Electronic Supplementary Information

Structural diversity of transition-metal complexes derived from *N*-propionic acid functionalized 1,4,7-triazacyclononane: From enchanting cluster motifs to unprecedented homometallic polymeric networks

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Contents

Table S1 Selected bond lengths (Å), angles (º) and hydrogen bonding for complex **1**

Cu(1)–O(1)	2.099(4)	Cu(1)–N(1)	2.120(5)
Cu(2)–O(2)	1.959(4)	Cu(2)–O(3)	1.936(5)
Cu(2)–O(1)	2.511(4)		
O(1)–Cu(1)–N(1)	89.29(19)	O(1)–Cu(1)–N(1)^{i}	171.0(2)
O(1)–Cu(1)–N(1)^{ii}	101.4(2)	O(1)–Cu(1)–O(1)^{i}	85.71(17)
N(1)–Cu(1)–N(1)^{i}	84.4(2)	O(1)–Cu(2)–O(2)	56.49(15)
O(1)–Cu(2)–O(3)	90.1(2)	O(1)–Cu(2)–O(1)^{ii}	150.37(13)
O(1)–Cu(2)–O(2)^{ii}	100.99(15)	O(1)–Cu(2)–O(3)^{ii}	110.6(2)
O(2)–Cu(2)–O(3)	90.3(3)	O(2)–Cu(2)–O(2)^{ii}	90.00(19)
O(2)–Cu(2)–O(3)^{ii}	166.8(3)	O(3)–Cu(2)–O(3)^{ii}	92.3(3)

D–H···A	d(D–H)	d(H···A)	D(D···A)	∠(D–H···A)
O(3)–H(3C)···O(2)^{iii}	0.85	2.05	2.678(8)	130
O(3)–H(3C)···O(12)	0.85	2.56	3.167(10)	129
O(3)–H(3D)···O(22)	0.85	2.17	2.695(15)	120

Symmetry codes: i) 1–y,x–y,z; ii) y,x,1/2–z; iii) 1–y,1+x–y,z.

Table S2 Selected bond lengths (Å), angles (º) and hydrogen bonding for complex **2**

Zn(2)–N(1)	2.099(3)	Zn(2)–N(2)	2.093(3)
Zn(2)–N(3)	2.087(3)	Zn(2)–O(1)	2.080(2)
Zn(2)–O(3)	2.059(3)	Zn(2)–O(5)	2.068(2)
Zn(1)–O(2)	2.049(2)	Zn(1)–O(7)	2.110(3)
Zn(3)–O(6)	2.063(2)	Zn(3)–O(11)	2.076(4)
Zn(3)–O(12)	2.062(3)	Zn(3)–O(13)	2.107(4)
Zn(4)–O(4)	2.074(3)	Zn(4)–O(8)	2.083(4)
Zn(4)–O(9)	2.031(4)	Zn(4)–O(10)	2.074(3)
O(2)–Zn(1)–O(7)	86.09(11)	O(7)–Zn(1)–O(7)^{i}	180.00
O(2)–Zn(1)–O(7)^{i}	93.91(11)	O(2)–Zn(1)–O(2)^{i}	90.77(11)
O(2)–Zn(1)–O(2)^{ii}	180.00	O(2)–Zn(1)–O(2)^{iii}	89.23(11)
O(1)–Zn(2)–O(3)	86.64(11)	O(1)–Zn(2)–O(5)	87.96(10)
O(1)–Zn(2)–N(1)	91.03(11)	O(1)–Zn(2)–N(2)	175.41(11)
O(1)–Zn(2)–N(3)	95.45(11)	O(3)–Zn(2)–O(5)	85.90(11)
O(3)–Zn(2)–N(1)	96.80(13)	O(3)–Zn(2)–N(2)	92.13(11)
O(3)–Zn(2)–N(3)	176.64(12)	O(5)–Zn(2)–N(1)	177.06(13)
O(5)–Zn(2)–N(2)	96.37(11)	O(5)–Zn(2)–N(3)	91.54(11)
N(1)–Zn(2)–N(2)	84.72(12)	N(1)–Zn(2)–N(3)	85.81(13)
N(2)–Zn(2)–N(3)	85.98(12)	O(6)–Zn(3)–O(11)	94.29(10)
O(11)–Zn(3)–O(12)	88.58(10)	O(11)–Zn(3)–O(13)	175.91(14)
O(6)–Zn(3)–O(12)	91.11(10)	O(6)–Zn(3)–O(13)	88.68(10)
O(6)–Zn(3)–O(6)^{iii}	87.11(10)	O(6)–Zn(3)–O(12)^{iii}	176.73(11)
O(12)–Zn(3)–O(13)	88.54(10)	O(12)–Zn(3)–O(12)^{iii}	90.54(11)
O(8)–Zn(4)–O(9)	179.21(13)	O(4)–Zn(4)–O(8)	93.70(10)
O(4)–Zn(4)–O(9)	86.85(10)	O(8)–Zn(4)–O(10)	88.34(10)
O(4)–Zn(4)–O(10)	177.27(11)	O(9)–Zn(4)–O(10)	91.09(10)
O(4)–Zn(4)–O(10)^{iii}	89.71(11)	O(4)–Zn(4)–O(4)^{iii}	91.97(11)
O(10)–Zn(4)–O(10)^{iii}	88.52(12)		

