

New heterometallic frameworks with flexible sulfonate-carboxylate
ligand: syntheses, structures, and properties

Electronic Supplementary Information

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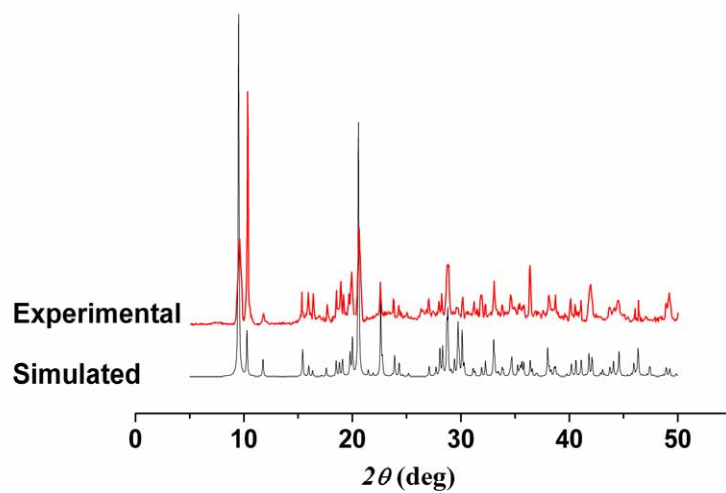
Table S1 Selected Bond Lengths (Å) and Bond Angles (deg) of compounds **1** and **2**^a

Compound 1			
Na(1)–O(6A)	2.295(2)	O(6A)–Na(1)–O(8)	98.99(8)
Na(1)–O(10)	2.315(3)	O(10)–Na(1)–O(8)	85.77(11)
Na(1)–O(7B)	2.381(2)	O(7B)–Na(1)–O(8)	160.62(8)
Na(1)–O(9)	2.422(3)	O(9)–Na(1)–O(8)	91.33(9)
Na(1)–O(2C)	2.486(2)	O(2C)–Na(1)–O(8)	72.11(7)
Na(1)–O(8)	2.568(2)	O(3)–Zn(1)–O(3A)	180.000(1)
Zn(1)–O(3)	2.0680(18)	O(3)–Zn(1)–O(1)	90.31(7)
Zn(1)–O(3A)	2.0680(18)	O(3A)–Zn(1)–O(1)	89.69(7)
Zn(1)–O(1)	2.0827(17)	O(3)–Zn(1)–O(1A)	89.69(7)
Zn(1)–O(1A)	2.0827(17)	O(3A)–Zn(1)–O(1A)	90.31(7)
Zn(1)–O(5A)	2.0980(18)	O(1)–Zn(1)–O(1A)	180.000(1)
Zn(1)–O(5)	2.0980(18)	O(3)–Zn(1)–O(5A)	93.40(7)
Zn(2)–O(8D)	1.9284(18)	O(3A)–Zn(1)–O(5A)	86.60(7)
Zn(2)–O(8)	1.9655(18)	O(1)–Zn(1)–O(5A)	89.10(7)
Zn(2)–O(4)	1.982(2)	O(1A)–Zn(1)–O(5A)	90.90(7)
Zn(2)–O(2C)	2.0079(19)	O(3)–Zn(1)–O(5)	86.60(7)
O(6A)–Na(1)–O(10)	174.91(13)	O(3A)–Zn(1)–O(5)	93.40(7)
O(6A)–Na(1)–O(7B)	89.53(8)	O(1)–Zn(1)–O(5)	90.90(7)
O(10)–Na(1)–O(7B)	86.48(12)	O(1A)–Zn(1)–O(5)	89.10(7)
O(6A)–Na(1)–O(9)	87.83(11)	O(5A)–Zn(1)–O(5)	180.00(4)
O(10)–Na(1)–O(9)	90.28(15)	O(8D)–Zn(2)–O(8)	124.71(4)
O(7B)–Na(1)–O(9)	106.44(10)	O(8D)–Zn(2)–O(4)	105.94(8)
O(6A)–Na(1)–O(2C)	93.83(8)	O(8)–Zn(2)–O(4)	108.11(8)
O(10)–Na(1)–O(2C)	89.32(13)	O(8D)–Zn(2)–O(2C)	109.30(8)
O(7B)–Na(1)–O(2C)	90.07(8)	O(8)–Zn(2)–O(2C)	96.97(8)
O(9)–Na(1)–O(2C)	163.43(10)	O(4)–Zn(2)–O(2C)	111.50(8)
Compound 2			
Zn(1)–O(9A)	1.972(3)	O(6D)–Na(1)–O(4A)	172.99(15)
Zn(1)–O(4A)	1.977(3)	O(14E)–Na(1)–O(4A)	89.57(12)
Zn(1)–O(10)	1.996(3)	O(10)–Na(1)–O(4A)	75.07(11)
Zn(1)–O(1)	2.002(3)	O(13C)–Na(1)–O(2)	162.01(13)
Na(1)–O(13C)	2.292(4)	O(6D)–Na(1)–O(2)	109.72(13)
Na(1)–O(6D)	2.324(4)	O(14E)–Na(1)–O(2)	80.07(12)
Na(1)–O(14E)	2.330(4)	O(10)–Na(1)–O(2)	81.39(12)
Na(1)–O(10)	2.410(3)	O(4A)–Na(1)–O(2)	76.24(11)
Na(1)–O(4A)	2.491(3)	O(15)–Na(2)–O(3)	114.8(3)
Na(1)–O(2)	2.570(4)	O(15)–Na(2)–O(11)	119.7(2)
Na(2)–O(15)	2.274(11)	O(3)–Na(2)–O(11)	96.05(15)
Na(2)–O(3)	2.297(4)	O(15)–Na(2)–O(16B)	91.3(3)
Na(2)–O(11)	2.334(4)	O(3)–Na(2)–O(16B)	160.2(2)
Na(2)–O(16B)	2.437(5)	O(11)–Na(2)–O(16B)	77.30 (15)
Na(2)–O(17F)	2.489(4)	O(15)–Na(2)–O(17F)	75.3(2)

