SUPPLEMENTARY MATERIALS SECTION

Hexnuclear Cadmium(II) Cluster Constructed from Tris(2-methylpyridyl)amine (TPA) and Azides

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X-ray crystal structure analysis

The X-ray single-crystal data of the title compound were collected on a Bruker-AXS APEX II CCD diffractometer at 100(2) K. The crystallographic data, conditions retained for the intensity data collection and some features of the structure refinements are listed in Table S1. The intensities were collected with Mo-Kα radiation (λ= 0.71073 Å). Data processing, Lorentz-polarization and absorption corrections were performed using APEX and the SADABS computer programs [S1]. The structures were solved by direct methods and refined by full-matrix least-squares methods on F^2, using the SHELX [S2] program library. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were located from difference Fourier maps, assigned with isotropic displacement factors and included in the final refinement cycles by use of geometrical constraints. Molecular plots were performed with the Mercury program. [S3]. Water molecules show twofold disorder with split occupancies of 0.778(7) for O1A and 0.222(7) for O1B, respectively.

References

[S1] (a) Bruker APEX, SAINT; (2006); Bruker AXS Inc. Madison, Wisconsin, USA;
(b) G.M. Sheldrick (2001), SADABS v. 2. University of Goettingen, Germany.

[S2] (a) G.M. Sheldrick, Acta Crystallogr. A64 (2008) 112;
(b) G.M. Sheldrick, Acta Crystallogr. C71 (2015) 3.

[S3] C.F. Macrae, P.R. Edington, P. McCabe, E. Pidcock, G.P. Shields, R. Taylor, T. Towler, J. van de Streek, J. Appl. Cryst. 39 (2006) 453.

Table S1. Crystallographic data and processing parameters

Empirical formula	$C_{72}H_{76}Cd_6Cl_2N_{46}O_{10}$
Formula mass	2491.15
System	Monoclinic
Space group	$P2_1/c$
a (Å)	12.747(3)
b (Å)	22.488(5)
c (Å)	16.219(3)
α (°)	90
β (°)	94.512(9)
γ (°)	90
V (Å^3)	4634.8(17)
Z	2
T (K)	100(2)
μ (mm^{-1})	1.490
D_{calc} (Mg/m^3)	1.785
Crystal size (mm)	0.23 × 0.18 × 0.15
θ max (°)	27.000
Data collected	186288
Unique refl. / R_{int}	10097 / 0.1091
Parameters	629
Goodness-of-Fit on F^2	1.056
R1 / wR2 (all data)	0.0363 / 0.1001

Table S2. Selected bond lengths (Å) and angles (°)

Cd1-N2	2.325(3)	Cd1-N3	2.356(3)
Cd1-N8	2.371(3)	Cd1-N4	2.392(3)
Cd1-N1	2.505(3)	Cd1-N19′	2.530(3)
Cd1-N5	2.607(3)	Cd2-N8	2.287(3)
Cd2-N14	2.298(3)	Cd2-N5	2.344(3)
Cd2-N11′	2.374(3)	Cd2-N11	2.378(3)
Cd2-N17′	2.418(3)	Cd3-N23	2.333(3)
Cd3-N22	2.382(3)	Cd3-N22	2.382(3)
Cd3-N21	2.392(3)	Cd3-N14	2.404(3)
Cd3-N17	2.406(4)	Cd3-N20	2.482(3)
Cd3-N13	2.547(3)	N5-N6	1.195(5)
N6-N7	1.163(5)	N8-N9	1.205(5)
N9-N10	1.146(5)	N11-N12	1.211(5)
N12-N13	1.164(5)	N14-N15	1.2218(5)
N15-N16	1.151(5)	N17-N18	1.194(4)
N18-N19	1.162(4)		
Cd1-N5-N6	135.6(3)	Cd2-N5-N6	117.0(3)
Cd1-N5-Cd2	98.86(12)	N5-N6-N7	179.6(5)
Cd2-N8-N9	126.7(3)	Cd1-N8-N9	118.5(2)
Cd1-N8Cd2	107.82(13)	N8-N9-N10	178.1(4)
Cd2′-N11-N12	112.2(2)	Cd2-N11-N12	107.3(2)
Cd2-N11-Cd2′	95.86(12)	N11-N12-N13	178.5(4)
Cd2-N14-N15	118.0(3)	Cd3-N14-N15	108.7(2)
Cd2-N14-Cd3	132.84(14)	N14-N15-N16	179.0(4)
Cd2′-N17-N18	107.0(2)	Cd3-N17-N18	120.4(3)
Cd2′-N17-Cd3	132.52(14)	N17-N18-N19	178.6(4)
Cd1′-N19-N18	107.1(3)	Cd3-N13-N12	106.0(2)
N8-Cd2-N11′	169.51(12)	N5-Cd2-N11	171.99(11)
N14-Cd2-N17′	169.11(11)	N11′-Cd2-N17′	82.59(11)
N8-Cd2-N14	103.28(12)	N1-Cd1-N3	68.99(11)
N3-Cd1-N19	164.04(11)	N20-Cd3-N21	69.38(11)
N14-Cd3-N22	162.41(11)		

Symmetry code: (′) 1-x,1-y,1-z.

