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Chemical bonding in complexes with high coordination numbers: a charge density study

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Experimental

X-ray structure analysis. A colorless crystal of tris(pyridine)bis(*o*-hydroxybenzoato)cadmium(II) (M = 623.92) having the shape of prism with edge lengths of 0.60x0.59x0.28 mm^3 was found to be monoclinic, space group $P2_1/n$, at 100(2) K: a = 10.116(2), b = 14.666(3), c = 17.715(4) Å, β = 93.66(3)°, V = 2622.8(9) $Å^3$, Z = 4, d_{calc} = 1.580 $g\cdot cm^{-3}$, μ(MoKα) = 8.82 cm^{-1}, F(000) = 1264. Intensities of 214045 reflections were measured with a “Bruker SMART APEX2” CCD diffractometer using MoKα radiation (λ = 0.71073 Å) and reduced to structure factors to supply a data set with a maximum resolution of 1.13 $Å^{-1}$. The absorption correction was performed empirically using APEX2 (Bruker, 2005) software and gave minimum and maximum transmission coefficients of 0.594 and 0.784, correspondingly. 18622 independent reflections [R_{int} = 0.0315] were used in further refinement. The refinement converged to wR2 = 0.0531 and GOF = 1.000 for all independent reflections (R1 = 0.0213 was calculated against F for 16347 observed reflections with I > 2σ(I)). All calculations were performed using SHELXTL PLUS 5.0.[1] Atomic coordinates, bond lengths and angles and thermal parameters have been deposited at the Cambridge Crystallographic Data Centre (CCDC) with CCDC number 798772.

The experimental charge density in the crystal was obtained by the multipole refinement based on the Hansen-Coppens formalism[2] using the XD program package.[3] Before the refinement, the C-H bond distances were normalized to the ideal value of 1.08 Å; the O−H bond distances, to the values obtained from quantum chemical calculations. The refinement was carried out with electroneutrality constraints. The multipole expansion was truncated to hexadecapole for Cd atom, octopole for carbon, oxygen and nitrogen atoms and dipole for H atoms. The multipole occupancies of all atoms were refined without any local symmetry constrains. The refinement was carried out as follows: we first performed the high-angle refinement (sinθ/λ > 0.7 $Å^{-1}$) of the positional and thermal parameters of all non-hydrogen atoms and then included the lower-angle data to refine multipoles, gradually adding the monopoles and two Kappa values with the repetition of multipole refinement. Scale factor was refined in the last cycle. Weights were taken as $1/(\sigma^2(F_o^2)+(1/3a\, F_o^2)^2+1/3b\, F_o^2)$, where a = 0.01, b = 0.4. The refinement was carried out against *F* and converged to $R = 0.0169$, $wR = 0.0176$ and GOF = 1.0512 for 16268 merged reflections with $I>3\sigma(I)$. The average difference of the mean square displacement amplitudes (the Hirshfeld rigid-bond criteria[4]) along the bonds between non-metal atoms was not more than $11 \cdot 10^{-4}$ Å^2. The residual electron density was not more that 0.6 eÅ^{-3}. Analysis of topology of the $\rho(\mathbf{r})$ function was carried out using the WINXPRO program package.[5] The kinetic energy ($g(\mathbf{r})$) was estimated from experimental diffraction data within the Kirzhnits's approximation,[6] which relates it to values of $\rho(\mathbf{r})$ and its derivatives: $g(\mathbf{r}) = (3/10)(3\pi^2)^{2/3}[\rho(\mathbf{r})]^{5/3} + (1/72)|\nabla\rho(\mathbf{r})|^2/\rho(\mathbf{r}) + 1/6\nabla^2\rho(\mathbf{r})$. Use of this relationship in conjunction with the virial theorem $[2g(\mathbf{r}) + v(\mathbf{r}) = 1/4\nabla^2\rho(\mathbf{r})]$ provided values of the potential energy density $v(\mathbf{r})$ at the bond critical points. The final residual Fourier maps were flat and featureless (see supporting information). The kappa and kappa' values as well as the multipole populations are summarized in the supplementary data.

Quantum Chemical Calculations. The optimizations of tris(pyridine)bis(*o*-hydroxybenzoato)-cadmium(II) and tris(pyridine)bis(benzoato)cadmium(II) molecules were performed with the Gaussian 98 programme package.[7] The DFT calculation was carried out at the PBE1PBE level using a DGDZVP basis set. As convergence criteria, the extremely tight threshold limits of $2 \cdot 10^{-6}$ and $6 \cdot 10^{-6}$ au were applied for the maximum force and displacement, respectively. To enhance the accuracy in the DFT calculation, the pruned (99,590) grid (keyword Grid=Ultrafine) has been used. The topological analysis of the $\rho(\mathbf{r})$ functions was performed using the AIMAll program package,[8] based on the wave functions obtained from the above calculations.

CSD search. The data were recovered from the November 2009 update release of the CSD (version 1.12).[9] Both neutral and charged species were considered. Only entries presenting atomic coordinates and where R<0.10 were taken into account. The results of the search are discussed above and are presented in the graphic form (see S2). $CdN_3(COO)_2$ moiety was used as a query for the search. In order to run comparative analysis of the distributions of Cd-O and Cd-N distances, the subset of structural data was created.

The second search (see S3) included coordination complexes with coordination number of Cd atom varying from 3 to 7. Atoms bound to Cd were allowed to be oxygen or nitrogen; one of Cd-O distances was set as the defined parameter. The histograms including this bond length are presented as ESI.

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Table S1. Bond lengths (*d*) and topological parameters of ρ(r) at the BCPs for **1**, **1a** and **2.**