Na(2)–O(15F)	2.659(11)	O(3)–Na(2)–O(17F)	83.23(14)
Na(3)–O(16)	2.344(4)	O(11)–Na(2)–O(17F)	137.79(18)
Na(3)–O(5)	2.367(4)	O(16B)–Na(2)–O(17F)	89.30(15)
Na(3)–O(9E)	2.382(3)	O(15)–Na(2)–O(15F)	23.9(4)
Na(3)–O(14E)	2.427(4)	O(15)–Na(2)–O(1)	67.0(3)
Na(3)–O(11G)	2.522(4)	O(3)–Na(2)–O(1)	75.85(12)
Na(3)–O(2)	2.560(4)	O(11)–Na(2)–O(1)	73.10(12)
Na(4)–O(8A)	2.288(4)	O(16B)–Na(2)–O(1)	118.73(14)
Na(4)–O(7)	2.362(4)	O(17F)–Na(2)–O(1)	144.94(15)
Na(4)–O(17)	2.437(4)	O(16)–Na(3)–O(5)	140.15(16)
Na(4)–O(7H)	2.446(4)	O(16)–Na(3)–O(9E)	115.25(16)
Na(4)–O(18)	2.637(5)	O(5)–Na(3)–O(9E)	93.75(13)
Na(4)–O(1)	2.695(4)	O(16)–Na(3)–O(14E)	93.75(13)
O(4)–Zn(11)	1.977(3)	O(5)–Na(3)–O(14E)	130.47(14)
O(4)–Na(11)	2.491(3)	O(9E)–Na(3)–O(14E)	80.53(11)
O(6)–Na(1J)	2.330(4)	O(16)–Na(3)–O(11G)	75.47(13)
O(7)–Na(4H)	2.446(4)	O(5)–Na(3)–O(11G)	85.12(13)
O(8)–Na(4I)	2.288(4)	O(9E)–Na(3)–O(11G)	78.29(11)
O(9)–Zn(1I)	1.972(3)	O(14E)–Na(3)–O(11G)	139.56(14)
O(9)–Na(3K)	2.382(3)	O(16)–Na(3)–O(2)	93.33(14)
O(11)–Na(3B)	2.522(4)	O(5)–Na(3)–O(2)	76.72(12)
O(13)–Na(1C)	2.292(4)	O(9E)–Na(3)–O(2)	141.97(12)
O(14)–Na(1K)	2.330(3)	O(14E)–Na(3)–O(2)	78.53(11)
O(14)–Na(3K)	2.427(4)	O(11G)–Na(3)–O(2)	135.78(12)
O(16)–Na(2G)	2.437(5)	O(8A)–Na(4)–O(7)	154.93(14)
O(17)–Na(2F)	2.489(4)	O(8A)–Na(4)–O(17)	89.28(14)
O(15)–Na(2F)	2.274(11)	O(7)–Na(4)–O(17)	103.79(15)
O(9A)–Zn(1)–O(4A)	119.61(12)	O(8A)–Na(4)–O(7H)	124.05(13)
O(9A)–Zn(1)–O(10)	112.46(13)	O(7)–Na(4)–O(7H)	79.20(12)
O(4A)–Zn(1)–O(10)	97.46(12)	O(17)–Na(4)–O(7H)	83.77(14)
O(9A)–Zn(1)–O(1)	111.15(13)	O(8A)–Na(4)–O(18)	94.15(14)
O(4A)–Zn(1)–O(1)	105.20(12)	O(7)–Na(4)–O(18)	75.37(14)
O(10)–Zn(1)–O(1)	109.92(12)	O(17)–Na(4)–O(18)	172.97(15)
O(13C)–Na(1)–O(6D)	88.11(14)	O(7H)–Na(4)–O(18)	89.22(13)
O(13C)–Na(1)–O(14E)	96.38(13)	O(8A)–Na(4)–O(1)	75.66(11)
O(6D)–Na(1)–O(14E)	95.06(14)	O(7)–Na(4)–O(1)	79.97(11)
O(13C)–Na(1)–O(10)	97.76(13)	O(17)–Na(4)–O(1)	107.71(13)
O(6D)–Na(1)–O(10)	101.79(13)	O(7H)–Na(4)–O(1)	158.13(12)
O(14E)–Na(1)–O(10)	158.17(17)	O(18)–Na(4)–O(1)	79.12(12)
O(13C)–Na(1)–O(4A)	86.14(12)		

