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An Unusual Member of the Solid Solution Series Between Cristobalite and Potassium Ferrate(III) Obtained from Hydroflux

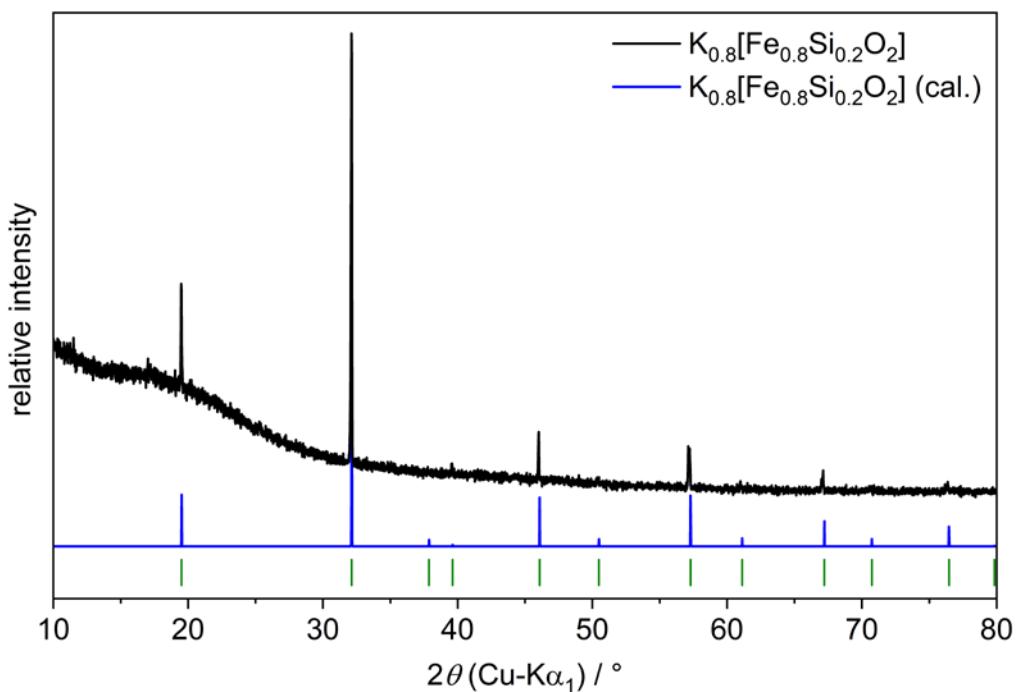


Fig S1: Powder X-ray diffractogram of hydroflux-grown $\text{K}_{0.8}[\text{Fe}_{0.8}\text{Si}_{0.2}\text{O}_2]$ and the simulated pattern based on the single-crystal structure determination.

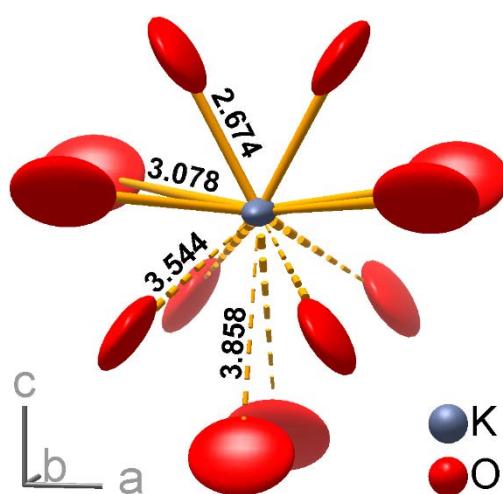


Fig S2: Coordination of the potassium cation in the tetragonal structure of $\text{K}_{0.8}[\text{Fe}_{0.8}\text{Si}_{0.2}\text{O}_2]$. Interatomic distances are given in Å. Ellipsoids enclose 50 % of the probability density of the atoms.

Synopsis of refinement results

Space group $F\bar{4}_1/d\bar{3}2/m$ (no. 227) origin choice 2

6 parameters

$R_1(F_o < 4\sigma(F_o)) = 0.109$

$wR_2(\text{all } F_o) = 0.257$

Atom	Wyckoff	Symm.	x	y	z	U_{eq}	u_{11}	u_{22}	u_{33}
K	8b	$\bar{4}3m$	3/8	3/8	3/8	700(20)	695	695	695
Fe	8a	$\bar{4}3m$	1/8	1/8	1/8	320(20)	309	309	309
O	16c	. $\bar{3}m$	0	0	0	2100(200)	2963	2963	351

Space group $F4_132$ (no. 210)