	d, Å[a)]	$\rho(\mathbf{r})$, eÅ^{-3}	$\nabla^2\rho(\mathbf{r})$, eÅ^{-5}	$V(\mathbf{r})$, a.u.	$h_e(\mathbf{r})$, a.u.	E_{int}, kcal/mol
Cd(1)-O(1)	2.3869(9)	0.281	4.12	-0.0430	-0.0001	13.5
	2.478	0.243	3.82	-0.0418	-0.0011	13.1
	2.512	0.223	3.54	-0.0376	-0.0038	11.8
Cd(1)-O(2)	2.5132(8)	0.231	3.38	-0.0324	0.0013	10.2
	2.393	0.290	4.59	-0.0406	-0.0036	17.2
	2.368	0.310	4.87	-0.0594	-0.0043	18.6
Cd(1)-O(4)	2.5191(9)	0.218	2.87	-0.0287	0.0005	9.0
	2.488	0.238	3.74	-0.5590	-0.0009	12.7
	2.512	0.223	3.54	-0.0376	-0.0038	11.8
Cd(1)-O(5)	2.3490(8)	0.295	4.30	-0.0461	-0.0008	14.5
	2.386	0.294	4.66	-0.0563	-0.0038	17.5
	2.368	0.310	4.87	-0.0594	-0.0043	18.6
Cd(1)-N(1)	2.3488(8)	0.379	5.01	-0.0646	-0.0063	20.3
	2.419	0.314	4.17	-0.0557	-0.0065	17.7
	2.433	0.303	4.05	-0.0537	-0.0058	16.8
Cd(1)-N(2)	2.3677(8)	0.357	4.58	-0.0587	-0.0056	18.4
	2.422	0.311	4.14	-0.0556	-0.0063	17.5
	2.433	0.303	4.05	-0.0537	-0.0058	16.8
Cd(1)-N(3)	2.3594(7)	0.354	4.52	-0.0577	-0.0054	18.1
	2.464	0.282	3.80	-0.0489	-0.0047	17.3
	2.481	0.271	3.66	-0.0463	-0.0041	14.5
C(7)-O(1)	1.2612(10)	2.686	-32.06	-1.1263	-0.7294	
	1.261	2.460	-10.56	-1.0165	-0.5630	
	1.266	2.430	-10.60	-0.9952	-0.5523	
C(7)-O(2)	1.2787(10)	2.515	-29.24	-1.0069	-0.6551	
	1.286	2.338	-11.84	-0.9144	-0.5186	
	1.267	2.430	-10.99	-0.9927	-0.5533	
C(14)-O(4)	1.2516(10)	2.738	-33.49	-1.1615	-0.7544	
	1.260	2.463	-10.51	-1.0191	-0.5641	
	1.266	2.430	-10.60	-0.9952	-0.5523	
C(14)-O(5)	1.2894(10)	2.377	-24.44	-0.9242	-0.5889	
	1.286	2.334	-11.85	-0.9119	-0.5174	
	1.267	2.430	-10.99	-0.9927	-0.5533	
O(3)...O(2)	2.5723(12)[156(2)°]	0.338	5.49	-0.0580	-0.0005	18.2
	2.565[148.8°]	0.353	3.88	-0.0536	-0.0067	16.8
O(6)...O(5)	2.5438(11)[156(2)°]	0.381	4.92	-0.0646	-0.0068	20.3
	2.566[148.8°]	0.352	3.88	-0.0535	-0.0066	16.8
C(15)-H(15A)…O(4)	3.2707(13) [131°]	0.054	0.80	-0.0046	0.0018	1.5
	3.191 [124.2°]	0.066	0.97	-0.0064	0.0018	2.0
	3.170 [124.1°]	0.069	1.01	-0.0067	0.0019	2.1
C(19)-H(19A)…O(2)						
	3.237 [130.0°]	0.070	0.97	-0.0067	0.0017	2.1
	3.165 [131.0°]	0.082	1.16	-0.0080	0.0020	2.5
C(20)-H(20A)…O(5)	3.2231(12) [123.3°]	0.067	0.91	-0.0058	0.0018	1.8
	3.224 [129.9°]	0.072	1.00	-0.0069	0.0017	2.2
	3.165 [131.0°]	0.082	1.16	-0.0080	0.0020	2.5

C(24)-H(24A)…O(1)	3.2342(12) [124.3°]	0.059	0.82	-0.0050	0.0018	1.6
	3.196 [124.6°]	0.067	0.96	-0.0064	0.0018	2.0
	3.170 [124.1°]	0.069	1.01	-0.0067	0.0018	2.1
C(25)-H(25A)…O(4)	3.1287(12) [133°]	0.075	1.20	-0.0073	0.0026	2.3
	3.040 [129.6°]	0.094	1.51	-0.0104	0.0027	3.3
	3.023 [130.4°]	0.100	1.60	-0.0112	0.0027	3.5
C(29)-H(29A)…O(1)	3.1205(12) [131°]	0.071	1.09	-0.0067	0.0023	2.1
	3.036 [129.8°]	0.095	1.54	-0.0105	0.0027	3.3
	3.023 [130.4°]	0.100	1.60	-0.0112	0.0027	3.5

[a] the values in the first lines are from the experiment and those in the second and third lines are from the gas-phase DFT calculation

=== INTEGRATED PROPERTY WITHIN ATOMIC BASIN ===

The accuracy of the obtained charges can in part be justified by the values of the Lagrangian [$L(r) = -1/4\nabla^2\rho(\mathbf{r})$] and volumes, obtained by the analogous procedure. In particular, the L(**r**) value for the Cd(1) atom is quite small, namely $1.85 \cdot 10^{-4}$ (A.M. Grana, R.A. Mosquera, *J. Chem. Phys.* 1999, 110, 6606). In turn, the sum of the atomic volumes in the crystal (653.5 $Å^3$) reproduces well the volume of the independent part of the unit cell (655.7(9) $Å^3$) with an error being only 0.3%.

Table S2

num	atom	nTheta	nPhi	RHO	CPU time (sec)
1	Cd(1)	48	64	46.169314	2005.86
2	O(1)	48	64	8.983936	1423.00
3	O(2)	48	64	8.882073	1442.64
4	O(3)	48	64	8.900723	1665.56
5	O(4)	48	64	8.928242	1488.23
6	O(5)	48	64	8.867325	1344.95
7	O(6)	48	64	8.769033	1600.06
8	N(1)	48	64	7.911792	1252.61
9	N(2)	48	64	7.930179	1258.02
10	N(3)	48	64	7.928786	1376.38
11	C(1)	48	64	6.247330	1251.73
12	C(2)	48	64	5.587250	1473.08
13	C(3)	48	64	5.998587	1071.97
14	C(4)	48	64	6.043124	1349.12
15	C(5)	48	64	6.003982	1483.31
16	C(6)	48	64	6.086550	1487.72
17	C(7)	48	64	4.761141	1326.08
18	C(8)	48	64	6.125805	1380.06
19	C(9)	48	64	5.639866	1545.23
20	C(10)	48	64	6.072991	1239.27
21	C(11)	48	64	6.017800	1313.59
22	C(12)	48	64	6.088821	1150.53
23	C(13)	48	64	6.037215	1329.08
24	C(14)	48	64	4.630266	1354.56
25	C(15)	48	64	5.704207	1272.94
26	C(16)	48	64	6.098250	1280.98
27	C(17)	48	64	6.021230	1439.14
28	C(18)	48	64	6.069811	1495.45
29	C(19)	48	64	5.690471	1534.11
30	C(20)	48	64	5.674769	1458.34
31	C(21)	48	64	6.057257	1465.27
32	C(22)	48	64	6.085971	1459.00
33	C(23)	48	64	6.103274	1696.98
34	C(24)	48	64	5.648085	1453.91
35	C(25)	48	64	5.665197	1717.52
36	C(26)	48	64	6.092006	1693.03
37	C(27)	48	64	6.061551	1566.66
38	C(28)	48	64	6.044281	1374.19
39	C(29)	48	64	5.710920	1418.28
40	H(3A)	48	64	0.899185	930.62
41	H(4A)	48	64	0.976293	1076.78
42	H(5A)	48	64	0.936992	1273.84
43	H(6A)	48	64	0.913086	1296.75
44	H(10A)	48	64	0.986800	1047.50
45	H(11A)	48	64	0.954602	1114.34
46	H(12A)	48	64	0.951634	895.88
47	H(13A)	48	64	0.974051	1258.75
48	H(15A)	48	64	0.921742	1215.00

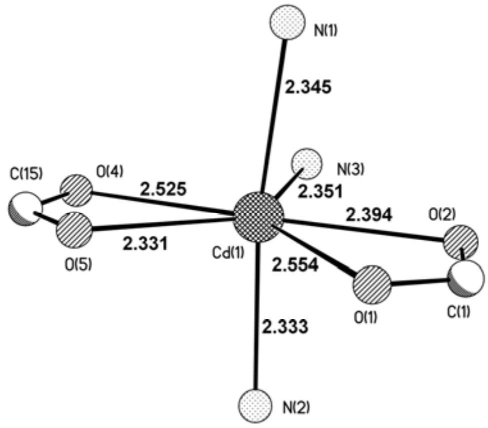
49	H(16A)	48	64	0.913717	1091.66
50	H(17A)	48	64	0.981058	863.70
51	H(18A)	48	64	0.955850	1395.00
52	H(19A)	48	64	0.877352	1312.95
53	H(20A)	48	64	0.963573	1207.75
54	H(21A)	48	64	0.941346	1329.75
55	H(22A)	48	64	0.938367	1113.58
56	H(23A)	48	64	0.905475	1561.70
57	H(24A)	48	64	0.956180	1405.42
58	H(25A)	48	64	0.931520	1388.47
59	H(26A)	48	64	0.921322	1375.69
60	H(27A)	48	64	0.957868	1167.66
61	H(28A)	48	64	0.896451	1501.97
62	H(29A)	48	64	0.876590	1485.61
63	H(3O)	48	64	0.610045	1361.36
64	H(6O)	48	64	0.618784	1164.20