D–H···A	d(D–H)	d(H···A)	D(D···A)	∠(D–H···A)
O(7)–H(7C)···O(1)^{i}	0.85	2.00	2.686(3)	137
O(7)–H(7D)···O(1)^{ii}	0.85	2.08	2.686(3)	128
O(6)–H(8C)···O(3)	0.85	1.88	2.636(3)	147

O(8)–H(8D)···O(3) [iii]	0.85	1.89	2.636(3)	145
O(9)–H(9C)···O(16)	0.85	2.39	2.721(6)	104
O(9)–H(9D)···O(16)	0.85	2.26	2.721(6)	114
O(10)–H(10D)···O(14)[iv]	0.85	2.29	2.770(4)	116
O(10)–H(10C)···O(33)[v]	0.85	2.45	3.093(4)	133
O(11)–H(11C)···O(5)	0.85	1.92	2.678(3)	148
O(11)–H(11D)···O(5)[iii]	0.85	2.00	2.678(3)	136
O(12)–H(12C)···O(15)	0.85	2.34	2.737(4)	109
O(12)–H(12D)···O(15)	0.85	2.33	2.737(4)	110
O(13)–H(13D)···O(13)[vi]	0.85	2.54	3.095(5)	117
O(13)–H(13C)···O(9)[vii]	0.85	2.50	3.095(5)	128
O(13)–H(13D)···O(13)[vii]	0.85	2.33	3.032(5)	140
O(13)–H(13D)···O(6)[viii]	0.85	2.23	2.884(4)	134
O(15)–H(15C)···O(31)	0.85	2.34	3.093(4)	147

Symmetry codes: i) 2–x,y,2–z; ii) 2–x,–y,2–z; iii) x,–y,z; iv) x,–1+y,z; v) 1–x,–y,1–z; vi) 1–x,y,1–z; vii) 2–x,y,1–z; viii) 2–x,–y,1–z.

Table S3 Selected bond lengths (Å), angles (º) and hydrogen bonding for complex **3**

