SUPPLEMENTARY MATERIALS

Trans-catena-poly[[(bis-(μ-N,N'-bis[(pyridin-3-yl)methyl] ethanediamide))diaqua-cadmium(II)] bis(nitrate) tetrahydrate)]

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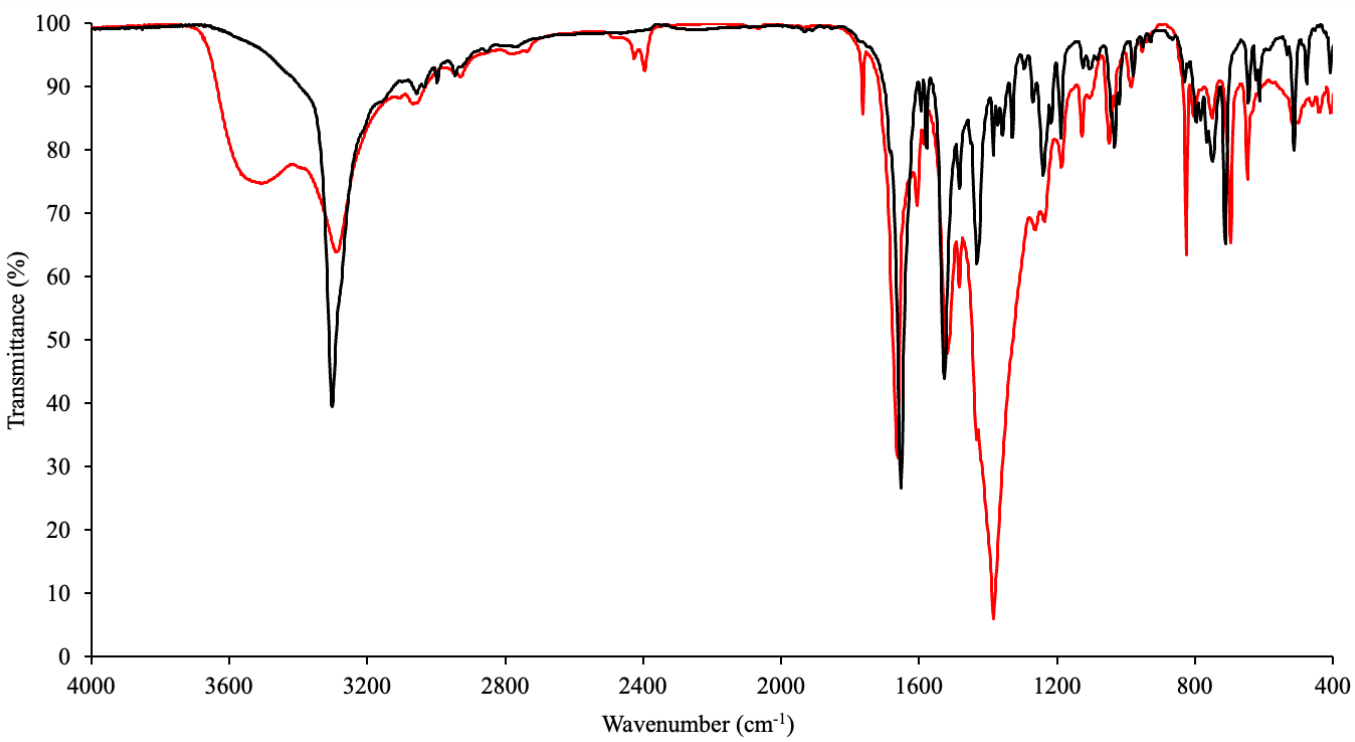

Figure S1. FT-IR spectrum (400–4000 cm^{-1}) recorded at r.t. for **L** (black) and compound **1** (red; KBr pellet).

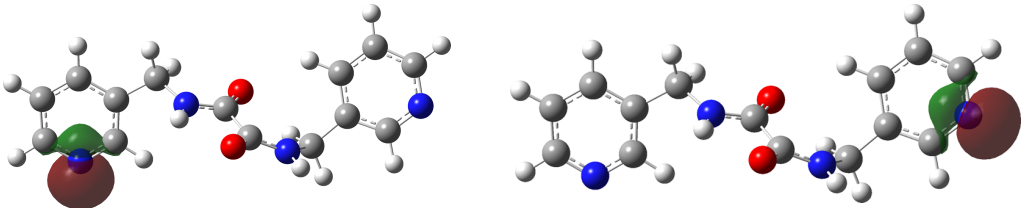

Figure S2. Natural bonding orbitals (NBOs) localized on the pyridine N-atoms of the donor **L**.