Table S3

num	atom	nTheta	nPhi	VOLUME	CPU time (sec)
1	Cd(1)	48	64	16.861151	1.11
2	O(1)	48	64	16.936603	1.31
3	O(2)	48	64	15.077463	1.38
4	O(3)	48	64	17.135763	1.44
5	O(4)	48	64	17.175108	1.50
6	O(5)	48	64	14.266337	1.52
7	O(6)	48	64	18.450254	1.56
8	N(1)	48	64	13.694704	1.58
9	N(2)	48	64	13.908895	1.56
10	N(3)	48	64	13.542602	1.05
11	C(1)	48	64	11.183834	1.19
12	C(2)	48	64	10.039013	1.23
13	C(3)	48	64	14.128160	1.30
14	C(4)	48	64	12.664053	1.34
15	C(5)	48	64	11.754904	1.31
16	C(6)	48	64	11.699044	1.33
17	C(7)	48	64	6.564701	1.36
18	C(8)	48	64	10.946710	1.41
19	C(9)	48	64	8.665155	1.41
20	C(10)	48	64	12.037339	1.47
21	C(11)	48	64	11.859142	1.50
22	C(12)	48	64	13.731846	1.58
23	C(13)	48	64	13.806717	1.48
24	C(14)	48	64	5.834952	1.55
25	C(15)	48	64	10.408333	1.55
26	C(16)	48	64	12.178435	1.56
27	C(17)	48	64	13.720908	1.61
28	C(18)	48	64	14.215616	1.61
29	C(19)	48	64	12.292099	1.64
30	C(20)	48	64	9.799025	1.66
31	C(21)	48	64	11.182516	1.67
32	C(22)	48	64	11.913248	1.67
33	C(23)	48	64	12.553418	1.75
34	C(24)	48	64	10.659082	1.75
35	C(25)	48	64	11.498380	1.92
36	C(26)	48	64	12.783851	1.97
37	C(27)	48	64	11.845043	1.94
38	C(28)	48	64	11.940791	2.03

39	C(29)	48	64	10.905637	2.11
40	H(3A)	48	64	6.722225	1.84
41	H(4A)	48	64	7.296233	1.72
42	H(5A)	48	64	7.443064	1.88
43	H(6A)	48	64	6.061536	1.88
44	H(10A)	48	64	6.074981	2.06
45	H(11A)	48	64	6.850729	2.02
46	H(12A)	48	64	6.474109	1.94
47	H(13A)	48	64	6.874393	1.94
48	H(15A)	48	64	6.305271	2.03
49	H(16A)	48	64	6.970164	1.95
50	H(17A)	48	64	7.305756	2.00
51	H(18A)	48	64	7.615216	2.09
52	H(19A)	48	64	6.377388	2.00
53	H(20A)	48	64	6.684554	2.09
54	H(21A)	48	64	7.380522	2.25
55	H(22A)	48	64	6.741835	2.12
56	H(23A)	48	64	7.174610	2.11
57	H(24A)	48	64	7.007533	2.20
58	H(25A)	48	64	6.264141	2.30
59	H(26A)	48	64	6.256176	2.56
60	H(27A)	48	64	8.199798	2.41
61	H(28A)	48	64	7.707939	2.62
62	H(29A)	48	64	5.997374	2.42
63	H(3O)	48	64	3.025005	2.44
64	H(6O)	48	64	2.806609	2.52

Figure S1. The distribution of Cd-O and Cd-N bond lengths in the relative compounds with $Cd(COO)_2N_3$ moiety (CSD reference codes are placed under each figure) and in the calculation data (ligands characterized by linear O-Cd-O disposition with the respective angle close to 180° are located on the backward of all the pictures).



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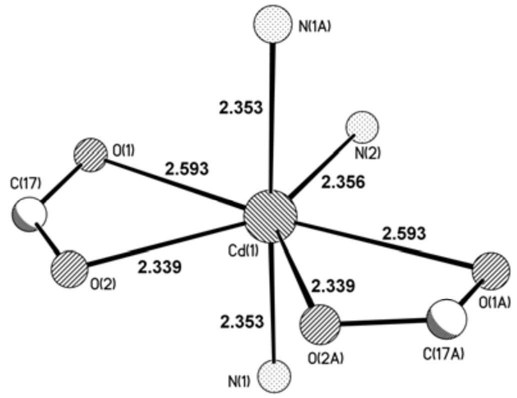

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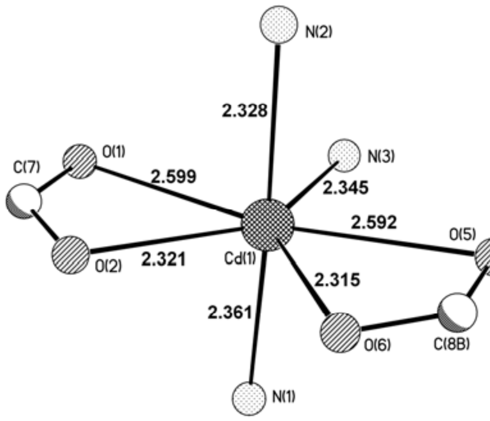

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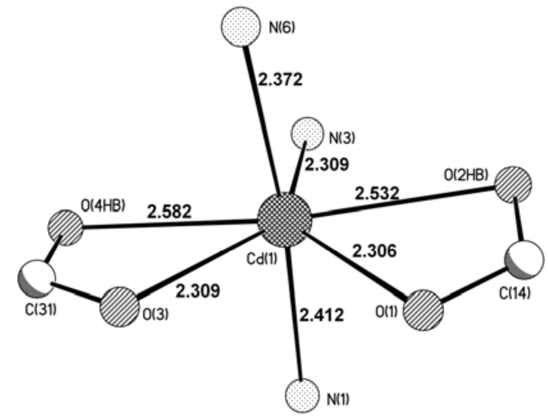

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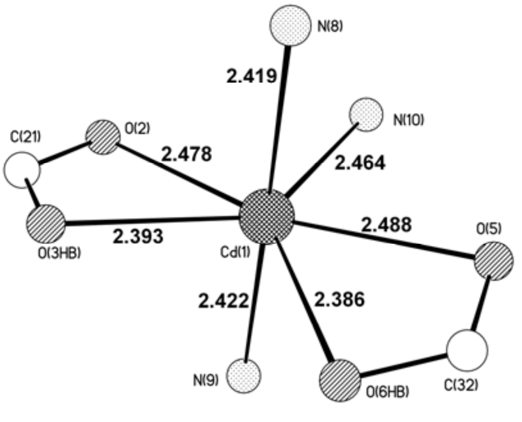
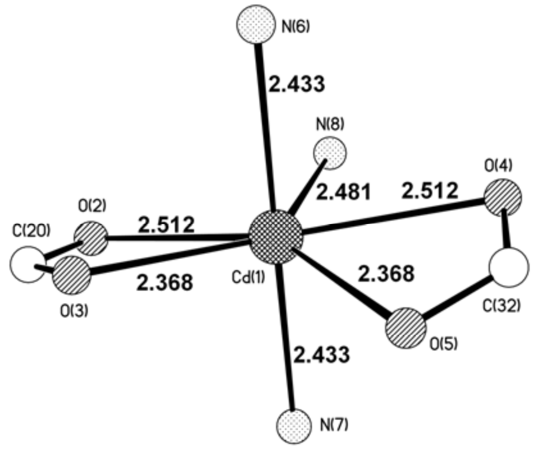
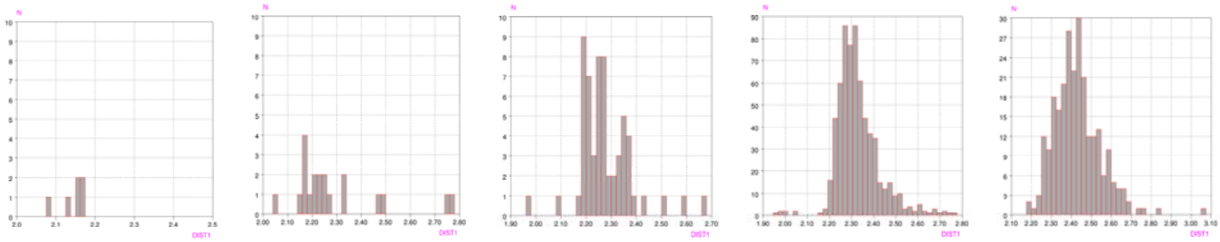


