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Hydrothermal Syntheses and Structures of Three Novel Coordination Polymers Assembled from 1,2,3-Triazolate Ligands

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Supporting Information

Table S1. Selected Bond Lengths (Å) and Angles (°) for Complex **1**[a]

Cd(1)–N(3)	2.284(5)	Cd(1)–N(4)	2.292(5)
Cd(1)–N(2e)	2.339(5)	Cd(1)–Cl(2)	2.650(1)
Cd(1)–Cl(2b)	2.729(1)	Cd(1)–Cl(1)	2.739(1)
Cd(2)–N(1d)	2.269(5)	Cd(2)–N(1f)	2.269(5)
Cd(2)–N(5)	2.371(7)	Cd(2)–Cl(2)	2.706(1)
Cd(2)–Cl(2a)	2.706(1)	Cd(2)–Cl(1c)	2.711(2)
N(3)–Cd(1)–N(4)	170.5(2)	N(3)–Cd(1)–N(2e)	86.5(2)
N(4)–Cd(1)–N(2e)	84.1(2)	N(3)–Cd(1)–Cl(2)	97.3(1)
N(4)–Cd(1)–Cl(2)	92.2(1)	N(2e)–Cd(1)–Cl(2)	170.4(1)
N(3)–Cd(1)–Cl(2b)	91.1(1)	N(4)–Cd(1)–Cl(2b)	89.9(1)
N(2e)–Cd(1)–Cl(2b)	87.0(1)	Cl(2)–Cd(1)–Cl(2b)	84.10(5)
N(3)–Cd(1)–Cl(1)	89.7(1)	N(4)–Cd(1)–Cl(1)	88.7(1)
N(2e)–Cd(1)–Cl(1)	89.0(1)	Cl(2)–Cd(1)–Cl(1)	99.79(4)
Cl(2b)–Cd(1)–Cl(1)	175.90(4)	N(1d)–Cd(2)–N(1f)	168.2(2)
N(1d)–Cd(2)–N(5)	84.1(1)	N(1d)–Cd(2)–Cl(2)	90.7(1)
N(1f)–Cd(2)–Cl(2)	88.8(1)	N(5)–Cd(2)–Cl(2)	87.52(3)
Cl(2)–Cd(2)–Cl(2a)	175.05(6)	N(1d)–Cd(2)–Cl(1c)	95.9(1)
N(5)–Cd(2)–Cl(1c)	180.0	Cl(2)–Cd(2)–Cl(1c)	92.48(3)
N(1d)–Cd(2)–Cl(2a)	88.8(1)	N(1f)–Cd(2)–Cl(2a)	90.7(1)
N(1f)–Cd(2)–N(5)	84.1(1)	N(1f)–Cd(2)–Cl(1c)	95.9(1)
N(5)–Cd(2)–Cl(2a)	87.52(3)	Cl(2a)–Cd(2)–Cl(1c)	92.48(3)
Cd(2c)–Cl(1)–Cd(1)	136.35(3)	Cd(2c)–Cl(1)–Cd(1e)	136.35(3)
Cd(1)–Cl(1)–Cd(1e)	87.29(6)	Cd(1)–Cl(2)–Cd(2)	135.20(6)
Cd(1)–Cl(2)–Cd(1b)	95.90(5)	Cd(2)–Cl(2)–Cd(1b)	89.83(4)

[a] Symmetry codes: a: $1 - x$, y, $2.5 - z$; b: $0.5 - x$, $0.5 - y$, $2 - z$; c: $1 - x$, $-y$, $2 - z$; d: $-0.5 + x$, $0.5 - y$, $0.5 + z$; e: $1 - x$, y, $1.5 - z$; f: $1.5 - x$, $0.5 - y$, $2 - z$.