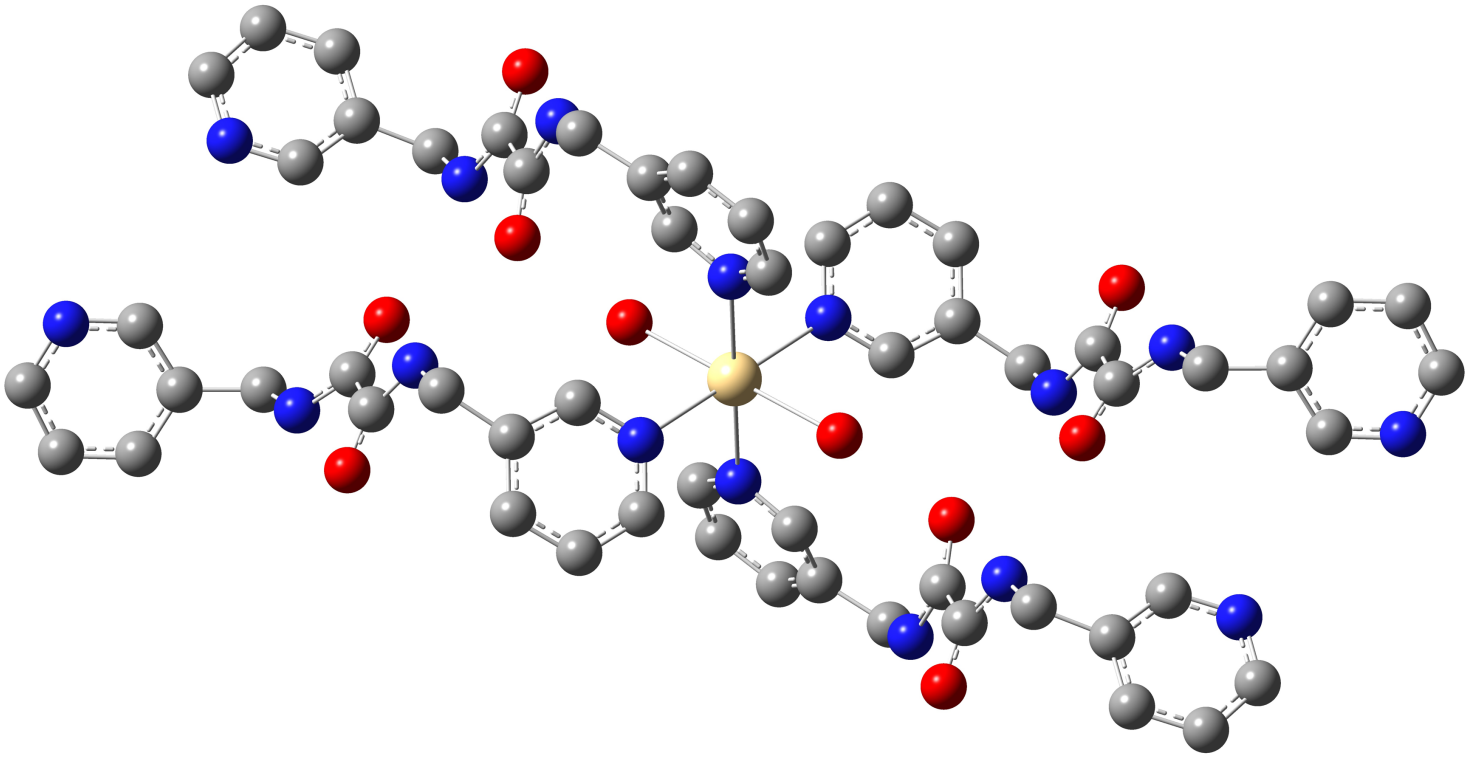

Figure S3. Model cation $[Cd(\mathbf{L})_4(OH_2)_2]^{2+}$ optimized at hybrid-DFT level (mPW1PW/def2SVP). Cd, pale yellow; C, gray; N, blue; O, red. Hydrogen atoms were omitted for clarity.

Table S1. Crystal data and refinement parameters for compound **1**.

Formula	$C_{28}H_{40}CdN_{10}O_{16}$
$\rho_{calc.}$/ g cm^{-3}	1.621
μ/mm^{-1}	0.688
Formula Weight	885.10
Colour	colourless
Shape	block-shaped
Size/mm^3	0.20×0.18×0.10
T/K	100(2)
Crystal System	triclinic
Space Group	$P\bar{1}$
a/Å	9.1489(9)
b/Å	9.2546(9)
c/Å	11.6226(12)
α/°	91.023(4)
β/°	112.441(4)
γ/°	93.497(4)
V/Å^3	906.96(16)
Z	1
Z'	0.5
Wavelength/Å	0.71073
Radiation type	MoK_α
θ_{min}/°	2.433
θ_{max}/°	28.699
Measured Refl's.	44270
Indep't Refl's	4674
Refl's I≥2 σ(I)	4618
R_{int}	0.0390
Parameters	276
Restraints	0
Largest Peak	0.425
Deepest Hole	-0.266
GooF	1.065
wR_2 (all data)	0.0425
wR_2	0.0424
R_1 (all data)	0.0170
R_1	0.0167

Table S2. Bond lengths (Å) for compound **1**. Atom labelling scheme as in Figure 1.

