Electronic Supplementary Material (ESI) for Chemical Communications.

Crystal Structure, magnetism and superconductivity of $[(Li_{0.8}Fe_{0.2})OH]Fe(S_{1-x}Se_x)$

Supplementary

I. Crystallographic data of $[(Li_{0.8}Fe_{0.2})OH]FeS$

	$[(Li_{0.8}Fe_{0.2})OH]FeS$
Formula	$[(Li_{0.828(5)}Fe_{0.172(5)})OH]FeS$
Formula weight /g mol^{-1}	120.3
Crystal System	Tetragonal
Space group	*P4/nmm* O1 (No. 129)
a, *c* /pm	370.38(2), 888.5(1)
V /nm^3	0.12189(1)
Z	2
d_{calc} /gcm^3	3.2758
μ (Mo-K$_\alpha$) /mm^{-1}	7.642
Crystal Size /μm^3	30 × 20 × 5
Temperature /K	293
Radiation /pm	Mo-K$_\alpha$ λ = 71.073
θ range /deg.	4.6 – 30.4
hkl range	-4 → +5; -4 → +5; -11 → +12
Tot., Uniq. Data, R_{int}	1694, 143, 0.0522
N_{Refl}, N_{Par}	143, 15
*R*1, wR_2, *S*	0.0336, 0.0444, 1.21
$\Delta\rho_{min}$, $\Delta\rho_{max}$, /eÅ^{-3}	-0.50, 0.80

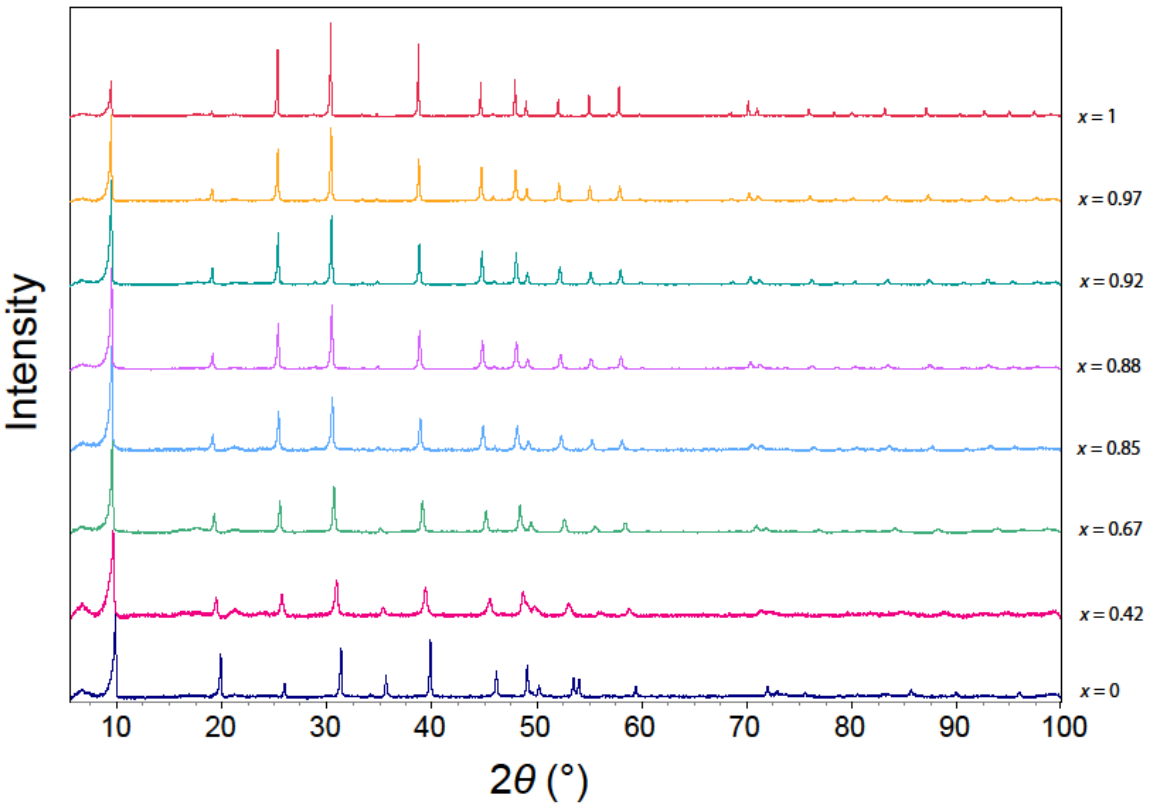
Atomic positions and equivalent displacement parameters