Cd(1)–O(3)	2.356(4)	Cd(1)–O(3)^{i}	2.301(4)
Cd(1)–O(4)^{i}	2.626(5)	Cd(1)–O(5)	2.306(4)
Cd(1)–N(1)	2.380(5)	Cd(1)–N(2)	2.412(5)
Cd(1)–N(3)	2.353(5)		
N(1)–Cd(1)–N(2)	76.6(2)	N(1)–Cd(1)–N(3)	77.97(18)
N(2)–Cd(1)–N(3)	76.29(19)	O(3)–Cd(1)–N(1)	106.31(17)
O(3)–Cd(1)–N(2)	79.62(18)	O(3)–Cd(1)–N(3)^{i}	130.95(16)
O(3)^{i}–Cd(1)–N(1)	93.70(17)	O(3)^{i}–Cd(1)–N(2)	149.1(2)
O(3)^{i}–Cd(1)–N(3)	130.95(18)	O(4)^{i}–Cd(1)–N(1)	105.29(18)
O(4)^{i}–Cd(1)–N(2)	162.52(19)	O(4)^{i}–Cd(1)–N(3)	87.02(18)
O(5)–Cd(1)–N(1)	159.67(18)	O(5)–Cd(1)–N(2)	95.25(19)
O(5)–Cd(1)–N(3)	82.00(17)	O(3)–Cd(1)–O(3)^{i}	75.10(17)
O(3)–Cd(1)–O(4)^{i}	115.63(15)	O(3)–Cd(1)–O(5)	90.18(16)
O(3)^{i}–Cd(1)–O(4)^{i}	48.26(16)	O(3)^{i}–Cd(1)–O(5)	102.17(16)
O(4)^{i}–Cd(1)–O(5)	77.01(17)		

D–H···A	d(D–H)	d(H···A)	D(D···A)	∠(D–H···A)
O(1)–H(1C)···O(10)^{ii}	0.85	2.11	2.900 (7)	154
O(6)–H(6C)···O(4)^{ii}	0.85	2.28	2.938(7)	135

Symmetry codes: i) 2–x,1–y,2–z; ii) 2–x,1–y,1–z; iii) x,–1+y,z.

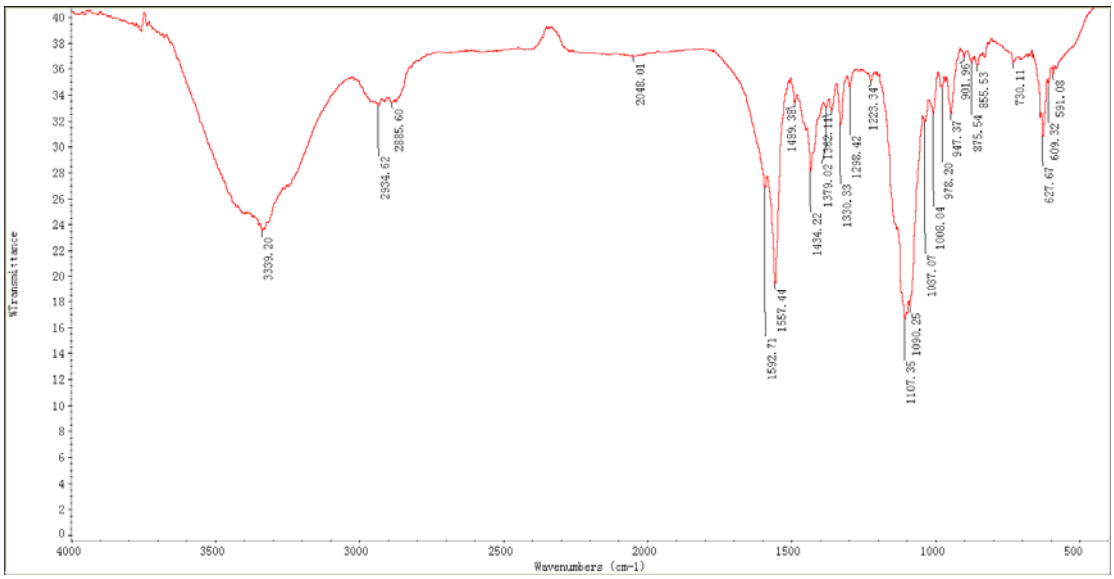
Table S4 Selected bond lengths (Å), angles (º) and hydrogen bonding for complex **4**