Atom	Atom	Length/Å
Cd1	O8^{ii}	2.2991(9)
Cd1	O8	2.2991(9)
Cd1	N1	2.3365(10)
Cd1	N1^{ii}	2.3365(10)
Cd1	N4^{iii}	2.3766(10)
Cd1	N4^{i}	2.3766(10)
O1	C7	1.2286(14)
O2	C8	1.2325(14)
N1	C1	1.3439(15)
N1	C5	1.3427(14)
N2	C6	1.4507(15)
N2	C7	1.3254(14)
N3	C8	1.3303(14)
N3	C9	1.4514(14)
N4	C11	1.3430(14)
N4	C12	1.3457(14)
C1	C2	1.3801(17)
C2	C3	1.3860(19)
C3	C4	1.3810(17)
C4	C5	1.3906(15)
C4	C6	1.5126(16)
C7	C8	1.5334(16)
C9	C10	1.5094(15)
C10	C11	1.3877(15)
C10	C14	1.3912(15)
C12	C13	1.3838(16)
C13	C14	1.3888(16)
O3	N5	1.2574(12)
O4	N5	1.2449(13)
O5	N5	1.2574(13)

Symmetry codes: ^{i} = +*x*, +*y*, 1+*z*; ^{ii} = 1−*x*, 1−*y*, 2−*z*; ^{iii} = 1−*x*, 1−*y*, 1−*z*.

Table S3. Bond angles (°) for compound **1**. Atom labelling scheme as in Figure 1.

Atom	Atom	Atom	Angle/°
O8^{ii}	Cd1	O8	180.0
O8	Cd1	N1^{ii}	88.99(3)
O8^{ii}	Cd1	N1	89.00(3)
O8	Cd1	N1	91.01(3)
O8^{ii}	Cd1	N1^{ii}	91.00(3)
O8	Cd1	N4^{iii}	91.16(3)
O8^{ii}	Cd1	N4^{i}	91.16(3)
O8^{ii}	Cd1	N4^{iii}	88.84(3)
O8	Cd1	N4^{i}	88.84(3)
N1	Cd1	N1^{ii}	180.00(4)
N1^{ii}	Cd1	N4^{iii}	90.28(3)
N1	Cd1	N4^{i}	90.28(3)
N1	Cd1	N4^{iii}	89.72(3)
N1^{ii}	Cd1	N4^{i}	89.72(3)
N4^{iii}	Cd1	N4^{i}	180.0
C1	N1	Cd1	119.59(8)
C5	N1	Cd1	121.99(7)
C5	N1	C1	118.26(10)
C7	N2	C6	121.41(10)
C8	N3	C9	122.77(10)
C11	N4	Cd1^{iv}	116.79(7)
C11	N4	C12	117.79(10)
C12	N4	Cd1^{iv}	124.13(7)
N1	C1	C2	122.16(11)
C1	C2	C3	119.02(11)
C4	C3	C2	119.69(11)
C3	C4	C5	117.71(11)
C3	C4	C6	121.97(10)
C5	C4	C6	120.30(10)
N1	C5	C4	123.15(10)
N2	C6	C4	112.26(9)
O1	C7	N2	125.40(11)
O1	C7	C8	121.16(10)
N2	C7	C8	113.43(10)
O2	C8	N3	125.03(11)
O2	C8	C7	121.72(10)
N3	C8	C7	113.25(10)
N3	C9	C10	114.26(9)
C11	C10	C9	121.62(10)
C11	C10	C14	117.63(10)
C14	C10	C9	120.68(10)
N4	C11	C10	123.71(10)
N4	C12	C13	122.53(10)
C12	C13	C14	118.94(10)
C13	C14	C10	119.38(10)
O4	N5	O3	120.10(10)
O4	N5	O5	119.85(9)
O5	N5	O3	120.04(10)

Symmetry codes: ^{i} = +*x*, +*y*, 1+*z*; ^{ii} = 1−*x*, 1−*y*, 2−*z*; ^{iii} = 1−*x*, 1−*y*, 1−*z*, ^{iv} = +*x*, +*y*, −1+*z*.

Table S4. Torsion angles (°) for compound **1**. Atom labelling scheme as in Figure 1.

