Supporting Information

STRUCTURAL DIVERSITY OF CADMIUM COORDINATION POLYMERS BASED ON THE EXTENDED ANILATE-TYPE LIGAND

Olesya Yu. Trofimova,[a] Irina N. Meshcheryakova,[a] Nikolai O. Druzhkov,[a] Irina V. Ershova,[a] Arina V. Maleeva,[a] Anton V. Cherkasov,[a] Ilya A. Yakushev,[b] Pavel V. Dorovatovskii[c], Rinat R. Aysin [d] and Alexandr V. Piskunov *[a]

[a] *G. A. Razuvaev Institute of Organometallic Chemistry of the Russian Academy of Sciences, Tropinin str., 49, Nizhny Novgorod, 603137, Russian Federation.*
[b] *Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences, Leninskii prosp., bld. 31, Moscow, 119991, Russian Federation.*
[c] *National Research Center «Kurchatov Institute», 1, Akademika Kurchatova pl., Moscow, 123182, Russian Federation*
[d] *A.N. Nesmeyanov Institute of Organometallic Chemistry of Russian Academy of Sciences, ul. Vavilova, 28 str 1, Moscow, 119991, Russian Federation.*
Electronic Supplementary Information (ESI) available: Crystal and structure refinement data. Experimental details and characteristics. See DOI: 10.1039/x0xx00000x

Table S1. Crystal data and structure refinement for **1**-**5**.

Compound	**1**	**2A**	**2B**	**3**	**4**	**5**
Formula	$C_{37}H_{49}CdN_3O_5$	$C_{53}H_{70}CdN_6O_6$	$C_{50}H_{63}CdN_5O_5$	$C_{42}H_{53}CdN_4O_5$	$C_{42}H_{58}CdN_4O_6$	$C_{80}H_{110}CdN_{12}O_8$
Formula weight	728.19	999.55	926.45	806.28	827.32	1480.19
Crystal system	Monoclinic	Triclinic	Monoclinic	Triclinic	Monoclinic	Triclinic
Space group	$P2_1/n$	P-1	$P2_1/c$	P -1	$P2_1/c$	P -1
a, Å	16.372(8)	12.4450(12)	10.0955(4)	10.0555(7)	10.664(3)	10.7318(12)
b , Å	10.139(3)	15.1029(14)	40.9697(15)	13.6937(10)	42.973(5)	14.1110(16)
c, Å	22.227(4)	15.5578(15)	11.4889(4)	17.1536(12)	9.228(2)	14.3004(17)
α, °	90	94.759(3)	90	92.456(2)	90	64.885(2)
β, °	101.261(15)	113.190(3)	98.1390(10)	106.837(2)	97.349(15)	72.876(8)
γ, °	90	103.711(3)	90	106.896(2)	90	75.908(5)
V, Å^3	3619(2)	2559.9(4)	4704.1(3)	2142.2(3)	4194.1(16)	1856.3(4)
Z	4	2	4	2	4	1
ρ, g/cm^3	1.337	1.297	1.308	1.250	1.310	1.324
θ range, °	1.915 – 30.970	2.453 – 27.485	2.098 – 27.997	2.231 – 25.084	2.539 – 28.922	1.798 – 30.556
Crystal size, mm	0.12 × 0.10 × 0.05	0.45 × 0.14 × 0.13	0.48 × 0.31 × 0.19	0.15 × 0.14 × 0.12	0.10 × 0.03 × 0.02	0.10 × 0.07 × 0.02
μ, mm^{-1}	0.868	0.480	0.515	0.554	0.763	0.479
Reflections Collected / unique	53524/8220	30652 / 11662	61434 / 11332	26806 / 7552	7894 / 7894	29459 / 8132
R_{int}	0.1102	0.0477	0.0265	0.0438	0.0635	0.0283
GOF on F^2	1.016	1.053	1.052	1.017	1.045	1.033
R_1, wR_2 [$I > 2\sigma(I)$]	0.0456, 0.0922	0.0448, 0.0911	0.0310, 0.0673	0.0482, 0.1036	0.0808, 0.1807	0.0437, 0.1139
R_1, wR_2 (all data)	0.0833, 0.1070	0.0660, 0.0990	0.0339, 0.0684	0.0655, 0.1108	0.1130, 0.1977	0.0483, 0.1170
$\Delta\rho_{max}/\Delta\rho_{min}$, e/Å^3	0.807 / -1.118	0.975 / -1.517	0.389 / -0.910	0.879 / -0.745	1.361 / -1.772	1.235 / -0.900

