3)	3.069(4)	163	167
N6c–H6cA···N7a^{viii}	2.13	2.04	2.987(3)	3.001(4)	177	165
N6c–H6cB···N1a^{ix}	2.14	2.01	2.945(3)	2.949(4)	156	161
C8a–H8a···O2^{x}	2.46	2.18	3.229(3)	3.236(3)	140	149
C8c–H8c···O6w^{iii}	2.64	2.67	3.518(3)	3.520(4)	158	143

[a]Symmetry: (i) x, –1 + y, z; (ii) 1 – x, 1 – y, – z ; (iii) 1 – x, 1 – y, 1 – z; (iv) 1 – x, – y, 1 – z; (v) –1 + x, y, z; (vi) –1 + x, 1+ y, z; (vii) 1 + x, 1 + y, z; (viii) 1 + x, –1 + y, z; (ix) 1 + x, y, z; (x) x, 1 + y, z. [b]D = donor; A = acceptor.

Table S4. - stacking parameters in compounds **5** and **6**[a]

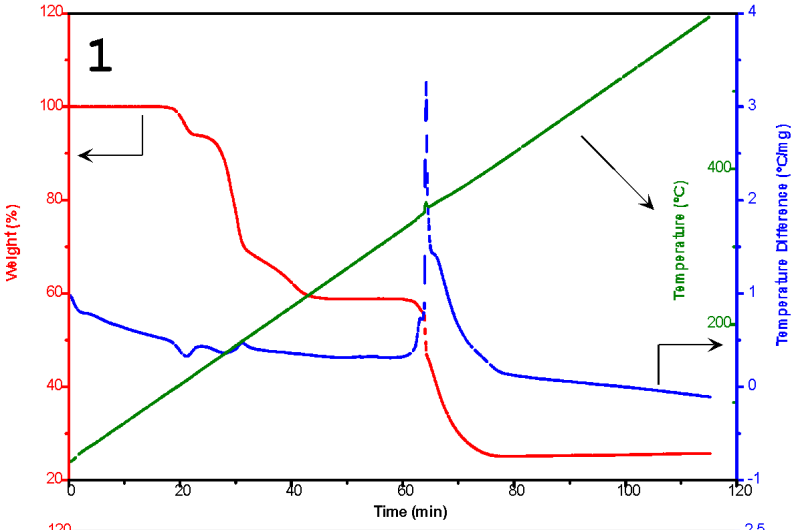
Ring···Ring[b,c]		Angle	DC	α	DZ	DXY	Dist.
adeAp–adeBp^{i}	**5**	12.2	3.56	23.7	3.26	1.43	3.09–3.65
	6	11.9	3.56	23.4	3.27	1.41	3.11–3.64
adeAp–adeBp	**5**	12.2	3.95	36.2	3.18	2.33	3.12–3.80
	6	11.9	3.97	36.1	3.21	2.34	3.19–4.03
adeAh– adeBp^{i}	**5**	13.1	3.37	14.8	3.26	0.86	3.09–3.38
	6	12.1	3.38	15.3	3.26	0.89	3.11–3.40
adeCp–adeCh^{ii}	**5**	0.28	3.70	18.8	3.50	1.19	3.46–3.97
	6	0.28	3.71	18.5	3.52	1.18	3.56–3.68
adeCp–adeCh^{iii}	**5**	0.28	3.79	25.3	3.43	1.62	3.46–3.83
	6	0.28	3.80	25.1	3.44	1.61	3.46–3.70

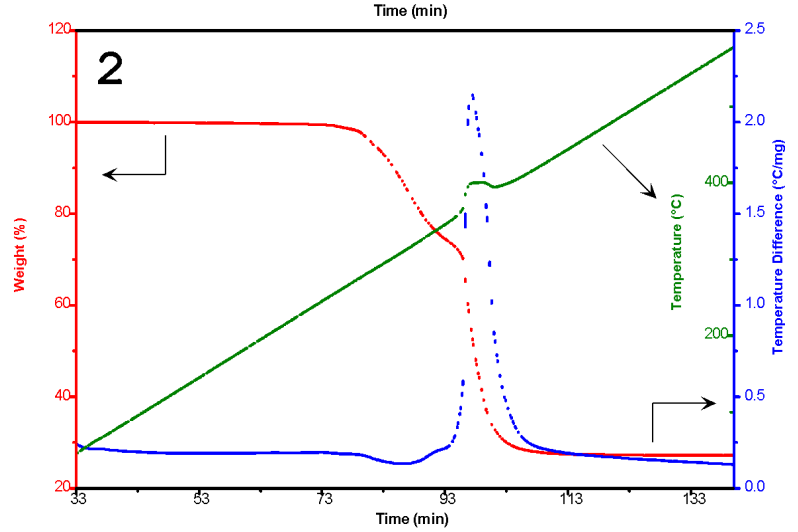
[a] Symmetry: (i) – 1 + x, y, z; (ii) 1 – x, – y, 1 – z; (iii) 2 – x; – y; 1 – z.

