

Supporting Information

Hydrothermal Synthesis of Benzothiazole-carboxylic Cadmium(II) Coordination

Networks: pH-controlled topologies and compositional distributions

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Table S1. Selected bond lengths [Å] and angles [°] for compounds **1** and **2**

1	Cd(1)-O(2)	2.209(3)	Cd(1)-O(4)	2.276(3)	Cd(1)-O(3)	2.424(3)	
	Cd(1)-N(3)	2.279(3)	Cd(1)-O(1)	2.298(3)	Cd(1)-C(17)	2.695(3)	
	O(2)-Cd(1)-O(4)	107.50(11)	O(2)-Cd(1)-N(3)	105.16(10)	O(2)-Cd(1)-C(17)	126.92(11)	
	O(4)-Cd(1)-N(3)	144.94(10)	O(2)-Cd(1)-O(1)	112.48(10)	N(3)-Cd(1)-C(17)	118.25(10)	
	O(4)-Cd(1)-O(1)	92.30(11)	N(3)-Cd(1)-O(1)	86.76(11)	O(3)-Cd(1)-C(17)	27.95(10)	
	O(2)-Cd(1)-O(3)	136.90(11)	O(4)-Cd(1)-O(3)	55.45(9)	O(4)-Cd(1)-C(17)	27.60(10)	
	N(3)-Cd(1)-O(3)	91.55(9)	O(1)-Cd(1)-O(3)	107.81(10)	O(1)-Cd(1)-C(17)	99.58(11)	
2	Cd(1)-N(1)	2.270(4)	Cd(1)-N(1) ^{#1}	2.270(4)	Cd(1)-C(1) ^{#1}	2.712(5)	
	Cd(1)-O(2) ^{#1}	2.302(4)	Cd(1)-O(2)	2.302(4)	Cd(1)-C(1)	2.712(5)	
	Cd(1)-O(1) ^{#1}	2.412(4)	Cd(1)-O(1)	2.412(4)			
	N(1)-Cd(1)-N(1) ^{#1}	92.5(2)	N(1)-Cd(1)-O(2) ^{#1}	98.97(17)	O(2)-Cd(1)-C(1) ^{#1}	90.14(17)	
	N(1) ^{#1} -Cd(1)-O(2) ^{#1}	147.75(16)	N(1)-Cd(1)-O(2)	147.75(16)	O(1)-Cd(1)-C(1) ^{#1}	119.30(17)	
	N(1) ^{#1} -Cd(1)-O(2)	98.97(17)	O(2) ^{#1} -Cd(1)-O(2)	87.2(3)	N(1) ^{#1} -Cd(1)-C(1)	109.84(17)	
	N(1)-Cd(1)-O(1) ^{#1}	113.61(16)	N(1) ^{#1} -Cd(1)-O(1) ^{#1}	92.73(15)	O(2)-Cd(1)-C(1)	27.45(15)	
	O(2) ^{#1} -Cd(1)-O(1) ^{#1}	55.06(14)	O(2)-Cd(1)-O(1) ^{#1}	95.95(16)	O(1)-Cd(1)-C(1)	27.71(15)	
	N(1)-Cd(1)-O(1)	92.73(15)	N(1) ^{#1} -Cd(1)-O(1)	113.61(16)	O(1) ^{#1} -Cd(1)-C(1) ^{#1}	27.71(15)	
	O(2) ^{#1} -Cd(1)-O(1)	95.95(16)	O(2)-Cd(1)-O(1)	55.06(14)	N(1)-Cd(1)-C(1)	120.42(16)	
	O(1) ^{#1} -Cd(1)-O(1)	142.2(2)	N(1)-Cd(1)-C(1) ^{#1}	109.84(17)	O(2) ^{#1} -Cd(1)-C(1)	90.14(17)	
	N(1) ^{#1} -Cd(1)-C(1) ^{#1}	120.42(16)	O(2) ^{#1} -Cd(1)-C(1) ^{#1}	27.45(15)	O(1) ^{#1} -Cd(1)-C(1)	119.30(17)	
	C(1) ^{#1} -Cd(1)-C(1)	104.6(2)					
	Symmetry code: #1 -x, y, -z+1/2; #2 x-1/2, y+1/2, z; #3 x+1/2, y-1/2, z.						

