

Structural and zeolitic features of a series of heterometallic supramolecular porous architectures based on tetrahedral $\{M(C_2O_4)_4\}^{4-}$ primary building units.

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Supplementary Information

Figure SI1. Thermogravimetric analysis for $[K_2MnU(C_2O_4)_4] \cdot 9H_2O$, **SPA-1**.

Figure SI2. Thermogravimetric analysis for $[K_2CdU(C_2O_4)_4] \cdot 9H_2O$, **SPA-2**.

Figure SI3. Temperature dependences of the X-ray powder diffractograms recorded for $[K_2MnU(C_2O_4)_4] \cdot 9H_2O$, **SPA-1** and $[K_2Mg_2U_2(C_2O_4)_7] \cdot 11H_2O$, **SPA-3**.

Figure SI4. Thermogravimetric analysis for EtOH@**SPA-3**.

Table SI1. Atomic coordinates and equivalent isotropic and anisotropic displacement parameters for $[K_2CdU(C_2O_4)_4] \cdot 9H_2O$, **SPA-2**.

Figure SI4. ORTEP plot (30% probability level) for the asymmetric unit of $[K_2CdU(C_2O_4)_4] \cdot 9H_2O$, **SPA-2**.

Table SI2. Bond lengths in Å for $[K_2CdU(C_2O_4)_4] \cdot 9H_2O$, **SPA-2**.

Table SI3. Angles in ° for $[K_2CdU(C_2O_4)_4] \cdot 9H_2O$, **SPA-2**.

Table SI4. Atomic coordinates, equivalent isotropic and anisotropic displacement parameters for $[K_2Mg_2U_2(C_2O_4)_7] \cdot 11H_2O$, **SPA-3**.

Figure SI5. ORTEP plot (30% probability level) for the asymmetric unit of $[K_2Mg_2U_2(C_2O_4)_7] \cdot 11H_2O$, **SPA-3**.

Table SI5. Distances in Å for $[K_2Mg_2U_2(C_2O_4)_7] \cdot 11H_2O$, **SPA-3**.

Table SI6. Angles in ° for $[K_2Mg_2U_2(C_2O_4)_7] \cdot 11H_2O$, **SPA-3**.

Table SI7. Atomic coordinates equivalent isotropic and anisotropic displacement parameters for $[K_2ZrMn(C_2O_4)_4] \cdot 8H_2O$, **SPA-4**.

Figure SI6. ORTEP plot (30% probability level) for the asymmetric unit of $[K_2Mn\{Zr(C_2O_4)_4\}] \cdot 8H_2O$, **SPA-4**.

Table SI8. Distances in Å for $[K_2ZrMn(C_2O_4)_4] \cdot 7H_2O$, **SPA-4**.

Table SI9. Angles in ° for $[K_2ZrMn(C_2O_4)_4] \cdot 7H_2O$, **SPA-4**.

Figure S11. Thermogravimetric analysis for $[K_2MnU(C_2O_4)_4] \cdot 9H_2O$, SPA-1.

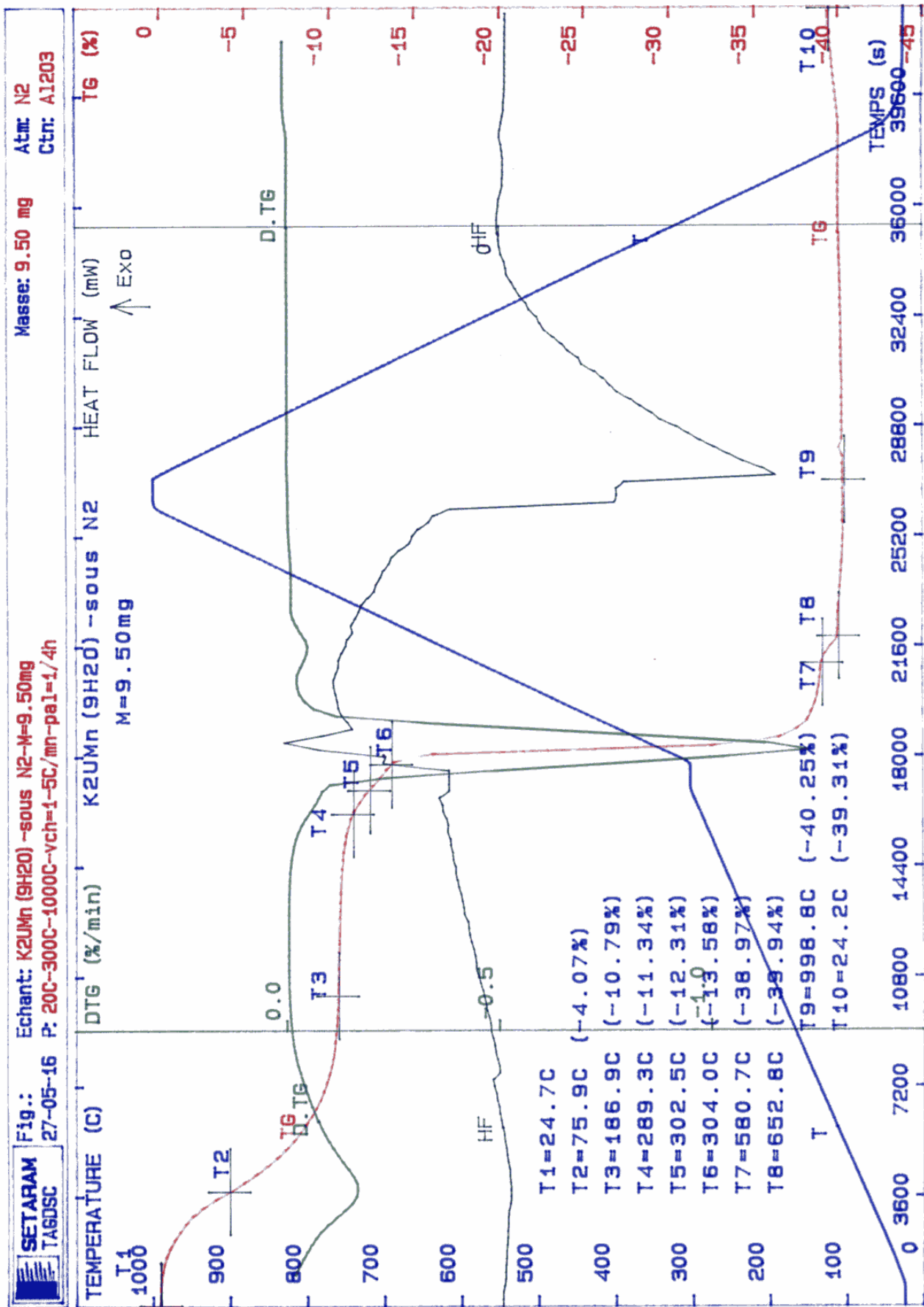


Figure SI2. Themogravimetric analysis for $[\text{K}_2\text{CdU}(\text{C}_2\text{O}_4)_4]\cdot 9\text{H}_2\text{O}$, SPA-2

