

# **Synthesis of Two Triarylboron-Functionalized Metal-Organic Frameworks: in Situ Decarboxylic Reaction, Structure, Photoluminescence, and Gas Adsorption Properties**

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**Table S1.** Selected bond length (Å) and angles (°) for **complexes 1 and 2.**

## Complex 1

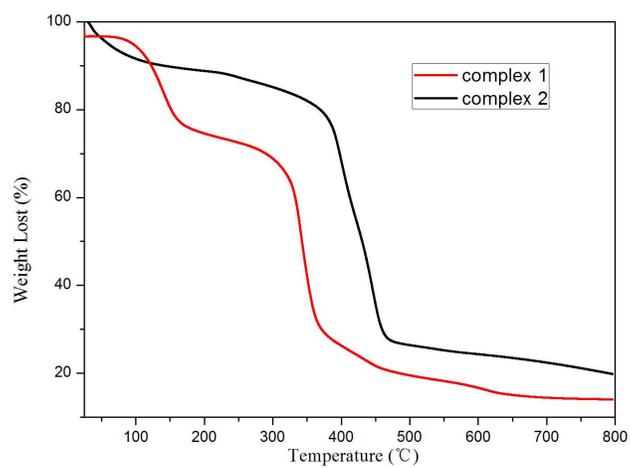
Cd1—O3	2.240 (6)	Cd2—O8 <sup>vi</sup>	2.350 (6)
Cd1—O3 <sup>i</sup>	2.240 (6)	Cd2—C20	2.675 (8)
Cd1—O5 <sup>ii</sup>	2.193 (5)	O1—C20	1.255 (11)
Cd1—O5 <sup>iii</sup>	2.193 (5)	O2—C20	1.267 (10)
Cd1—O8	2.356 (5)	O3—C9	1.283 (10)
Cd1—O8 <sup>i</sup>	2.356 (5)	O4—Cd2 <sup>vii</sup>	2.193 (5)
Cd2—O1	2.386 (5)	O4—C9	1.244 (10)
Cd2—O2	2.299 (5)	O5—Cd1 <sup>viii</sup>	2.193 (5)
Cd2—O4 <sup>iv</sup>	2.193 (5)	O8—Cd2 <sup>x</sup>	2.350 (6)
Cd2—O6 <sup>v</sup>	2.210 (6)	O6—Cd2 <sup>ix</sup>	2.210 (6)
O3—Cd1—O3 <sup>i</sup>	180.0 (3)	O2—Cd2—O1	56.0 (2)
O3 <sup>i</sup> —Cd1—O8 <sup>i</sup>	93.3 (2)	O2—Cd2—O7	91.2 (2)
O3—Cd1—O8 <sup>i</sup>	86.7 (2)	O2—Cd2—O8 <sup>vi</sup>	97.1 (2)
O3—Cd1—O8	93.3 (2)	O2—Cd2—C20	28.2 (2)
O3 <sup>i</sup> —Cd1—O8	86.7 (2)	O4 <sup>iv</sup> —Cd2—O1	148.8 (2)
O5 <sup>iii</sup> —Cd1—O3 <sup>i</sup>	90.8 (2)	O4 <sup>iv</sup> —Cd2—O2	92.8 (2)
O5 <sup>ii</sup> —Cd1—O3	90.8 (2)	O4 <sup>iv</sup> —Cd2—O6 <sup>v</sup>	115.5 (2)
O5 <sup>iii</sup> —Cd1—O3	89.2 (2)	O4 <sup>iv</sup> —Cd2—O7	92.4 (3)
O5 <sup>ii</sup> —Cd1—O3 <sup>i</sup>	89.2 (2)	O4 <sup>iv</sup> —Cd2—O8 <sup>vi</sup>	92.8 (2)
O5 <sup>ii</sup> —Cd1—O5 <sup>iii</sup>	180.000 (2)	O4 <sup>iv</sup> —Cd2—C20	120.9 (3)
O5 <sup>iii</sup> —Cd1—O8	93.4 (2)	O6 <sup>v</sup> —Cd2—O1	95.4 (2)
O5 <sup>iii</sup> —Cd1—O8 <sup>i</sup>	86.6 (2)	O6 <sup>v</sup> —Cd2—O2	150.4 (2)
O5 <sup>ii</sup> —Cd1—O8 <sup>i</sup>	93.4 (2)	O6 <sup>v</sup> —Cd2—O7	80.0 (2)
O5 <sup>ii</sup> —Cd1—O8	86.6 (2)	O2—Cd2—O1	56.0 (2)
O8 <sup>i</sup> —Cd1—O8	180.000 (1)	O2—Cd2—O7	91.2 (2)
O1—Cd2—C20	28.0 (2)	O2—Cd2—O8 <sup>vi</sup>	97.1 (2)