Table S2. Hydrogen bonding geometry (Å, °) for compounds **1 - 4**.

	D-H1...A	D-H	H...A	D...A	D-H1...A
1	N4-H1 ...N1 ^I	0.83(4)	2.08(5)	2.907(4)	178(4)
	N2-H3 ...O4 ^{II}	0.89(6)	2.22(6)	3.086(5)	164(5)
	N4-H2... O3	0.78(5)	2.10(5)	2.863(5)	167(5)
Symmetry code:(I) -x+1, -y+1, -z+2; (II) x, y, z+1.					
2	N2-H2A...O1 ^I	0.88	2.01	2.857(6)	162.4
	N2-H2B...O2 ^{II}	0.88	2.01	2.781(6)	145.8
(I)x-1/2, y+1/2, z; x-1/2, (II)-y+1/2, z-1/2.					

Table S3. Photoluminescent data for ABTC in DMSO and compounds **1-4** in the solid state.

compound	excitation λ/nm	emission λ/nm
1	354	425
2	365	443

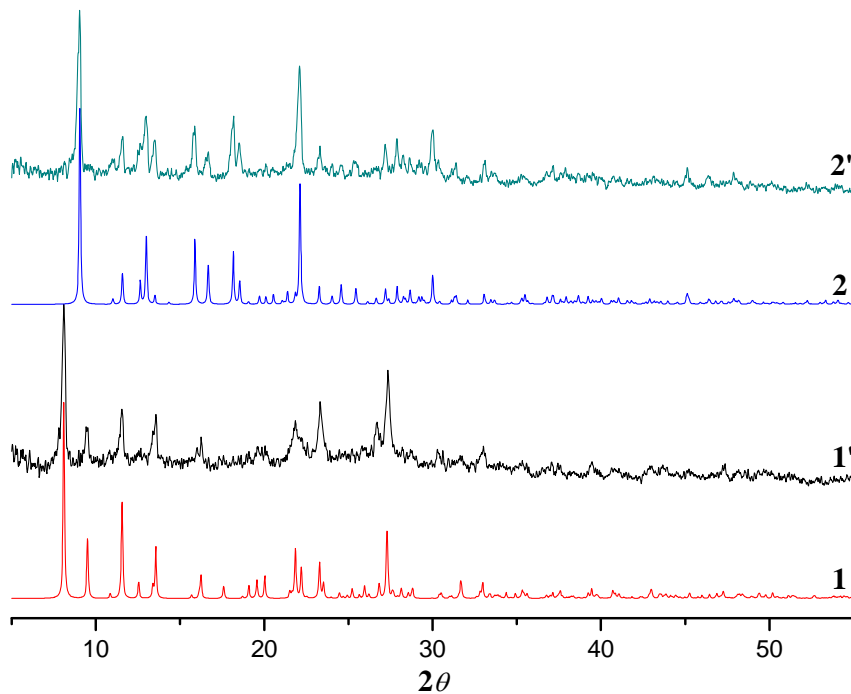


Figure S1. X-ray powder diffraction patterns for compounds **1** and **2**: complex **a**, simulated from single-crystal X-ray data; complex **a'**, experimental data.