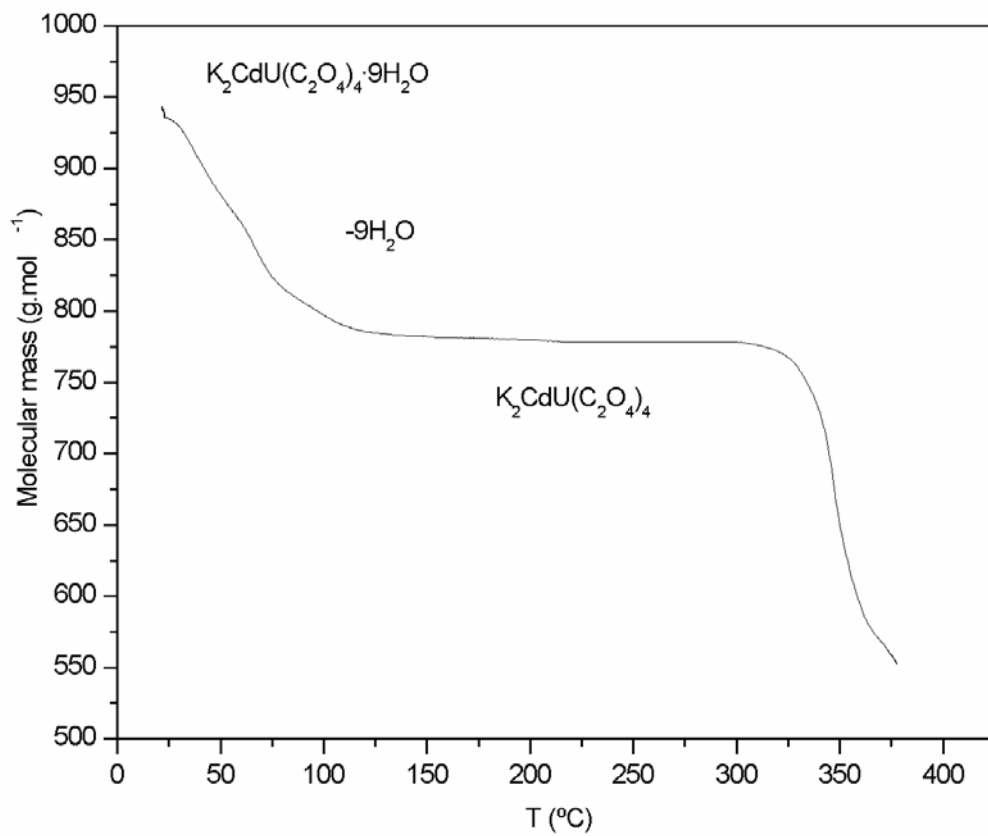
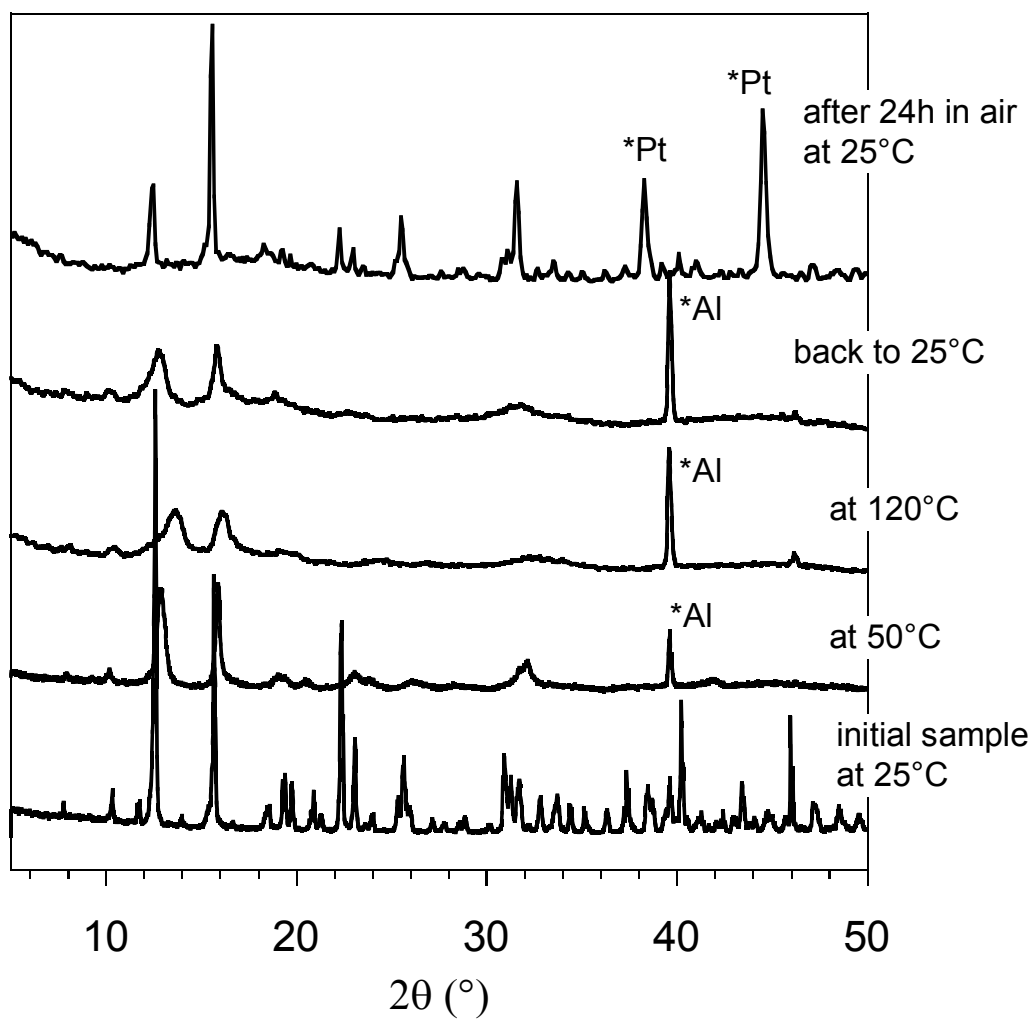


Figure SI3. Temperature dependences of the X-ray powder diffractograms recorded for:

a) $[\text{K}_2\text{MnU}(\text{C}_2\text{O}_4)_4]\cdot 9\text{H}_2\text{O}$, SPA-1. (*Pt and *Al mark the picks due to the sample holder)



b) $[\text{K}_2\text{Mg}_2\text{U}_2(\text{C}_2\text{O}_4)_7] \cdot 11\text{H}_2\text{O}$, SPA-3.

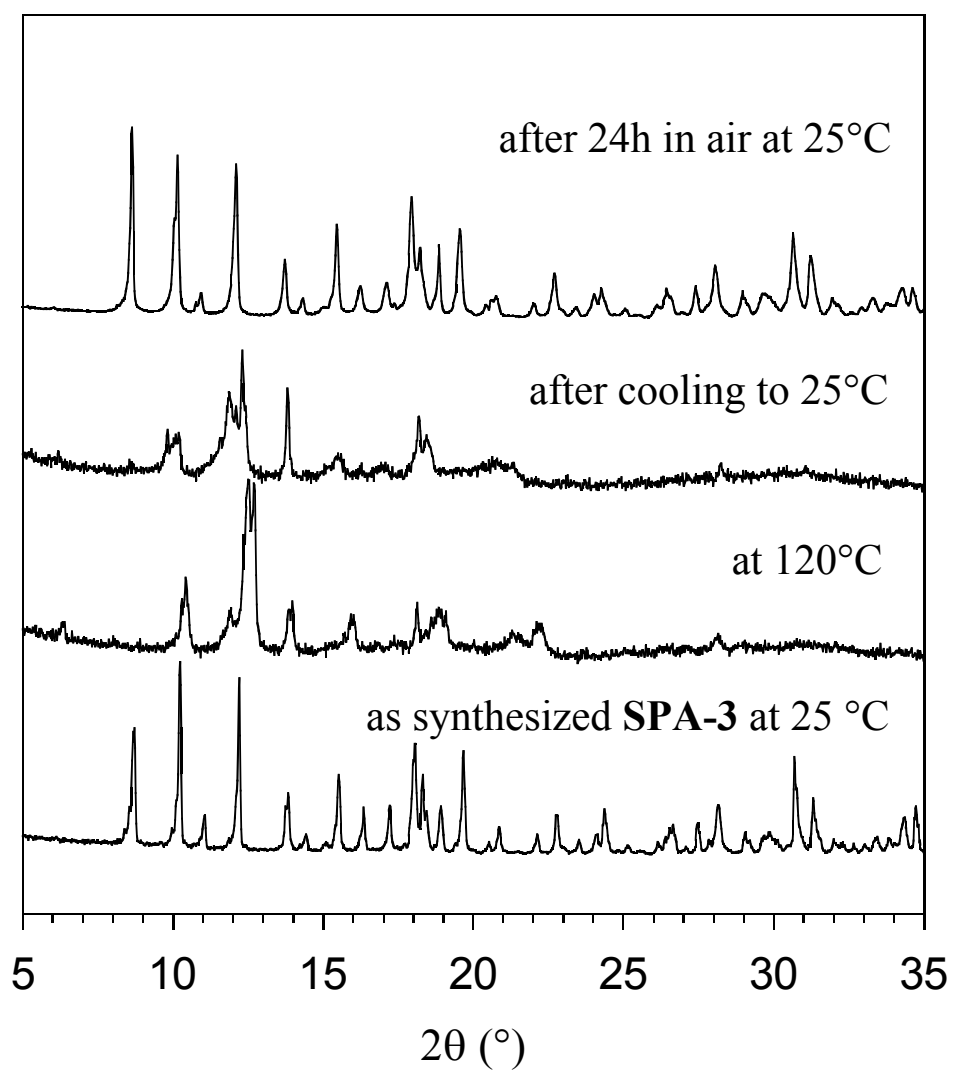


Figure SI4. Thermogravimetric analysis for EtOH@SPA-3.

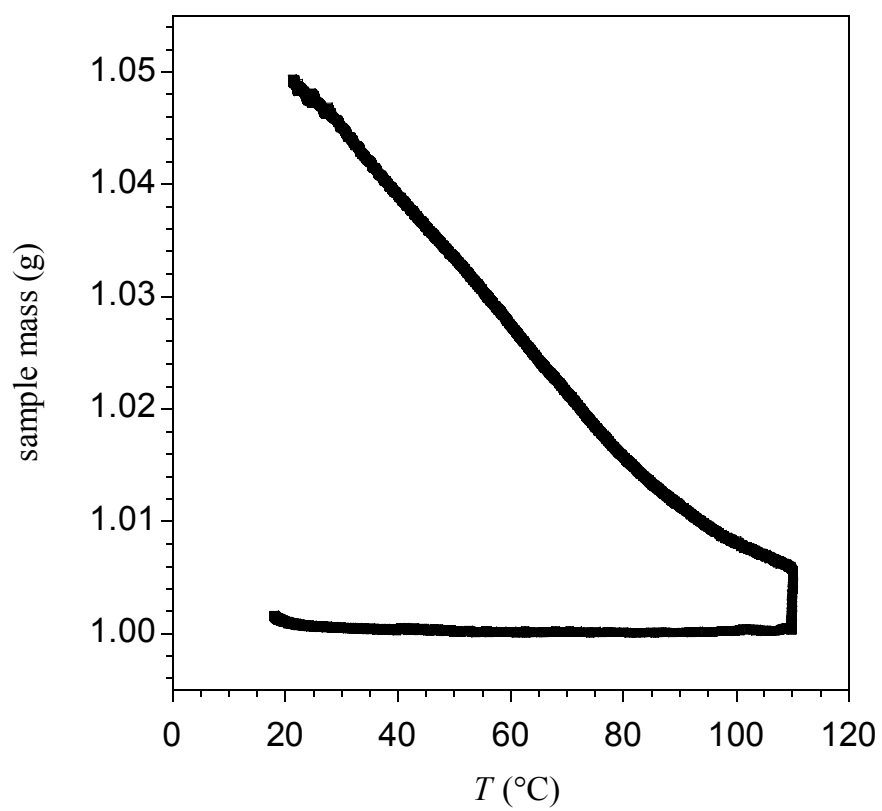


Table SII(a). Atomic coordinates and equivalent isotropic displacement parameters for $[\text{K}_2\text{CdU}(\text{C}_2\text{O}_4)_4]\cdot 9\text{H}_2\text{O}$, SPA-2.