Symmetry codes: (i)  $x+1, y, z$ ; (ii)  $x+1/2, -y+3/2, z+1/2$ ; (iii)  $-x+2, -y+2, -z+1$ ; (iv)  $-x+3/2, y+1/2, -z+1/2$ ; (v)  $x-1, y, z$ ; (vi)  $x-1/2, -y+3/2, z-1/2$ ; (vii)  $-x+3/2, y-1/2, -z+1/2$ .

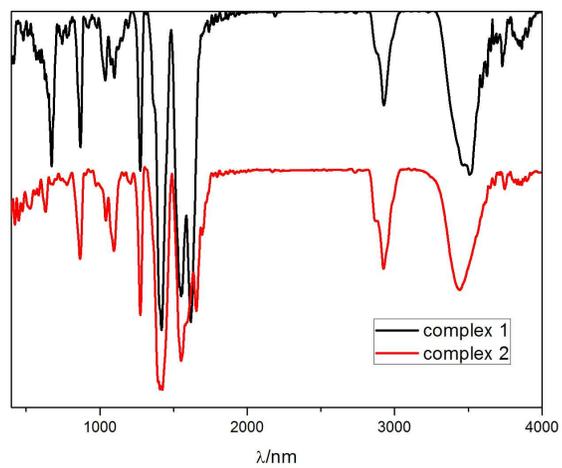
### Complex 2

Zn1—O1i	2.078 (5)	Zn2—O2v	1.900 (6)
Zn1—O1ii	2.078 (5)	Zn2—O2	1.900 (6)
Zn1—O1iii	2.078 (5)	Zn2—O1W	2.152 (11)
Zn1—O1	2.078 (5)	C12—B1	1.565 (13)
Zn1—O1iv	2.078 (5)	B1—C5vi	1.596 (8)
Zn1—O1v	2.078 (5)	C5—B1	1.596 (8)
Zn2—O2iii	1.900 (6)	O1—C1	1.283 (11)
O1i—Zn1—O1ii	91.1 (2)	O1iv—Zn1—O1v	88.9 (2)
O1ii—Zn1—O1	88.9 (2)	O1i—Zn1—O1iii	88.9 (2)
O1—Zn1—O1v	91.1 (2)	O1i—Zn1—O1	88.9 (2)
O1—Zn1—O1iii	91.1 (2)	O1ii—Zn1—O1iii	180.0 (3)
O1iv—Zn1—O1	180.0 (4)	O2iii—Zn2—O2	116.09 (19)
O1iii—Zn1—O1v	91.1 (2)	O2iii—Zn2—O2v	116.1 (2)
O1i—Zn1—O1iv	91.1 (2)	O2—Zn2—O2v	116.09 (19)
O1iv—Zn1—O1iii	88.9 (2)	O2iii—Zn2—O1W	101.6 (3)
O1i—Zn1—O1v	180.000 (1)	O2v—Zn2—O1W	101.6 (3)
O1ii—Zn1—O1v	88.9 (2)	O2—Zn2—O1W	101.6 (3)
O1ii—Zn1—O1iv	91.1 (2)	C1—O1—Zn1	141.8 (4)
C6—C5—B1	120.6 (6)	C1—O2—Zn2	122.8 (8)
C4—C5—B1	120.5 (5)	C13—C12—B1	120.5 (5)
C13vi—C12—B1	120.5 (5)	C5vi—B1—C5	119.6 (8)
C12—B1—C5	120.2 (4)	C12—B1—C5vi	120.2 (4)