Cd(1)–O(1)	2.321(8)	Cd(1)–O(2)^{i}	2.267(8)
Cd(1)–O(3)	2.313(9)	Cd(1)–N(1)	2.414(9)
Cd(1)–N(2)	2.340(10)	Cd(1)–N(3)	2.376(11)
O(1)–Cd(1)–O(2)^{i}	84.3(3)	O(1)–Cd(1)–O(3)	85.4(3)
O(2)^{i}–Cd(1)–O(3)	93.0(3)	N(1)–Cd(1)–N(2)	76.0(3)
N(1)–Cd(1)–N(3)	75.0(3)	N(2)–Cd(1)–N(3)	76.6(4)
O(1)–Cd(1)–N(1)	81.3(3)	O(1)–Cd(1)–N(2)	157.2(3)
O(1)–Cd(1)–N(3)	95.4(3)	O(2)^{i}–Cd(1)–N (1)	161.3(3)
O(2)^{i}–Cd(1)–N (2)	117.3(3)	O(2)^{i}–Cd(1)–N (3)	94.7(3)
O(3)–Cd(1)–N(1)	97.6(3)	O(3)–Cd(1)–N(2)	99.8(4)
O(3)–Cd(1)–N(1)	172.4(3)		

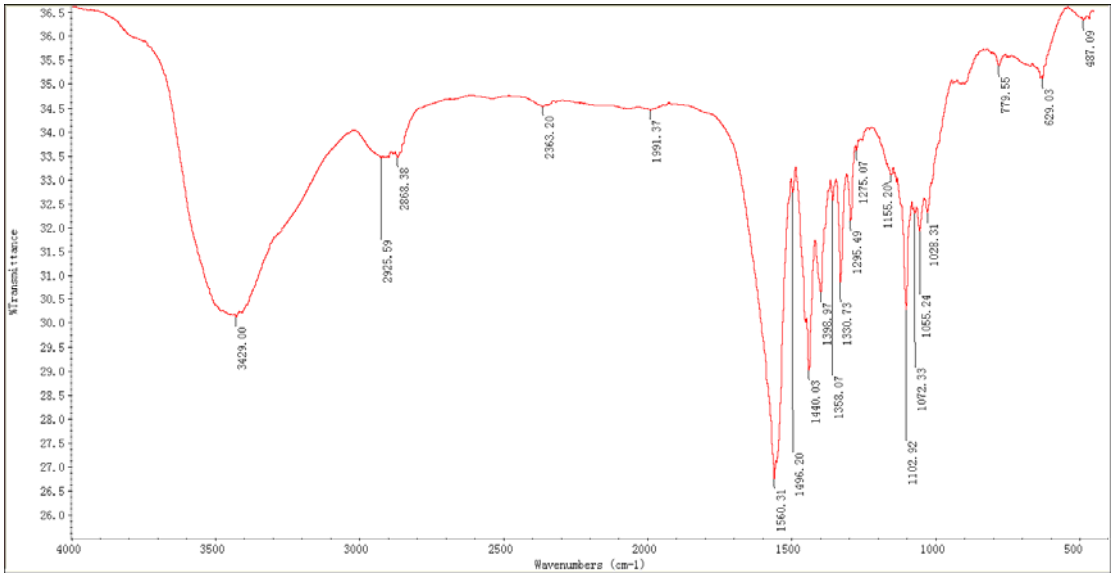
D–H···A	d(D–H)	d(H···A)	D(D···A)	∠(D–H···A)
N2–H2C···O2^{ii}	0.91	2.11	3.013(13)	172
N3–H3C···O4^{iii}	0.91	2.48	3.275(18)	147
O4–H4C···O2^{ii}	0.85	2.00	2.760(13)	149
O3–H3D···O4	0.85	1.90	2.652(13)	147

Symmetry codes: i) 1/2–x,–1/2+y,1/2–z; ii) x,–1+y,z; iii) 1/2–x,1/2+y,1/2–z.