^a symmetry transformation for equivalent atoms: Compound **1**, A: $-x + 1, -y, -z + 2$; B: $x - 1/2, -y - 1/2, z + 1/2$; C: $-x + 1, -y - 1, -z + 2$; D: $-x + 3/2, y - 1/2, -z + 5/2$. Compound **2**, A: $x - 1/2, -y + 1/2, z - 1/2$; B: $x + 1/2, -y + 1/2, z - 1/2$; C: $-x + 2, -y, -z + 2$; D: $-x + 3/2, y - 1/2, -z + 5/2$; E: $x - 1, y, z$; F: $-x + 2, -y + 1, -z + 2$; G: $x - 1/2, -y + 1/2, z + 1/2$; H: $-x + 1, -y + 1, -z + 2$; I: $x + 1/2, -y + 1/2, z + 1/2$.

Compound 1



Compound 2

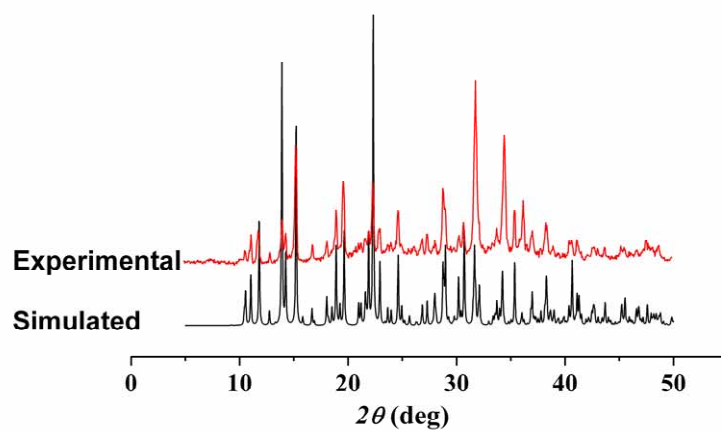


Fig. S1 The PXRD patterns for compounds **1** and **2**.

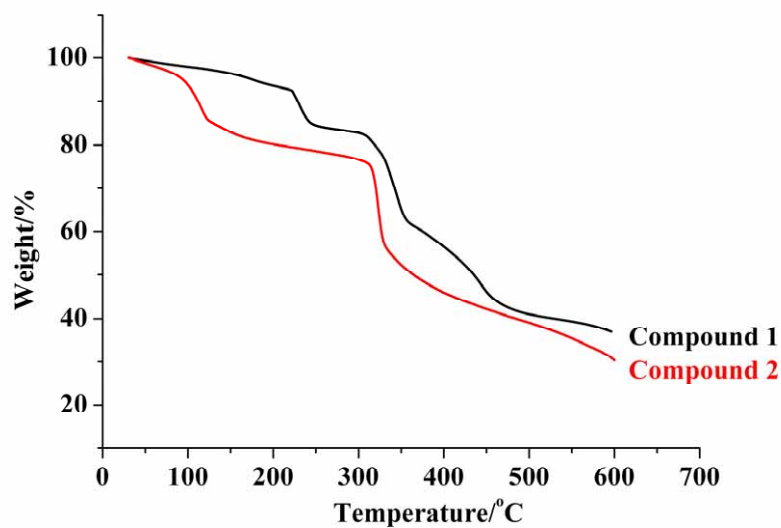


Fig. S2 TGA curve of compounds 1 and 2.