PBE1PBE/DGDZVP (H-bonded)



PBE1PBE/DGDZVP

Figure S2. The distribution of Cd-O bond lengths in cadmium complexes with different coordination number (the coordination number of metal atom is shown under each figure) according to Cambridge Structural Database. Average Cd-O bond length increases with the increase of coordination number.



3 4 5 6 7

Figure S3. Molecular graph of the tris(pyridine)bis(*o*-hydroxybenzoato)cadmium(II) molecule. BCPs (bond critical points) – red points, RCPs (ring critical points) – orange points.

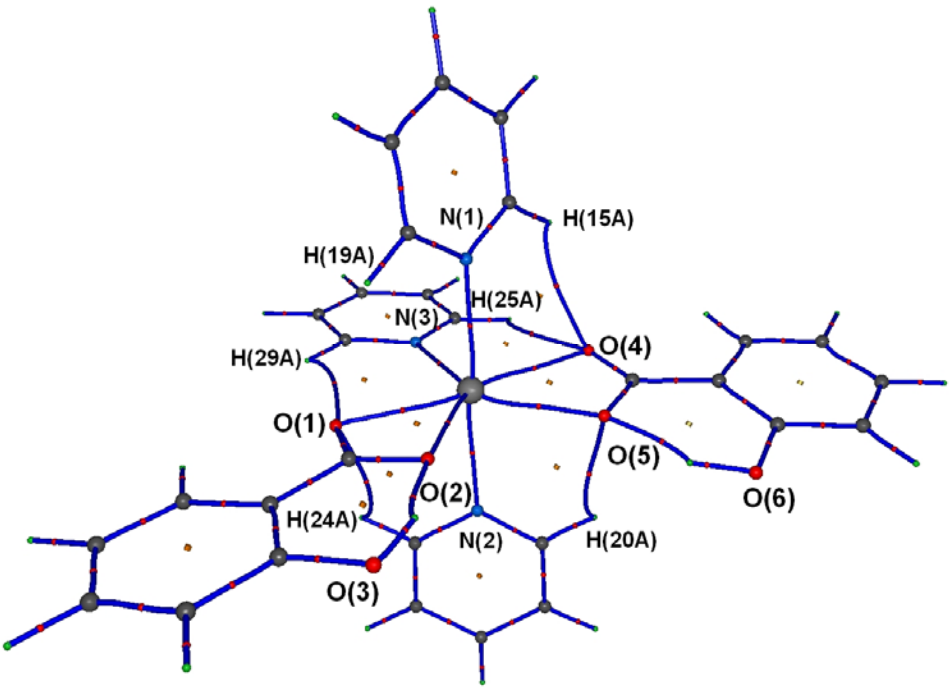


Figure S4. Stacking interactions in the crystal of **1** (hydrogen atoms are omitted for clarity).

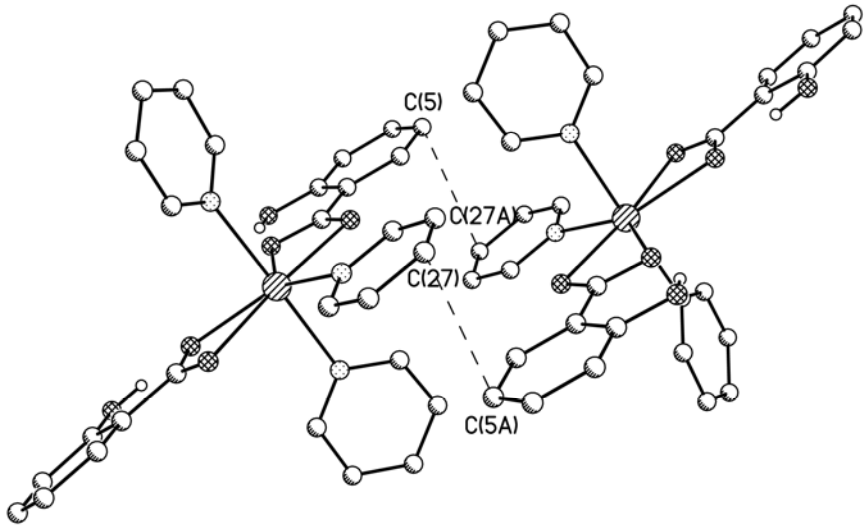


Table S4. The conformation of metallacycles in **1**, **1a** and **2.**

Angle	**1**	**1a**	**2**
O(1)-Cd(1)-O(2)	53.72(2)	54.1	54.1
O(4)-Cd(1)-O(5)	53.96(3)	54.0	54.1
O(1)-Cd(1)-O(4)	170.01(2)	145.8	157.8
N(3)-Cd(1)-O(1)	85.71(3)	79.9	78.9
N(3)-Cd(1)-O(4)	84.42(3)	79.7	78.9
N(1)-Cd(1)-O(1)-C(7)	87.80(5)	83.8	79.9
N(2)-Cd(1)-O(5)-C(14)	94.47(5)	102.8	104.7

Table S5. Optimized geometry for **1a** (Atom number and x,y,z coordinates).

Cd1	0.00000	0.00000	0.00000
O1	2.43800	0.10030	0.43370
O2	1.72880	-0.32470	-1.62170
O3	3.38490	-0.87460	-3.50230
O4	-2.44680	0.24380	0.37650
O5	-1.72680	-0.84040	-1.41650
O6	-3.37360	-1.73520	-3.16889
N1	-0.18640	2.25390	-0.85720
N2	0.21160	-2.26680	0.82660
N3	-0.00630	0.84760	2.31390
C1	4.07600	-0.33620	-1.24840
C2	4.35040	-0.67720	-2.59250
C3	5.68380	-0.81800	-3.00590
H3A	5.87450	-1.08210	-4.04210
C4	6.71950	-0.62341	-2.10570
H4A	7.74640	-0.73660	-2.44510
C5	6.45830	-0.28501	-0.77170
H5A	7.27540	-0.13350	-0.07220
C6	5.14260	-0.14670	-0.35900
H6A	4.90030	0.11480	0.66710
C7	2.68190	-0.17700	-0.77180
C8	-4.07570	-0.58490	-1.16100
C9	-4.34360	-1.25880	-2.37439
C10	-5.67500	-1.44480	-2.77619