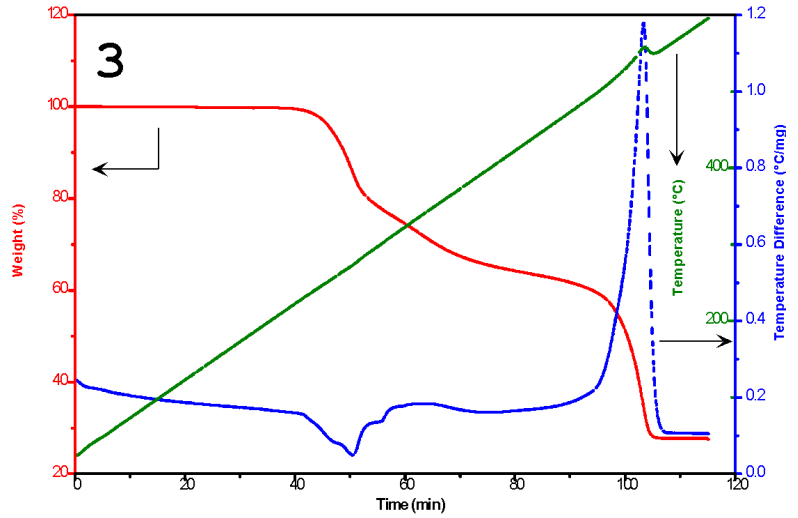
[b]Angle: dihedral angle between the rings (°), DC: distance between the centroids of the rings (Å), α: angle between the perpendicular to the first ring and the DC vector (°), DZ: distance between planes (Å), DXY: lateral displacement (Å), Dist: shortest distances between the non-hydrogen atoms from the two rings (Å).

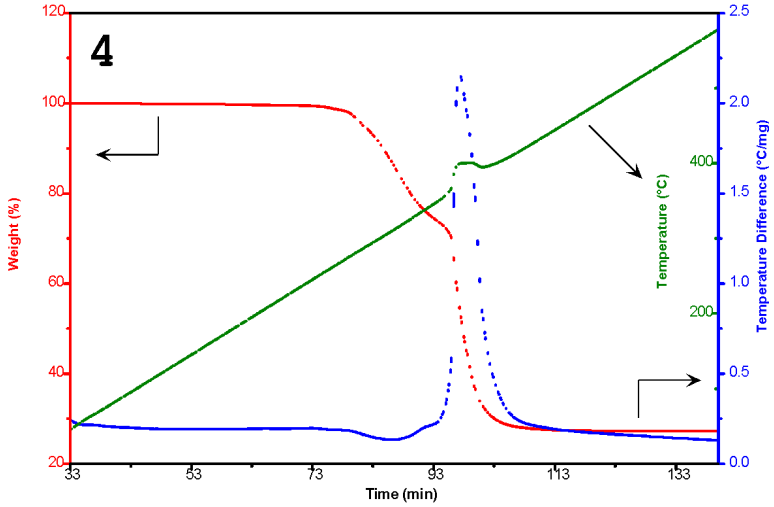
[c]*adeAp* (Adenine A, pentagonal ring): C4a, C5a, N7a, C8a, N9a; *adeAh* (Adenine A, hexagonal ring): N1a, C2a, N3a, C4a, C5a, C6a; *adeBp* (Adenine B, pentagonal ring): C4b, C5b, N7b, C8b, N9b; *adeBh* (Adenine B, hexagonal ring): N1b, C2b, N3b, C4b, C5b, C6b; *adeCp* (Adenine C, pentagonal ring): C4c, C5c, N7c, C8c, N9c; *adeCh* (Adenine C, hexagonal ring): N1c, C2c, N3c, C4c, C5c, C6c.

