STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 79 (2023)

Supporting information for article:

New iron(II) oxalate potassium salt structure K2Fe[(C2O4)2(H2O)2]·0.18H2O

Sara Amanchar, Thierry Schweitzer, Thomas Mazet, Bernard Malaman, Leopold V. B Diop and Michel Francois

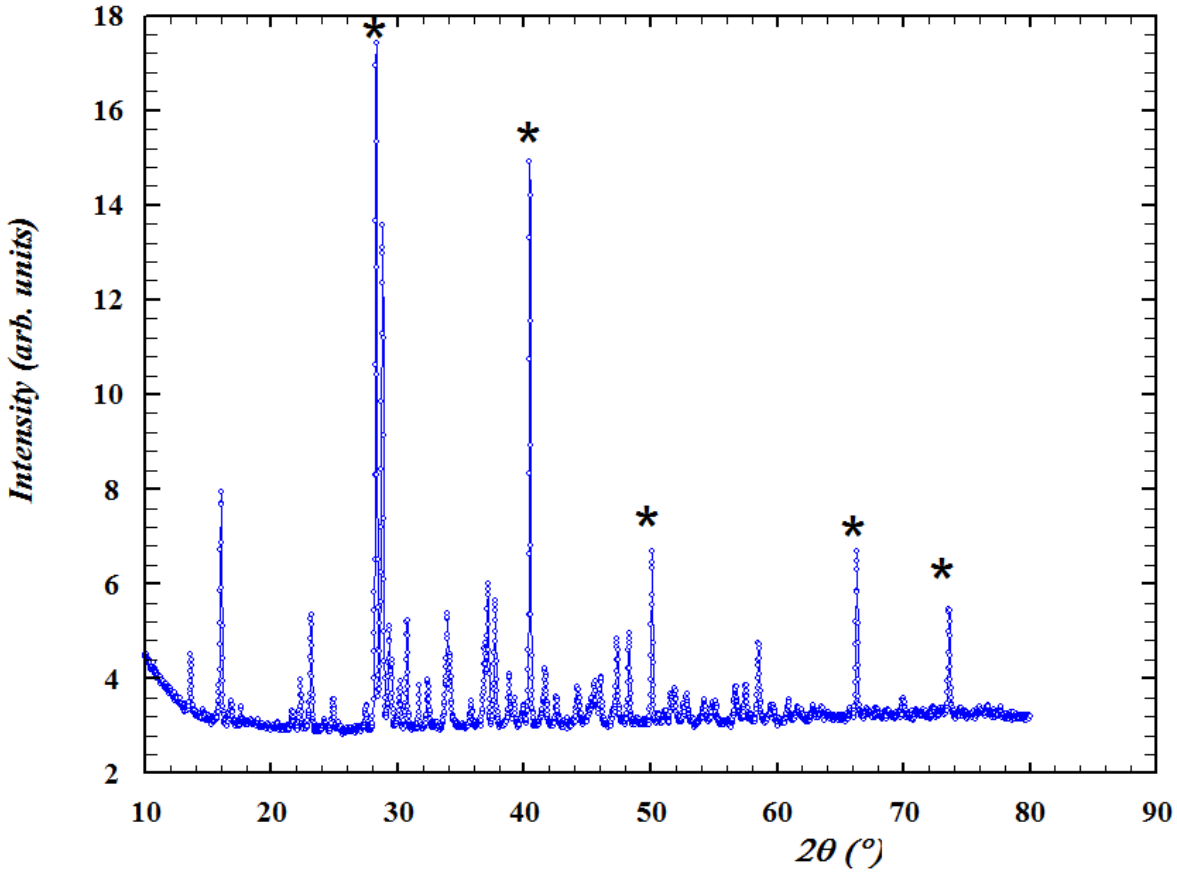

Figure S1: Raw PXRD pattern for the mixing obtained after the reaction. Asterisks correspond to the KCl phase.