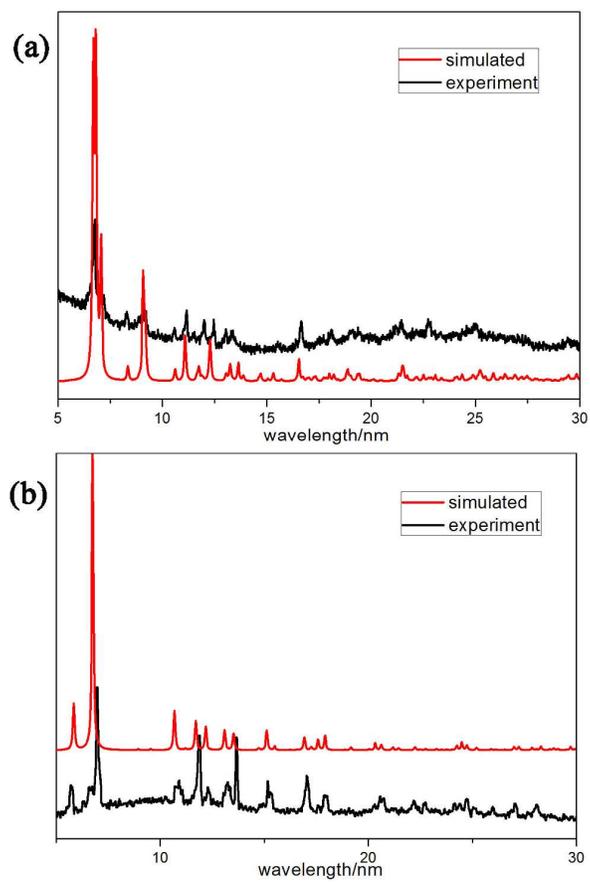
Symmetry codes: (i)  $-y+1, -z+1, -x+1$ ; (ii)  $-z+1, -x+1, -y+1$ ; (iii)  $z, x, y$ ; (iv)  $-x+1, -y+1, -z+1$ ; (v)  $y, z, x$ ; (vi)  $z-1/4, -y+3/4, x+1/4$ .



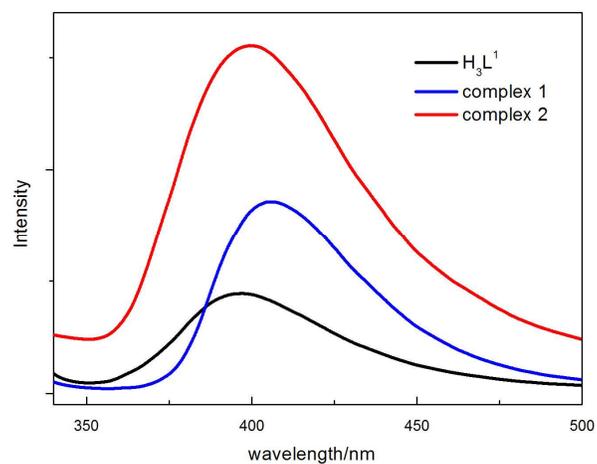
**Figure S1.** TGA curves of complexes **1** and **2**.



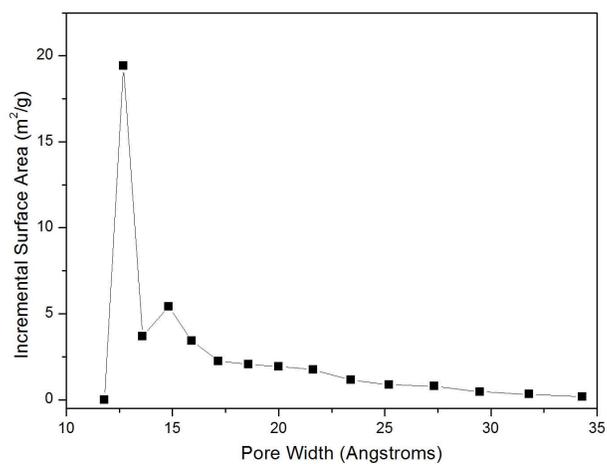
**Figure S2.** IR of complexes **1** and **2**.