Atom	x	y	z	U (eq) [Ang ²]
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U1	0.28702 (1)	0.76383 (4)	0.28280 (1)	0.0088 (1)
Cd1	0.77568 (4)	1.01890 (4)	0.22672 (4)	0.0115 (1)
K1	0.26564 (13)	0.2708 (3)	0.26944 (13)	0.0279 (4)
K2	0.77802 (16)	0.5195 (3)	0.21895 (16)	0.0283 (4)
O1	0.5747 (4)	1.0839 (5)	0.2383 (4)	0.0207 (12)
O2	0.6509 (4)	0.8028 (5)	0.1972 (4)	0.0213 (14)
O3	0.4683 (4)	0.7201 (5)	0.2048 (4)	0.0195 (12)
O4	0.4023 (4)	0.9858 (5)	0.2722 (4)	0.0181 (11)
O5	0.2406 (4)	0.4551 (5)	0.5757 (4)	0.0222 (14)
O6	0.2154 (4)	0.7405 (5)	0.6517 (4)	0.0199 (13)
O7	0.2617 (4)	0.5462 (5)	0.3991 (4)	0.0184 (11)
O8	0.2380 (4)	0.8219 (5)	0.4727 (4)	0.0164 (11)
O9	-0.1051 (4)	0.7942 (5)	0.2407 (5)	0.0251 (15)
O10	-0.0219 (4)	1.0760 (5)	0.2496 (4)	0.0203 (14)
O11	0.0810 (4)	0.7102 (5)	0.2541 (4)	0.0197 (13)
O12	0.1612 (4)	0.9850 (5)	0.2651 (4)	0.0155 (11)
O13	0.2398 (4)	0.4596 (5)	-0.0263 (4)	0.0235 (14)
O14	0.2191 (4)	0.7428 (6)	-0.1063 (4)	0.0226 (13)
O15	0.2695 (4)	0.5493 (5)	0.1567 (4)	0.0158 (11)
O16	0.2398 (4)	0.8235 (5)	0.0792 (4)	0.0204 (11)
O17	0.4653 (4)	0.7420 (7)	0.4390 (4)	0.0291 (16)
O19	0.0534 (6)	0.3159 (8)	0.1159 (7)	0.057 (2)
O20	0.3833 (6)	0.2290 (7)	0.0680 (5)	0.049 (2)
O21	0.5060 (5)	0.3474 (7)	0.3378 (5)	0.0387 (17)
O22	0.5532 (6)	0.4762 (8)	0.0835 (7)	0.051 (2)
O23	0.9767 (5)	0.5115 (8)	0.4020 (7)	0.050 (2)
O24	0.9033 (6)	0.5572 (7)	0.0257 (5)	0.0460 (19)
O25	0.6877 (5)	0.6168 (7)	0.4366 (6)	0.0458 (19)
C1	0.5060 (5)	0.9788 (7)	0.2443 (5)	0.0149 (16)
C2	0.5469 (5)	0.8215 (7)	0.2119 (5)	0.0141 (16)
C3	0.2455 (5)	0.5581 (7)	0.5057 (5)	0.0143 (16)
C4	0.2310 (5)	0.7209 (6)	0.5498 (5)	0.0118 (14)
C5	0.0504 (5)	0.9724 (6)	0.2538 (5)	0.0134 (16)
C6	0.0026 (5)	0.8122 (6)	0.2480 (5)	0.0134 (16)
C7	0.2346 (5)	0.7231 (6)	0.0009 (5)	0.0132 (16)
C8	0.2484 (5)	0.5627 (6)	0.0464 (5)	0.0129 (16)
O18	0.0807 (6)	0.2346 (7)	0.4457 (6)	0.051 (2)
H17A	0.53250	0.71290	0.40300	0.0130
H17B	0.44980	0.66910	0.49580	0.0130
H19A	0.00260	0.23150	0.11910	0.0130
H19C	0.01420	0.40400	0.13940	0.0130
H20B	0.45150	0.29300	0.07430	0.0130
H20C	0.33130	0.25510	-0.00070	0.0130
H21B	0.51070	0.43880	0.38130	0.0130
H21C	0.54480	0.35990	0.26920	0.0130
H22A	0.50540	0.56200	0.09240	0.0130
H22C	0.56440	0.46570	0.00260	0.0130
H23A	0.98110	0.60360	0.44410	0.0130
H23B	1.04770	0.49720	0.36710	0.0130
H24A	0.92820	0.65970	0.02270	0.0130
H24B	0.85230	0.53430	-0.04510	0.0130
H25A	0.70260	0.72160	0.44810	0.0130
H25B	0.72770	0.56240	0.50180	0.0130
H18B	0.00320	0.24930	0.40520	0.0130
H18C	0.09600	0.30740	0.50700	0.0130

Table S11(b). Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{K}_2\text{CdU}(\text{C}_2\text{O}_4)_4 \cdot 9\text{H}_2\text{O}$, **SPA-2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hk a^* b^* U_{12}]$

Atom	U(1,1)	or U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
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U1	0.0084(1)	0.0101(1)	0.0081(1)	-0.0002(1)	0.0022(1)	-0.0002(1)
Cd1	0.0109(2)	0.0135(2)	0.0104(2)	-0.0005(2)	0.0022(2)	-0.0006(2)
K1	0.0313(6)	0.0166(7)	0.0356(7)	0.0014(9)	0.0038(5)	-0.0028(10)
K2	0.0313(8)	0.0201(7)	0.0330(8)	-0.0035(8)	0.0026(7)	-0.0014(7)
O1	0.012(2)	0.017(2)	0.033(2)	-0.0002(19)	0.0029(18)	-0.0026(16)
O2	0.0128(19)	0.023(3)	0.029(2)	-0.0048(17)	0.0061(16)	-0.0005(15)
O3	0.016(2)	0.015(2)	0.029(2)	-0.0092(16)	0.0091(17)	-0.0052(15)
O4	0.0125(19)	0.015(2)	0.028(2)	-0.0006(17)	0.0075(17)	-0.0003(16)
O5	0.036(3)	0.018(2)	0.012(2)	0.0021(17)	0.0010(18)	-0.0049(19)
O6	0.028(2)	0.019(3)	0.0136(17)	-0.0023(17)	0.0067(16)	0.0039(18)
O7	0.029(2)	0.014(2)	0.0124(19)	-0.0010(16)	0.0037(17)	-0.0009(17)
O8	0.024(2)	0.0146(19)	0.012(2)	-0.0007(15)	0.0072(16)	0.0029(16)
O9	0.0119(19)	0.017(3)	0.046(3)	-0.002(2)	0.0027(18)	-0.0031(16)
O10	0.013(2)	0.014(2)	0.034(3)	0.0004(18)	0.0031(18)	0.0030(16)
O11	0.009(2)	0.0126(18)	0.037(3)	-0.0015(18)	0.0015(17)	0.0016(15)
O12	0.0096(18)	0.012(2)	0.025(2)	0.0017(16)	0.0029(16)	-0.0015(15)
O13	0.039(3)	0.016(2)	0.015(2)	-0.0017(17)	0.0013(19)	0.0018(19)
O14	0.041(2)	0.016(3)	0.0101(17)	0.0036(18)	0.0005(17)	0.000(2)
O15	0.025(2)	0.013(2)	0.0094(18)	0.0003(15)	0.0025(16)	-0.0002(16)
O16	0.030(2)	0.0163(19)	0.014(2)	-0.0007(16)	0.0000(17)	0.0050(17)
O17	0.018(2)	0.045(4)	0.023(2)	0.003(2)	-0.0021(17)	0.004(2)
O19	0.039(3)	0.047(4)	0.085(5)	0.021(3)	0.013(3)	-0.012(3)
O20	0.063(4)	0.044(4)	0.037(3)	0.007(3)	-0.007(3)	0.020(3)
O21	0.033(3)	0.050(3)	0.032(3)	-0.008(3)	0.000(2)	0.005(3)
O22	0.044(3)	0.043(4)	0.069(4)	-0.018(3)	0.017(3)	0.004(3)
O23	0.036(3)	0.038(3)	0.077(5)	0.018(3)	0.012(3)	-0.001(3)
O24	0.060(4)	0.042(3)	0.033(3)	-0.001(2)	-0.005(3)	-0.019(3)
O25	0.038(3)	0.043(3)	0.057(4)	0.015(3)	0.009(3)	0.009(3)
C1	0.009(2)	0.018(3)	0.018(3)	0.002(2)	0.003(2)	-0.003(2)
C2	0.007(2)	0.022(3)	0.014(3)	-0.003(2)	0.004(2)	-0.003(2)
C3	0.014(3)	0.018(3)	0.011(2)	0.003(2)	0.002(2)	-0.005(2)
C4	0.011(2)	0.015(3)	0.009(2)	0.0008(19)	-0.0002(19)	0.0010(18)
C5	0.013(2)	0.015(3)	0.013(3)	0.000(2)	0.005(2)	0.001(2)
C6	0.008(2)	0.014(3)	0.018(3)	-0.0022(19)	0.001(2)	0.0000(19)
C7	0.016(3)	0.015(3)	0.008(2)	0.0003(19)	-0.001(2)	-0.0007(19)
C8	0.011(2)	0.015(3)	0.013(3)	0.000(2)	0.003(2)	0.001(2)
O18	0.062(4)	0.027(4)	0.058(4)	-0.013(3)	-0.013(3)	0.002(3)

Figure SI4. ORTEP plot (30% probability level) for the assymmetric unit of $[\text{K}_2\text{CdU}(\text{C}_2\text{O}_4)_4]\cdot 9\text{H}_2\text{O}$, SPA-2.

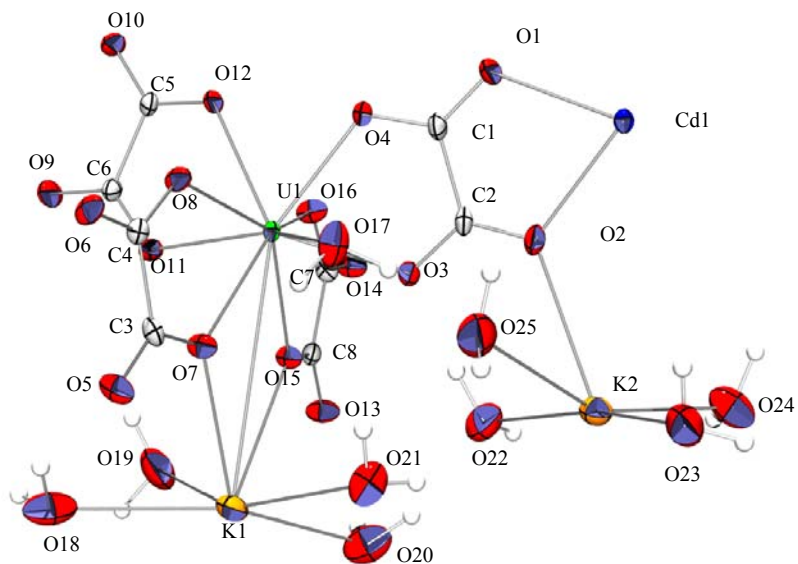


Table SI2. Bond lengths in Å for [K₂CdU(C₂O₄)₄];9H₂O, SPA-2.