THERMOANALITIC CURVES (TG AND DTA)





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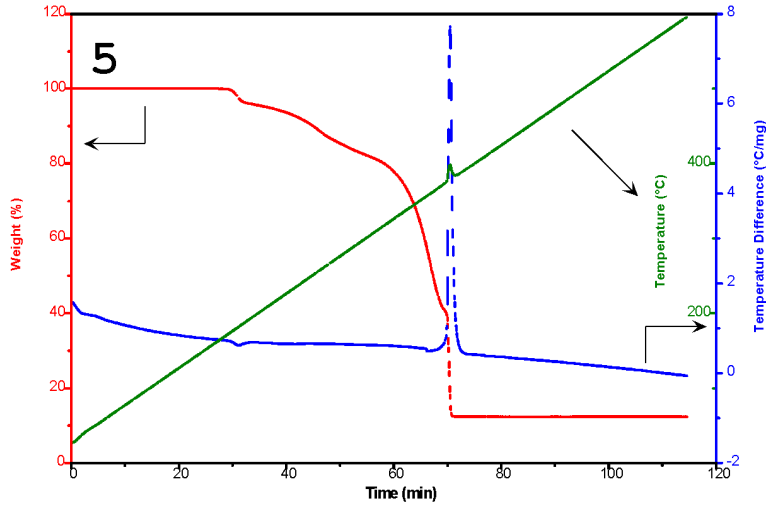
Weight (%)
Temperature (°C)
Temperature Difference (°C/mg)
Time (min)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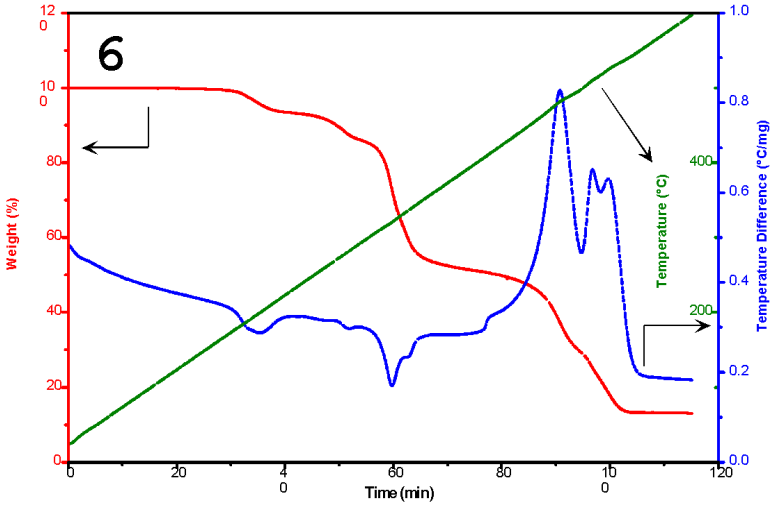
Temperature (°C)
Temperature Difference (°C/mg)
Time (min)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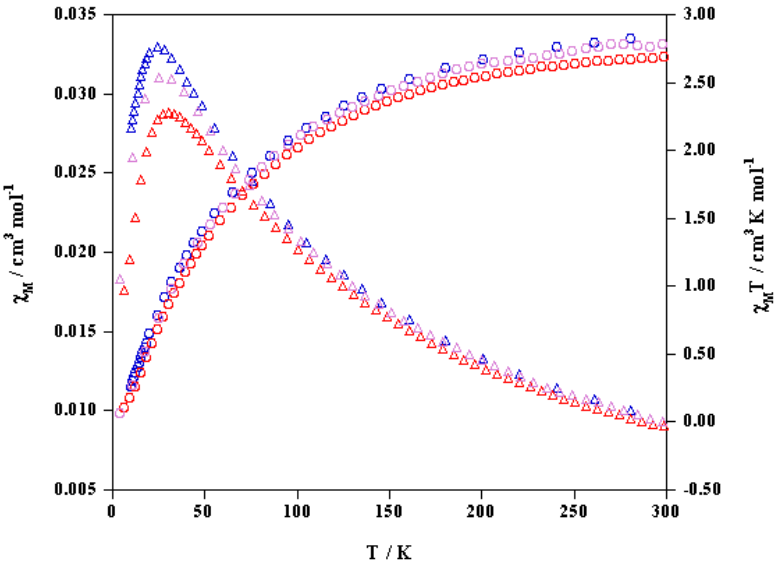
Weight (%)
Temperature (°C)
Temperature Difference (°C/mg)
Time (min)

MAGNETIC PROPERTIES



Thermal dependence of χ_M(Δ) and $\chi_M T$ (O) for compounds: **2** (blue), **4** (purple), **5** (red)