Two Tartratoborates with Hybrid Anionic Groups from Unusual Condensation Reactions

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Table S1. Hydrogen bonds for compounds **1** and **2**.

D-H···A	*d*(D-H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(DHA) (*deg.*)
$K_2[(C_4H_2O_6)(B_3O_4H)](H_2O)$ (**1**)				
O(7)-H(7A)...O(1W)	0.820	2.068	2.884(3)	173.33
$KCu_2[(C_4H_2O_6)_2B](H_2O)_{2.5}$ (**2**)				
O(1W)-H(1WA)...O(10)	0.850	1.850	2.687(5)	168.10
O(1W)-H(1WB)...O(7)	0.850	1.740	2.532(5)	153.80
O(2W)-H(2WB)...O(3)	0.850	2.070	2.911(6)	168.20

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for compounds **1** and **2**.

$K_2[(C_4H_2O_6)(B_3O_4H)](H_2O)$ (**1**)				
	x	y	z	U(eq)
K(1)	2728(2)	4627(1)	769(1)	54(1)
Cu(1)	5040(1)	3392(1)	2690(1)	20(1)
Cu(2)	-195(1)	917(1)	1554(1)	18(1)
B(1)	2583(5)	2090(3)	2057(4)	17(1)
C(1)	1917(5)	3988(3)	3433(3)	20(1)
C(2)	1721(5)	2856(3)	3506(3)	19(1)
C(3)	119(5)	2467(3)	2990(3)	22(1)
C(4)	-632(5)	1536(4)	3434(4)	28(1)
C(5)	6388(5)	1999(3)	1347(3)	20(1)
C(6)	4645(5)	2049(3)	858(3)	18(1)
C(7)	3775(5)	1013(3)	939(3)	17(1)
C(8)	2518(5)	872(3)	123(3)	19(1)
O(1)	3290(4)	4329(2)	3117(3)	28(1)
O(2)	666(4)	4489(2)	3713(3)	28(1)
O(3)	-1097(6)	1568(3)	4270(3)	54(1)
O(4)	-803(4)	775(2)	2892(3)	27(1)
O(5)	6597(4)	2429(2)	2139(2)	27(1)
O(6)	7495(3)	1506(2)	918(2)	23(1)
O(7)	3166(4)	729(3)	-674(3)	34(1)
O(8)	918(3)	944(2)	290(2)	22(1)
O(9)	3477(3)	2685(2)	1356(2)	20(1)
O(10)	2979(3)	1045(2)	1847(2)	18(1)
O(11)	3114(3)	2370(2)	3045(2)	19(1)

O(12)	727(3)	2275(2)	2040(2)	20(1)
O(1W)	6063(6)	4524(3)	2024(3)	51(1)
O(2W)	6229(5)	3308(3)	4115(3)	47(1)
O(3W)	4938(5)	6192(3)	596(3)	76(3)
$KCu_2[(C_4H_2O_6)_2B](H_2O)_{2.5}$ (**2**)				
	x	y	z	U(eq)
K(1)	4530(1)	6382(1)	10736(1)	28(1)
K(2)	86(1)	6142(1)	-2688(1)	28(1)
C(1)	1261(2)	6156(2)	1612(3)	22(1)
C(2)	1801(2)	6558(2)	3477(3)	20(1)
C(3)	2753(2)	5782(2)	4584(3)	21(1)
C(4)	3203(2)	6103(2)	6509(3)	20(1)
B(1)	-450(2)	6376(2)	2789(3)	22(1)
B(2)	-2226(2)	5489(2)	3619(3)	21(1)
B(3)	-2557(3)	7144(2)	2203(3)	23(1)
O(1)	1891(2)	5965(1)	618(2)	30(1)
O(2)	33(2)	6028(1)	1226(2)	25(1)
O(3)	747(2)	6746(1)	4086(2)	24(1)
O(4)	2227(2)	4816(1)	4573(2)	23(1)
O(5)	2939(2)	5411(1)	7511(2)	25(1)
O(6)	3728(2)	6900(1)	7060(2)	27(1)
O(7)	-3439(2)	7874(1)	1410(3)	32(1)
O(8)	-2995(2)	6392(1)	3055(2)	23(1)
O(9)	-988(2)	5567(1)	3467(2)	25(1)
O(10)	-1351(2)	7196(1)	2111(2)	26(1)
O(1W)	3835(2)	4377(2)	11175(3)	47(1)

