Supporting Information

Energetic Nitrogen-rich Cu(II) and Cd(II) 5,5′-Azobis(tetrazolate) Complexes

Guo-Hong Tao, Brendan Twamley, and Jean'ne M. Shreeve*

Department of Chemistry, University of Idaho, Moscow, Idaho, 83844-2343, USA

jshreeve@uidaho.edu

Table of contents

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[Cu(NH_3)_4]ABT(H_2O)_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(3)	5868(1)	2911(3)	5762(2)	13(1)
C(8)	6638(1)	3716(3)	7876(2)	13(1)
C(16)	8364(1)	3721(3)	2593(2)	13(1)
C(20)	9124(1)	2880(3)	461(2)	12(1)
Cu(1)	4938(1)	2525(1)	2774(1)	13(1)
Cu(2)	7444(1)	4161(1)	5594(1)	13(1)
N(1)	5414(1)	2470(3)	4459(2)	14(1)
N(2)	5816(1)	3029(3)	4629(2)	15(1)
N(4)	5521(1)	2302(3)	6308(2)	15(1)
N(5)	5238(1)	2036(3)	5457(2)	15(1)
N(6)	6262(1)	3387(3)	6253(2)	14(1)
N(7)	6252(1)	3265(3)	7336(2)	14(1)
N(9)	7008(1)	4232(3)	7412(2)	14(1)
N(10)	7263(1)	4520(3)	8318(2)	16(1)
N(11)	7049(1)	4190(3)	9284(2)	16(1)
N(12)	6652(1)	3669(3)	9027(2)	16(1)
N(13)	7916(1)	4228(3)	3903(2)	14(1)
N(14)	7734(1)	4590(3)	2900(2)	16(1)
N(15)	8012(1)	4278(3)	2050(2)	15(1)
N(17)	8317(1)	3666(3)	3736(2)	15(1)
N(18)	8757(1)	3239(3)	2097(2)	14(1)
N(19)	8741(1)	3307(3)	1012(2)	14(1)
N(21)	9499(1)	2369(3)	919(2)	14(1)
N(22)	9751(1)	2143(3)	4(2)	15(1)
N(23)	9535(1)	2509(3)	-953(2)	15(1)
N(24)	9136(1)	2961(3)	-685(2)	15(1)
N(25)	5324(1)	575(3)	1982(2)	16(1)
N(26)	5260(1)	4752(3)	2067(2)	15(1)
N(27)	4563(1)	4489(3)	3598(2)	17(1)
N(28)	4614(1)	287(3)	3472(2)	16(1)
N(29)	7111(1)	1921(3)	4930(2)	15(1)

N(30)	7839(1)	2199(3)	6367(2)	14(1)
N(31)	7773(1)	6385(3)	6306(2)	16(1)
N(32)	7073(1)	6124(3)	4743(2)	16(1)
O(5)	6117(1)	4255(3)	929(2)	25(1)
O(6)	6473(1)	3465(3)	3061(2)	23(1)
O(7)	6386(1)	9483(3)	2519(2)	23(1)
O(8)	6057(1)	8156(3)	392(2)	24(1)

Table S2. Bond lengths [Å] and angles [°] for $[Cu(NH_3)_4]ABT(H_2O)_2$.