Atom	Atom	Atom	Atom	Angle/°
Cd1	N1	C1	C2	175.24(9)
Cd1	N1	C5	C4	-174.38(8)
Cd1^{iv}	N4	C11	C10	-165.69(8)
Cd1^{iv}	N4	C12	C13	165.47(8)
O1	C7	C8	O2	-174.70(10)
O1	C7	C8	N3	5.85(15)
N1	C1	C2	C3	-0.53(19)
N2	C7	C8	O2	4.57(15)
N2	C7	C8	N3	-174.88(9)
N3	C9	C10	C11	33.78(15)
N3	C9	C10	C14	-149.37(10)
N4	C12	C13	C14	-0.14(17)
C1	N1	C5	C4	0.98(16)
C1	C2	C3	C4	0.58(19)
C2	C3	C4	C5	0.10(17)
C2	C3	C4	C6	-178.29(11)
C3	C4	C5	N1	-0.92(17)
C3	C4	C6	N2	-131.29(12)
C5	N1	C1	C2	-0.24(17)
C5	C4	C6	N2	50.35(14)
C6	N2	C7	O1	0.24(17)
C6	N2	C7	C8	-178.99(9)
C6	C4	C5	N1	177.50(10)
C7	N2	C6	C4	78.86(13)
C8	N3	C9	C10	-86.13(13)
C9	N3	C8	O2	5.02(17)
C9	N3	C8	C7	-175.56(9)
C9	C10	C11	N4	175.60(10)
C9	C10	C14	C13	-176.96(10)
C11	N4	C12	C13	-1.10(16)
C11	C10	C14	C13	0.01(16)
C12	N4	C11	C10	1.87(16)
C12	C13	C14	C10	0.68(17)
C14	C10	C11	N4	-1.34(17)

Symmetry code: ^{iv} = $+x, +y, -1+z$.

Table S5. Optimized geometry at DFT level (mPW1PW/def2SVP) for **L** in Cartesian coordinate format.

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	6	4.969078	-0.790985	0.604069
2	6	3.678894	-0.534996	0.130927
3	6	3.558676	0.279946	-0.999324
4	6	4.711126	0.792594	-1.583025
5	6	5.946114	0.472758	-1.016226
6	1	5.106111	-1.435957	1.481090
7	1	2.568613	0.488493	-1.410216
8	1	4.659135	1.427563	-2.468699
9	1	6.871238	0.863680	-1.452857
10	7	6.077331	-0.304701	0.053300
11	6	2.465814	-1.105266	0.823956
12	1	1.771305	-1.517935	0.086685
13	1	2.778476	-1.920553	1.493780
14	7	1.750862	-0.123252	1.624818
15	1	2.194445	0.166760	2.490908
16	6	0.574964	0.505404	1.432004
17	7	-1.436007	0.779799	0.208793
18	1	-1.629815	1.273781	1.076903
19	6	-2.377716	0.767448	-0.878332
20	1	-1.922126	0.152274	-1.670157
21	1	-2.495917	1.781152	-1.296427
22	6	-3.733255	0.224693	-0.498634
23	6	-3.875054	-0.854534	0.382514
24	6	-4.902842	0.761303	-1.039658
25	1	-2.985040	-1.298423	0.840992
26	6	-6.130917	0.205199	-0.696184
27	1	-4.851861	1.611417	-1.724756
28	6	-6.146000	-0.872304	0.187852
29	1	-7.062512	0.602842	-1.101007
30	1	-7.094464	-1.334214	0.480773
31	7	-5.042675	-1.390966	0.719234
32	6	-0.197074	0.267386	0.115019
33	8	0.261935	-0.283867	-0.871958
34	8	0.096370	1.267932	2.256735

Table S6. Optimized geometry at DFT level (mPW1PW/def2SVP) the model cation $[Cd(\mathbf{L})_4(OH_2)_2]^{2+}$ in Cartesian coordinate format.

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	8	-5.187736	-4.518935	0.278367
2	8	-4.199177	-1.525422	-1.243082
3	7	-10.164486	-2.093813	0.152065
4	7	-5.929454	-2.409139	0.759362
5	1	-5.966850	-1.442011	0.425624
6	7	-3.832233	-3.710135	-1.796642
7	1	-4.076215	-4.641985	-1.453509
8	7	-0.090050	-1.710405	-1.641981
9	6	-10.867141	-3.178735	0.471650
10	1	-11.903415	-3.210771	0.122717
11	6	-10.335785	-4.234262	1.211633
12	1	-10.946694	-5.107648	1.442387
13	6	-9.015979	-4.146881	1.646853
14	1	-8.570497	-4.956438	2.229710
15	6	-8.272676	-3.010096	1.327958
16	6	-8.906465	-2.021588	0.568118
17	1	-8.352066	-1.120298	0.287401
18	6	-6.852043	-2.815191	1.806848
19	1	-6.472700	-3.749517	2.239014
20	1	-6.823599	-2.044636	2.591837
21	6	-5.229344	-3.317023	0.074908
22	6	-4.377284	-2.736995	-1.068686
23	6	-3.088928	-3.539133	-3.022861
24	1	-3.107660	-4.493383	-3.564442
25	1	-3.621889	-2.810466	-3.656932
26	6	-1.662893	-3.058986	-2.867784
27	6	-1.281024	-2.303535	-1.763623
28	1	-1.975927	-2.137569	-0.946107
29	6	0.824973	-1.902645	-2.598128
30	1	1.790089	-1.411911	-2.458909
31	6	0.562480	-2.689734	-3.714666
32	1	1.335567	-2.842160	-4.467942
33	6	-0.700923	-3.257246	-3.861960
34	1	-0.932925	-3.850092	-4.749803
35	8	-6.100317	3.244661	-1.772956
36	8	-6.564812	0.386786	0.191437
37	7	-1.038027	1.505716	-1.463960
38	7	-5.261589	1.151055	-2.070939
39	1	-5.226762	0.212468	-1.677458
40	7	-7.763505	2.336852	0.138332
41	1	-7.801689	3.218942	-0.368513
42	7	-12.180660	1.791998	-0.309687
43	6	-0.680213	2.796291	-1.532203
44	1	0.258349	3.076543	-1.050707
45	6	-1.462647	3.750632	-2.167472