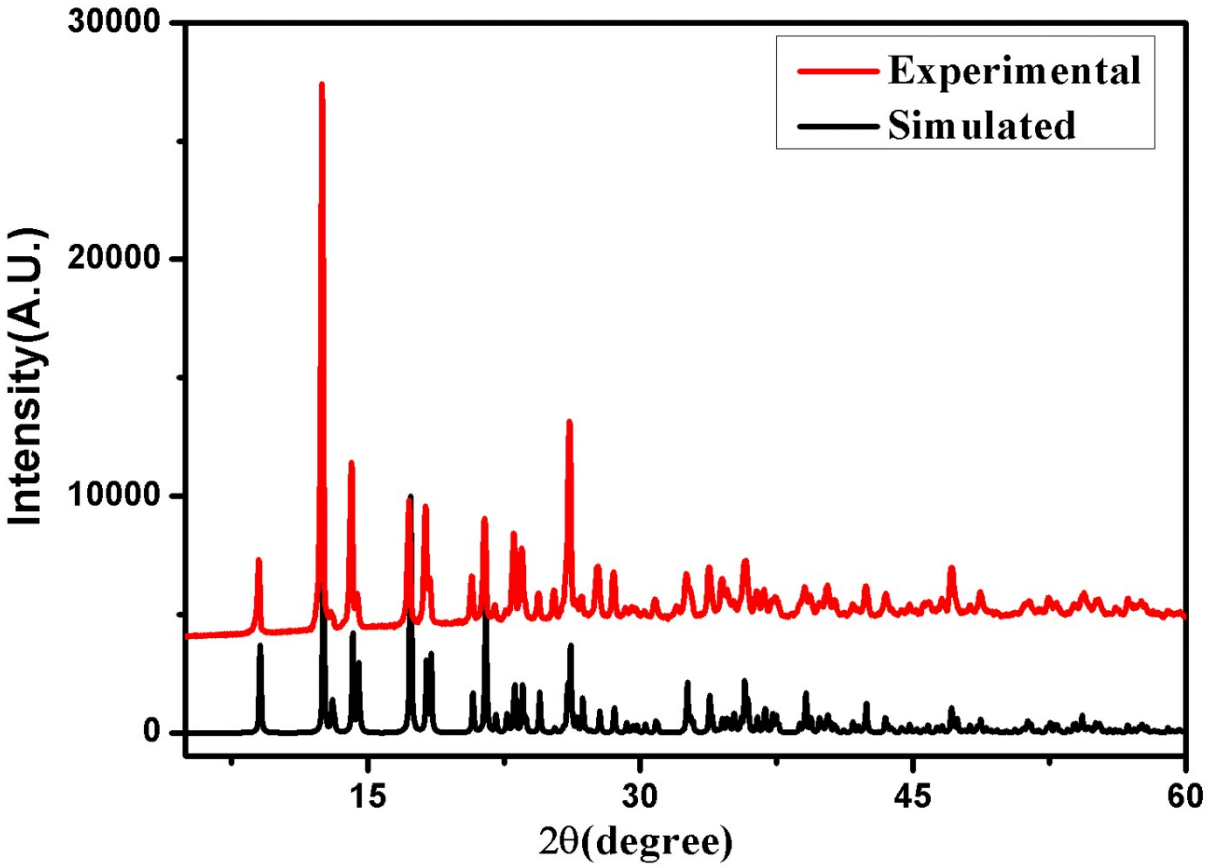

Figure S1. Experimental and simulated X-ray powder diffraction patterns for compound **2**.