Fig. S1 IR spectra of the complexes **!–4**



Complex 1



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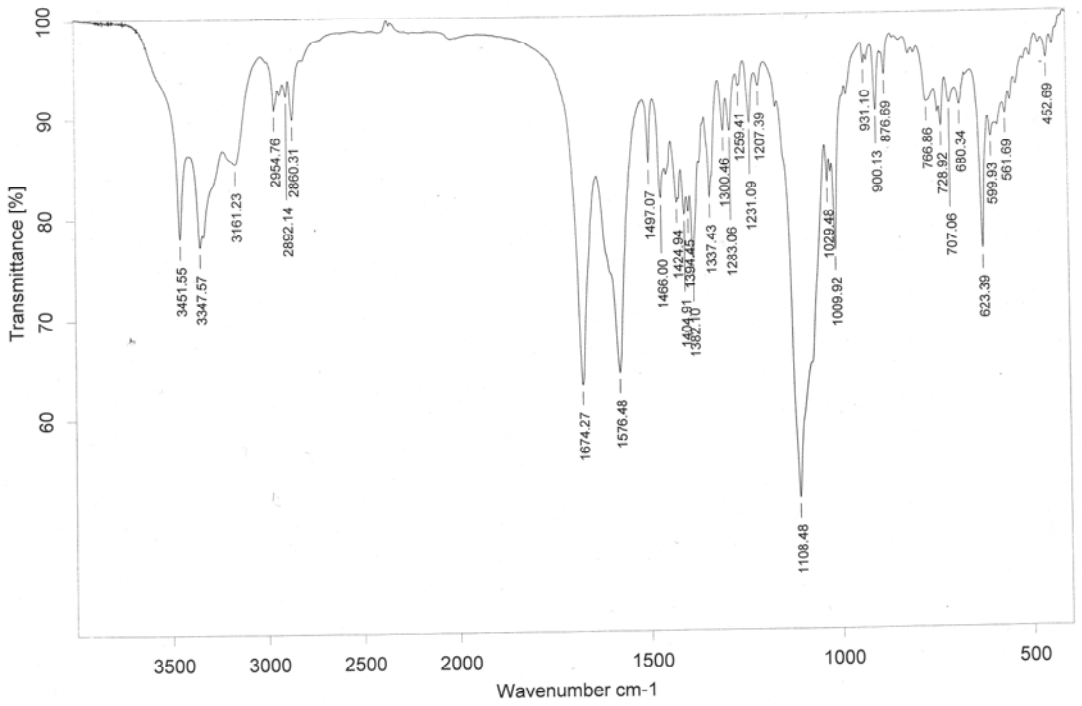
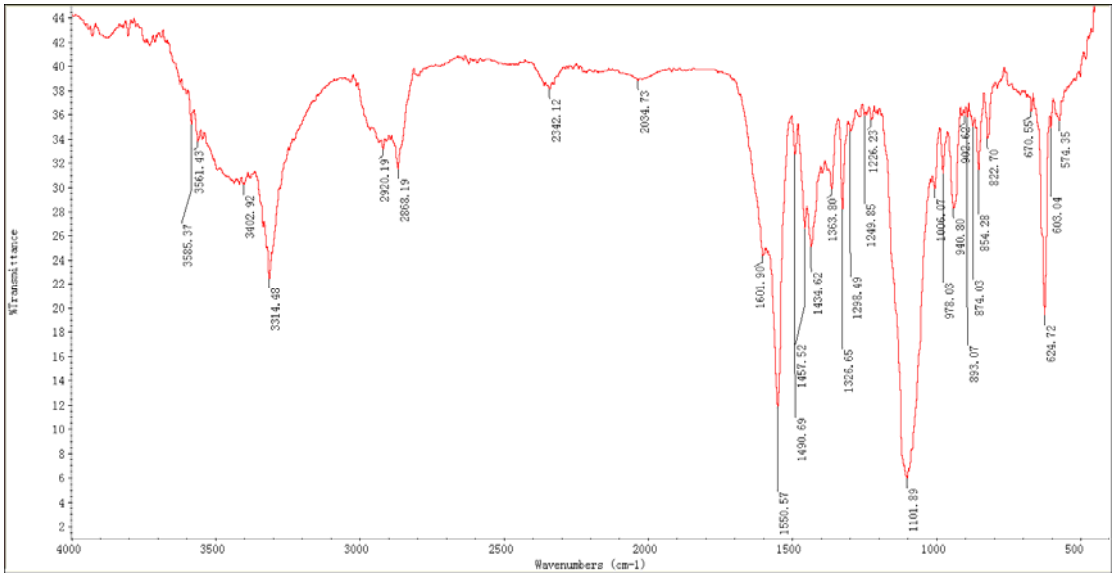


Complex 3



Complex 4