U1	-O3	2.402 (5)	K2	-O25	2.966 (7)
U1	-O4	2.402 (5)	K2	-O9 _d	2.801 (5)
U1	-O7	2.406 (5)	K2	-O14 _e	2.803 (6)
U1	-O8	2.386 (5)	K2	-O6 _f	2.908 (5)
U1	-O11	2.393 (5)	O1	-C1	1.236 (8)
U1	-O12	2.446 (5)	O2	-C2	1.238 (7)
U1	-O15	2.404 (5)	O3	-C2	1.276 (8)
U1	-O16	2.399 (5)	O4	-C1	1.274 (7)
U1	-O17	2.552 (5)	O5	-C3	1.232 (8)
Cd1	-O1	2.399 (5)	O6	-C4	1.223 (7)
Cd1	-O2	2.407 (5)	O7	-C3	1.271 (7)
Cd1	-O9 _d	2.429 (5)	O8	-C4	1.279 (7)
Cd1	-O10 _d	2.359 (5)	O9	-C6	1.238 (7)
Cd1	-O13 _g	2.354 (5)	O10	-C5	1.242 (7)
Cd1	-O14 _g	2.446 (5)	O11	-C6	1.278 (7)
Cd1	-O5 _h	2.378 (5)	O12	-C5	1.266 (7)
Cd1	-O6 _h	2.426 (5)	O13	-C8	1.243 (7)
K1	-O7	2.890 (5)	O14	-C7	1.238 (7)
K1	-O15	2.818 (5)	O15	-C8	1.269 (7)
K1	-O19	2.848 (8)	O16	-C7	1.271 (7)
K1	-O20	2.857 (6)	O17	-H17A	0.9578
K1	-O21	2.852 (6)	O17	-H17B	0.9579
K1	-O4 _b	2.997 (5)	O19	-H19C	0.9651
K1	-O12 _b	2.827 (5)	O19	-H19A	0.9589
K2	-O2	2.924 (5)	O20	-H20B	0.9655
K2	-O22	2.863 (8)	O20	-H20C	0.9567
K2	-O23	2.900 (7)	O21	-H21B	0.9587
K2	-O24	2.823 (6)	O21	-H21C	0.9627
O22	-H22C	0.9620	O25	-H25B	0.9612
O22	-H22A	0.9581	O18	-H18C	0.9613
O23	-H23B	0.9625	O18	-H18B	0.9584
O23	-H23A	0.9559	C1	-C2	1.548 (9)
O24	-H24B	0.9627	C3	-C4	1.562 (8)
O24	-H24A	0.9645	C5	-C6	1.536 (8)
O25	-H25A	0.9614	C7	-C8	1.532 (8)

Table SI3. Angles in ° for [K₂CdU(C₂O₄)₄];9H₂O, SPA-2.

O3	-U1	-O4	66.87 (15)	O11	-U1	-O16	79.37 (16)
O3	-U1	-O7	104.40 (15)	O11	-U1	-O17	140.31 (16)
O3	-U1	-O8	134.18 (16)	O12	-U1	-O15	126.61 (15)
O3	-U1	-O11	143.42 (15)	O12	-U1	-O16	71.42 (15)
O3	-U1	-O12	129.15 (15)	O12	-U1	-O17	122.12 (17)
O3	-U1	-O15	69.63 (15)	O15	-U1	-O16	66.21 (15)
O3	-U1	-O16	76.55 (16)	O15	-U1	-O17	111.21 (17)
O3	-U1	-O17	66.27 (15)	O16	-U1	-O17	140.00 (15)
O4	-U1	-O7	143.85 (15)	O1	-Cd1	-O2	69.22 (15)
O4	-U1	-O8	93.58 (15)	O1	-Cd1	-O9_d	137.31 (15)
O4	-U1	-O11	134.44 (15)	O1	-Cd1	-O10_d	151.69 (15)
O4	-U1	-O12	69.31 (15)	O1	-Cd1	-O13_g	99.11 (16)
O4	-U1	-O15	129.51 (15)	O1	-Cd1	-O14_g	85.78 (15)
O4	-U1	-O16	79.72 (15)	O1	-Cd1	-O5_h	79.05 (16)
O4	-U1	-O17	72.72 (17)	O1	-Cd1	-O6_h	74.80 (15)
O7	-U1	-O8	66.83 (15)	O2	-Cd1	-O9_d	70.18 (15)
O7	-U1	-O11	74.08 (15)	O2	-Cd1	-O10_d	138.53 (16)
O7	-U1	-O12	126.28 (15)	O2	-Cd1	-O13_g	73.23 (16)
O7	-U1	-O15	71.39 (15)	O2	-Cd1	-O14_g	129.68 (16)
O7	-U1	-O16	134.21 (15)	O2	-Cd1	-O5_h	79.79 (15)
O7	-U1	-O17	71.84 (17)	O2	-Cd1	-O6_h	136.13 (16)
O8	-U1	-O11	79.91 (16)	O9_d	-Cd1	-O10_d	68.59 (15)
O8	-U1	-O12	72.12 (15)	O9_d	-Cd1	-O13_g	81.26 (17)
O8	-U1	-O15	135.88 (15)	O9_d	-Cd1	-O14_g	131.59 (17)
O8	-U1	-O16	142.94 (15)	O5_h	-Cd1	-O9_d	81.39 (17)
O8	-U1	-O17	68.43 (15)	O6_h	-Cd1	-O9_d	131.29 (17)
O11	-U1	-O12	65.78 (15)	O10_d	-Cd1	-O13_g	96.14 (16)
O11	-U1	-O15	75.62 (15)	O10_d	-Cd1	-O14_g	77.83 (15)
O5_h	-Cd1	-O10_d	98.24 (16)	O4_b	-K1	-O12_b	56.42 (14)
O6_h	-Cd1	-O10_d	77.90 (16)	O2	-K2	-O22	70.55 (18)
O13_g	-Cd1	-O14_g	68.48 (16)	O2	-K2	-O23	114.86 (19)
O5_h	-Cd1	-O13_g	151.59 (16)	O2	-K2	-O24	97.33 (17)
O6_h	-Cd1	-O13_g	138.06 (15)	O2	-K2	-O25	65.92 (16)
O5_h	-Cd1	-O14_g	138.71 (16)	O2	-K2	-O9_d	58.07 (14)
O6_h	-Cd1	-O14_g	69.69 (16)	O2	-K2	-O14_e	139.93 (15)
O5_h	-Cd1	-O6_h	69.32 (15)	O2	-K2	-O6_f	140.44 (14)
O7	-K1	-O15	58.88 (14)	O22	-K2	-O23	164.0 (2)
O7	-K1	-O19	97.50 (19)	O22	-K2	-O24	95.8 (2)
O7	-K1	-O20	124.95 (18)	O22	-K2	-O25	96.5 (2)
O7	-K1	-O21	74.37 (16)	O9_d	-K2	-O22	123.7 (2)
O4_b	-K1	-O7	140.05 (14)	O14_e	-K2	-O22	72.01 (18)
O7	-K1	-O12_b	138.51 (14)	O6_f	-K2	-O22	97.16 (19)
O15	-K1	-O19	69.57 (18)	O23	-K2	-O24	98.3 (2)
O15	-K1	-O20	72.81 (16)	O23	-K2	-O25	73.73 (19)
O15	-K1	-O21	80.89 (17)	O9_d	-K2	-O23	68.55 (18)
O4_b	-K1	-O15	136.17 (14)	O14_e	-K2	-O23	105.06 (19)
O12_b	-K1	-O15	145.81 (14)	O6_f	-K2	-O23	68.90 (17)
O19	-K1	-O20	88.3 (2)	O24	-K2	-O25	154.3 (2)
O19	-K1	-O21	148.9 (2)	O9_d	-K2	-O24	71.24 (18)
O4_b	-K1	-O19	122.14 (19)	O14_e	-K2	-O24	72.72 (17)
O12_b	-K1	-O19	77.96 (18)	O6_f	-K2	-O24	121.69 (18)
O20	-K1	-O21	73.41 (18)	O9_d	-K2	-O25	83.17 (17)
O4_b	-K1	-O20	66.12 (16)	O14_e	-K2	-O25	132.72 (18)
O12_b	-K1	-O20	96.34 (17)	O6_f	-K2	-O25	78.96 (16)
O4_b	-K1	-O21	73.54 (16)	O9_d	-K2	-O14_e	141.82 (16)
O12_b	-K1	-O21	128.00 (18)	O6_f	-K2	-O9_d	136.93 (16)