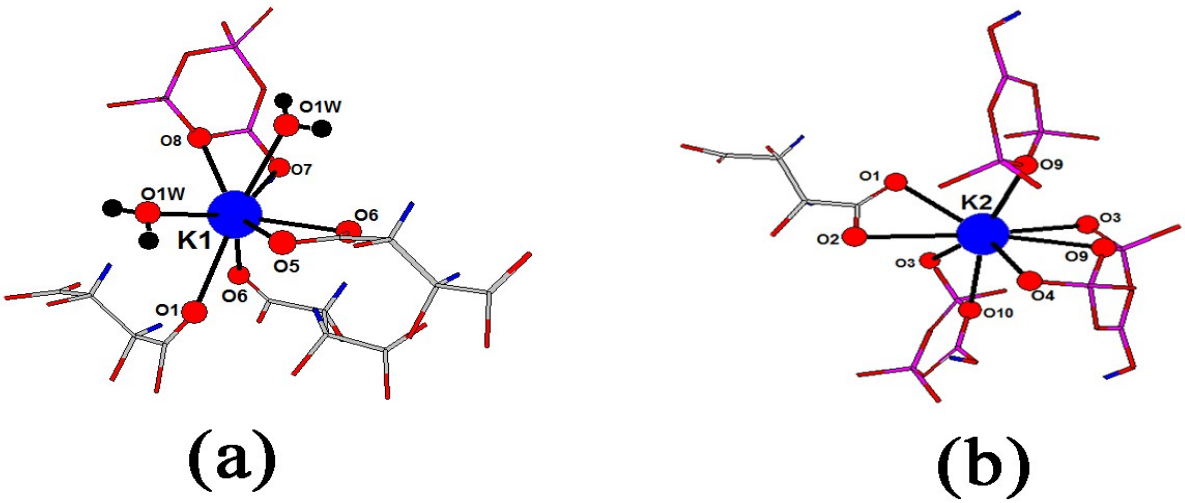

Figure S2. Coordination mode of K(1) (a), and K(2) (b) in compound **1**.

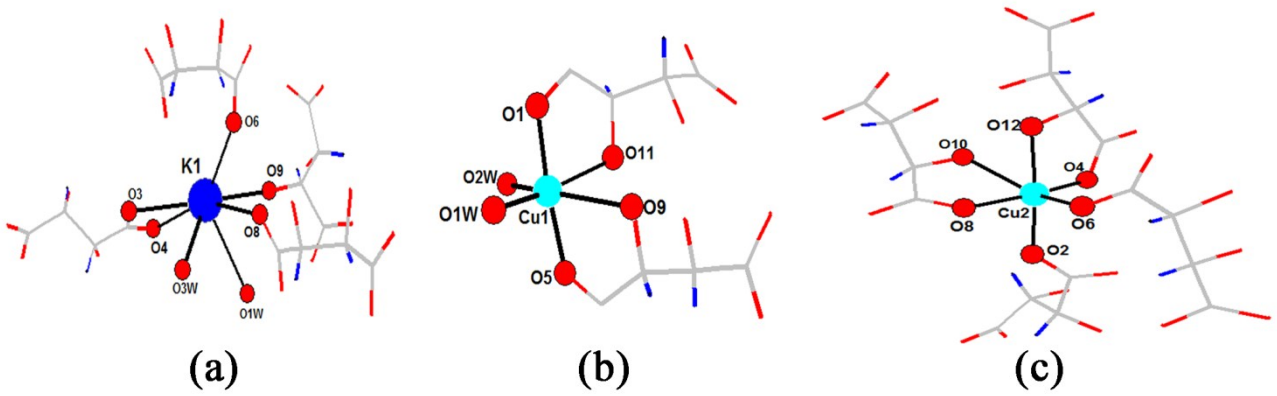

Figure S3. Coordination mode of K(1) (a), Cu(1) (b), and Cu(2) (c)) in compound **2**.