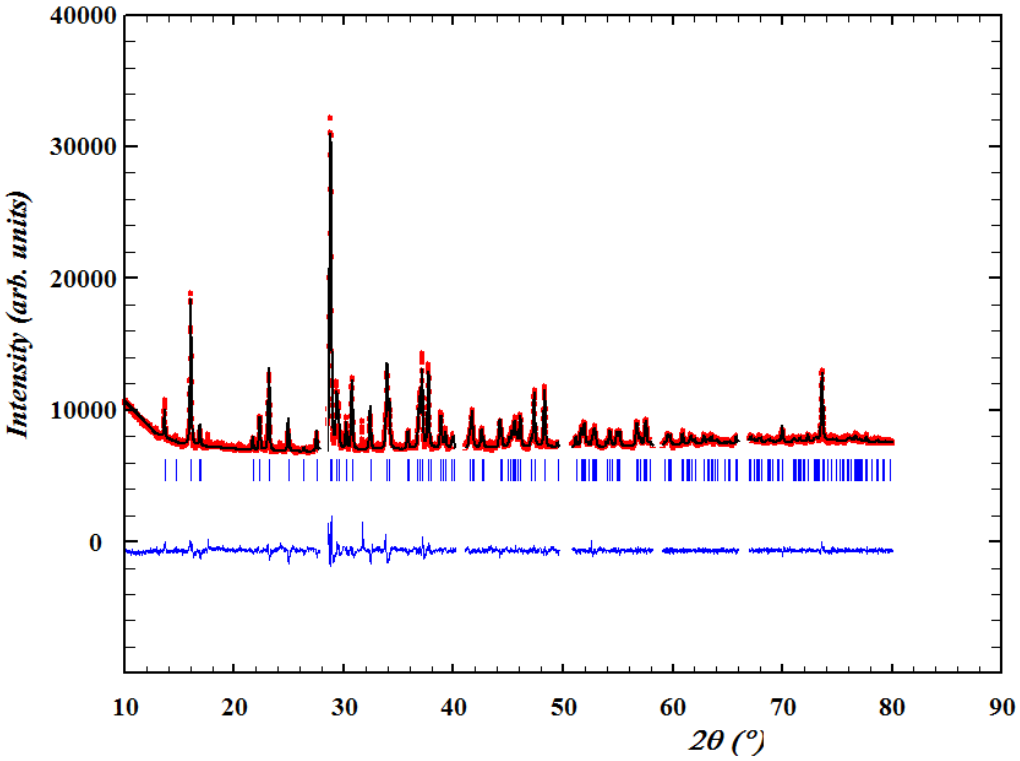

Figure S2: Le Bail plot of the orange mixing after the reaction, a = 7.6668(3) Å b = 12.0845(4) Å c = 10.5543(5) Å, SG: C m c 2_1

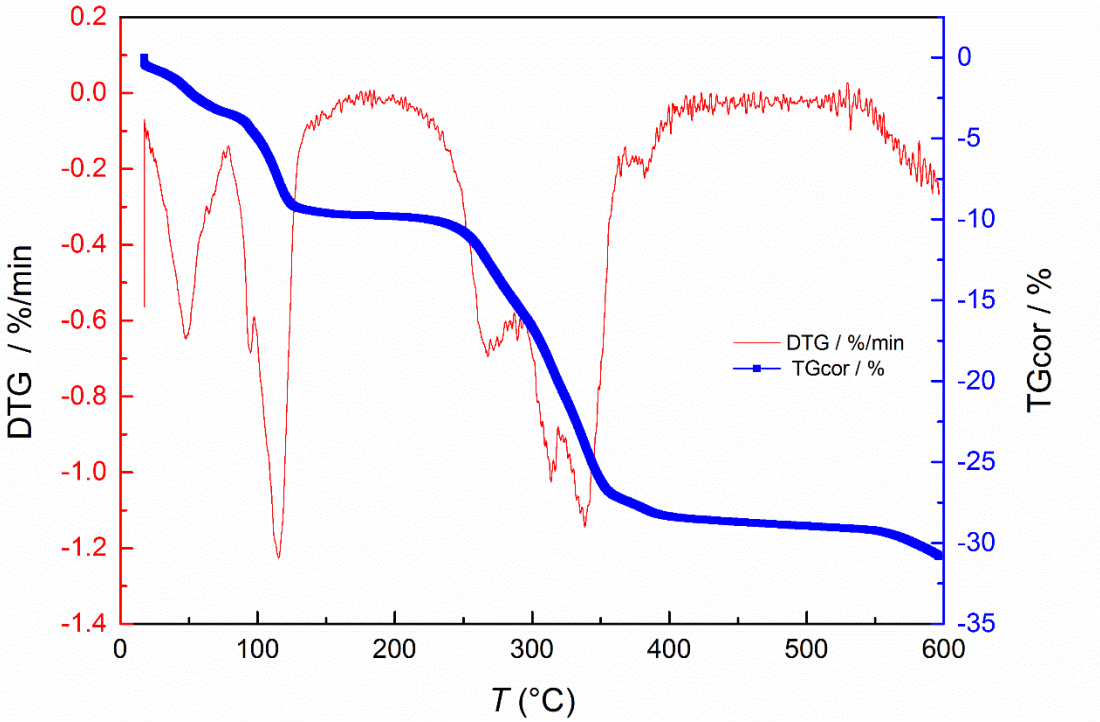

Figure S3: ATG of mixed phases $K_2[Fe(II)(C_2O_4)_2(H_2O)_2]\cdot 0.18H_2O$, 2 KCl under air