O6_f	-K2	-O14_e	58.31 (14)	Cd1_e	-O14	-K2_g	117.48 (18)
Cd1	-O1	-C1	116.3 (4)	U1	-O15	-K1	115.83 (18)
Cd1	-O2	-K2	113.98 (17)	U1	-O15	-C8	121.3 (4)
Cd1	-O2	-C2	116.0 (4)	K1	-O15	-C8	122.3 (4)
K2	-O2	-C2	125.8 (4)	U1	-O16	-C7	121.4 (4)
U1	-O3	-C2	119.9 (4)	U1	-O17	-H17B	109.37
U1	-O4	-C1	120.7 (4)	H17A	-O17	-H17B	109.94
U1	-O4	-K1_c	114.62 (17)	U1	-O17	-H17A	109.40
K1_c	-O4	-C1	123.0 (4)	H19A	-O19	-H19C	109.13
Cd1_f	-O5	-C3	117.5 (4)	K1	-O19	-H19A	109.82
Cd1_f	-O6	-C4	115.9 (4)	K1	-O19	-H19C	109.51
K2_h	-O6	-C4	128.2 (4)	H20B	-O20	-H20C	109.23
Cd1_f	-O6	-K2_h	114.35 (17)	K1	-O20	-H20C	109.31
U1	-O7	-K1_h	113.21 (17)	K1	-O20	-H20B	108.93
U1	-O7	-C3	120.9 (4)	K1	-O21	-H21B	109.71
K1	-O7	-C3	125.9 (4)	K1	-O21	-H21C	109.54
U1	-O8	-C4	121.7 (4)	H21B	-O21	-H21C	109.22
Cd1_a	-O9	-C6	116.4 (4)	K2	-O22	-H22A	108.69
K2_a	-O9	-C6	125.7 (4)	K2	-O22	-H22C	108.53
Cd1_a	-O9	-K2_a	117.70 (18)	H22A	-O22	-H22C	109.42
Cd1_a	-O10	-C5	119.0 (4)	K2	-O23	-H23A	109.44
U1	-O11	-C6	122.6 (4)	K2	-O23	-H23B	109.12
U1	-O12	-C5	120.7 (4)	H23A	-O23	-H23B	109.58
U1	-O12	-K1_c	119.31 (18)	K2	-O24	-H24A	109.02
K1_c	-O12	-C5	120.0 (4)	K2	-O24	-H24B	109.11
Cd1_e	-O13	-C8	118.9 (4)	H24A	-O24	-H24B	108.86
Cd1_e	-O14	-C7	116.0 (4)	H25A	-O25	-H25B	109.27
K2_g	-O14	-C7	125.4 (4)	K2	-O25	-H25A	109.20
K2	-O25	-H25B	109.15	O6	-C4	-O8	126.6 (5)
H18B	-O18	-H18C	109.52	O10	-C5	-C6	117.7 (5)
O4	-C1	-C2	115.4 (5)	O12	-C5	-C6	115.9 (5)
O1	-C1	-C2	117.8 (5)	O10	-C5	-O12	126.4 (5)
O1	-C1	-O4	126.9 (6)	O11	-C6	-C5	115.0 (5)
O2	-C2	-C1	119.0 (5)	O9	-C6	-C5	118.2 (5)
O2	-C2	-O3	125.5 (6)	O9	-C6	-O11	126.8 (5)
O3	-C2	-C1	115.6 (5)	O16	-C7	-C8	115.4 (5)
O5	-C3	-C4	118.2 (5)	O14	-C7	-C8	118.1 (5)
O5	-C3	-O7	126.5 (6)	O14	-C7	-O16	126.5 (5)
O7	-C3	-C4	115.4 (5)	O13	-C8	-O15	126.4 (5)
O6	-C4	-C3	118.8 (5)	O13	-C8	-C7	118.2 (5)
O8	-C4	-C3	114.7 (5)	O15	-C8	-C7	115.5 (5)

Table SI4 (a). Atomic coordinates ($\times 10^4$) and equivalent isotropic and anisotropic displacement parameters ($\text{\AA}^2 \times 10^2$) for $[\text{K}_2\text{Mg}_2\text{U}_2(\text{C}_2\text{O}_4)_7] \cdot 11\text{H}_2\text{O}$, **SPA-3**.

Atom	x	y	z	U (eq) [Ang ²]
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U1	0.80529 (1)	0.24889 (1)	0.21096 (1)	0.0144 (1)
K1	0.78770 (11)	0	0.43504 (13)	0.0321 (5)
K2	0.93868 (9)	0	0.59105 (14)	0.0308 (5)
Mg1	0.57814 (15)	0.2090 (3)	0.4333 (3)	0.0549 (10)
O1	0.9227 (2)	0.2238 (4)	0.2104 (3)	0.0265 (11)
O2	0.8526 (2)	0.1387 (4)	0.3299 (3)	0.0306 (14)
O3	0.9409 (3)	0.1165 (8)	0.4288 (5)	0.067 (3)
O4	1.0148 (2)	0.1617 (6)	0.2827 (4)	0.0512 (18)
O5'	0.7128 (2)	0.2751 (4)	0.2998 (3)	0.0244 (10)
O6	0.8287 (2)	0.3455 (4)	0.3480 (3)	0.0326 (14)
O7	0.6701 (2)	0.3668 (4)	0.4109 (4)	0.0372 (16)
O8	0.8012 (3)	0.3744 (5)	0.4912 (3)	0.0429 (16)
O9	0.8320 (2)	0.0871 (3)	0.1247 (3)	0.0279 (11)
O10	0.7389 (2)	0.0869 (3)	0.2412 (3)	0.0245 (10)
O11	0.8735 (2)	0.4125 (3)	0.1901 (3)	0.0264 (10)
O12	0.7433 (2)	0.4132 (3)	0.1694 (3)	0.0264 (10)
O13	0.7101 (2)	0.2203 (4)	0.0979 (3)	0.0241 (10)
O14	0.6726 (2)	0.2162 (4)	-0.0498 (3)	0.0235 (10)
O32	0.4613 (4)	0.1076 (7)	0.3970 (11)	0.120 (6)
C1	0.9552 (3)	0.1778 (5)	0.2761 (4)	0.0284 (16)
C2	0.9141 (3)	0.1404 (6)	0.3525 (4)	0.0324 (17)
C3	0.7880 (3)	0.3528 (5)	0.4095 (4)	0.0257 (14)
C4	0.7166 (3)	0.3309 (4)	0.3717 (4)	0.0231 (12)
C5	0.8119 (4)	0	0.1487 (5)	0.0200 (17)
C6	0.7580 (3)	0	0.2158 (5)	0.0190 (17)
C7	0.8460 (4)	1/2	0.1863 (5)	0.0194 (17)
C8	0.7708 (4)	1/2	0.1739 (5)	0.0204 (17)
C9	0.7160 (3)	0.2317 (4)	0.0138 (3)	0.0178 (11)
O30	0.88900 (17)	0.1568 (4)	0.8317 (3)	0.0287 (12)
O31	0.8939 (8)	0.366 (2)	0.756 (2)	0.35 (2)
O33	0.9338 (3)	0.1243 (9)	0.0074 (5)	0.076 (3)
O34	0.9603 (4)	0.3634 (9)	0.0614 (7)	0.097 (4)
O35	0.88300	1/2	0.96310	0.29 (3)
H32A	0.46780	0.03480	0.40710	0.1800
H32C	0.43080	0.13190	0.44270	0.1800
H30A	0.86690	0.10490	0.79020	0.0840
H30B	0.91000	0.09190	0.84720	0.0360
H31A	0.89150	0.40130	0.71400	0.0500
H31B	0.85140	0.34170	0.73950	2.0000
H33A	0.89450	0.13700	0.03700	2.0000
H33B	0.95150	0.13160	0.06870	0.1640
H34A	0.95010	0.34500	0.11360	0.1000
H34C	1.00090	0.34810	0.08480	0.0680
H35	0.90940	0.45240	0.98240	0.0050

Table SI4(b) (cont.): Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for $[\text{K}_2\text{Mg}_2\text{U}_2(\text{C}_2\text{O}_4)_7] \cdot 11\text{H}_2\text{O}$, **SPA-3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hk a^* b^* U_{12}]$

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
U1	0.0135(1)	0.0143(1)	0.0152(1)	0.0006(1)	0.0008(1)	0.0011(1)
K1	0.0409(10)	0.0330(9)	0.0242(8)	0	0.0147(7)	0
K2	0.0236(8)	0.0357(9)	0.0323(9)	0	-0.0025(6)	0
Mg1	0.0347(14)	0.0479(17)	0.078(2)	0.0126(16)	-0.0213(14)	-0.0166(13)
O1	0.0205(18)	0.0291(18)	0.030(2)	0.0085(17)	0.0032(15)	0.0017(16)
O2	0.0232(19)	0.041(3)	0.028(2)	0.0165(19)	0.0045(15)	0.0033(18)
O3	0.039(3)	0.116(7)	0.044(3)	0.040(4)	-0.005(2)	0.021(4)
O4	0.020(2)	0.079(4)	0.055(3)	0.018(3)	0.005(2)	0.013(3)
O5'	0.0205(17)	0.0277(18)	0.0254(18)	-0.0067(16)	0.0049(14)	-0.0028(15)
O6	0.0240(19)	0.046(3)	0.028(2)	-0.0133(19)	0.0029(15)	-0.0043(19)
O7	0.029(2)	0.042(3)	0.042(3)	-0.014(2)	0.0120(19)	0.003(2)
O8	0.033(2)	0.068(4)	0.027(2)	-0.016(2)	-0.0020(18)	0.003(2)
O9	0.037(2)	0.0187(17)	0.030(2)	0.0011(15)	0.0157(17)	-0.0013(16)
O10	0.0255(18)	0.0170(16)	0.032(2)	-0.0012(14)	0.0085(15)	0.0010(14)
O11	0.0193(17)	0.0198(17)	0.040(2)	0.0003(16)	0.0012(15)	0.0026(14)
O12	0.0203(17)	0.0173(16)	0.041(2)	0.0019(16)	-0.0004(15)	-0.0026(14)
O13	0.0247(18)	0.0297(18)	0.0179(16)	0.0022(15)	0.0016(13)	-0.0048(16)
O14	0.0201(16)	0.031(2)	0.0188(16)	0.0040(15)	-0.0016(13)	-0.0050(16)
O32	0.050(5)	0.054(5)	0.247(16)	0.005(7)	-0.052(7)	-0.004(4)
C1	0.018(2)	0.034(3)	0.033(3)	0.007(2)	0.0009(19)	0.006(2)
C2	0.028(3)	0.042(3)	0.027(3)	0.013(2)	0.001(2)	0.013(2)
C3	0.024(2)	0.028(3)	0.025(2)	-0.007(2)	0.0021(18)	0.005(2)
C4	0.024(2)	0.021(2)	0.025(2)	-0.0023(18)	0.0058(18)	0.0015(18)
C5	0.021(3)	0.020(3)	0.019(3)	0	0.001(2)	0
C6	0.016(3)	0.020(3)	0.021(3)	0	0.001(2)	0
C7	0.021(3)	0.017(3)	0.020(3)	0	0.000(2)	0
C8	0.022(3)	0.017(3)	0.022(3)	0	0.000(2)	0
C9	0.0162(18)	0.020(2)	0.0171(18)	0.0024(15)	-0.0001(14)	-0.0013(15)
O30	0.0057(13)	0.058(3)	0.0229(17)	-0.0060(18)	0.0040(11)	0.0074(15)
O31	0.082(10)	0.36(3)	0.63(5)	-0.38(4)	0.116(19)	-0.077(15)
O33	0.041(3)	0.139(8)	0.051(4)	0.012(5)	0.023(3)	0.007(4)
O34	0.078(6)	0.121(8)	0.101(7)	0.018(7)	0.060(5)	0.007(6)
O35	0.26(4)	0.25(4)	0.35(6)	0	0.02(4)	0