Table S2. Selected Bond Lengths (Å) and Angles (°) for Complex **2**[b]

Cd(1)–N(1)	2.339(4)	Cd(2)–N(2)	2.364(6)
N(1g)–Cd(1)–N(1)	89.8(1)	N(1f)–Cd(1)–N(1)	180.0
N(1b)–Cd(1)–N(1)	90.2(1)	N(2e)–Cd(2)–N(2)	90.0
N(2)–Cd(2)–N(2c)	180.0		

[b] Symmetry codes: a: z, $0.5 + x$, $-0.5 + y$; b: $-0.5 + y$, $0.5 + z$, x; c: $0.25 - x$, $1.25 - y$, z; d: z, $0.75 - x$, $0.75 - y$; e: $0.75 - y$, $0.5 + z$, $0.25 - x$; f: $-x$, $1 - y$, $-z$; g: $-z$, $0.5 - x$, $0.5 - y$; h: $0.5 - y$, $0.5 - z$, $-x$; i: $0.25 - x$, y, $0.25 - z$; j: $0.5 - y$, $0.75 + x$, $0.25 + z$; k: $-0.25 + y$, $0.5 - x$, $0.25 + z$.

Table S3. Selected Bond Lengths (Å) and Angles (°) for Complex **3**[c]

Cu(1)–N(1)	1.976(9)	Cu(1)–I(3)	2.643(2)
Cu(1)–I(4)	2.685(2)	Cu(1)–I(1)	2.746(2)
Cu(2)–N(2)	1.872(10)	Cu(2)–N(2a)	1.872(10)
Cu(3)–N(3)	1.900(10)	Cu(3)–N(4)	1.904(9)
Cu(4)–N(5b)	1.988(10)	Cu(4)–I(2b)	2.749(2)
Cu(4)–I(3)	2.630(2)	Cu(4)–I(4)	2.718(2)
Cu(5)–N(9)	1.990(9)	Cu(5)–I(1)	2.696(2)
Cu(5)–I(2b)	2.705(2)	Cu(5)–I(3)	2.653(2)
Cu(6)–N(6c)	1.904(10)	Cu(6)–N(7d)	1.906(10)
Cu(6)–I(5)	2.962(2)	Cu(7)–N(8a)	1.922(10)
Cu(7)–I(5)	2.877(3)	Cu(7)–N(8)	1.922(10)
N(1)–Cu(1)–I(3)	105.4(3)	I(3)–Cu(1)–I(4)	113.31(7)
N(1)–Cu(1)–I(4)	114.6(3)	I(3)–Cu(1)–I(1)	119.39(6)
N(1)–Cu(1)–I(1)	107.5(3)	I(4)–Cu(1)–I(1)	96.84(6)
N(2)–Cu(2)–N(2a)	174.4(6)	N(3)–Cu(3)–N(4)	161.5(5)
N(5b)–Cu(4)–I(3)	114.2(3)	I(3)–Cu(4)–I(4)	112.61(7)
N(5b)–Cu(4)–I(4)	109.6(3)	I(3)–Cu(4)–I(2b)	113.15(6)
N(5b)–Cu(4)–I(2b)	100.4(3)	I(4)–Cu(4)–I(2b)	105.94(7)
N(9)–Cu(5)–I(3)	106.2(3)	I(3)–Cu(5)–I(1)	120.88(6)
N(9)–Cu(5)–I(1)	108.0(3)	I(3)–Cu(5)–I(2b)	113.87(7)
N(9)–Cu(5)–I(2b)	107.1(3)	I(1)–Cu(5)–I(2b)	100.10(6)
N(6c)–Cu(6)–I(5)	103.8(3)	N(6c)–Cu(6)–N(7d)	153.8(5)
N(7d)–Cu(6)–I(5)	102.4(3)	N(8)–Cu(7)–I(5c)	102.4(3)
N(8)–Cu(7)–N(8a)	148.7(6)	N(8a)–Cu(7)–I(5c)	102.4(3)

[c] Symmetry codes: a: x, 0.5 – y, z; b: 0.5 + x, y, 0.5 – z; c: 0.5 + x, y, –0.5 – z; d: –0.5 + x, y, –0.5 – z; e; –0.5 + x, y, –0.5 – z; f: –0.5 + x, y, 1.5 – z; g: –1 + x, 0.5 – y, z; h: –1 + x, y, z.