Table S2. Selected bond lengths (Å) in **1.**

Bond	**1**	**Bond**	**1**
Cd(1)-O(1)	2.165(3)	C(2)-C(3)	1.464(5)
Cd(1)-O(4C)	2.239(3)	C(3)-C(4)	1.472(6)
Cd(1)-O(5)	2.285(3)	C(4)-C(5)	1.344(5)
Cd(1)-O(4B)	2.309(3)	C(5)-C(6)	1.482(5)
Cd(1)-O(3B)	2.342(3)	C(15)-C(20)	1.396(6)
Cd(1)-O(2)	2.383(3)	C(15)-C(16)	1.402(5)
O(1)-C(1)	1.301(4)	C(16)-C(17)	1.382(5)
O(2)-C(6)	1.243(4)	C(17)-C(18)	1.397(5)
O(3)-C(24)	1.239(4)	C(18)-C(19)	1.400(5)
O(4)-C(23)	1.327(4)	C(19)-C(20)	1.388(5)
N(1)-C(3)	1.304(5)	C(21)-C(26)	1.461(5)
N(1)-C(15)	1.406(5)	C(21)-C(22)	1.480(5)
N(2)-C(21)	1.306(5)	C(22)-C(23)	1.365(5)
N(2)-C(18)	1.416(4)	C(23)-C(24)	1.499(5)
C(1)-C(2)	1.383(5)	C(24)-C(25)	1.476(5)
C(1)-C(6)	1.514(5)	C(25)-C(26)	1.341(5)

Symmetry transformations used to generate equivalent atoms **1**: (A) x + 1, y, z; (B) −x + 1, −y, −z+1; (C) x-1, y, z; (D) –x+2, -y, -z+1.

Table S3. Selected bond lengths (Å) in **2A**.

Bond	2A	Bond	2A
Cd(1)-O(2)	2.196(2)	C(15)-C(16)	1.407(4)
Cd(1)-O(3A)	2.217(2)	C(15)-C(20)	1.398(4)
Cd(1)-N(3)	2.296(2)	C(16)-C(17)	1.380(4)
Cd(1)-O(4A)	2.385(2)	C(17)-C(18)	1.406(4)
Cd(1)-N(4B)	2.306(2)	C(18)-C(19)	1.409(4)
Cd(1)-O(1)	2.399(2)	C(19)-C(20)	1.385(4)
O(1)-C(1)	1.240(3)	C(21)-C(22)	1.454(3)
O(2)-C(2)	1.294(3)	C(21)-C(26)	1.479(3)
O(3)-C(23)	1.298(3)	C(22)-C(23)	1.383(4)
O(4)-C(24)	1.242(3)	C(23)-C(24)	1.510(3)
N(1)-C(4)	1.310(3)	C(24)-C(25)	1.466(3)
N(1)-C(15)	1.402(3)	C(25)-C(26)	1.334(4)
N(2)-C(21)	1.309(3)	C(35)-C(36)	1.385(4)
N(2)-C(18)	1.400(3)	C(36)-C(37)	1.388(4)
N(3)-C(39)	1.345(3)	C(37)-C(38)	1.388(4)
N(3)-C(35)	1.338(3)	C(37)-C(40)	1.499(4)
N(4)-C(47)	1.346(3)	C(38)-C(39)	1.375(4)
N(4)-C(45)	1.344(3)	C(40)-C(41)	1.530(4)
C(1)-C(6)	1.469(4)	C(41)-C(42)	1.528(4)
C(1)-C(2)	1.513(3)	C(42)-C(43)	1.509(4)
C(2)-C(3)	1.395(3)	C(43)-C(46)	1.395(4)
C(3)-C(4)	1.457(4)	C(43)-C(44)	1.383(4)
C(4)-C(5)	1.483(3)	C(44)-C(45)	1.380(4)
C(5)-C(6)	1.342(3)	C(46)-C(47)	1.382(4)

Symmetry transformations used to generate equivalent atoms **2A**: (A) –x+1, -y, -z+1; (B) -x+2, -y+1, -z.

Table S4. Selected bond lengths (Å) in **2B**.