46	1	-1.132645	4.789052	-2.202436
47	6	-2.678295	3.362395	-2.728575
48	1	-3.335394	4.097608	-3.196975
49	6	-3.057987	2.021550	-2.668324
50	6	-2.187230	1.134392	-2.035995
51	1	-2.457397	0.077700	-1.973808
52	6	-4.396569	1.519169	-3.164101
53	1	-4.892567	2.303107	-3.750925
54	1	-4.258850	0.645444	-3.815273
55	6	-6.021710	2.073220	-1.453471
56	6	-6.820059	1.497658	-0.272539
57	6	-8.730517	2.074822	1.191988
58	1	-8.449804	2.646494	2.091178
59	1	-8.651798	1.009768	1.442443
60	6	-10.130879	2.435584	0.768983
61	6	-10.954368	1.508648	0.114431
62	1	-10.613685	0.479343	-0.057463
63	6	-12.654043	3.016986	-0.100971
64	1	-13.666839	3.218049	-0.464345
65	6	-11.930455	4.015624	0.550539
66	1	-12.367497	5.001694	0.711592
67	6	-10.646637	3.714826	0.992222
68	1	-10.053071	4.468958	1.516200
69	48	0.000009	0.000025	-0.000001
70	8	6.100253	-3.244687	1.772930
71	8	6.564824	-0.386839	-0.191485
72	8	-2.329693	-0.585008	0.735822
73	1	-2.559268	-1.056188	1.545346
74	1	-3.109608	-0.686590	0.153247
75	7	1.038037	-1.505669	1.463962
76	7	5.261606	-1.151051	2.070923
77	1	5.226800	-0.212464	1.677442
78	7	7.763461	-2.336939	-0.138366
79	1	7.801625	-3.219021	0.368496
80	7	12.180614	-1.792024	0.309634
81	6	0.680216	-2.796242	1.532208
82	1	-0.258352	-3.076488	1.050720
83	6	1.462647	-3.750587	2.167474
84	1	1.132639	-4.789005	2.202441
85	6	2.678299	-3.362357	2.728572
86	1	3.335396	-4.097573	3.196970
87	6	3.057997	-2.021514	2.668320
88	6	2.187244	-1.134351	2.035993
89	1	2.457415	-0.077660	1.973809
90	6	4.396584	-1.519140	3.164091
91	1	4.892573	-2.303074	3.750929
92	1	4.258875	-0.645402	3.815248
93	6	6.021683	-2.073243	1.453442
94	6	6.820038	-1.497714	0.272498
95	6	8.730475	-2.074956	-1.192031
96	1	8.449770	-2.646675	-2.091193

97	1	8.651750	-1.009915	-1.442542
98	6	10.130840	-2.435683	-0.769005
99	6	10.954320	-1.508706	-0.114499
100	1	10.613631	-0.479395	0.057340
101	6	12.654008	-3.017019	0.100981
102	1	13.666805	-3.218055	0.464366
103	6	11.930429	-4.015697	-0.550478
104	1	12.367480	-5.001771	-0.711480
105	6	10.646608	-3.714932	-0.992178
106	1	10.053050	-4.469096	-1.516118
107	8	5.187772	4.518919	-0.278389
108	8	4.199194	1.525428	1.243096
109	7	10.164545	2.093693	-0.152218
110	7	5.929454	2.409111	-0.759381
111	1	5.966859	1.441988	-0.425629
112	7	3.832262	3.710152	1.796624
113	1	4.076251	4.641995	1.453477
114	7	0.090077	1.710456	1.641977
115	6	10.867109	3.178752	-0.471543
116	1	11.903373	3.210802	-0.122579
117	6	10.335675	4.234399	-1.211297
118	1	10.946513	5.107889	-1.441844
119	6	9.015884	4.147002	-1.646561
120	1	8.570339	4.956651	-2.229243
121	6	8.272677	3.010078	-1.327939
122	6	8.906541	2.021451	-0.568315
123	1	8.352210	1.120051	-0.287816
124	6	6.852058	2.815152	-1.806862
125	1	6.472713	3.749466	-2.239051
126	1	6.823636	2.044580	-2.591833
127	6	5.229356	3.317006	-0.074931
128	6	4.377301	2.736997	1.068677
129	6	3.088963	3.539172	3.022849
130	1	3.107700	4.493429	3.564418
131	1	3.621921	2.810509	3.656927
132	6	1.662926	3.059030	2.867779
133	6	1.281052	2.303583	1.763617
134	1	1.975955	2.137619	0.946101
135	6	-0.824944	1.902696	2.598127
136	1	-1.790061	1.411965	2.458909
137	6	-0.562446	2.689782	3.714666
138	1	-1.335530	2.842208	4.467944
139	6	0.700959	3.257292	3.861958
140	1	0.932965	3.850135	4.749802
141	8	2.329711	0.585061	-0.735832
142	1	2.559285	1.056244	-1.545355
143	1	3.109627	0.686643	-0.153259