H10A	-5.86050	-1.96390	-3.71209
C11	-6.71510	-0.97250	-1.99139
H11A	-7.74040	-1.12629	-2.31969
C12	-6.46040	-0.30240	-0.78799
H12A	-7.28070	0.06540	-0.17839
C13	-5.14670	-0.11610	-0.38789
H13A	-4.90930	0.39840	0.53881
C14	-2.68440	-0.37140	-0.69750
C15	-1.16240	3.05600	-0.41320
H15A	-1.84010	2.61730	0.31440
C16	-1.32430	4.36100	-0.86470
H16A	-2.13420	4.97070	-0.47620
C17	-0.43890	4.85290	-1.81940
H17A	-0.53820	5.86750	-2.19600
C18	0.57110	4.01850	-2.28810
H18A	1.28080	4.35300	-3.03830
C19	0.65960	2.72670	-1.78070
H19A	1.42150	2.03260	-2.12460
C20	-0.63730	-3.23140	0.45100
H20A	-1.41750	-2.93070	-0.24269
C21	-0.52960	-4.54320	0.90021
H21A	-1.24310	-5.28870	0.56381
C22	0.50530	-4.86820	1.77191
H22A	0.62090	-5.88440	2.13961
C23	1.39400	-3.86890	2.15760
H23A	2.22320	-4.07600	2.82700
C24	1.21080	-2.58370	1.66020
H24A	1.89050	-1.77440	1.91390
C25	-1.12450	0.82010	3.05210
H25A	-2.00560	0.42400	2.55490
C26	-1.16890	1.27910	4.36500
H26A	-2.09990	1.23180	4.92160
C27	-0.00830	1.79410	4.93470
H27A	-0.00890	2.16290	5.95720
C28	1.15290	1.82750	4.16850
H28A	2.08310	2.22040	4.56760
C29	1.11070	1.34180	2.86540
H29A	1.99220	1.33120	2.23030
H3O	2.52440	-0.73810	-3.01980
H6O	-2.51550	-1.49840	-2.72239

Table S6. Optimized geometry for **2.**

Cd1	0.00000	0.00000	0.00000
O1	-2.46290	0.10720	0.48380
O2	-1.74010	-0.37370	-1.56230
O3	2.46290	-0.10870	0.48380
O4	1.74020	0.37420	-1.56180
N1	0.23050	-2.42230	0.01590
N2	-0.23140	2.42220	0.01570
N3	0.00010	0.00010	2.48140
C1	-4.08860	-0.19150	-1.23680
C2	-4.34570	-0.42950	-2.58979
H2A	-3.50210	-0.57300	-3.25840
C3	-5.65690	-0.47340	-3.05639
H3A	-5.85300	-0.65660	-4.10989
C4	-6.71930	-0.28029	-2.17289
H4A	-7.74320	-0.31459	-2.53709
C5	-6.46690	-0.04129	-0.82160
H5A	-7.29460	0.11011	-0.13309

C6	-5.15540	0.00410	-0.35570
H6A	-4.93580	0.19020	0.69150
C7	-2.67550	-0.14780	-0.73800
C8	4.08870	0.19010	-1.23680
C9	4.34580	0.42910	-2.58960
H9A	3.50220	0.57380	-3.25800
C10	5.65690	0.47239	-3.05640
H10A	5.85310	0.65640	-4.10980
C11	6.71930	0.27780	-2.17310
H11A	7.74310	0.31169	-2.53750
C12	6.46690	0.03779	-0.82200
H12A	7.29460	-0.11480	-0.13381
C13	5.15550	-0.00700	-0.35600
H13A	4.93590	-0.19380	0.69100
C14	2.67570	0.14700	-0.73780
C15	1.20430	-3.00800	0.72340
H15A	1.86920	-2.33440	1.25780
C16	1.38100	-4.38700	0.75780
H16A	2.18830	-4.81440	1.34470
C17	0.51340	-5.19050	0.02350
H17A	0.62400	-6.27180	0.02631
C18	-0.49340	-4.58270	-0.72040
H18A	-1.18870	-5.16640	-1.31569
C19	-0.59770	-3.19550	-0.69710
H19A	-1.35500	-2.66730	-1.27070
C20	0.59660	3.19560	-0.69720
H20A	1.35450	2.66760	-1.27040
C21	0.49150	4.58270	-0.72100
H21A	1.18680	5.16660	-1.31630
C22	-0.51580	5.19020	0.02220
H22A	-0.62710	6.27140	0.02460
C23	-1.38330	4.38650	0.75650
H23A	-2.19100	4.81360	1.34300
C24	-1.20580	3.00750	0.72260
H24A	-1.87040	2.33370	1.25710
C25	1.12070	0.26330	3.16730
H25A	2.00400	0.45510	2.56420
C26	1.16420	0.27770	4.55830
H26A	2.09770	0.50030	5.06650
C27	0.00010	0.00050	5.26880
H27A	0.00020	0.00060	6.35580
C28	-1.16400	-0.27690	4.55840
H28A	-2.09740	-0.49940	5.06670
C29	-1.12050	-0.26300	3.16750
H29A	-2.00390	-0.45490	2.56440

Table S7. Monopole populations, radial parameters and net atomic charges.

Atom	Pval	Kappa	P00	Kappa'	Net charge
CD(1)	8.950	1.013	0.000	0.938	+1.05010
O(1)	6.155	0.994	0.000	1.056	-0.15510
O(2)	6.167	0.994	0.000	0.970	-0.16690
O(3)	6.116	0.990	0.000	0.954	-0.11620
O(4)	6.104	0.994	0.000	0.970	-0.10400
O(5)	6.136	0.994	0.000	1.056	-0.13640
O(6)	6.026	0.990	0.000	0.954	-0.02570
N(1)	5.105	0.991	0.000	0.926	-0.10500
N(2)	5.088	0.997	0.000	0.941	-0.08840

N(3)	5.065	0.998	0.000	0.948	-0.06540
C(1)	4.181	1.000	0.000	1.009	-0.18140
C(2)	4.095	0.990	0.000	1.012	-0.09530
C(3)	4.024	0.995	0.000	0.984	-0.02390
C(4)	4.031	0.995	0.000	0.984	-0.03100
C(5)	4.024	0.995	0.000	0.984	-0.02410
C(6)	4.121	0.995	0.000	0.984	-0.12140
C(7)	4.184	0.995	0.000	0.941	-0.18370
C(8)	4.081	1.000	0.000	1.009	-0.08070
C(9)	4.077	0.990	0.000	1.012	-0.07710
C(10)	4.084	0.995	0.000	0.984	-0.08400
C(11)	4.060	0.995	0.000	0.984	-0.06000
C(12)	4.083	0.995	0.000	0.984	-0.08330
C(13)	4.104	0.995	0.000	0.984	-0.10390
C(14)	4.066	0.995	0.000	0.941	-0.06560
C(15)	4.068	1.004	0.000	0.956	-0.06790
C(16)	4.032	1.001	0.000	0.997	-0.03150
C(17)	4.060	1.001	0.000	0.997	-0.05960
C(18)	3.982	1.001	0.000	0.997	+0.01810
C(19)	4.063	1.004	0.000	0.956	-0.06290
C(20)	4.066	1.004	0.000	0.956	-0.06610
C(21)	4.090	1.001	0.000	0.997	-0.09050
C(22)	4.117	1.001	0.000	0.997	-0.11700
C(23)	4.121	1.001	0.000	0.997	-0.12110
C(24)	4.064	1.004	0.000	0.956	-0.06370
C(25)	4.073	1.004	0.000	0.956	-0.07280
C(26)	4.045	1.001	0.000	0.997	-0.04460
C(27)	4.098	1.001	0.000	0.997	-0.09810
C(28)	4.037	1.001	0.000	0.997	-0.03680
C(29)	4.084	1.004	0.000	0.956	-0.08390
H(3A)	0.914	1.200	0.000	1.200	+0.08570
H(4A)	0.938	1.200	0.000	1.200	+0.06190
H(5A)	0.894	1.200	0.000	1.200	+0.10620
H(6A)	0.905	1.200	0.000	1.200	+0.09480
H(10A)	0.942	1.200	0.000	1.200	+0.05780
H(11A)	0.923	1.200	0.000	1.200	+0.07650
H(12A)	0.937	1.200	0.000	1.200	+0.06280
H(13A)	0.960	1.200	0.000	1.200	+0.04040
H(15A)	0.900	1.200	0.000	1.200	+0.10010
H(16A)	0.903	1.200	0.000	1.200	+0.09700
H(17A)	0.930	1.200	0.000	1.200	+0.06960
H(18A)	0.958	1.200	0.000	1.200	+0.04250
H(19A)	0.885	1.200	0.000	1.200	+0.11540
H(20A)	0.931	1.200	0.000	1.200	+0.06850
H(21A)	0.898	1.200	0.000	1.200	+0.10200
H(22A)	0.917	1.200	0.000	1.200	+0.08310
H(23A)	0.906	1.200	0.000	1.200	+0.09370
H(24A)	0.913	1.200	0.000	1.200	+0.08700
H(25A)	0.902	1.200	0.000	1.200	+0.09830
H(26A)	0.907	1.200	0.000	1.200	+0.09260
H(27A)	0.928	1.200	0.000	1.200	+0.07170
H(28A)	0.908	1.200	0.000	1.200	+0.09190
H(29A)	0.871	1.200	0.000	1.200	+0.12870
H(3O)	0.914	1.200	0.000	1.200	+0.08610
H(6O)	0.888	1.200	0.000	1.200	+0.11240

