Electronic Supplementary Information

Solvent-driven azide-induced mononuclear discrete versus one-dimensional polymeric aromatic Möbius cadmium(II) complexes of N_6 tetradentate helical ligand

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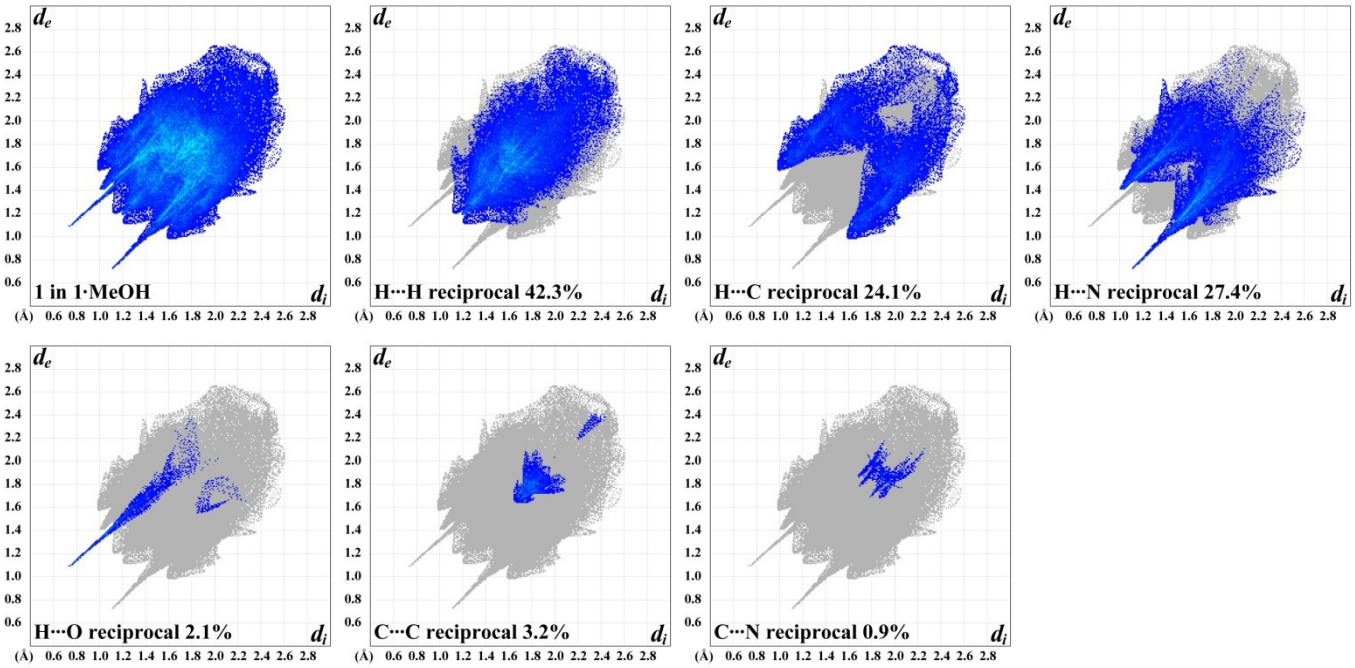

Fig. S1. 2D and decomposed 2D fingerprint plots of observed contacts for **1** in **1·MeOH**.