Table S7. Summary of natural population analysis (|e|) at the optimized geometry (mPW1PW/def2SVP) for **L**.

Atom	No	Natural Charge	Natural Population			
			Core	Valence	Rydberg	Total
C	1	0.05670	1.99897	3.91940	0.02494	5.94330
C	2	-0.10434	1.99886	4.08981	0.01567	6.10434
C	3	-0.18150	1.99889	4.16625	0.01636	6.18150
C	4	-0.26281	1.99896	4.24988	0.01397	6.26281
C	5	0.05530	1.99906	3.92137	0.02426	5.94470
H	6	0.20474	0.00000	0.79253	0.00273	0.79526
H	7	0.24920	0.00000	0.74684	0.00396	0.75080
H	8	0.23469	0.00000	0.76243	0.00288	0.76531
H	9	0.20944	0.00000	0.78781	0.00275	0.79056
N	10	-0.48260	1.99930	5.46561	0.01769	7.48260
C	11	-0.23942	1.99907	4.21958	0.02077	6.23942
H	12	0.26802	0.00000	0.72769	0.00429	0.73198
H	13	0.22638	0.00000	0.77056	0.00306	0.77362
N	14	-0.64091	1.99918	5.62912	0.01261	7.64091
H	15	0.41222	0.00000	0.58004	0.00774	0.58778
C	16	0.64697	1.99919	3.30748	0.04636	5.35303
N	17	-0.65110	1.99918	5.64035	0.01158	7.65110
H	18	0.43814	0.00000	0.55503	0.00683	0.56186
C	19	-0.23625	1.99911	4.21585	0.02130	6.23625
H	20	0.26099	0.00000	0.73351	0.00550	0.73901
H	21	0.22557	0.00000	0.77141	0.00302	0.77443
C	22	-0.10086	1.99888	4.08636	0.01562	6.10086
C	23	0.06310	1.99898	3.91357	0.02435	5.93690
C	24	-0.19337	1.99890	4.17920	0.01527	6.19337
H	25	0.21292	0.00000	0.78416	0.00292	0.78708
C	26	-0.26050	1.99896	4.24739	0.01415	6.26050
H	27	0.23129	0.00000	0.76584	0.00286	0.76871
C	28	0.05192	1.99905	3.92480	0.02422	5.94808
H	29	0.23585	0.00000	0.76128	0.00287	0.76415
H	30	0.21099	0.00000	0.78628	0.00273	0.78901
N	31	-0.47771	1.99930	5.46069	0.01772	7.47771
C	32	0.64157	1.99920	3.31228	0.04695	5.35843
O	33	-0.65768	1.99973	6.64740	0.01054	8.65768
O	34	-0.64698	1.99974	6.63685	0.01039	8.64698

Table S8. Summary of natural population analysis (|e|) at the optimized geometry (mPW1PW/def2SVP) for the model cation $[Cd(\mathbf{L})_4(OH_2)_2]^{2+}$.