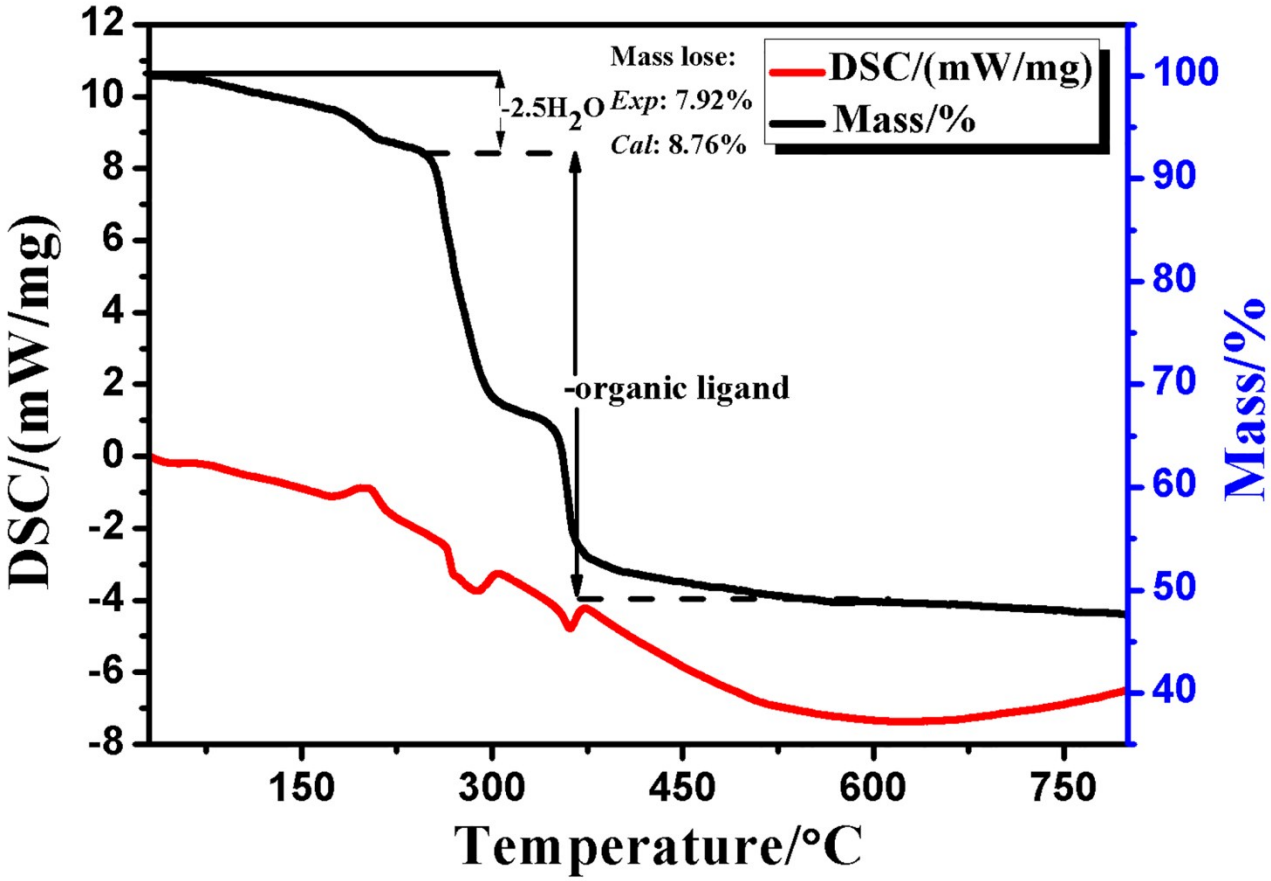

Figure S4. TGA and DSC curves for compound **2**.

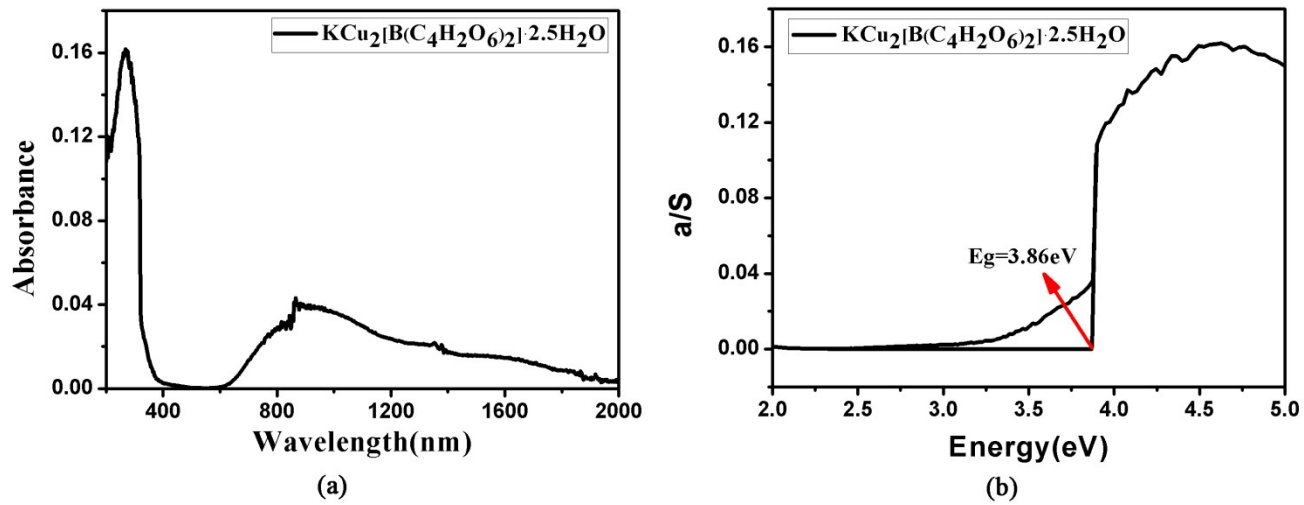

Figure S5. UV-vis Optical absorption spectra (a) and diffuse reflectance spectra (b) for compound **2**.