Thermogravimetric analysis were performed with a 'TG/ATD 92-16.18' SETARAM instrument between 20 and 650°C in air and using a heating rate of 1°C/min. Figure S3 shows the experimental measurement of weight loss as a function of temperature for a mixed phases $K_2[Fe(II)(C_2O_4)_2(H_2O)_2]\cdot 0.18H_2O$, 2 KCl.

A first mass loss of 8.5% from 20°C to 120°C, which represents the dehydration of the product by the departure of water molecules, which corresponds to the calculated mass loss (7.94%).

Table S1: Fractional atomic coordinates

code atom	Atom	x	y	Z
Fe1	F	0.57527(3)	0.37529(2)	0.41806(4)
Fe2	F	0.57584(3)	0.87864(2)	0.39496(3)
K1	K	0.15296(4)	1.00515(3)	0.08100(7)
K2	K	0.84231(4)	0.75030(3)	0.61398(6)
K3	K	0.34061(5)	0.75029(4)	0.61061(6)
K4	K	0.15658(5)	0.50195(3)	0.12461(7)
C1A	C	0.34303(19)	0.38627(16)	0.3362(2)
C2A	C	0.4084(2)	0.36038(17)	0.2160(2)

O1A	O	0.39588(16)	0.38205(11)	0.43982(17)
O2A	O	0.24528(18)	0.41121(17)	0.3216(2)
O3A	O	0.35460(18)	0.33417(17)	0.1228(2)
O4A	O	0.51306(17)	0.36704(13)	0.22508(19)
C1B	C	0.6017(2)	0.37194(14)	0.6988(2)
C2B	C	0.67172(19)	0.37729(14)	0.8230(2)
O1B	O	0.77576(16)	0.37112(12)	0.80943(19)
O2B	O	0.61993(16)	0.38686(13)	0.92450(18)
O3B	O	0.65585(16)	0.37712(12)	0.59543(17)
O4B	O	0.49970(17)	0.36274(14)	0.70862(19)
C1C	C	0.3417(2)	0.86090(16)	0.3233(2)
C2C	C	0.40106(19)	0.88501(15)	0.1980(2)
O1C	O	0.40172(16)	0.86431(13)	0.42287(18)
O2C	O	0.24256(18)	0.83954(18)	0.3192(2)
O3C	O	0.34115(17)	0.90514(15)	0.10561(19)
O4C	O	0.50599(15)	0.88356(12)	0.20109(17)
C1D	C	0.89776(19)	0.88001(13)	0.1809(2)
C2D	C	0.82378(19)	0.87185(14)	0.3017(2)
O1D	O	0.72217(16)	0.89200(14)	0.28778(19)
O2D	O	0.86779(17)	0.84462(15)	0.40071(19)
O3D	O	0.84677(16)	0.87663(11)	0.07576(18)
O4D	O	1.00011(16)	0.88804(13)	0.19609(18)
OW1	O	0.56748(15)	0.23819(13)	0.4300(2)
OW2	O	0.57196(15)	0.51244(13)	0.4287(2)
OW3	O	0.55566(18)	0.01555(12)	0.41170(18)
OW4	O	0.58754(18)	0.74056(13)	0.3998(2)
OW5	O	0.5716(10)	0.1224(7)	0.4001(19)
OW6	O	0.5710(8)	0.6262(6)	0.4076(15)

Table S2: Rietveld refinement parameters

compound	K_2 Fe $(C_2O_4)_2$ $(H_2O)_{2.18}$
System	Orthorhombic
Space group	P c a 2_1
Wavelength (Å)	1.54056
2θ range (°)	10.126669 - 80.005730
a (Å)	12.08378

b (Å)	15.32717
c (Å)	10.54829
R_p	20.5%
R_{wp}	14.9%
R_{Bragg}	14.7%
R_f	15.6%