C(3)-N(2)	1.332(3)	N(21)-N(22)	1.339(3)
C(3)-N(4)	1.336(3)	N(22)-N(23)	1.330(3)
C(3)-N(6)	1.407(3)	N(23)-N(24)	1.335(3)
C(8)-N(9)	1.337(3)	N(25)-H(25A)	0.9100
C(8)-N(12)	1.341(3)	N(25)-H(25B)	0.9100
C(8)-N(7)	1.405(3)	N(25)-H(25C)	0.9100
C(16)-N(15)	1.338(3)	N(26)-H(26A)	0.9100
C(16)-N(17)	1.339(3)	N(26)-H(26B)	0.9100
C(16)-N(18)	1.409(3)	N(26)-H(26C)	0.9100
C(20)-N(24)	1.335(3)	N(27)-H(27A)	0.9100
C(20)-N(21)	1.347(3)	N(27)-H(27B)	0.9100
C(20)-N(19)	1.400(3)	N(27)-H(27C)	0.9100
Cu(1)-N(26)	2.021(2)	N(28)-H(28A)	0.8547
Cu(1)-N(28)	2.026(2)	N(28)-H(28B)	0.8475
Cu(1)-N(25)	2.038(2)	N(28)-H(28C)	0.9236
Cu(1)-N(27)	2.041(2)	N(29)-H(29A)	0.9100
Cu(1)-N(1)	2.471(2)	N(29)-H(29B)	0.9100
Cu(2)-N(29)	2.025(2)	N(29)-H(29C)	0.9100
Cu(2)-N(31)	2.032(2)	N(30)-H(30A)	0.9100
Cu(2)-N(32)	2.049(2)	N(30)-H(30B)	0.9100
Cu(2)-N(30)	2.051(2)	N(30)-H(30C)	0.9100
Cu(2)-N(13)	2.469(2)	N(31)-H(31A)	0.9100
Cu(2)-N(9)	2.526(2)	N(31)-H(31B)	0.9100
N(1)-N(5)	1.322(3)	N(31)-H(31C)	0.9100
N(1)-N(2)	1.344(3)	N(32)-H(32A)	0.9100
N(4)-N(5)	1.346(3)	N(32)-H(32B)	0.9100
N(6)-N(7)	1.263(3)	N(32)-H(32C)	0.9100
N(9)-N(10)	1.341(3)	O(5)-H(5A)	0.8474
N(10)-N(11)	1.332(3)	O(5)-H(5B)	0.8505
N(11)-N(12)	1.339(3)	O(6)-H(6A)	0.8501
N(13)-N(14)	1.325(3)	O(6)-H(6B)	0.8463
N(13)-N(17)	1.341(3)	O(7)-H(7A)	0.8511
N(14)-N(15)	1.340(3)	O(7)-H(7B)	0.8495
N(18)-N(19)	1.264(3)	O(8)-H(8A)	0.8506