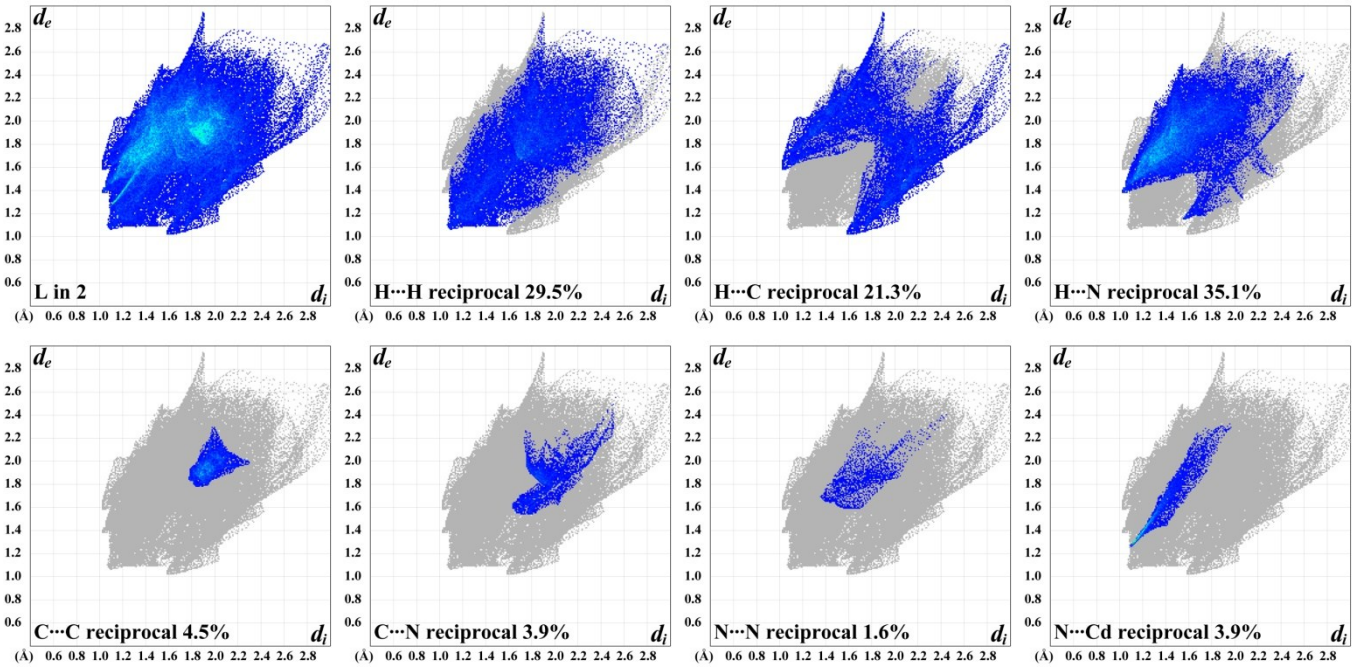

Figure S2. 2D and decomposed 2D fingerprint plots of observed contacts for **L** in **2**.

Table S1. Selected bond lengths (Å) and angles (°) for **1·MeOH** and **2**

	Complex 1·MeOH	**Complex 2**
Bond lengths		
$Cd–N_{Py}$	2.372(2), 2.378(2)	2.3512(14), 2.3866(14)
$Cd–N_{imine}$	2.480(2), 2.533(2)	2.3874(13), 2.3894(13)
$Cd–N_{azide}$	2.270(2), 2.327(2)	2.283(2), 2.304(2)
$Cd–O_{methanol}$	2.539(2)	—
Cd(L)···Cd(L)	7.941 (the shortest separation)	8.912
$Cd(L)\cdots Cd(N_{azide})_6$	—	5.618, 5.892
$Cd(N_{azide})_6\cdots Cd(N_{azide})_6$	—	3.538, 5.404
$Cd–\mu_{1,3}\text{-}N_{azide}(–CdL)$	—	2.320(2), 2.330(2)
$Cd–\mu_{1,1}\text{-}N_{azide}$	—	2.2702(13), 2.2801(13)
$Cd–\mu_{1,1,1}\text{-}N_{azide}$	—	2.3933(13), 2.4033(12), 2.4428(13)
$Cd–\mu_{1,3}\text{-}N_{azide}$	—	2.304(2), 2.308(2)
$Cd–\mu_{1,1,3}\text{-}N_{azide}$	—	2.3359(14), 2.363(2), 2.4329(13)
Bond Angles		
$N_{Py}–Cd–N_{Py}$	168.91(6)	163.35(5)
$N_{Py}–Cd–N_{imine}$	65.56(6), 66.53(6), 124.03(6), 124.08(6)	67.72(4), 67.81(5), 124.96(5), 128.45(5)
$N_{Py}–Cd–N_{azide}$	85.57(6), 88.26(7), 88.76(7), 93.18(6)	81.09(6), 87.08(6), 87.27(6), 90.04(6)
$N_{Py}–Cd–O_{methanol}$	82.04(6), 87.00(6)	—
$N_{imine}–Cd–N_{imine}$	168.91(6)	77.52(4)
$N_{imine}–Cd–N_{azide}$	77.25(6), 82.64(6), 118.28(7), 119.03(6)	88.06(6), 93.05(5), 130.95(6), 139.09(5)
$N_{imine}–Cd–O_{methanol}$	140.16(6), 146.41(6)	—
$N_{azide}–Cd(L)–N_{azide}$	157.64(7)	125.13(6)
$N_{azide}–Cd–O_{methanol}$	75.03(6), 83.21(6)	—
$N_{azide}–Cd–N_{azide}$	—	75.94(4), 77.58(4), 79.66(4), 80.01(5), 81.28(5), 85.89(5), 86.10(6), 87.86(5), 89.99(5), 90.01(7), 90.16(4), 90.28(5), 90.80(6), 91.37(6), 92.50(6), 92.73(6), 93.45(5), 93.58(5), 94.71(5), 94.88(6), 96.70(6), 96.76(5), 103.96(5), 105.75(7), 162.69(6), 163.23(5), 167.72(5), 169.94(6), 174.49(5), 176.08(6)
Torsion angles		
N–C(Ph)–C(Ph)–N	75.03(6)	76.5(2)
C(Ph)–N–N–C	121.7(2), 137.72(19)	119.18(15), 125.21(16)
Py···Py	69.00(10)	60.47(9)
Py···Ph	51.00(10), 68.65(10), 68.79(10), 76.56(10)	62.21(9), 66.81(9), 67.46(9), 83.39(10)
Ph···Ph	86.46(10)	88.44(9)