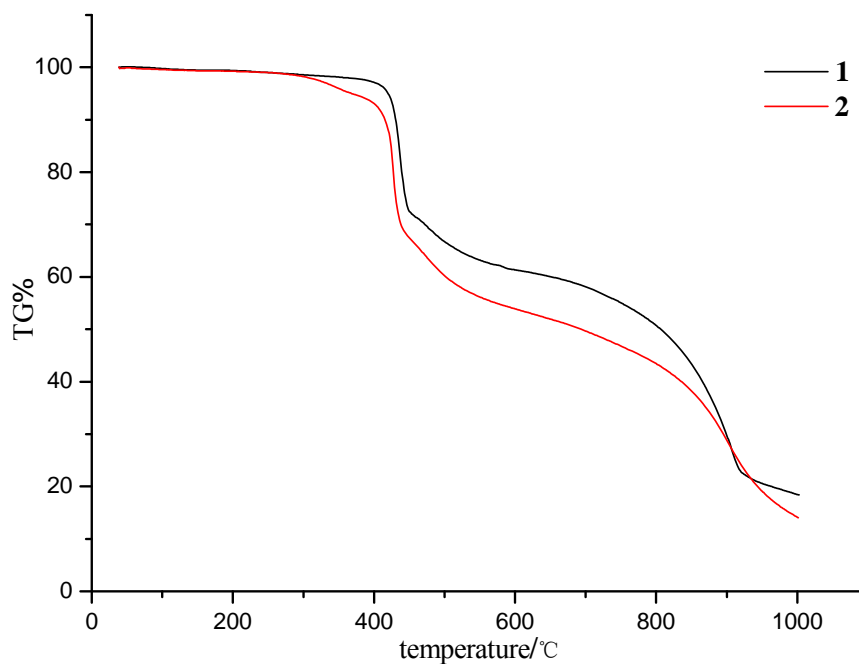


Figure S2. TGA profiles for compounds **1** and **2**.

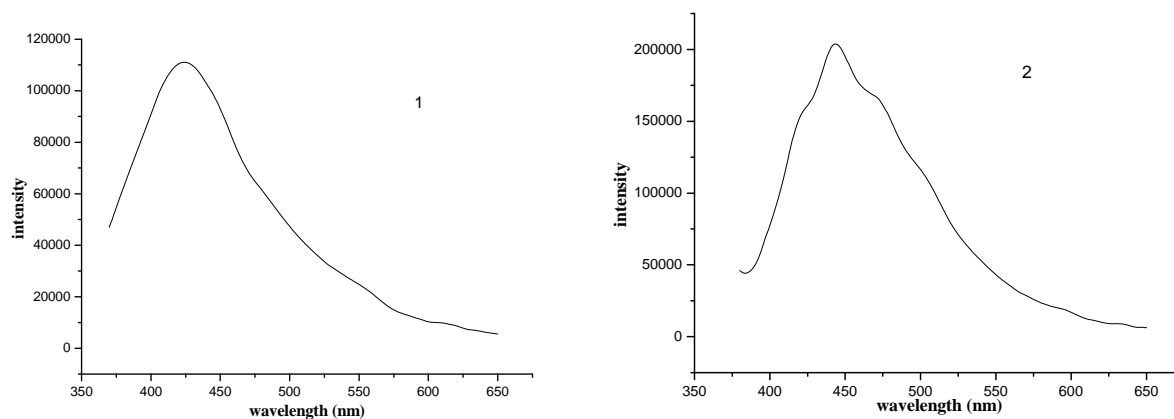


Figure S3. Emission spectrum of compounds 1 and 2 in solid state and ABTC in solution at room temperature