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
O	1	-0.63849	1.99974	6.62841	0.01034	8.63849
O	2	-0.74030	1.99970	6.73120	0.00939	8.74030
N	3	-0.49126	1.99930	5.47353	0.01843	7.49126
N	4	-0.65328	1.99916	5.64243	0.01169	7.65328
H	5	0.45591	0.00000	0.53734	0.00674	0.54409
N	6	-0.62838	1.99915	5.61850	0.01073	7.62838
H	7	0.45647	0.00000	0.53666	0.00687	0.54353
N	8	-0.59856	1.99931	5.57783	0.02142	7.59856
C	9	0.06663	1.99905	3.91010	0.02421	5.93337
H	10	0.22391	0.00000	0.77352	0.00256	0.77609
C	11	-0.25158	1.99896	4.23846	0.01416	6.25158
H	12	0.24612	0.00000	0.75116	0.00272	0.75388
C	13	-0.18333	1.99890	4.16905	0.01538	6.18333
H	14	0.23852	0.00000	0.75878	0.00270	0.76148
C	15	-0.11176	1.99886	4.09755	0.01535	6.11176
C	16	0.05349	1.99896	3.92262	0.02493	5.94651
H	17	0.20752	0.00000	0.78812	0.00436	0.79248
C	18	-0.23552	1.99910	4.21487	0.02154	6.23552
H	19	0.25007	0.00000	0.74569	0.00424	0.74993
H	20	0.24185	0.00000	0.75513	0.00302	0.75815
C	21	0.62938	1.99915	3.32481	0.04667	5.37062
C	22	0.66723	1.99915	3.28722	0.04640	5.33277
C	23	-0.24016	1.99911	4.21967	0.02138	6.24016
H	24	0.26108	0.00000	0.73652	0.00240	0.73892
H	25	0.25644	0.00000	0.73948	0.00408	0.74356
C	26	-0.07183	1.99885	4.05771	0.01526	6.07183
C	27	0.06127	1.99893	3.91479	0.02502	5.93873
H	28	0.22042	0.00000	0.77396	0.00562	0.77958
C	29	0.07636	1.99901	3.90079	0.02384	5.92364
H	30	0.22666	0.00000	0.76888	0.00446	0.77334
C	31	-0.23414	1.99897	4.22087	0.01430	6.23414
H	32	0.26067	0.00000	0.73689	0.00244	0.73933
C	33	-0.15300	1.99890	4.13863	0.01547	6.15300
H	34	0.25550	0.00000	0.74196	0.00254	0.74450
O	35	-0.63612	1.99974	6.62608	0.01030	8.63612
O	36	-0.72132	1.99970	6.71170	0.00993	8.72132
N	37	-0.61222	1.99931	5.59094	0.02197	7.61222
N	38	-0.66611	1.99916	5.65543	0.01151	7.66611
H	39	0.44617	0.00000	0.54715	0.00668	0.55383
N	40	-0.61234	1.99915	5.60163	0.01156	7.61234
H	41	0.43907	0.00000	0.55447	0.00646	0.56093
N	42	-0.47089	1.99930	5.45398	0.01761	7.47089
C	43	0.06795	1.99901	3.91017	0.02287	5.93205
H	44	0.21523	0.00000	0.78081	0.00396	0.78477
C	45	-0.23610	1.99896	4.22279	0.01435	6.23610
H	46	0.25903	0.00000	0.73851	0.00245	0.74097
C	47	-0.13997	1.99889	4.12472	0.01636	6.13997
H	48	0.26378	0.00000	0.73340	0.00281	0.73622
C	49	-0.06673	1.99886	4.05176	0.01611	6.06673
C	50	0.08408	1.99891	3.89314	0.02387	5.91592
H	51	0.21782	0.00000	0.77736	0.00483	0.78218
C	52	-0.24121	1.99911	4.21836	0.02374	6.24121
H	53	0.25982	0.00000	0.73587	0.00431	0.74018
H	54	0.24413	0.00000	0.75295	0.00292	0.75587
C	55	0.64435	1.99919	3.30874	0.04771	5.35565
C	56	0.66141	1.99915	3.29491	0.04453	5.33859
C	57	-0.23468	1.99909	4.21333	0.02227	6.23468
H	58	0.23317	0.00000	0.76375	0.00308	0.76683
H	59	0.24727	0.00000	0.74803	0.00470	0.75273
C	60	-0.12639	1.99886	4.11208	0.01545	6.12639
C	61	0.07297	1.99895	3.90232	0.02576	5.92703
H	62	0.22485	0.00000	0.77008	0.00507	0.77515
C	63	0.06846	1.99906	3.90850	0.02399	5.93154
H	64	0.21964	0.00000	0.77767	0.00270	0.78036
C	65	-0.25632	1.99896	4.24301	0.01435	6.25632
H	66	0.24340	0.00000	0.75380	0.00280	0.75660
C	67	-0.19599	1.99890	4.18145	0.01564	6.19599