Bond	2B	Bond	2B
Cd(1)-O(2)	2.190(2)	C(15)-C(16)	1.404(2)
Cd(1)-O(3A)	2.215(2)	C(15)-C(20)	1.404(2)
Cd(1)-N(3)	2.276(2)	C(16)-C(17)	1.383(2)
Cd(1)-O(4A)	2.358(2)	C(17)-C(18)	1.405(2)
Cd(1)-N(4C)	2.358(2)	C(18)-C(19)	1.403(2)
Cd(1)-O(1)	2.390(2)	C(19)-C(20)	1.386(2)
O(1)-C(1)	1.239(2)	C(21)-C(22)	1.458(2)
O(2)-C(2)	1.295(2)	C(21)-C(26)	1.473(2)
O(3)-C(23)	1.297(2)	C(22)-C(23)	1.390(2)
O(4)-C(24)	1.240(2)	C(23)-C(24)	1.516(2)
N(1)-C(4)	1.304(2)	C(24)-C(25)	1.469(2)
N(1)-C(15)	1.399(2)	C(25)-C(26)	1.338(2)
N(2)-C(21)	1.311(2)	C(35)-C(36)	1.377(3)
N(2)-C(18)	1.397(2)	C(36)-C(37)	1.389(3)
N(3)-C(39)	1.340(2)	C(37)-C(38)	1.392(3)
N(3)-C(35)	1.346(2)	C(37)-C(40)	1.509(3)
N(4)-C(47)	1.339(2)	C(38)-C(39)	1.384(2)
N(4)-C(45)	1.345(2)	C(40)-C(41)	1.532(3)
C(1)-C(6)	1.467(2)	C(41)-C(42)	1.529(3)
C(1)-C(2)	1.513(2)	C(42)-C(43)	1.510(3)
C(2)-C(3)	1.391(2)	C(43)-C(46)	1.387(3)
C(3)-C(4)	1.457(2)	C(43)-C(44)	1.396(2)
C(4)-C(5)	1.474(2)	C(44)-C(45)	1.380(3)
C(5)-C(6)	1.341(2)	C(46)-C(47)	1.387(3)

Symmetry transformations used to generate equivalent atoms **2B**: (A) –x, -y+1, -z+1; (B) x+1, -y+1/2, z+1/2; (C) x-1, -y+1/2, z-1/2.

Table S5. Selected bond lengths (Å) in **3.**

Bond	3	Bond	3
Cd(1)-O(1)	2.187(3)	C(4)-C(5)	1.379(6)
Cd(1)-O(4)	2.194(3)	C(6)-C(7)	1.383(6)
Cd(1)-N(1)	2.302(3)	C(6)-C(11)	1.522(5)
Cd(1)-O(5)	2.326(3)	C(7)-C(8)	1.444(6)
Cd(1)-O(2)	2.342(3)	C(8)-C(9)	1.474(5)
Cd(1)-O(3)	2.350(3)	C(9)-C(10)	1.329(6)
N(1)-C(5)	1.304(5)	C(10)-C(11)	1.463(6)
N(1)-C(1)	1.311(5)	C(20)-C(22B)	1.397(8)
N(2)-C(8)	1.308(6)	C(20)-C(21)	1.400(7)
N(2)-C(20)	1.422(6)	C(21)-C(22)	1.364(6)
N(3)-C(26)	1.300(5)	C(23)-C(24)	1.454(6)
N(3)-C(37)	1.395(5)	C(23)-C(28)	1.521(5)
O(1)-C(6)	1.295(5)	C(24)-C(25)	1.336(6)
O(2)-C(11)	1.241(5)	C(25)-C(26)	1.476(5)
O(3)-C(23)	1.246(5)	C(26)-C(27)	1.453(5)
O(4)-C(28)	1.287(4)	C(27)-C(28)	1.392(5)
C(1)-C(2)	1.377(6)	C(37)-C(39C)	1.399(5)
C(2)-C(3)	1.354(6)	C(37)-C(38)	1.400(5)
C(3)-C(4)	1.358(5)	C(38)-C(39)	1.375(5)
C(3)-C(3A)	1.487(7)		

Symmetry transformations used to generate equivalent atoms **3**: (A) –x+2, -y+1, -z+1; (B) –x, -y+2, -z+1; (C) –x, -y, -z.

Table S6. Selected bond lengths (Å) in **4**.