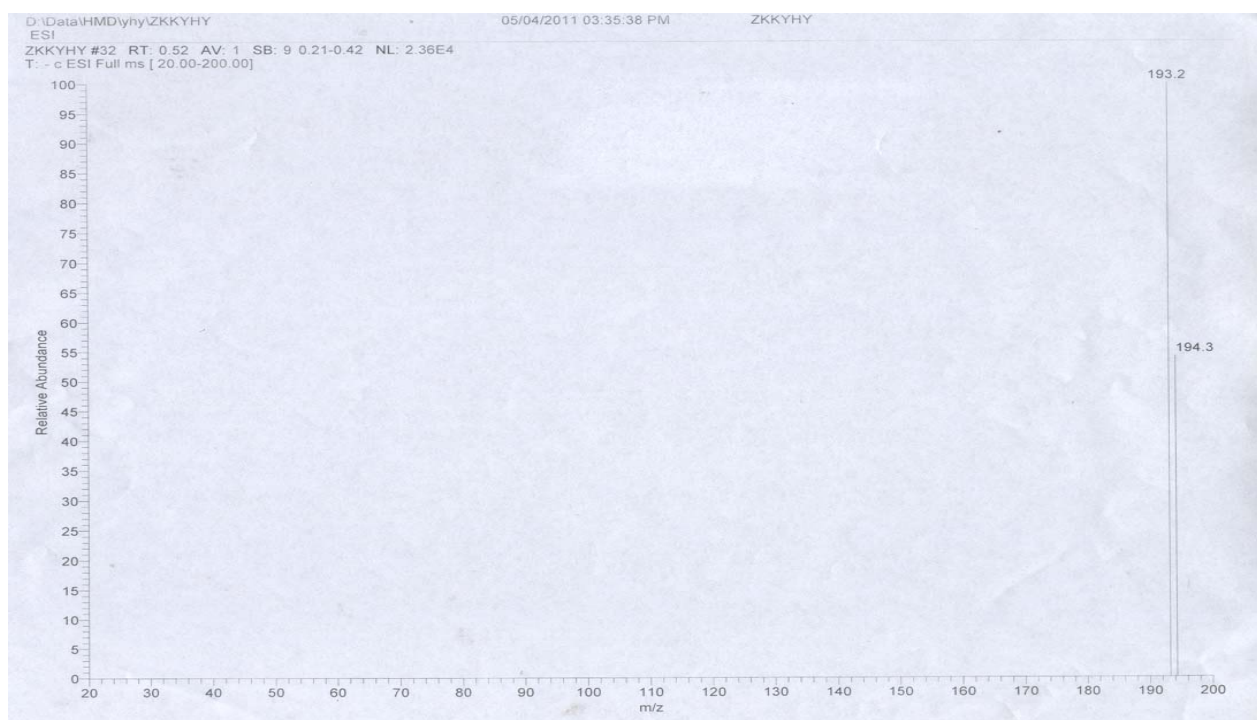


Figure S4. Mass spectra of ABTC

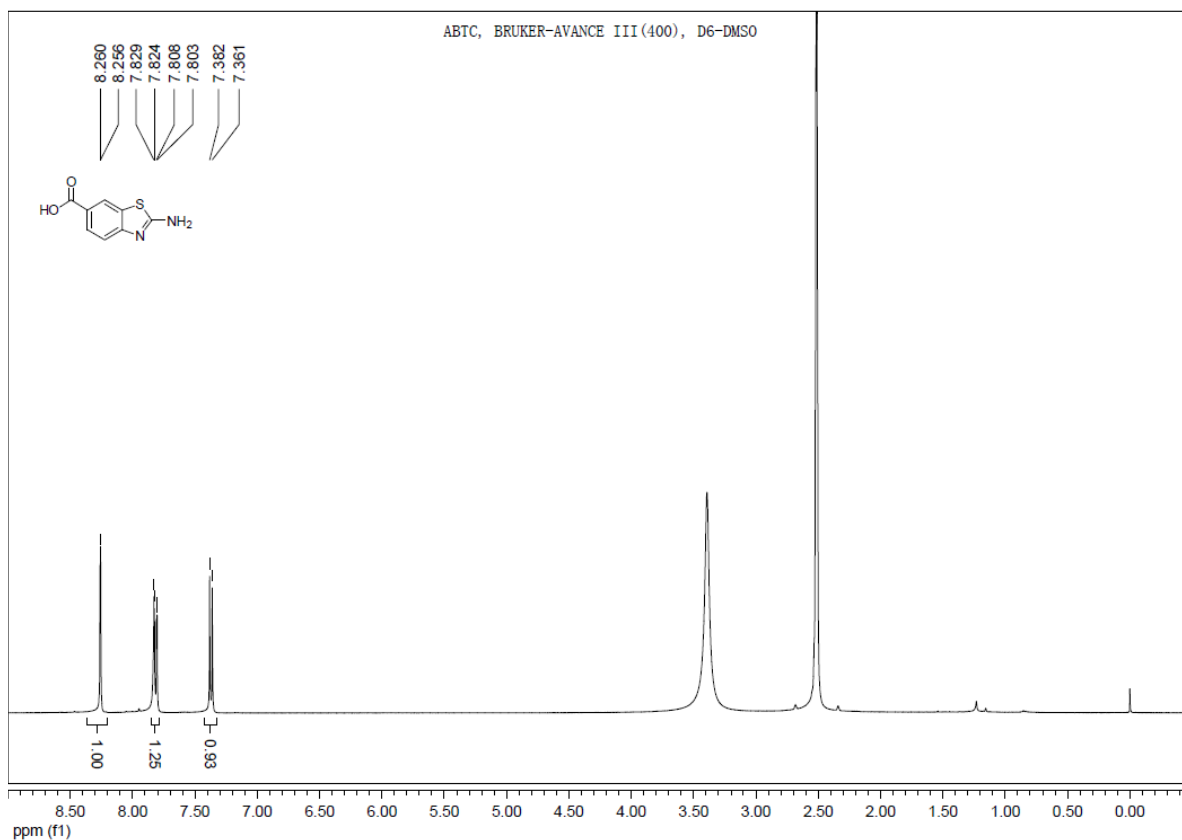