Figure S15. ORTEP plot (30% probability level) for the asymmetric unit of $[\text{K}_2\text{Mg}_2\text{U}_2(\text{C}_2\text{O}_4)_7] \cdot 11\text{H}_2\text{O}$, **SPA-3**.

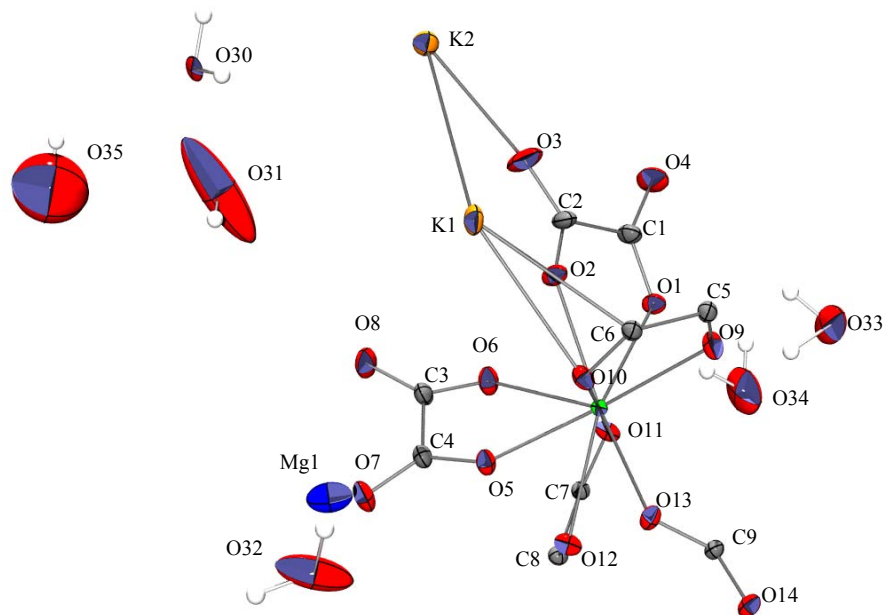


Table SI5. Distances in Å for [K₂Mg₂U₂(C₂O₄)₇];11H₂O, SPA-3.

U1	-O1	2.422 (4)	O2	-C2	1.274 (7)
U1	-O2	2.386 (5)	O3	-C2	1.242 (9)
U1	-O5'	2.400 (4)	O4	-C1	1.232 (7)
U1	-O6	2.372 (5)	O5'	-C4	1.269 (7)
U1	-O9	2.512 (4)	O6	-C3	1.275 (7)
U1	-O10	2.541 (4)	O7	-C4	1.237 (8)
U1	-O11	2.553 (4)	O8	-C3	1.235 (7)
U1	-O12	2.511 (4)	O9	-C5	1.251 (5)
U1	-O13	2.478 (4)	O10	-C6	1.248 (5)
U1	-O14_h	2.474 (4)	O11	-C7	1.256 (5)
K1	-O2	2.759 (5)	O12	-C8	1.248 (5)
K1	-O2_c	2.759 (5)	O13	-C9	1.253 (6)
K1	-O7_f	2.904 (6)	O14	-C9	1.249 (7)
K1	-O8_f	2.715 (6)	O32	-H32C	0.9988
K1	-O7_i	2.904 (6)	O32	-H32A	0.9541
K1	-O8_i	2.715 (6)	O30	-H30B	0.9564
K2	-O3	2.807 (8)	O30	-H30A	0.9863
K2	-O3_a	2.914 (8)	O31	-H31A	0.7615
K2	-O4_a	2.888 (7)	O31	-H31B	0.9364
K2	-O3_b	2.914 (8)	O33	-H33A	0.9558
K2	-O4_b	2.888 (7)	O33	-H33B	0.9440
K2	-O3_c	2.807 (8)	O34	-H34C	0.8940
K2	-O7_f	2.803 (5)	O34	-H34A	0.8404
K2	-O7_i	2.803 (5)	O35	-H35_k	0.8487
Mg1	-O7	2.800 (6)	O35	-H35	0.8487
Mg1	-O32	2.735 (9)	C1	-C2	1.527 (9)
Mg1	-O8_i	2.831 (7)	C3	-C4	1.545 (9)
O1	-C1	1.269 (8)	C5	-C6	1.531 (10)
C7	-C8	1.533 (12)	C9	-C9_h	1.550 (8)

Table SI6. Angles in ° for [K₂Mg₂U₂(C₂O₄)₇];11H₂O, SPA-3.

O1	-U1	-O2	65.09(15)	O6	-U1	-O13	137.37(15)
O1	-U1	-O5'	147.50(15)	O6	-U1	-O14_h	132.00(16)
O1	-U1	-O6	86.47(15)	O9	-U1	-O10	63.29(13)
O1	-U1	-O9	68.52(15)	O9	-U1	-O11	118.58(13)
O1	-U1	-O10	115.75(15)	O9	-U1	-O12	134.34(14)
O1	-U1	-O11	63.81(15)	O9	-U1	-O13	74.52(15)
O1	-U1	-O12	126.31(15)	O9	-U1	-O14_h	66.98(15)
O1	-U1	-O13	134.74(15)	O10	-U1	-O11	176.84(14)
O1	-U1	-O14_h	76.44(14)	O10	-U1	-O12	117.63(13)
O2	-U1	-O5'	88.87(15)	O10	-U1	-O13	65.98(15)
O2	-U1	-O6	69.63(17)	O10	-U1	-O14_h	117.00(15)
O2	-U1	-O9	77.50(15)	O11	-U1	-O12	63.22(13)
O2	-U1	-O10	65.11(14)	O11	-U1	-O13	116.72(15)
O2	-U1	-O11	112.41(15)	O11	-U1	-O14_h	66.09(15)
O2	-U1	-O12	147.38(15)	O12	-U1	-O13	66.96(15)
O2	-U1	-O13	130.50(16)	O12	-U1	-O14_h	75.17(15)
O2	-U1	-O14_h	135.00(15)	O13	-U1	-O14_h	65.47(14)
O5'	-U1	-O6	65.48(15)	O2	-K1	-O2_c	80.40(15)
O5'	-U1	-O9	126.80(15)	O2	-K1	-O7_f	133.28(15)
O5'	-U1	-O10	64.32(15)	O2	-K1	-O8_f	166.05(17)
O5'	-U1	-O11	114.21(15)	O2	-K1	-O7_i	85.71(14)
O5'	-U1	-O12	66.99(15)	O2	-K1	-O8_i	101.75(16)
O5'	-U1	-O13	76.77(14)	O2_c	-K1	-O7_f	85.71(14)
O5'	-U1	-O14_h	134.46(15)	O2_c	-K1	-O8_f	101.75(16)
O6	-U1	-O9	144.95(15)	O2_c	-K1	-O7_i	133.28(15)
O6	-U1	-O10	110.86(15)	O2_c	-K1	-O8_i	166.05(17)
O6	-U1	-O11	66.09(15)	O7_f	-K1	-O8_f	60.63(15)
O6	-U1	-O12	80.16(15)	O7_f	-K1	-O7_i	72.18(16)
O7_f	-K1	-O8_i	102.08(16)	O4_b	-K2	-O7_i	131.76(16)
O7_i	-K1	-O8_f	102.08(16)	O3_c	-K2	-O7_f	74.45(19)
O8_f	-K1	-O8_i	72.88(19)	O3_c	-K2	-O7_i	112.5(2)
O7_i	-K1	-O8_i	60.63(15)	O7_f	-K2	-O7_i	75.20(15)
O3	-K2	-O3_a	64.7(2)	O7	-Mg1	-O32	154.9(3)
O3	-K2	-O4_a	97.5(2)	O7	-Mg1	-O8_i	75.36(18)
O3	-K2	-O3_b	96.9(2)	O8_i	-Mg1	-O32	128.0(3)
O3	-K2	-O4_b	153.7(2)	U1	-O1	-C1	121.3(4)
O3	-K2	-O3_c	64.4(3)	U1	-O2	-K1	127.12(17)
O3	-K2	-O7_f	112.5(2)	U1	-O2	-C2	120.9(4)
O3	-K2	-O7_i	74.45(19)	K1	-O2	-C2	112.0(4)
O3_a	-K2	-O4_a	57.08(19)	K2	-O3	-C2	148.8(6)
O3_a	-K2	-O3_b	61.8(3)	K2	-O3	-K2_a	83.1(2)
O3_a	-K2	-O4_b	101.2(2)	K2_a	-O3	-C2	110.7(5)
O3_a	-K2	-O3_c	96.9(2)	K2_a	-O4	-C1	116.4(5)
O3_a	-K2	-O7_f	170.9(2)	U1	-O5'	-C4	121.9(4)
O3_a	-K2	-O7_i	111.2(2)	U1	-O6	-C3	122.3(4)
O3_b	-K2	-O4_a	101.2(2)	Mg1	-O7	-C4	109.4(4)
O4_a	-K2	-O4_b	91.9(2)	K1_g	-O7	-Mg1	119.8(2)
O3_c	-K2	-O4_a	153.7(2)	K2_g	-O7	-Mg1	84.47(14)
O4_a	-K2	-O7_f	131.76(16)	K1_g	-O7	-C4	112.7(4)
O4_a	-K2	-O7_i	77.80(15)	K2_g	-O7	-C4	149.4(5)
O3_b	-K2	-O4_b	57.08(19)	K1_g	-O7	-K2_g	80.52(15)
O3_b	-K2	-O3_c	64.7(2)	K1_g	-O8	-C3	114.5(5)
O3_b	-K2	-O7_f	111.2(2)	Mg1_i	-O8	-C3	114.2(5)
O3_b	-K2	-O7_i	170.9(2)	K1_g	-O8	-Mg1_i	131.3(2)
O3_c	-K2	-O4_b	97.5(2)	U1	-O9	-C5	120.6(4)
O4_b	-K2	-O7_f	77.80(15)	U1	-O10	-C6	119.8(4)