O(8)-H(8B)	0.8494	N(32)-Cu(2)-N(9)	94.56(8)
		N(30)-Cu(2)-N(9)	88.70(8)
N(2)-C(3)-N(4)	112.8(2)	N(13)-Cu(2)-N(9)	175.37(7)
N(2)-C(3)-N(6)	119.8(2)	N(5)-N(1)-N(2)	109.4(2)
N(4)-C(3)-N(6)	127.3(2)	N(5)-N(1)-Cu(1)	116.54(15)
N(9)-C(8)-N(12)	112.3(2)	N(2)-N(1)-Cu(1)	133.45(16)
N(9)-C(8)-N(7)	129.6(2)	C(3)-N(2)-N(1)	104.2(2)
N(12)-C(8)-N(7)	118.1(2)	C(3)-N(4)-N(5)	103.8(2)
N(15)-C(16)-N(17)	112.7(2)	N(1)-N(5)-N(4)	109.74(18)
N(15)-C(16)-N(18)	127.4(2)	N(7)-N(6)-C(3)	111.57(19)
N(17)-C(16)-N(18)	119.9(2)	N(6)-N(7)-C(8)	114.21(19)
N(24)-C(20)-N(21)	112.3(2)	C(8)-N(9)-N(10)	104.4(2)
N(24)-C(20)-N(19)	118.3(2)	C(8)-N(9)-Cu(2)	144.10(17)
N(21)-C(20)-N(19)	129.3(2)	N(10)-N(9)-Cu(2)	109.52(14)
N(26)-Cu(1)-N(28)	179.58(10)	N(11)-N(10)-N(9)	109.54(19)
N(26)-Cu(1)-N(25)	91.06(9)	N(10)-N(11)-N(12)	109.3(2)
N(28)-Cu(1)-N(25)	88.79(9)	N(11)-N(12)-C(8)	104.5(2)
N(26)-Cu(1)-N(27)	88.70(9)	N(14)-N(13)-N(17)	109.6(2)
N(28)-Cu(1)-N(27)	91.46(9)	N(14)-N(13)-Cu(2)	116.45(14)
N(25)-Cu(1)-N(27)	178.55(9)	N(17)-N(13)-Cu(2)	132.98(16)
N(26)-Cu(1)-N(1)	91.66(8)	N(13)-N(14)-N(15)	109.77(19)
N(28)-Cu(1)-N(1)	88.72(8)	C(16)-N(15)-N(14)	104.0(2)
N(25)-Cu(1)-N(1)	89.15(8)	C(16)-N(17)-N(13)	104.0(2)
N(27)-Cu(1)-N(1)	89.43(8)	N(19)-N(18)-C(16)	111.52(19)
N(29)-Cu(2)-N(31)	178.34(9)	N(18)-N(19)-C(20)	114.6(2)
N(29)-Cu(2)-N(32)	91.44(8)	N(22)-N(21)-C(20)	103.8(2)
N(31)-Cu(2)-N(32)	89.35(8)	N(23)-N(22)-N(21)	109.80(19)
N(29)-Cu(2)-N(30)	88.71(9)	N(22)-N(23)-N(24)	109.4(2)
N(31)-Cu(2)-N(30)	90.58(9)	N(23)-N(24)-C(20)	104.6(2)
N(32)-Cu(2)-N(30)	176.72(9)	Cu(1)-N(25)-H(25A)	109.5
N(29)-Cu(2)-N(13)	91.35(8)	Cu(1)-N(25)-H(25B)	109.5
N(31)-Cu(2)-N(13)	90.15(8)	H(25A)-N(25)-H(25B)	109.5
N(32)-Cu(2)-N(13)	87.03(8)	Cu(1)-N(25)-H(25C)	109.5
N(30)-Cu(2)-N(13)	89.69(8)	H(25A)-N(25)-H(25C)	109.5
N(29)-Cu(2)-N(9)	92.95(8)	H(25B)-N(25)-H(25C)	109.5
N(31)-Cu(2)-N(9)	85.53(7)	Cu(1)-N(26)-H(26A)	109.5

Cu(1)-N(26)-H(26B)	109.5	Cu(2)-N(30)-H(30A)	109.5
H(26A)-N(26)-H(26B)	109.5	Cu(2)-N(30)-H(30B)	109.5
Cu(1)-N(26)-H(26C)	109.5	H(30A)-N(30)-H(30B)	109.5
H(26A)-N(26)-H(26C)	109.5	Cu(2)-N(30)-H(30C)	109.5
H(26B)-N(26)-H(26C)	109.5	H(30A)-N(30)-H(30C)	109.5
Cu(1)-N(27)-H(27A)	109.5	H(30B)-N(30)-H(30C)	109.5
Cu(1)-N(27)-H(27B)	109.5	Cu(2)-N(31)-H(31A)	109.5
H(27A)-N(27)-H(27B)	109.5	Cu(2)-N(31)-H(31B)	109.5
Cu(1)-N(27)-H(27C)	109.5	H(31A)-N(31)-H(31B)	109.5
H(27A)-N(27)-H(27C)	109.5	Cu(2)-N(31)-H(31C)	109.5
H(27B)-N(27)-H(27C)	109.5	H(31A)-N(31)-H(31C)	109.5
Cu(1)-N(28)-H(28A)	110.4	H(31B)-N(31)-H(31C)	109.5
Cu(1)-N(28)-H(28B)	113.5	Cu(2)-N(32)-H(32A)	109.5
H(28A)-N(28)-H(28B)	116.9	Cu(2)-N(32)-H(32B)	109.5
Cu(1)-N(28)-H(28C)	121.9	H(32A)-N(32)-H(32B)	109.5
H(28A)-N(28)-H(28C)	98.5	Cu(2)-N(32)-H(32C)	109.5
H(28B)-N(28)-H(28C)	94.6	H(32A)-N(32)-H(32C)	109.5
Cu(2)-N(29)-H(29A)	109.5	H(32B)-N(32)-H(32C)	109.5
Cu(2)-N(29)-H(29B)	109.5	H(5A)-O(5)-H(5B)	101.8
H(29A)-N(29)-H(29B)	109.5	H(6A)-O(6)-H(6B)	94.0
Cu(2)-N(29)-H(29C)	109.5	H(7A)-O(7)-H(7B)	100.6
H(29A)-N(29)-H(29C)	109.5	H(8A)-O(8)-H(8B)	113.7
H(29B)-N(29)-H(29C)	109.5		