Table S8. Dipole population parameters.

Atom	D11+	D11-	D10	Kappa'
CD(1)	0.115(9)	-0.037(8)	0.059(9)	0.938
O(1)	0.012(9)	-0.086(9)	-0.040(10)	1.056
O(2)	0.009(10)	-0.059(10)	-0.054(11)	0.970
O(3)	0.002(11)	-0.022(11)	0.011(12)	0.954
O(4)	0.011(11)	-0.042(11)	-0.101(11)	0.970
O(5)	0.000(9)	0.007(9)	-0.041(10)	1.056
O(6)	0.019(11)	-0.039(11)	-0.032(11)	0.954
N(1)	-0.036(13)	-0.122(14)	-0.026(15)	0.926
N(2)	0.025(13)	-0.065(13)	-0.049(14)	0.941
N(3)	-0.004(12)	-0.111(13)	-0.041(14)	0.948
C(1)	0.030(14)	0.045(16)	-0.024(16)	1.009
C(2)	0.011(15)	0.013(17)	-0.029(16)	1.012
C(3)	0.024(17)	-0.028(19)	0.064(18)	0.984
C(4)	-0.049(17)	0.101(19)	-0.165(18)	0.984
C(5)	0.015(16)	0.009(19)	-0.086(18)	0.984
C(6)	-0.018(15)	0.038(17)	0.025(17)	0.984
C(7)	0.000(15)	0.001(16)	0.045(16)	0.941
C(8)	-0.018(15)	-0.041(16)	0.011(17)	1.009
C(9)	-0.005(15)	-0.007(17)	-0.047(16)	1.012
C(10)	-0.010(16)	0.013(18)	-0.062(18)	0.984
C(11)	-0.076(16)	-0.064(19)	-0.091(18)	0.984
C(12)	0.167(17)	0.042(19)	-0.099(18)	0.984
C(13)	-0.096(16)	-0.032(18)	-0.022(17)	0.984
C(14)	-0.009(15)	-0.055(17)	0.068(17)	0.941
C(15)	0.030(16)	0.054(19)	-0.128(19)	0.956
C(16)	-0.081(16)	0.072(19)	-0.152(18)	0.997
C(17)	-0.002(17)	-0.146(20)	-0.055(18)	0.997
C(18)	-0.057(18)	-0.058(19)	-0.007(18)	0.997
C(19)	0.131(17)	-0.011(19)	0.040(19)	0.956
C(20)	0.006(16)	0.010(18)	-0.016(17)	0.956
C(21)	-0.013(15)	0.035(17)	-0.058(17)	0.997
C(22)	-0.032(15)	-0.021(18)	-0.013(17)	0.997
C(23)	0.009(15)	-0.035(18)	-0.006(17)	0.997
C(24)	-0.009(16)	-0.055(18)	-0.011(18)	0.956
C(25)	-0.027(16)	-0.013(18)	-0.047(17)	0.956
C(26)	-0.079(16)	-0.060(18)	-0.079(17)	0.997
C(27)	0.018(15)	0.051(18)	-0.034(17)	0.997
C(28)	-0.016(16)	-0.014(18)	-0.037(17)	0.997
C(29)	-0.016(16)	0.000(18)	-0.043(18)	0.956
H(3A)	0.000	0.000	0.141(19)	1.200
H(4A)	0.000	0.000	0.139(18)	1.200
H(5A)	0.000	0.000	0.139(17)	1.200
H(6A)	0.000	0.000	0.120(17)	1.200
H(10A)	0.000	0.000	0.132(17)	1.200
H(11A)	0.000	0.000	0.171(18)	1.200
H(12A)	0.000	0.000	0.154(18)	1.200
H(13A)	0.000	0.000	0.164(17)	1.200
H(15A)	0.000	0.000	0.152(16)	1.200
H(16A)	0.000	0.000	0.174(18)	1.200
H(17A)	0.000	0.000	0.083(18)	1.200
H(18A)	0.000	0.000	0.105(19)	1.200
H(19A)	0.000	0.000	0.177(18)	1.200
H(20A)	0.000	0.000	0.107(16)	1.200
H(21A)	0.000	0.000	0.074(17)	1.200

H(22A)	0.000	0.000	0.120(17)	1.200
H(23A)	0.000	0.000	0.118(17)	1.200
H(24A)	0.000	0.000	0.101(17)	1.200
H(25A)	0.000	0.000	0.139(16)	1.200
H(26A)	0.000	0.000	0.152(17)	1.200
H(27A)	0.000	0.000	0.110(17)	1.200
H(28A)	0.000	0.000	0.149(17)	1.200
H(29A)	0.000	0.000	0.157(17)	1.200
H(3O)	0.000	0.000	0.152(19)	1.200
H(6O)	0.000	0.000	0.109(20)	1.200

Table S9. Quadrupole population parameters.