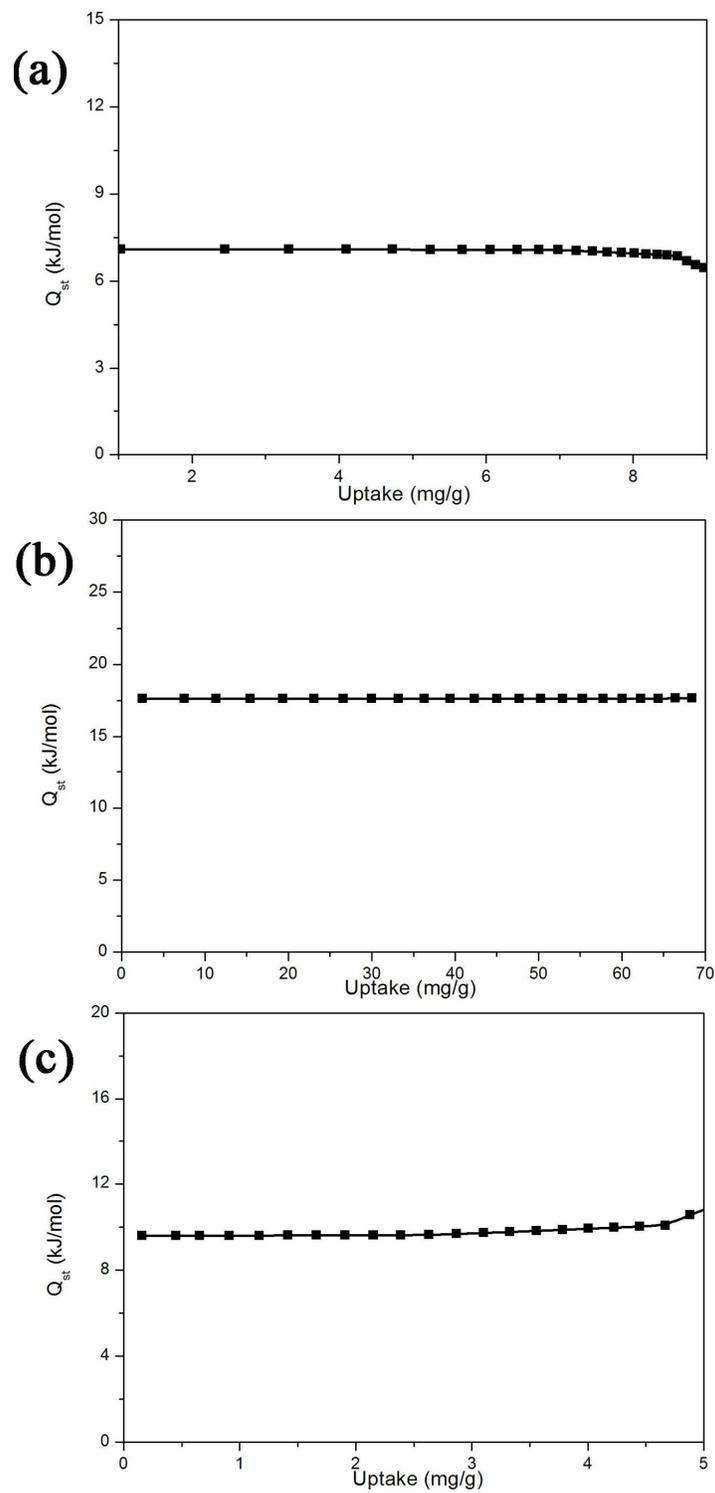
**Figure S3.** XRD of complexes **1** (a) and **2** (b).



**Figure S4.** Solid-state emission spectra of free ligand  $H_3L^1$  and complexes **1** and **2**.



**Figure S5.** Density functional theory pore size distribution of **2** determined from the N<sub>2</sub> adsorption isotherms at 77 K.



**Figure S6.** The  $Q_{st}$  of **2** for  $H_2$  (a),  $CO_2$  (b), and  $CH_4$  (c).