U1	-O11	-C7	119.7 (4)	O6	-C3	-O8	126.4 (6)
U1	-O12	-C8	121.4 (4)	O5'	-C4	-C3	113.2 (5)
U1	-O13	-C9	120.4 (4)	O7	-C4	-C3	120.3 (5)
U1_h	-O14	-C9	120.5 (4)	O5'	-C4	-O7	126.5 (6)
H32A	-O32	-H32C	106.82	O9	-C5	-C6	116.6 (4)
Mg1	-O32	-H32A	109.13	O9	-C5	-O9_c	126.7 (7)
Mg1	-O32	-H32C	107.63	O9_c	-C5	-C6	116.6 (4)
H30A	-O30	-H30B	74.46	O10	-C6	-C5	116.6 (3)
H31A	-O31	-H31B	89.50	O10	-C6	-O10_c	126.8 (6)
H33A	-O33	-H33B	80.00	O10_c	-C6	-C5	116.6 (3)
H34A	-O34	-H34C	83.12	O11	-C7	-C8	116.5 (4)
H35	-O35	-H35_k	92.14	O11_d	-C7	-C8	116.5 (4)
O4	-C1	-C2	119.2 (6)	O11_d	-C7	-O11_d	127.0 (7)
O1	-C1	-O4	126.3 (6)	O12	-C8	-O12_d	126.6 (7)
O1	-C1	-C2	114.5 (5)	O12_d	-C8	-C7	116.7 (4)
O2	-C2	-C1	113.8 (5)	O12	-C8	-C7	116.7 (4)
O3	-C2	-C1	120.4 (6)	O13	-C9	-C9_h	116.6 (5)
O2	-C2	-O3	125.8 (6)	O14	-C9	-C9_h	117.0 (4)
O6	-C3	-C4	112.6 (5)	O13	-C9	-O14	126.4 (6)
O8	-C3	-C4	121.0 (6)				

Table SI7 (a). Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^2$) for $[\text{K}_2\text{ZrMn}(\text{C}_2\text{O}_4)_4] \cdot 8\text{H}_2\text{O}$, SPA-4.

Zr1	0.67327 (3)	0.56068 (3)	0.79184 (3)	0.0192 (1)
Mn1	0.76678 (10)	0.50272 (12)	1.06775 (9)	0.0576 (4)
O1	0.8406 (3)	0.6135 (3)	0.7756 (3)	0.0280 (9)
O2	0.8153 (3)	0.4640 (3)	0.8831 (2)	0.0258 (8)
O3	1.0369 (4)	0.5993 (4)	0.8190 (4)	0.0429 (13)
O4	1.0066 (3)	0.4181 (3)	0.9218 (3)	0.0322 (10)
O5	0.6821 (4)	0.7990 (3)	0.9962 (3)	0.0370 (11)
O6	0.6039 (5)	0.8889 (3)	0.8138 (3)	0.0463 (13)
O7	0.6360 (3)	0.7310 (3)	0.7584 (2)	0.0281 (9)
O8	0.7030 (3)	0.6485 (3)	0.9238 (2)	0.0287 (9)
O9	0.6415 (3)	0.5843 (3)	0.6369 (2)	0.0270 (9)
O10	0.6380 (4)	0.4087 (3)	0.7215 (2)	0.0302 (10)
O11	0.5861 (4)	0.3169 (3)	0.5861 (3)	0.0377 (13)
O12	0.6314 (4)	0.5044 (3)	0.4985 (3)	0.0366 (11)
O13	0.3070 (5)	0.5092 (6)	0.7573 (5)	0.071 (2)
O14	0.4368 (5)	0.3875 (6)	0.9075 (6)	0.081 (3)
O15	0.5996 (3)	0.4584 (3)	0.8855 (3)	0.0274 (9)
O16	0.4795 (3)	0.5748 (3)	0.7472 (3)	0.0324 (10)
C1	0.9406 (4)	0.5715 (4)	0.8213 (4)	0.0274 (12)
C2	0.9241 (4)	0.4754 (4)	0.8822 (3)	0.0238 (10)
C3	0.6751 (4)	0.7467 (4)	0.9252 (3)	0.0253 (11)
C4	0.6340 (4)	0.7963 (4)	0.8251 (3)	0.0257 (11)
C5	0.6160 (4)	0.3986 (4)	0.6310 (3)	0.0251 (11)
C6	0.6301 (4)	0.5035 (4)	0.5811 (3)	0.0258 (11)
C7	0.4158 (5)	0.5150 (6)	0.7843 (4)	0.0400 (16)
C8	0.4889 (5)	0.4475 (5)	0.8672 (4)	0.0362 (16)
*O24B	0.4095 (16)	0.9107 (19)	0.0782 (14)	0.035 (6)
*O24C	0.4003 (9)	0.9863 (9)	0.0410 (10)	0.049 (4)
O20	0.8260 (6)	0.2190 (6)	1.0601 (5)	0.074 (2)
O21	0.3155 (8)	0.8062 (10)	0.7266 (6)	0.117 (4)
O22	0.6156 (9)	0.3178 (9)	0.0813 (6)	0.105 (4)
O23	0.6376 (3)	0.8359 (4)	0.1694 (3)	0.0434 (13)
*O24A	0.5357 (8)	0.8880 (8)	0.0272 (7)	0.031 (3)
K1	0.42759 (11)	0.71203 (9)	0.59627 (8)	0.0329 (3)
K2	0.71767 (13)	0.26285 (9)	0.86488 (9)	0.0389 (3)

Table SI7 (b). Anisotropic displacement parameters (\AA^2) for $[\text{K}_2\text{ZrMn}(\text{C}_2\text{O}_4)_4]\cdot 8\text{H}_2\text{O}$, SPA-4. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hk a^* b^* U_{12}]$

Atom	U(1,1)	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
----	-----	-----	-----	-----	-----	-----
Zr1	0.0172(2)	0.0206(2)	0.0185(2)	0.0020(1)	0.0031(1)	-0.0001(1)
Mn1	0.0403(6)	0.0839(9)	0.0478(6)	0.0188(6)	0.0117(5)	0.0056(6)
O1	0.0193(14)	0.0289(15)	0.0341(17)	0.0081(13)	0.0048(12)	0.0009(12)
O2	0.0189(14)	0.0292(15)	0.0270(15)	0.0055(12)	0.0031(11)	0.0010(12)
O3	0.0215(17)	0.048(2)	0.058(3)	0.010(2)	0.0097(17)	-0.0040(16)
O4	0.0246(16)	0.0325(17)	0.0358(18)	0.0016(14)	0.0027(14)	0.0069(13)
O5	0.047(2)	0.0358(19)	0.0297(17)	-0.0071(15)	0.0136(16)	-0.0004(17)
O6	0.069(3)	0.0263(18)	0.041(2)	0.0009(16)	0.012(2)	0.0129(19)
O7	0.0340(18)	0.0243(15)	0.0229(14)	0.0022(11)	0.0031(13)	0.0039(13)
O8	0.0331(17)	0.0274(16)	0.0235(14)	0.0037(12)	0.0047(12)	0.0039(13)
O9	0.0333(18)	0.0250(14)	0.0215(14)	0.0005(11)	0.0058(13)	-0.0033(13)
O10	0.040(2)	0.0248(14)	0.0244(15)	0.0021(12)	0.0071(14)	0.0024(14)
O11	0.054(3)	0.0262(17)	0.0310(18)	-0.0085(14)	0.0093(17)	-0.0022(16)
O12	0.049(2)	0.041(2)	0.0219(15)	-0.0006(14)	0.0136(15)	0.0021(18)
O13	0.027(2)	0.106(5)	0.078(4)	0.034(4)	0.012(2)	0.003(3)
O14	0.035(3)	0.104(5)	0.110(5)	0.071(4)	0.029(3)	0.001(3)
O15	0.0224(15)	0.0323(16)	0.0288(15)	0.0059(13)	0.0093(12)	-0.0014(12)
O16	0.0192(15)	0.044(2)	0.0342(18)	0.0114(15)	0.0081(13)	0.0072(14)
C1	0.023(2)	0.028(2)	0.030(2)	-0.0003(16)	0.0057(16)	0.0009(16)
C2	0.0197(18)	0.0246(18)	0.0247(18)	-0.0026(15)	0.0027(14)	0.0025(14)
C3	0.0232(19)	0.0255(19)	0.0268(19)	-0.0020(15)	0.0068(15)	-0.0019(15)
C4	0.0222(19)	0.0254(18)	0.028(2)	0.0010(15)	0.0049(15)	0.0009(15)
C5	0.025(2)	0.026(2)	0.0223(18)	-0.0011(15)	0.0038(15)	0.0040(15)
C6	0.023(2)	0.032(2)	0.0228(18)	0.0004(15)	0.0075(15)	0.0023(16)
C7	0.024(2)	0.055(3)	0.043(3)	0.017(3)	0.013(2)	0.005(2)
C8	0.027(2)	0.043(3)	0.040(3)	0.014(2)	0.012(2)	0.002(2)
O24B	0.024(8)	0.051(12)	0.036(9)	-0.027(9)	0.017(7)	-0.011(8)
O24C	0.029(5)	0.035(5)	0.085(9)	-0.033(6)	0.022(5)	0.004(4)
O20	0.063(4)	0.079(4)	0.080(4)	-0.012(4)	0.021(3)	0.004(3)
O21	0.104(6)	0.186(10)	0.061(4)	-0.004(5)	0.024(4)	0.080(7)
O22	0.101(6)	0.135(8)	0.080(5)	-0.004(5)	0.029(5)	0.007(6)
O23	0.0212(15)	0.067(3)	0.051(2)	-0.048(2)	0.0248(15)	-0.0229(17)
O24A	0.027(4)	0.037(5)	0.034(4)	-0.006(4)	0.015(4)	0.001(4)
K1	0.0344(5)	0.0337(5)	0.0259(4)	0.0019(4)	0.0014(4)	0.0025(4)
K2	0.0501(7)	0.0280(5)	0.0386(6)	-0.0024(4)	0.0128(5)	0.0081(5)