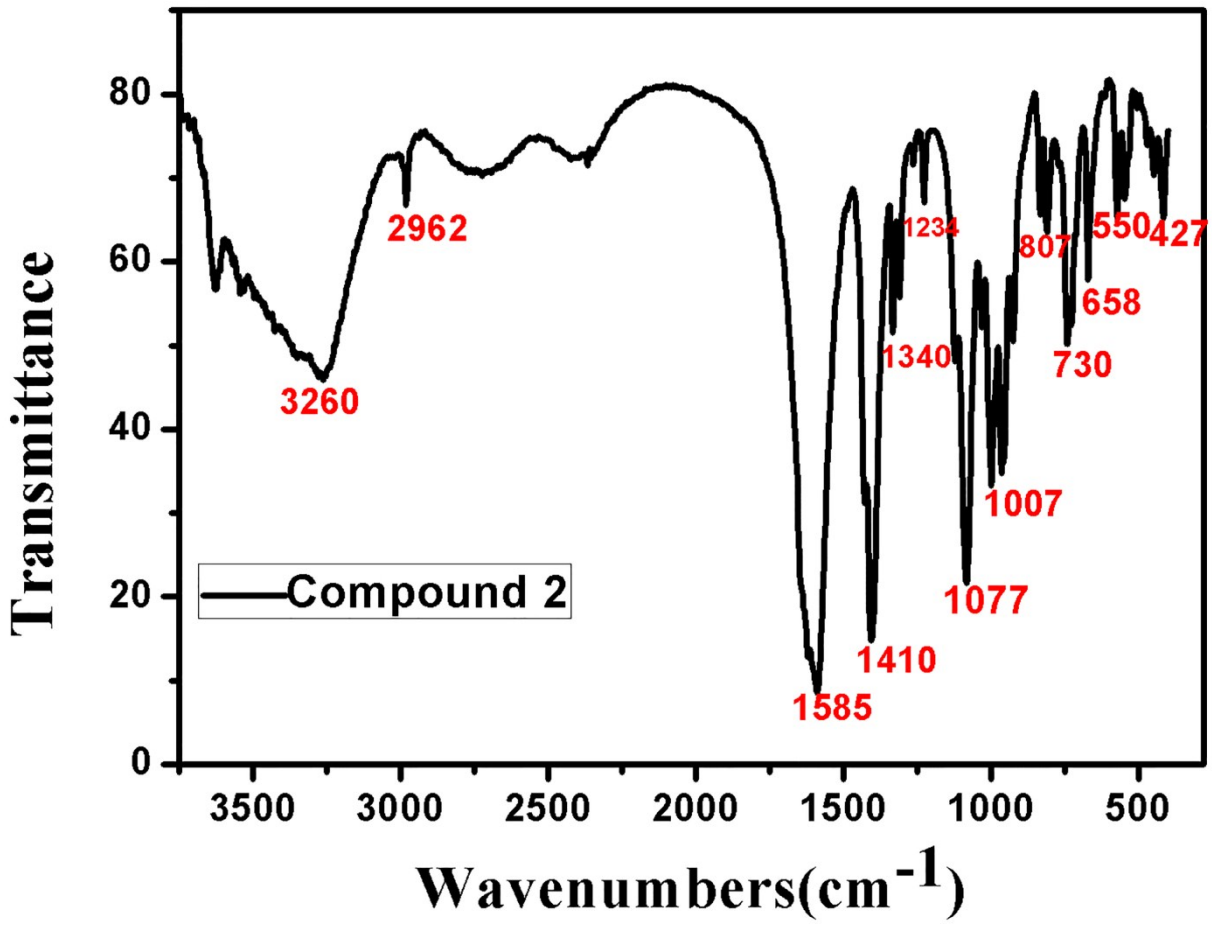

Figure S6. IR spectra for compound **2**.