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Cu(NH_3)_4]ABT(H_2O)_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(3)	15(1)	10(1)	14(1)	0(1)	-1(1)	2(1)
C(8)	15(1)	11(1)	11(1)	-1(1)	1(1)	-1(1)
C(16)	12(1)	11(1)	15(1)	-2(1)	-1(1)	-1(1)
C(20)	12(1)	11(1)	14(1)	-1(1)	2(1)	-2(1)
Cu(1)	13(1)	13(1)	14(1)	-1(1)	2(1)	0(1)
Cu(2)	14(1)	13(1)	13(1)	0(1)	-2(1)	0(1)
N(1)	14(1)	15(1)	13(1)	1(1)	-1(1)	-1(1)
N(2)	15(1)	15(1)	14(1)	-2(1)	-2(1)	-1(1)
N(4)	15(1)	17(1)	14(1)	0(1)	-2(1)	-2(1)
N(5)	14(1)	19(1)	14(1)	1(1)	-1(1)	-1(1)
N(6)	15(1)	13(1)	13(1)	0(1)	-1(1)	1(1)
N(7)	15(1)	13(1)	13(1)	0(1)	1(1)	-1(1)
N(9)	14(1)	14(1)	12(1)	-2(1)	-2(1)	0(1)
N(10)	16(1)	17(1)	15(1)	-2(1)	-1(1)	-2(1)
N(11)	16(1)	15(1)	15(1)	-1(1)	-1(1)	-2(1)
N(12)	17(1)	16(1)	15(1)	0(1)	1(1)	-2(1)
N(13)	12(1)	15(1)	15(1)	0(1)	1(1)	2(1)
N(14)	15(1)	17(1)	15(1)	1(1)	3(1)	2(1)
N(15)	14(1)	18(1)	12(1)	-2(1)	2(1)	2(1)
N(17)	14(1)	17(1)	15(1)	0(1)	1(1)	0(1)
N(18)	14(1)	12(1)	14(1)	1(1)	0(1)	-1(1)
N(19)	13(1)	14(1)	13(1)	-1(1)	1(1)	2(1)
N(21)	15(1)	13(1)	14(1)	-1(1)	1(1)	2(1)
N(22)	14(1)	17(1)	15(1)	-1(1)	2(1)	-1(1)
N(23)	18(1)	15(1)	12(1)	-1(1)	2(1)	1(1)
N(24)	17(1)	15(1)	14(1)	-1(1)	2(1)	3(1)
N(25)	16(1)	18(1)	14(1)	-2(1)	-1(1)	2(1)
N(26)	15(1)	17(1)	14(1)	0(1)	-1(1)	-2(1)
N(27)	17(1)	18(1)	16(1)	-2(1)	0(1)	1(1)
N(28)	15(1)	18(1)	15(1)	1(1)	-1(1)	-1(1)
N(29)	15(1)	16(1)	15(1)	0(1)	0(1)	2(1)

N(30)	14(1)	16(1)	13(1)	1(1)	1(1)	0(1)
N(31)	15(1)	16(1)	15(1)	1(1)	1(1)	0(1)
N(32)	14(1)	17(1)	16(1)	0(1)	2(1)	2(1)
O(5)	24(1)	33(1)	18(1)	2(1)	5(1)	4(1)
O(6)	16(1)	35(1)	18(1)	5(1)	2(1)	2(1)
O(7)	24(1)	28(1)	19(1)	2(1)	7(1)	-2(1)
O(8)	16(1)	35(1)	20(1)	0(1)	5(1)	0(1)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Cu(NH_3)_4]ABT(H_2O)_2$.