H	68	0.23110	0.00000	0.76610	0.00280	0.76890
Cd	69	1.36204	35.99815	10.62743	0.01239	46.63796
O	70	-0.63612	1.99974	6.62608	0.01030	8.63612
O	71	-0.72132	1.99970	6.71170	0.00993	8.72132
O	72	-0.95045	1.99980	6.93987	0.01079	8.95045
H	73	0.49761	0.00000	0.49638	0.00601	0.50239
H	74	0.52060	0.00000	0.47232	0.00709	0.47940
N	75	-0.61222	1.99931	5.59094	0.02197	7.61222
N	76	-0.66611	1.99916	5.65543	0.01151	7.66611
H	77	0.44617	0.00000	0.54715	0.00668	0.55383
N	78	-0.61234	1.99915	5.60163	0.01156	7.61234
H	79	0.43907	0.00000	0.55447	0.00646	0.56093
N	80	-0.47089	1.99930	5.45398	0.01761	7.47089
C	81	0.06795	1.99901	3.91017	0.02287	5.93205
H	82	0.21523	0.00000	0.78081	0.00396	0.78477
C	83	-0.23610	1.99896	4.22279	0.01435	6.23610
H	84	0.25903	0.00000	0.73851	0.00245	0.74097
C	85	-0.13997	1.99889	4.12472	0.01636	6.13997
H	86	0.26378	0.00000	0.73340	0.00281	0.73622
C	87	-0.06673	1.99886	4.05177	0.01611	6.06673
C	88	0.08408	1.99891	3.89314	0.02387	5.91592
H	89	0.21782	0.00000	0.77736	0.00483	0.78218
C	90	-0.24121	1.99911	4.21836	0.02374	6.24121
H	91	0.25982	0.00000	0.73587	0.00431	0.74018
H	92	0.24413	0.00000	0.75295	0.00292	0.75587
C	93	0.64435	1.99919	3.30874	0.04771	5.35565
C	94	0.66141	1.99915	3.29491	0.04453	5.33859
C	95	-0.23468	1.99909	4.21333	0.02227	6.23468
H	96	0.23317	0.00000	0.76375	0.00308	0.76683
H	97	0.24726	0.00000	0.74804	0.00470	0.75274
C	98	-0.12639	1.99886	4.11208	0.01545	6.12639
C	99	0.07297	1.99895	3.90231	0.02576	5.92703
H	100	0.22485	0.00000	0.77008	0.00507	0.77515
C	101	0.06846	1.99906	3.90850	0.02399	5.93154
H	102	0.21964	0.00000	0.77767	0.00270	0.78036
C	103	-0.25632	1.99896	4.24301	0.01435	6.25632
H	104	0.24340	0.00000	0.75380	0.00280	0.75660
C	105	-0.19599	1.99890	4.18145	0.01564	6.19599
H	106	0.23110	0.00000	0.76610	0.00280	0.76890
O	107	-0.63849	1.99974	6.62841	0.01034	8.63849
O	108	-0.74030	1.99970	6.73120	0.00939	8.74030
N	109	-0.49126	1.99930	5.47353	0.01843	7.49126
N	110	-0.65328	1.99916	5.64243	0.01169	7.65328
H	111	0.45591	0.00000	0.53734	0.00674	0.54409
N	112	-0.62838	1.99915	5.61850	0.01073	7.62838
H	113	0.45647	0.00000	0.53666	0.00687	0.54353
N	114	-0.59856	1.99931	5.57783	0.02142	7.59856
C	115	0.06664	1.99905	3.91010	0.02421	5.93336
H	116	0.22392	0.00000	0.77352	0.00256	0.77608
C	117	-0.25158	1.99896	4.23846	0.01416	6.25158
H	118	0.24612	0.00000	0.75116	0.00272	0.75388
C	119	-0.18333	1.99890	4.16905	0.01538	6.18333
H	120	0.23852	0.00000	0.75878	0.00270	0.76148
C	121	-0.11177	1.99886	4.09755	0.01535	6.11177
C	122	0.05350	1.99896	3.92261	0.02493	5.94650
H	123	0.20752	0.00000	0.78813	0.00436	0.79248
C	124	-0.23552	1.99910	4.21487	0.02154	6.23552
H	125	0.25007	0.00000	0.74569	0.00424	0.74993
H	126	0.24185	0.00000	0.75513	0.00302	0.75815
C	127	0.62937	1.99915	3.32481	0.04667	5.37063
C	128	0.66723	1.99915	3.28722	0.04640	5.33277
C	129	-0.24015	1.99911	4.21967	0.02138	6.24015
H	130	0.26108	0.00000	0.73652	0.00240	0.73892
H	131	0.25644	0.00000	0.73948	0.00408	0.74356
C	132	-0.07183	1.99885	4.05771	0.01526	6.07183
C	133	0.06127	1.99893	3.91479	0.02502	5.93873
H	134	0.22042	0.00000	0.77396	0.00562	0.77958
C	135	0.07636	1.99901	3.90079	0.02384	5.92364
H	136	0.22666	0.00000	0.76888	0.00446	0.77334
C	137	-0.23414	1.99897	4.22087	0.01430	6.23414
H	138	0.26067	0.00000	0.73689	0.00244	0.73933
C	139	-0.15300	1.99890	4.13863	0.01547	6.15300
H	140	0.25550	0.00000	0.74196	0.00254	0.74450
O	141	-0.95045	1.99980	6.93987	0.01079	8.95045
H	142	0.49761	0.00000	0.49638	0.00601	0.50239
H	143	0.52059	0.00000	0.47232	0.00709	0.47941