Table S2. Classic hydrogen bond lengths (Å) and angles (°) for **1·MeOH**

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(DHA)
O(1)–H(1)···O(2)[a]	0.88(4)	1.93(4)	2.781(2)	164(3)
O(2)–H(2)···N(4)	0.88(4)	1.94(4)	2.787(3)	161(4)

[a]Symmetry transformations used to generate equivalent atoms: –*x*, 1 – *y*, 1 – *z*.

Table S3. π···π interaction distances (Å) and angles (°) for **1·MeOH** and **2**[a]

Complex	Cg(*I*)	Cg(*J*)	*d*[Cg(*I*)–Cg(*J*)]	α	β	γ	slippage
1·MeOH[b]	Cg(1)	Cg(1)$^{\#1}$	3.6360(12)	0.02(10)	20.9	20.9	1.298
	Cg(2)	Cg(2)$^{\#2}$	3.7038(12)	0.00(10)	25.5	25.5	1.592
2[c]	Cg(15)	Cg(16)$^{\#1}$	3.7242(11)	0.00(10)	12.1	12.1	0.783
	Cg(16)	Cg(15)$^{\#2}$	3.7003(10)	0.00(8)	14.9	14.9	0.954

[a]Cg(*I*)–Cg(*J*): distance between ring centroids; α: dihedral angle between planes Cg(*I*) and Cg(*J*); β: angle Cg(*I*) → Cg(*J*) vector and normal to plane *I*; γ: angle Cg(*I*) → Cg(*J*) vector and normal to plane *J*; slippage: distance between Cg(*I*) and perpendicular projection of Cg(*J*) on ring *I*.
[b]Symmetry transformations used to generate equivalent atoms: #1 –*x*, 1 – *y*, –*z*; #2 1 – *x*, 1 – *y*, 1 – *z*. Cg(1): N(11)–C(12)–C(13)–C(14)–C(15)–C(16), Cg(2): N(30)–C(25)–C(26)–C(27)–C(28)–C(29).
[c]Symmetry transformations used to generate equivalent atoms: #1 1 – *x*, 1 – *y*, 1 – *z*; #2 1 – *x*, –*y*, 1 – *z*. Cg(15): N(1)–C(2)–C(3)–C(4)–C(5)–C(6), Cg(16): N(6)–C(24)–C(25)–C(26)–C(27)–C(28).

Table S4. C–H···π and N–N···π interaction distances (Å) and angles (°) for **1·MeOH** and **2**[a]

Complex	X–Y(*I*)	Cg(*J*)	*d*[Y(*I*)–Cg(*J*)]	*d*[X–Cg(*J*)]	∠ XYCg)	γ
1·MeOH[b]	C(13)–H(13)	Cg(4)$^{\#1}$	2.48	3.320(2)	147	7.97
	C(33)–H(33)	Cg(2)$^{\#2}$	2.76	3.655(2)	156	11.62
	C(40)–H(40)	Cg(3)$^{\#3}$	2.70(3)	3.604(2)	163(3)	8.84
2[c]	C(2)–H(2)	Cg(18)$^{\#1}$	2.70	3.589(2)	158	14.83
	N(17)–N(18)	Cg(17)$^{\#2}$	3.580(2)	3.9426(17)	100.04(12)	28.11

[a]Y(*I*)–Cg(*J*): distance of Y to ring centroid; X–Cg(*J*): distance of X to ring centroid; ∠(XYCg): angle X–Y–Cg; γ: angle Y(*I*) → Cg(*J*) vector and normal to plane *J*.
[b]Symmetry transformations used to generate equivalent atoms: #1 –*x*, 1 – *y*, –*z*; #2 *x*, –1 + *y*, *z*; #3 1 – *x*, –*y*, –*z*. Cg(2): N(30)–C(25)–C(26)–C(27)–C(28)–C(29), Cg(3): C(31)–C(32)–C(33)–C(34)–C(35)–C(36), Cg(4): C(37)–C(38)–C(39)–C(40)–C(41)–C(42).
[c]Symmetry transformations used to generate equivalent atoms: #1 2 – *x*, 1 – *y*, 1 – *z*; #2 1 – *x*, –*y*, 1 – *z*. Cg(17): C(9)–C(10)–C(11)–C(12)–C(13)–C(14); Cg(18): C(16)–C(17)–C(18)–C(19)–C(20)–C(21).