	x	y	z	U(eq)
H(25A)	5179	-29	1410	24
H(25B)	5414	-318	2503	24
H(25C)	5552	1200	1680	24
H(26A)	5482	4285	1652	23
H(26B)	5359	5541	2633	23
H(26C)	5085	5434	1596	23
H(27A)	4442	5291	3072	26
H(27B)	4723	5195	4095	26
H(27C)	4357	3855	3994	26
H(28A)	4482	-339	2949	24
H(28B)	4758	-370	3945	24
H(28C)	4390	480	3970	24
H(29A)	7268	1323	4379	23
H(29B)	6867	2370	4615	23
H(29C)	7049	1062	5498	23
H(30A)	7695	1547	6921	22
H(30B)	8062	2833	6690	22
H(30C)	7936	1347	5832	22
H(31A)	7843	7253	5750	23
H(31B)	8012	5921	6641	23
H(31C)	7610	6977	6847	23
H(32A)	6912	6785	5260	24
H(32B)	6901	5491	4241	24
H(32C)	7240	6968	4352	24
H(5A)	6193	3769	293	37
H(5B)	6097	5448	760	37
H(6A)	6246	3554	3447	34
H(6B)	6370	4015	2474	34
H(7A)	6247	9031	3084	35
H(7B)	6396	10674	2698	35
H(8A)	6227	8401	-156	35

H(8B)	6124	8699	1021	35

Table S5. Hydrogen bonds for $[Cu(NH_3)_4]ABT(H_2O)_2$ [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(25)-H(25A)...N(5)#1	0.91	2.21	3.093(3)	163
N(25)-H(25B)...N(23)#2	0.91	2.35	3.235(3)	165
N(26)-H(26A)...O(5)	0.91	2.18	3.034(3)	157
N(26)-H(26B)...N(23)#3	0.91	2.16	3.060(3)	169
N(26)-H(26C)...N(5)#4	0.91	2.42	3.305(3)	164
N(26)-H(26C)...N(4)#4	0.91	2.50	3.320(3)	151
N(27)-H(27A)...N(7)#4	0.91	2.56	3.348(3)	146
N(27)-H(27B)...N(22)#3	0.91	2.39	3.277(3)	166
N(27)-H(27C)...O(8)#5	0.91	2.51	3.398(3)	166
N(28)-H(28A)...N(4)#1	0.85	2.34	3.120(3)	151
N(28)-H(28B)...N(22)#2	0.85	2.62	3.454(3)	167
N(28)-H(28C)...O(8)#5	0.92	2.37	3.262(3)	162
N(29)-H(29A)...N(10)#6	0.91	2.30	3.192(3)	168
N(29)-H(29A)...N(11)#6	0.91	2.62	3.342(3)	137
N(29)-H(29B)...O(6)	0.91	2.32	3.153(3)	152
N(29)-H(29C)...N(15)#2	0.91	2.19	3.094(3)	170
N(30)-H(30A)...N(14)#2	0.91	2.23	3.118(3)	166
N(30)-H(30B)...O(7)#2	0.91	2.30	3.207(3)	179
N(30)-H(30C)...N(11)#6	0.91	2.34	3.214(3)	161
N(31)-H(31A)...N(11)#7	0.91	2.20	3.101(3)	173
N(31)-H(31B)...O(7)#2	0.91	2.38	3.284(3)	176
N(31)-H(31C)...N(14)#3	0.91	2.44	3.304(3)	159
N(31)-H(31C)...N(15)#3	0.91	2.54	3.300(3)	142
N(32)-H(32A)...N(19)#3	0.91	2.48	3.328(3)	156
N(32)-H(32B)...O(6)	0.91	2.38	3.287(3)	173
O(5)-H(5A)...N(12)#8	0.85	2.07	2.815(3)	147
O(5)-H(5B)...O(8)	0.85	1.92	2.774(3)	179
O(6)-H(6A)...N(2)	0.85	1.97	2.781(3)	160
O(6)-H(6B)...O(5)	0.85	1.98	2.778(3)	158
O(7)-H(7A)...N(24)#3	0.85	2.02	2.865(3)	174
O(7)-H(7B)...O(6)#9	0.85	1.99	2.837(3)	175
O(8)-H(8A)...N(17)#7	0.85	1.94	2.784(3)	170