Figure S5. ¹H NMR of ABTC

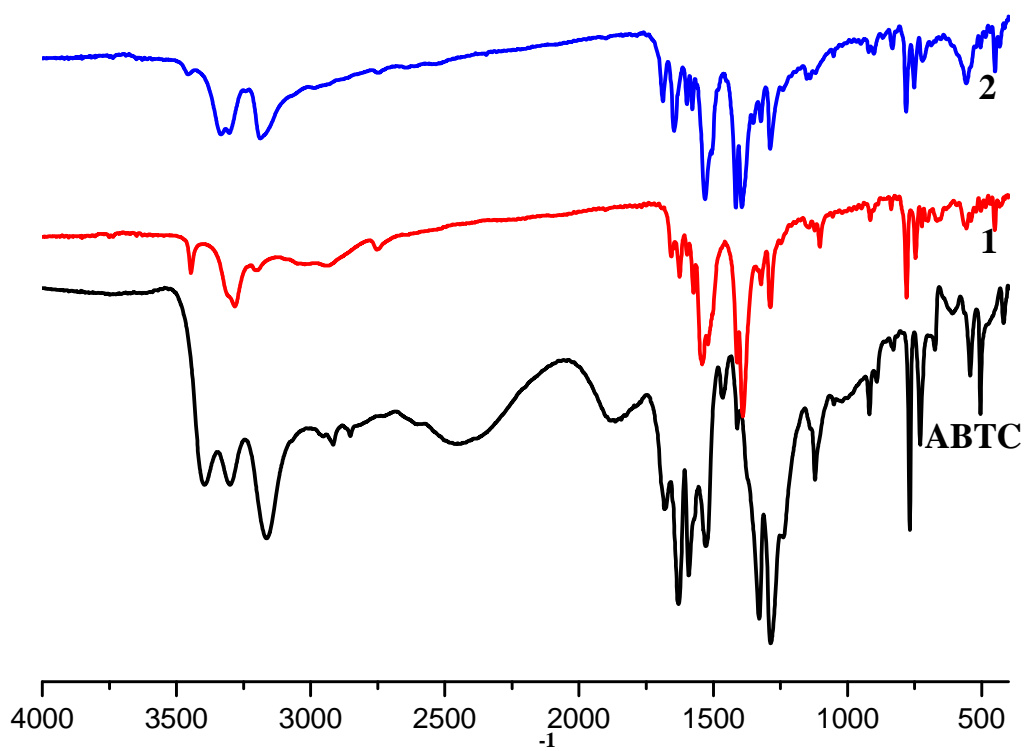


Figure S6. FT-IR of ABTC and compounds 1 and 2