Atom	Q20	Q21+	Q21-	Q22+	Q22-	Kappa'
CD(1)	0.122(10)	-0.123(10)	0.003(10)	0.033(10)	0.037(10)	0.938
O(1)	-0.082(12)	0.022(12)	-0.013(12)	-0.100(11)	-0.042(11)	1.056
O(2)	-0.082(13)	0.009(12)	-0.005(13)	-0.100(12)	0.014(12)	0.970
O(3)	0.009(14)	0.002(13)	0.018(13)	0.057(13)	-0.027(13)	0.954
O(4)	-0.031(13)	-0.002(13)	0.019(13)	-0.081(12)	0.013(12)	0.970
O(5)	0.024(11)	-0.039(11)	-0.031(11)	-0.003(11)	0.032(11)	1.056
O(6)	0.011(13)	0.018(12)	0.037(12)	0.065(13)	-0.004(13)	0.954
N(1)	0.025(16)	-0.008(15)	0.063(16)	-0.126(14)	-0.010(14)	0.926
N(2)	0.051(15)	-0.018(14)	0.048(15)	-0.127(13)	0.005(13)	0.941
N(3)	0.024(15)	-0.041(14)	0.002(14)	-0.103(13)	0.019(13)	0.948
C(1)	0.136(17)	0.023(15)	-0.053(17)	-0.103(15)	0.006(15)	1.009
C(2)	0.070(18)	0.007(16)	-0.022(18)	-0.177(16)	-0.011(16)	1.012
C(3)	0.034(19)	0.003(17)	-0.007(19)	-0.133(19)	0.003(20)	0.984
C(4)	0.096(19)	0.049(17)	-0.035(20)	-0.197(19)	-0.019(20)	0.984
C(5)	0.009(19)	0.019(16)	-0.023(19)	-0.180(18)	0.001(19)	0.984
C(6)	0.151(18)	-0.012(15)	0.039(18)	-0.162(17)	-0.011(17)	0.984
C(7)	0.195(18)	0.038(16)	-0.031(18)	-0.230(16)	0.020(16)	0.941
C(8)	0.144(17)	0.012(16)	-0.036(17)	-0.087(15)	-0.004(15)	1.009
C(9)	0.108(18)	-0.013(15)	-0.021(17)	-0.189(15)	0.013(16)	1.012
C(10)	-0.001(19)	0.006(16)	-0.081(19)	-0.178(17)	-0.018(18)	0.984
C(11)	0.014(19)	0.002(16)	0.006(20)	-0.169(18)	-0.032(19)	0.984
C(12)	0.059(19)	-0.035(17)	-0.023(19)	-0.104(18)	-0.028(19)	0.984
C(13)	0.060(18)	0.003(16)	-0.011(18)	-0.118(17)	0.037(18)	0.984
C(14)	0.244(18)	0.001(17)	-0.038(18)	-0.197(16)	-0.026(16)	0.941
C(15)	0.041(19)	-0.019(16)	0.015(19)	-0.205(17)	0.036(18)	0.956
C(16)	0.104(19)	0.036(16)	-0.012(19)	-0.169(18)	-0.044(18)	0.997
C(17)	0.078(19)	-0.030(17)	0.087(20)	-0.212(19)	-0.025(20)	0.997
C(18)	0.033(20)	-0.003(18)	0.033(20)	-0.127(19)	0.024(20)	0.997
C(19)	0.014(20)	0.017(17)	0.012(20)	-0.163(18)	-0.004(19)	0.956
C(20)	0.084(18)	-0.017(16)	0.027(18)	-0.140(17)	-0.018(17)	0.956
C(21)	0.078(18)	0.014(15)	0.007(18)	-0.137(16)	0.002(17)	0.997
C(22)	0.076(18)	0.005(15)	0.004(18)	-0.134(17)	0.030(18)	0.997
C(23)	0.062(18)	0.001(16)	0.020(18)	-0.140(17)	-0.006(18)	0.997
C(24)	0.049(18)	0.001(16)	0.073(18)	-0.204(17)	-0.013(18)	0.956
C(25)	0.056(18)	-0.035(16)	0.017(18)	-0.197(17)	-0.020(18)	0.956
C(26)	0.069(18)	-0.021(16)	0.010(18)	-0.128(17)	0.004(18)	0.997
C(27)	0.042(18)	-0.007(16)	-0.048(19)	-0.194(18)	0.024(19)	0.997
C(28)	0.071(18)	-0.003(16)	-0.003(19)	-0.138(17)	0.024(18)	0.997
C(29)	0.076(18)	0.018(16)	0.026(18)	-0.190(17)	-0.018(17)	0.956

Table S10. Octupole population parameters.

Atom	O30	O31+	O31-	O32+	O32-	O33+	O33-	Kappa'
CD(1)	-0.005(12)	-0.007(11)	0.023(11)	0.006(11)	-0.002(11)	0.033(11)	-0.012(11)	0.938
O(1)	0.054(16)	0.018(16)	0.034(16)	0.033(16)	-0.009(16)	-0.008(15)	0.021(15)	1.056
O(2)	0.041(17)	0.021(17)	0.013(17)	0.051(16)	0.012(16)	-0.005(15)	0.018(15)	0.970
O(3)	0.014(19)	0.044(18)	-0.072(17)	0.046(18)	-0.001(18)	-0.026(18)	-0.028(17)	0.954
O(4)	0.024(17)	0.018(18)	0.018(17)	0.041(17)	0.005(17)	-0.009(16)	-0.011(16)	0.970
O(5)	0.047(16)	0.017(15)	-0.027(15)	0.029(15)	0.006(15)	-0.004(14)	0.013(14)	1.056
O(6)	0.072(18)	0.007(17)	-0.011(17)	0.024(17)	-0.018(17)	-0.004(17)	0.011(17)	0.954
N(1)	0.110(20)	0.008(20)	-0.010(22)	0.046(19)	0.022(20)	0.036(18)	0.013(18)	0.926
N(2)	0.167(19)	0.004(19)	0.016(21)	0.080(18)	-0.024(19)	-0.005(17)	-0.021(17)	0.941
N(3)	0.128(18)	0.004(18)	0.012(20)	0.076(18)	-0.001(18)	0.016(17)	-0.012(17)	0.948
C(1)	0.175(21)	0.003(21)	0.044(27)	0.154(20)	-0.006(22)	-0.001(20)	-0.011(20)	1.009
C(2)	0.267(23)	0.001(22)	-0.041(27)	0.151(21)	0.033(23)	0.006(21)	-0.043(21)	1.012
C(3)	0.107(24)	0.028(22)	0.004(27)	0.054(23)	0.070(25)	-0.014(26)	0.002(25)	0.984
C(4)	0.146(24)	0.035(22)	-0.013(27)	0.148(23)	-0.048(26)	0.042(27)	-0.006(25)	0.984
C(5)	0.212(23)	0.004(21)	-0.002(26)	0.170(22)	-0.035(24)	0.002(24)	0.003(23)	0.984
C(6)	0.143(22)	0.037(20)	-0.016(25)	0.085(20)	-0.042(22)	-0.015(22)	-0.005(21)	0.984
C(7)	0.275(23)	0.003(23)	0.022(28)	0.225(22)	-0.010(23)	0.005(22)	-0.009(21)	0.941
C(8)	0.160(21)	0.006(21)	0.009(27)	0.113(20)	0.035(22)	-0.046(20)	-0.002(20)	1.009
C(9)	0.284(22)	0.003(21)	-0.014(26)	0.164(20)	0.020(22)	-0.003(20)	-0.009(20)	1.012
C(10)	0.169(23)	0.021(21)	0.004(26)	0.138(21)	0.019(23)	0.060(23)	-0.008(22)	0.984
C(11)	0.202(23)	0.050(21)	-0.020(27)	0.108(22)	0.038(25	0.035(25)	0.001(24)	0.984
C(12)	0.132(24)	0.031(22)	0.008(27)	0.131(22)	0.082(25)	0.002(25)	-0.015(24)	0.984
C(13)	0.175(23)	0.005(21)	-0.074(25)	0.151(21)	-0.008(24	-0.050(24)	-0.018(23)	0.984
C(14)	0.269(23)	0.041(24)	0.010(29)	0.183(23)	0.017(24)	-0.030(21)	-0.011(21)	0.941
C(15)	0.191(23)	0.009(21)	0.061(27)	0.181(22)	-0.020(24)	-0.016(24)	-0.010(22)	0.956
C(16)	0.198(23)	0.032(21)	0.043(27)	0.115(22)	-0.033(24)	-0.014(24)	-0.014(23)	0.997
C(17)	0.186(24)	0.034(22)	-0.002(28)	0.133(23)	0.021(26	0.093(26)	0.009(25)	0.997
C(18)	0.070(25)	0.011(23)	-0.097(28)	0.155(23)	0.073(27	-0.006(27)	-0.063(26	0.997
C(19)	0.205(24)	0.034(22)	0.056(27)	0.169(23)	-0.002(25)	0.065(26)	-0.001(25)	0.956
C(20)	0.181(22)	0.014(20)	0.069(25)	0.162(21)	0.001(23)	0.007(23)	0.002(22)	0.956
C(21)	0.208(22)	0.028(20)	0.008(25)	0.141(20)	-0.006(23)	-0.022(22)	-0.025(22)	0.997
C(22)	0.174(22)	-0.006(20)	-0.015(25)	0.115(21)	0.009(23)	0.002(23)	0.016(22)	0.997
C(23)	0.153(22)	-0.009(21)	0.012(25)	0.099(21)	-0.033(24)	0.017(23)	0.003(22)	0.997
C(24)	0.221(23)	0.002(21)	0.026(26)	0.183(22)	0.021(24)	-0.003(23)	-0.017(22)	0.956
C(25)	0.235(23)	-0.004(20)	0.091(25)	0.246(21)	0.006(23)	-0.009(23)	0.004(22	0.956
C(26)	0.163(22)	-0.035(21)	0.022(26)	0.109(21)	0.016(24)	0.019(24)	0.018(23)	0.997
C(27)	0.188(23)	0.011(21)	-0.021(26)	0.150(21)	-0.024(24)	-0.011(24)	-0.021(23)	0.997
C(28)	0.139(23)	0.020(21)	0.007(25)	0.116(21)	0.005(24)	0.005(24)	-0.008(23)	0.997
C(29)	0.203(23)	-0.004(21)	0.076(26)	0.197(21)	0.002(23)	0.003(23)	-0.007(22)	0.956