Table S3. π···π ring···ring interactions [a)]

		Symmetry ring B	Cg…Cg (Å)	Alpha (°)
ring 2	ring 4	[1-x,1-y,2-z]	4.223(3)	35.5(2)
ring 2	ring 5	[x,3/2-y,1/2+z]	4.475(3)	36.4(2)
ring 3	ring 5	[x,3/2-y,1/2+z]	4.594(3)	52.1(2)
ring 3	ring 6	[-x,1-y,1-z]	4.650(3)	58.0(2)
ring 3	ring 7		4.566(3)	25.1(2)

[a)] Cg = center of gravity of ring, Alpha = dihedral angle between planes of rings.
Ring 2: [N2,C2-C6], ring 3: [N3,C8-C12], ring 4: [N4,C14-C18], ring 5: [N21,C20-C24], ring 6: [N22,C26-C30], ring 7: [N23,C32-C36]

Table S4. Possible hydrogen bonds

D-H…A[1)]	Symmetry of A	D..A (Å)	D-H..A (°)
O1A-H1AA…N7		2.934(7)	103.4
O1A-H2AA…O1		2.844(6)	166.8
C6-H6…N6		3.178(5)	121.3
C7-H7A…O4	[-1+x,3/2-y,1/2+z]	3.433(5)	163.4
C9-H9…O2	[-1+x,3/2-y,1/2+z]	3.516(5)	175.2
C11-H11…O4	[-1+x,y,z]	3.392(5)	143.5
C12-H12…N15		3.366(5)	148.8
C25-H25B…N10	[-x,1-y,1-z]	3.356(6)	133.8
C28-H28…O3	[1-x,-1/2+y,1/2-z]	3.385(6)	166.0
C36-H36…N13		3.287(5)	127.3

[1)] D = donor atom, A = acceptor atom,

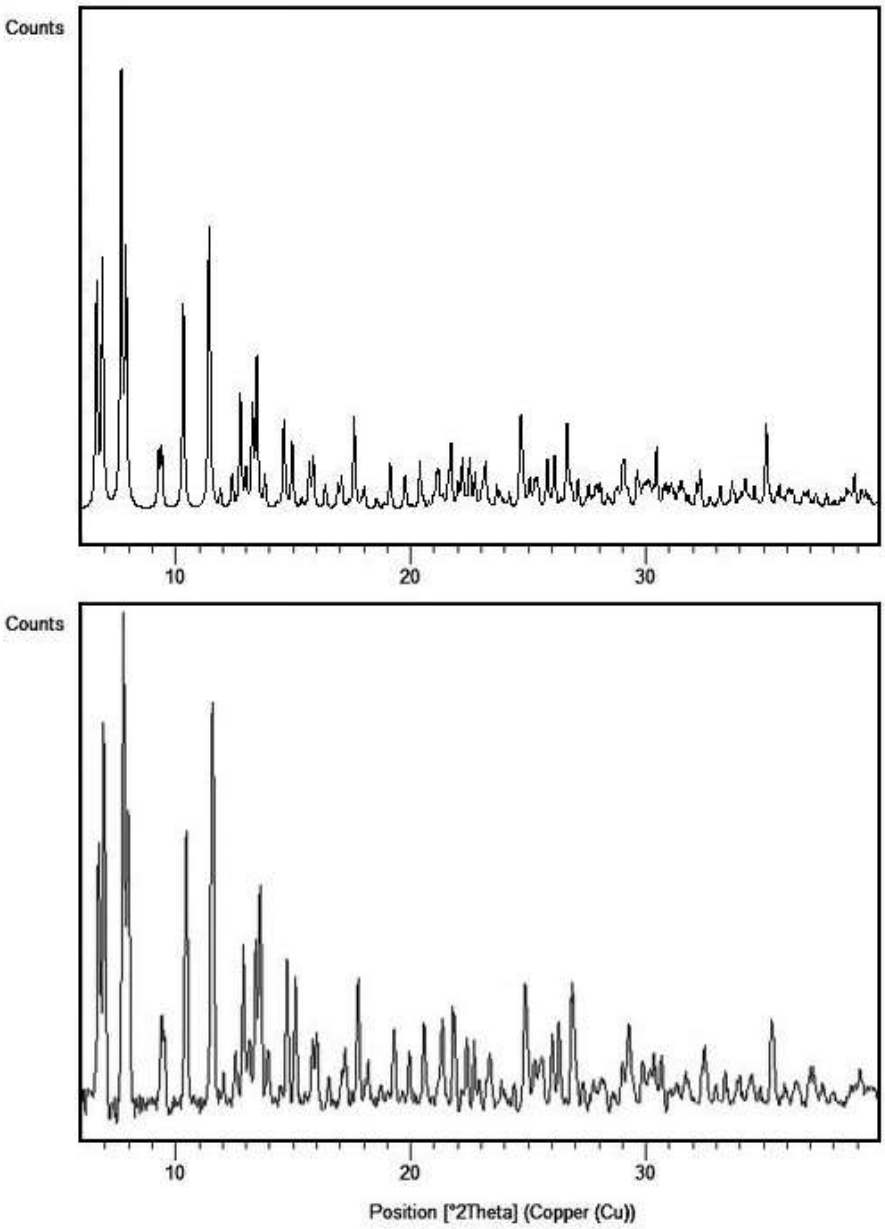

Figure S1. Observed (bottom) and simulated (top) X-ray powder pattern of the title complex. BRUKER D8 ADVANCE (Copper-Kα 2-Theta: 6-40°; 0.02°/step). PANALYTICAL X'PERT Highscore Plus full-pattern profile refinement: a = 12.802(2), b = 22.873(3), c = 16.296(2) Å, β = 94.254(8)°.