6 parameters

Inversion twin, equal twin volumes

$R_1(F_o < 4\sigma(F_o)) = 0.114$

$wR_2(\text{all } F_o) = 0.256$

Atom	Wyckoff	Symm.	x	y	z	U_{eq}	u_{11}	u_{22}	u_{33}
K	8b	23.	1/2	1/2	1/2	700(20)	695	695	695
Fe	8a	23.	1/4	1/4	1/4	310(10)	310	310	310
O	16c	.32	0	0	0	2100(200)	2964	2964	351

Space group $I4_1/amd$ (no. 141) origin choice 2

no additional degree of freedom for the atomic positions

Atom	Wyckoff	Symm.	x	y	z
K	4b	$\bar{4}m2$	0	1/4	3/8
Fe	4a	$\bar{4}m2$	0	3/4	1/8
O	8c	.2/m.	0	1/2	0

Space group $I4_122$ (no. 98)

13 parameters (damping needed → e.s.d.s are not reliable)

Twinning along threefold axis of cF cell, inversion twin, equal twin volumes

$R_1(F_o < 4\sigma(F_o)) = 0.108$

$wR_2(\text{all } F_o) = 0.249$

Atom	Wyckoff	Symm.	x	y	z	U_{eq}	U_{11}	U_{22}	U_{33}
K	4b	2.22	0	0	1/2	700(10)	969	685	450
Fe	4a	2.22	0	1/2	1/4	329(7)	447	306	234
O	8b	.2.	-0.014(7)	1/4	1/8	2100(100)	3038	2751	361

Space group $\bar{I}4_2d$ (no. 122)

11 parameters (damping needed → e.s.d.s are not reliable)

Twinning along threefold axis of cF cell, inversion twin, equal twin volumes

$R_1(F_o < 4\sigma(F_o)) = 0.103$

$wR_2(\text{all } F_o) = 0.254$

Atom	Wyckoff	Symm.	x	y	z	U_{eq}	U_{11}	U_{22}	U_{33}
K	4b	$\bar{4}$	0	0	1/2	700(10)	705	705	676
Fe	4a	$\bar{4}$	0	1/2	1/4	309(7)	309	308	308
O	8d	.2.	-0.02(1)	1/4	1/8	2000(200)	2959	2610	361

Space group $\bar{I}4m2$ (no. 119)

11 parameters

Twinning along threefold axis of cF cell, inversion twin, equal twin volumes

$R_1(F_o < 4\sigma(F_o)) = 0.108$

$wR_2(\text{all } F_o) = 0.244$

Atom	Wyckoff	Symm.	x	y	z	U_{eq}	U_{11}	U_{22}	U_{33}
K1	2b	$\bar{4}m2$	0	0	1/2	800(30)	931	732	732
K2	2d	$\bar{4}m2$	0	1/2	3/4	600(30)	729	729	229
Fe1	2a	$\bar{4}m2$	0	1/2	1/4	440(20)	698	316	316
Fe2	2c	$\bar{4}m2$	0	0	0	283(9)	296	296	258
O	8i	.m.	0	0.265(5)	0.132(4)	2000(100)	2798	2788	302

Space group $I4_1/a$ (no. 88) origin choice 1

no additional degree of freedom for the atomic positions

Atom	Wyckoff	Symm.	x	y	z
K	4b	$\bar{4}$	0	3/4	3/8
Fe	4a	$\bar{4}$	0	1/4	1/8
O	8c	$\bar{1}$	0	0	0

Space group $I4_1md$ (no. 109)

16 parameters

Twinning along threefold axis of cF cell, inversion twin, equal twin volumes $R_1(F_o < 4\sigma(F_o)) = 0.061$ $wR_2(\text{all } F_o) = 0.144$

Atom	Wyckoff	Symm.	x	y	z	U_{eq}	u_{11}	u_{22}	u_{33}
K	4a	$2mm$	0	0	0.5209(6)	610(10)	1212	346	280
Fe	4a	$2mm$	0	1/2	0.2500(4)	319(7)	377	369	210
O	8b	.m.	0	0.257(4)	0.082(4)	1790(90)	2724	2476	163

Space group $I4_1$ (no. 80)

21 parameters (damping needed → e.s.d.s are not reliable)

Twinning along threefold axis of cF cell, inversion twin, equal twin volumes $R_1(F_o < 4\sigma(F_o)) = 0.064$ $wR_2(\text{all } F_o) = 0.147$

Atom	Wyckoff	Symm	x	y	z	U_{eq}	u_{11}	u_{22}	u_{33}
K	4a	2..	0	0	0.5213(3)	605(10)	1156	356	303
Fe	4a	2..	0	1/2	0.2506(4)	314(4)	397	343	202
O	8b	1	-0.016(4)	0.273(3)	0.075(2)	1580(60)	2708	1819	208