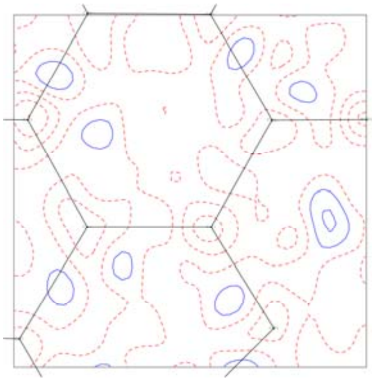
Table S11. Hexadecapole population parameters.

Atom	H40	H41+	H41-	H42+	H42-	H43+	H43-	H44+	H44-	Kappa'
CD(1)	-0.142(16)	0.021(13)	0.190(14)	-0.168(14)	0.011(14)	0.139(14)	0.231(14)	0.065(13)	-0.154(13)	0.938

Table S12. Differences of Mean-Squares Displacement Amplitudes (DMSDA) (1.E4 A**2) along interatomic vectors (*bonds)

ATOM-->	ATOM /	DIST	DMSDA	ATOM /	DIST	DMSDA	ATOM /	DIST	DMSDA
O(1)	O(2)	2.2143	-4	C(1)	2.3834	-6	C(7)	* 1.2619	-6
O(2)	O(3)	2.5696	7	C(1)	2.3833	-2	C(7)	* 1.2762	6
O(3)	C(1)	2.4172	-2	C(2)	* 1.3574	0	C(3)	2.3745	9
O(4)	O(5)	2.2111	-11	C(8)	2.3919	0	C(14)	* 1.2510	4
O(5)	O(6)	2.5413	10	C(8)	2.3780	-3	C(14)	* 1.2883	7
O(6)	C(8)	2.4176	-4	C(9)	* 1.3536	1	C(10)	2.3564	3
N(1)	C(15)	* 1.3471	2	C(16)	2.4048	9	C(17)	2.7951	11
	C(18)	2.3987	5	C(19)	* 1.3397	0			
N(2)	C(20)	* 1.3463	4	C(21)	2.4055	7	C(22)	2.7921	3
	C(23)	2.4005	4	C(24)	* 1.3417	3			
N(3)	C(25)	* 1.3462	7	C(26)	2.4027	6	C(27)	2.7964	6
	C(28)	2.4026	2	C(29)	* 1.3431	3			
C(1)	C(2)	* 1.4085	1	C(3)	2.4314	10	C(4)	2.7971	10
	C(5)	2.4314	8	C(6)	* 1.4003	2	C(7)	* 1.4904	-1
C(2)	C(3)	* 1.4044	11	C(4)	2.4205	5	C(6)	2.4200	1
	C(7)	2.5260	-6						
C(3)	C(4)	* 1.3893	-4	C(5)	2.4217	7	C(6)	2.7812	-3
C(4)	C(5)	* 1.3967	2	C(6)	2.3996	-6			
C(5)	C(6)	* 1.3869	-1						
C(6)	C(7)	2.5013	-7						
C(8)	C(9)	* 1.4088	3	C(10)	2.4315	6	C(11)	2.7997	9
	C(12)	2.4290	6	C(13)	* 1.4024	4	C(14)	* 1.4894	0
C(9)	C(10)	* 1.3980	3	C(11)	2.4119	10	C(12)	2.7979	5
	C(13)	2.4214	4	C(14)	2.5215	-5			
C(10)	C(11)	* 1.3847	6	C(12)	2.4189	-1	C(13)	2.7877	-1
C(11)	C(12)	* 1.4020	-5	C(13)	2.4113	-4			
C(12)	C(13)	* 1.3899	-2						
C(13)	C(14)	2.5070	-3						
C(15)	C(16)	* 1.3943	3	C(17)	2.3981	3	C(18)	2.7307	-3
	C(19)	2.3047	-2						
C(16)	C(17)	* 1.3884	0	C(18)	2.3935	4	C(19)	2.7302	-1
C(17)	C(18)	* 1.3974	11	C(19)	2.4007	-2			
C(18)	C(19)	* 1.3907	-5						
C(20)	C(21)	* 1.3900	4	C(22)	2.3916	1	C(23)	2.7289	1
	C(24)	2.3047	5						
C(21)	C(22)	* 1.3914	2	C(23)	2.3992	2	C(24)	2.7356	2
C(22)	C(23)	* 1.3965	2	C(24)	2.3998	-1			
C(23)	C(24)	* 1.3925	-9						
C(25)	C(26)	* 1.3912	8	C(27)	2.4002	8	C(28)	2.7312	-2
	C(29)	2.3060	-2						
C(26)	C(27)	* 1.3947	-2	C(28)	2.3935	-4	C(29)	2.7305	-2
C(27)	C(28)	* 1.3914	2	C(29)	2.3991	-3			
C(28)	C(29)	* 1.3932	-5						

Figure S6. The residual electron density map in the plane of phenyl ring. Contours are drawn with 0.05 eÅ^{-3} step, the negative and zero contours are dashed.



The residual electron density map in the area of cadmium atoms. Contours are drawn with 0.05 eÅ^{-3} step, the negative and zero contours are dashed.

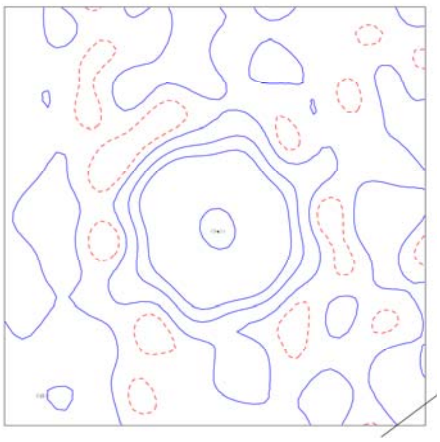


Figure S7. Scatter plots of the scale factor versus resolution.