O(8)-H(8B)...O(7)	0.85	2.01	2.839(3)	166

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+1,-y+1,z-1/2 #5 -x+1,-y+1,z+1/2 #6 -x+3/2,y-1/2,z-1/2

#7 -x+3/2,y+1/2,z-1/2 #8 x,y,z-1 #9 x,y+1,z

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[Cd(NH_3)_2(H_2O)_2]$ABT. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cd(1A)	-1727(1)	1336(1)	1175(1)	14(1)
N(1)	-1682(5)	-422(2)	1301(2)	16(1)
N(2)	-2361(5)	-940(3)	802(2)	16(1)
N(3)	-2138(5)	-1882(2)	928(2)	16(1)
N(4)	-1326(5)	-2001(2)	1510(2)	16(1)
C(5)	-1065(6)	-1091(3)	1723(2)	16(1)
N(6)	-232(4)	-803(2)	2311(1)	13(1)
N(7)	220(4)	-1513(2)	2668(2)	13(1)
C(8)	1042(6)	-1213(3)	3256(2)	16(1)
N(9)	1643(4)	-1874(3)	3684(2)	16(1)
N(10)	2311(5)	-1352(2)	4178(2)	16(1)
N(11)	2109(5)	-408(2)	4046(2)	16(1)
N(12)	1317(5)	-304(2)	3463(2)	16(1)
N(13)	158(5)	1347(2)	431(2)	18(1)
N(14)	-4469(5)	1346(2)	466(2)	20(1)
O(1)	940(5)	1345(2)	1903(2)	34(1)
O(2)	-3777(5)	1346(2)	1900(2)	28(1)
Cd(1B)	1719(10)	980(6)	3823(3)	20(2)
N(1B)	1660(30)	-779(6)	3678(7)	16(1)
N(2B)	2370(50)	-1305(7)	4169(9)	16(1)
N(3B)	2150(60)	-2238(7)	4040(12)	16(1)
N(4B)	1300(50)	-2349(7)	3460(12)	16(1)
C(5B)	1030(40)	-1440(7)	3255(8)	16(1)
N(6B)	160(30)	-1134(11)	2672(7)	13(1)
N(7B)	-310(40)	-1829(14)	2311(9)	13(1)
C(8B)	-1170(40)	-1528(18)	1729(9)	16(1)
N(9B)	-1790(50)	-2170(20)	1297(11)	16(1)
N(10B)	-2490(60)	-1630(30)	810(10)	16(1)
N(11B)	-2270(60)	-700(20)	952(8)	16(1)
N(12B)	-1460(50)	-610(20)	1531(7)	16(1)

Table S7. Bond lengths [Å] and angles [°] for $[Cd(NH_3)_2(H_2O)_2]ABT$.