Figure S18. ORTEP plot (30% probability level) for the assymmetric unit of $[\text{K}_2\text{Mn}\{\text{Zr}(\text{C}_2\text{O}_4)_4\}]\cdot 8\text{H}_2\text{O}$, SPA-4.

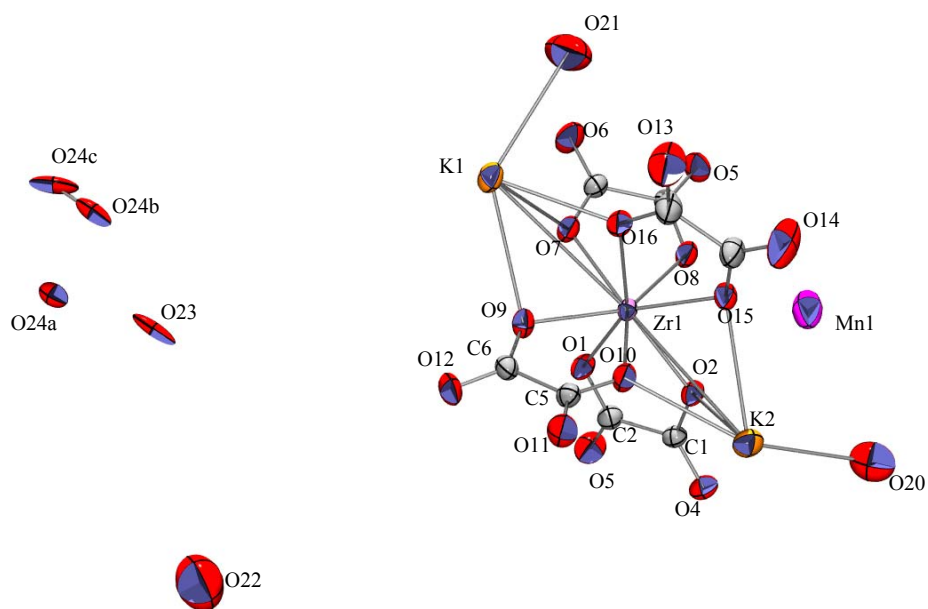


Table SI8. Bond Distances (Angstrom) for $[\text{K}_2\text{ZrMn}(\text{C}_2\text{O}_4)_4]\cdot 8\text{H}_2\text{O}$, SPA-4

Zr1	-O1	2.165 (4)	O4	-C2	1.219 (6)
Zr1	-O2	2.193 (4)	O5	-C3	1.218 (6)
Zr1	-O7	2.222 (4)	O6	-C4	1.220 (6)
Zr1	-O8	2.173 (3)	O7	-C4	1.287 (6)
Zr1	-O9	2.219 (3)	O8	-C3	1.285 (6)
Zr1	-O10	2.163 (4)	O9	-C6	1.292 (6)
Zr1	-O15	2.239 (4)	O10	-C5	1.286 (5)
Zr1	-O16	2.200 (4)	O11	-C5	1.221 (6)
Mn1	-O2	2.972 (4)	O12	-C6	1.219 (6)
Mn1	-O8	2.741 (4)	O13	-C7	1.234 (9)
Mn1	-O15	2.888 (4)	O14	-C8	1.231 (10)
Mn1	-O13_a	2.948 (7)	O15	-C8	1.265 (7)
Mn1	-O14_a	2.890 (7)	O16	-C7	1.293 (8)
Mn1	-O3_b	2.754 (6)	O24B	-O24C	1.09 (3)
Mn1	-O4_b	2.821 (4)	C1	-C2	1.554 (7)
O1	-C1	1.293 (7)	C3	-C4	1.543 (6)
O2	-C2	1.298 (6)	C5	-C6	1.547 (7)
O3	-C1	1.201 (7)	C7	-C8	1.533 (9)

Table SI9. Angles (degrees) for $[\text{K}_2\text{ZrMn}(\text{C}_2\text{O}_4)_4]\cdot 8\text{H}_2\text{O}$, SPA-4.

O1	-Zr1	-O2	71.13 (14)	O2	-Mn1	-O8	59.21 (10)
O1	-Zr1	-O7	78.84 (14)	O2	-Mn1	-O15	51.80 (10)
O1	-Zr1	-O8	91.35 (15)	O2	-Mn1	-O13_a	166.37 (17)
O1	-Zr1	-O9	74.62 (15)	O2	-Mn1	-O14_a	125.52 (19)
O1	-Zr1	-O10	106.08 (16)	O2	-Mn1	-O3_b	97.13 (14)
O1	-Zr1	-O15	140.83 (15)	O2	-Mn1	-O4_b	71.20 (11)
O1	-Zr1	-O16	147.96 (15)	O8	-Mn1	-O15	56.77 (11)
O2	-Zr1	-O7	137.92 (13)	O8	-Mn1	-O13_a	128.53 (17)
O2	-Zr1	-O8	80.80 (13)	O8	-Mn1	-O14_a	73.82 (18)
O2	-Zr1	-O9	125.15 (13)	O3_b	-Mn1	-O8	140.97 (14)
O2	-Zr1	-O10	78.83 (14)	O4_b	-Mn1	-O8	81.33 (12)
O2	-Zr1	-O15	70.58 (14)	O13_a	-Mn1	-O15	120.26 (16)
O2	-Zr1	-O16	140.79 (14)	O14_a	-Mn1	-O15	80.68 (18)
O7	-Zr1	-O8	70.98 (12)	O3_b	-Mn1	-O15	134.56 (14)
O7	-Zr1	-O9	71.26 (12)	O4_b	-Mn1	-O15	120.26 (12)
O7	-Zr1	-O10	139.00 (12)	O13_a	-Mn1	-O14_a	56.5 (2)
O7	-Zr1	-O15	127.38 (13)	O3_b	-Mn1	-O13_a	81.87 (18)
O7	-Zr1	-O16	74.50 (14)	O4_b	-Mn1	-O13_a	119.06 (16)
O8	-Zr1	-O9	141.57 (14)	O3_b	-Mn1	-O14_a	137.3 (2)
O8	-Zr1	-O10	147.01 (13)	O4_b	-Mn1	-O14_a	129.42 (17)
O8	-Zr1	-O15	74.76 (14)	O3_b	-Mn1	-O4_b	60.79 (14)
O8	-Zr1	-O16	96.38 (14)	Zr1	-O1	-C1	122.9 (3)
O9	-Zr1	-O10	71.12 (13)	Zr1	-O2	-Mn1	98.72 (13)
O9	-Zr1	-O15	136.72 (14)	Zr1	-O2	-C2	121.2 (3)
O9	-Zr1	-O16	80.19 (14)	Mn1	-O2	-C2	116.4 (3)
O10	-Zr1	-O15	74.12 (14)	Mn1_b	-O3	-C1	119.1 (4)
O10	-Zr1	-O16	83.62 (16)	Mn1_b	-O4	-C2	115.6 (3)
O15	-Zr1	-O16	70.98 (15)	Zr1	-O7	-C4	119.9 (3)
Zr1	-O8	-Mn1	106.49 (15)	O5	-C3	-C4	121.5 (5)
Zr1	-O8	-C3	122.1 (3)	O8	-C3	-C4	112.8 (4)
Mn1	-O8	-C3	130.6 (3)	O6	-C4	-O7	125.4 (4)
Zr1	-O9	-C6	120.1 (3)	O6	-C4	-C3	121.2 (4)
Zr1	-O10	-C5	122.4 (3)	O7	-C4	-C3	113.4 (4)
Mn1_a	-O13	-C7	105.4 (5)	O10	-C5	-O11	125.7 (5)
Mn1_a	-O14	-C8	108.4 (5)	O10	-C5	-C6	112.9 (4)
Zr1	-O15	-Mn1	100.09 (14)	O11	-C5	-C6	121.4 (4)
Zr1	-O15	-C8	119.6 (4)	O9	-C6	-O12	126.6 (5)
Mn1	-O15	-C8	127.4 (4)	O9	-C6	-C5	112.4 (4)
Zr1	-O16	-C7	120.6 (4)	O12	-C6	-C5	121.0 (4)
O1	-C1	-O3	126.7 (5)	O13	-C7	-O16	125.4 (6)
O1	-C1	-C2	111.8 (4)	O13	-C7	-C8	121.3 (6)
O3	-C1	-C2	121.5 (5)	O16	-C7	-C8	113.4 (5)
O2	-C2	-O4	126.0 (5)	O14	-C8	-O15	126.5 (6)
O2	-C2	-C1	112.5 (4)	O14	-C8	-C7	118.7 (6)
O4	-C2	-C1	121.5 (4)	O15	-C8	-C7	114.8 (5)
O5	-C3	-O8	125.7 (4)				