Bond	4	Bond	4
Cd(1)-O(1)	2.200(5)	N(4)-C(21)	1.308(9)
Cd(1)-O(6A)	2.261(6)	N(4)-C(18)	1.42(2)
Cd(1)-O(5)	2.293(5)	C(1)-C(2)	1.40(2)
Cd(1)-N(1)	2.322(6)	C(1)-C(6)	1.51(2)
Cd(1)-O(2)	2.332(4)	C(2)-C(3)	1.446(9)
Cd(1)-O(5A)	2.532(5)	C(3)-C(4)	1.47(2)
O(5)-Cd(1A)	2.532(5)	C(4)-C(5)	1.35(2)
O(6)-Cd(1A)	2.261(6)	C(5)-C(6)	1.468(9)
O(1)-C(1)	1.294(8)	C(15)-C(20)	1.39(2)
O(2)-C(6)	1.245(8)	C(15)-C(16)	1.41(2)
O(3)-C(23)	1.321(8)	C(16)-C(17)	1.36(2)
O(3)-H(3)	0.77(8)	C(17)-C(18)	1.40(2)
O(4)-C(24)	1.243(8)	C(18)-C(19)	1.40(2)
O(5)-C(41)	1.29(2)	C(19)-C(20)	1.36(2)
O(6)-C(41)	1.24(2)	C(21)-C(22)	1.465(9)
N(1)-C(38)	1.45(2)	C(21)-C(26)	1.47(2)
N(1)-C(35)	1.47(2)	C(22)-C(23)	1.359(9)
N(1)-C(40)	1.48(2)	C(23)-C(24)	1.49(2)
N(2)-C(37)	1.42(2)	C(24)-C(25)	1.466(9)
N(2)-C(36)	1.44(2)	C(25)-C(26)	1.35(2)
N(2)-C(39)	1.47(2)	C(35)-C(36)	1.59(2)
N(3)-C(3)	1.311(9)	C(37)-C(38)	1.57(2)
N(3)-C(15)	1.41(2)	C(39)-C(40)	1.56(2)

Symmetry transformations used to generate equivalent atoms **4**: (A) x, -y+1/2, z-1/2.

Table S7. Selected bond lengths (Å) in **5**.

Bond	5	Bond	5
Cd(1)-O(2A)	2.243(2)	N(3)-C(21)	1.473(4)
Cd(1)-O(2)	2.243(2)	N(4)-C(20)	1.463(4)
Cd(1)-O(1A)	2.304(2)	N(4)-C(22)	1.472(3)
Cd(1)-O(1)	2.304(2)	N(4)-C(21)	1.474(4)
Cd(1)-N(1)	2.422(2)	N(5)-C(4)	1.315(3)
O(1)-C(1)	1.259(3)	N(5)-C(15)	1.407(4)
O(2)-C(6)	1.282(3)	C(1)-C(2)	1.448(3)
N(1)-C(23)	1.484(3)	C(1)-C(6)	1.504(3)
N(1)-C(18)	1.484(3)	C(2)-C(3)	1.369(3)
N(1)-C(22)	1.493(3)	C(3)-C(4)	1.459(3)
N(2)-C(19)	1.463(4)	C(4)-C(5)	1.431(3)
N(2)-C(23)	1.468(3)	C(5)-C(6)	1.419(3)
N(2)-C(20)	1.473(4)	C(15)-C(16)	1.395(5)
N(3)-C(18)	1.467(3)	C(15)-C(17)	1.414(5)
N(3)-C(19)	1.471(4)	C(16)-C(17B)	1.382(5)

Symmetry transformations used to generate equivalent atoms: **5**: (A): -x+1, -y+1, -z+1; (B) –x, -y, -z+2.

Table S8. Hydrogen bonds for **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3)...N(2)#3	0.77(8)	1.96(8)	2.686(9)	155(9)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z+1/2 #2 x,-y+1/2,z-1/2 #3 -x+1,y+1/2,-z+3/2

Table S9. Hydrogen bonds for **5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3)#1...O(4)	0.86(4)	2.00(4)	2.547(3)	121(3)
O(3)-H(3)#1...N(4)	0.86(4)	2.47(4)	3.234(3)	148(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x,-y,-z+2 #3 -x+1,-y,-z

Fig. S1. PXRD patterns for **1-5**.