Cd(1A)-N(13)	2.310(3)	N(2B)-N(3B)	1.3138
Cd(1A)-O(1)	2.316(4)	N(3B)-N(4B)	1.3486
Cd(1A)-N(14)	2.333(3)	N(4B)-C(5B)	1.3296
Cd(1A)-O(2)	2.361(3)	C(5B)-N(6B)	1.4154
Cd(1A)-N(1)	2.422(3)	N(6B)-N(7B)	1.2569
Cd(1A)-N(9)#1	2.470(3)	N(7B)-C(8B)	1.4090
N(1)-C(5)	1.337(5)	C(8B)-N(9B)	1.3310
N(1)-N(2)	1.344(5)	C(8B)-N(12B)	1.3384
N(2)-N(3)	1.324(5)	N(9B)-N(10B)	1.3433
N(3)-N(4)	1.346(5)	N(9B)-Cd(1B)#2	2.54(3)
N(4)-C(5)	1.335(5)	N(10B)-N(11B)	1.3228
C(5)-N(6)	1.410(5)	N(11B)-N(12B)	1.3383
N(6)-N(7)	1.265(5)		
N(7)-C(8)	1.413(5)	N(13)-Cd(1A)-O(1)	88.98(12)
C(8)-N(12)	1.331(5)	N(13)-Cd(1A)-N(14)	92.79(12)
C(8)-N(9)	1.336(5)	O(1)-Cd(1A)-N(14)	178.11(11)
N(9)-N(10)	1.336(5)	N(13)-Cd(1A)-O(2)	177.22(11)
N(9)-Cd(1A)#2	2.470(3)	O(1)-Cd(1A)-O(2)	93.71(12)
N(10)-N(11)	1.328(5)	N(14)-Cd(1A)-O(2)	84.52(12)
N(11)-N(12)	1.342(5)	N(13)-Cd(1A)-N(1)	95.23(11)
N(13)-H(13A)	0.9061	O(1)-Cd(1A)-N(1)	85.97(11)
N(13)-H(13B)	0.9104	N(14)-Cd(1A)-N(1)	94.51(11)
N(13)-H(13C)	0.9124	O(2)-Cd(1A)-N(1)	85.71(10)
N(14)-H(14A)	0.9010	N(13)-Cd(1A)-N(9)#1	94.53(11)
N(14)-H(14B)	0.9096	O(1)-Cd(1A)-N(9)#1	84.55(11)
N(14)-H(14C)	0.9125	N(14)-Cd(1A)-N(9)#1	94.66(11)
O(1)-H(1A)	0.8534	O(2)-Cd(1A)-N(9)#1	84.99(10)
O(1)-H(1B)	0.8523	N(1)-Cd(1A)-N(9)#1	166.25(11)
O(2)-H(2A)	0.8560	C(5)-N(1)-N(2)	105.0(3)
O(2)-H(2B)	0.8578	C(5)-N(1)-Cd(1A)	139.3(3)
Cd(1B)-N(1B)	2.4287	N(2)-N(1)-Cd(1A)	115.6(2)
Cd(1B)-N(9B)#1	2.543(5)	N(3)-N(2)-N(1)	108.7(3)
N(1B)-C(5B)	1.3325	N(2)-N(3)-N(4)	110.0(3)
N(1B)-N(2B)	1.3414	C(5)-N(4)-N(3)	104.2(3)

N(4)-C(5)-N(1)	112.0(4)	H(1A)-O(1)-H(1B)	115.7
N(4)-C(5)-N(6)	127.3(4)	Cd(1A)-O(2)-H(2A)	106.3
N(1)-C(5)-N(6)	120.6(4)	Cd(1A)-O(2)-H(2B)	104.2
N(7)-N(6)-C(5)	113.6(3)	H(2A)-O(2)-H(2B)	118.3
N(6)-N(7)-C(8)	113.0(3)	N(1B)-Cd(1B)-N(9B)#1	166.3(8)
N(12)-C(8)-N(9)	111.8(4)	C(5B)-N(1B)-N(2B)	104.9
N(12)-C(8)-N(7)	127.6(4)	C(5B)-N(1B)-Cd(1B)	139.7
N(9)-C(8)-N(7)	120.6(3)	N(2B)-N(1B)-Cd(1B)	115.2
C(8)-N(9)-N(10)	105.2(3)		
C(8)-N(9)-Cd(1A)#2	139.5(3)		
N(10)-N(9)-Cd(1A)#2	115.2(2)	N(3B)-N(2B)-N(1B)	108.9
N(11)-N(10)-N(9)	108.8(3)	N(2B)-N(3B)-N(4B)	109.9
N(10)-N(11)-N(12)	109.5(3)	C(5B)-N(4B)-N(3B)	104.1
C(8)-N(12)-N(11)	104.7(3)	N(4B)-C(5B)-N(1B)	112.1
Cd(1A)-N(13)-H(13A)	117.3	N(4B)-C(5B)-N(6B)	127.7
Cd(1A)-N(13)-H(13B)	106.4	N(1B)-C(5B)-N(6B)	120.1
H(13A)-N(13)-H(13B)	109.3	N(7B)-N(6B)-C(5B)	113.6
Cd(1A)-N(13)-H(13C)	127.3	N(6B)-N(7B)-C(8B)	113.8
H(13A)-N(13)-H(13C)	100.4	N(9B)-C(8B)-N(12B)	111.6
H(13B)-N(13)-H(13C)	93.0	N(9B)-C(8B)-N(7B)	121.4
Cd(1A)-N(14)-H(14A)	111.0	N(12B)-C(8B)-N(7B)	127.0
Cd(1A)-N(14)-H(14B)	114.0	C(8B)-N(9B)-N(10B)	105.1
H(14A)-N(14)-H(14B)	114.6	C(8B)-N(9B)-Cd(1B)#2	136.5(9)
Cd(1A)-N(14)-H(14C)	111.1	N(10B)-N(9B)-Cd(1B)#2	118.2(9)
H(14A)-N(14)-H(14C)	115.4	N(11B)-N(10B)-N(9B)	108.9
H(14B)-N(14)-H(14C)	89.1	N(10B)-N(11B)-N(12B)	109.6
Cd(1A)-O(1)-H(1A)	113.2	N(11B)-N(12B)-C(8B)	104.7
Cd(1A)-O(1)-H(1B)	113.4		

Symmetry transformations used to generate equivalent atoms:

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

Table S8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Cd(NH_3)_2(H_2O)_2]ABT$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cd(1A)	16(1)	14(1)	11(1)	0(1)	-1(1)	0(1)
N(13)	19(2)	23(2)	11(2)	0(1)	1(1)	-1(1)
N(14)	23(2)	24(2)	9(2)	-1(1)	-3(1)	5(1)
O(1)	30(2)	38(2)	31(2)	-1(1)	0(2)	1(1)
O(2)	37(2)	21(2)	30(2)	1(1)	13(2)	4(1)

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Cd(NH_3)_2(H_2O)_2]$ABT.

	x	y	z	U(eq)
H(13A)	958	1856	429	22
H(13B)	821	779	472	22
H(13C)	-204	1259	23	22
H(14A)	-5195	1861	525	24
H(14B)	-4279	1263	76	24
H(14C)	-5048	752	448	24
H(1A)	1537	805	1925	50
H(1B)	764	1589	2241	50
H(2A)	-4369	803	1859	42
H(2B)	-4403	1877	1826	42

Table S10. Hydrogen bonds for $[Cd(NH_3)_2(H_2O)_2]ABT$ [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(13)-H(13A)...N(3)#3	0.91	2.37	3.200(5)	152
N(13)-H(13B)...N(11)#4	0.91	2.35	3.211(5)	158
N(13)-H(13C)...N(10)#5	0.91	2.39	3.196(5)	147
N(14)-H(14A)...N(3)#6	0.90	2.48	3.362(5)	167
N(14)-H(14B)...N(10)#5	0.91	2.46	3.328(5)	159
N(14)-H(14C)...N(11)#7	0.91	2.56	3.356(5)	146
O(1)-H(1A)...N(12)#4	0.85	2.43	3.196(5)	150
O(1)-H(1B)...O(2)#7	0.85	2.59	3.303(5)	141
O(2)-H(2A)...N(12)#7	0.86	2.12	2.943(5)	163
O(2)-H(2B)...N(4)#6	0.86	2.12	2.961(5)	168

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+1/2,y+1/2,z

#4 -x+1/2,y+0,-z+1/2 #5 x-1/2,-y,z-1/2 #6 x-1/2,y+1/2,z

#7 -x-1/2,y+0,-z+1/2

Figure S1. IR spectra of **2** and **4**