Atom	*Wyck.*	*x*	*y*	*z*	occ.	U_{eq}
Li	4*f*	0	0	0.061(6)	0.828(5)	0.035(5)
Fe[a]	2*a*	0	0	0	0.172(5)	0.035(5)
O	2*c*	0	1/2	0.0798(6)	1.0	0.024(1)
H	2*c*	0	1/2	0.0160(9)	1.0	0.02
Fe	2*b*	0	0	1/2	1.0	0.0115(2)
S	2*c*	1/2	0	0.3546(1)	1.0	0.0120(3)

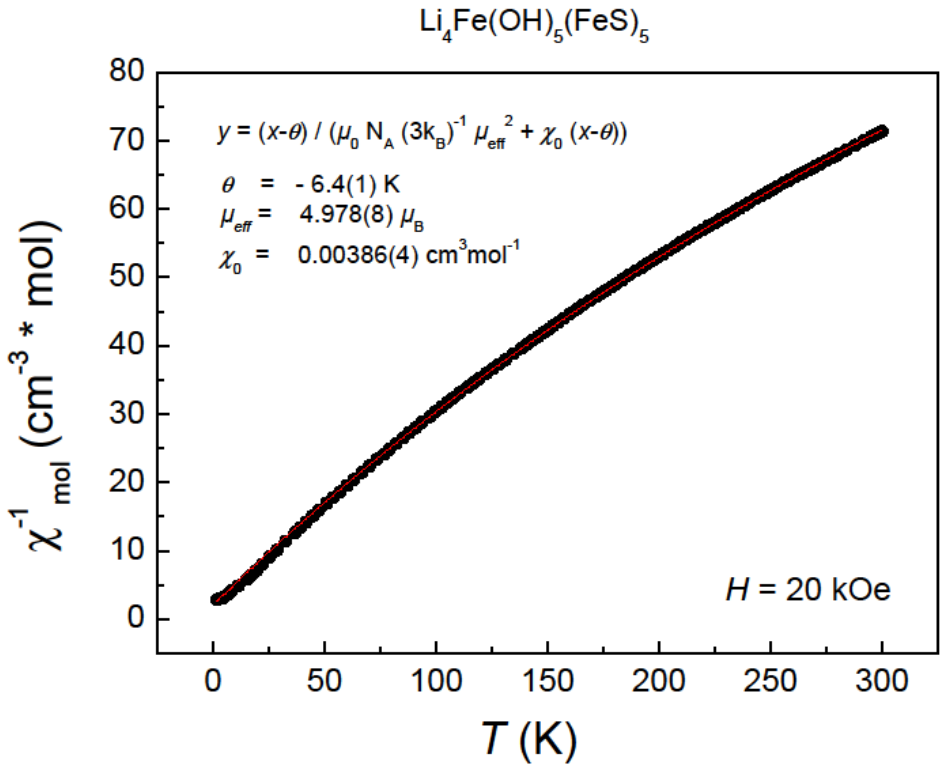
Selected bond lengths (/pm) and angles (/deg)

Li-O	185.9(4) ×2	223(3) ×2	O-Li-O	170(1)	112(1)	92.8(1) ×4
Fe[a]-O	198.3(1) ×4		O-Fe[a]-O	138.1(1) ×2	97.3(1) ×4	
Fe-S	225.79(9) ×4		S-Fe-S	110.20(1) ×2	109.11(1) ×4	

II. X-ray powder patterns of $[(Li_{0.8}Fe_{0.2})OH]Fe(S_{1-x}Se_x)]$ $(0 \leq x \leq 1)$

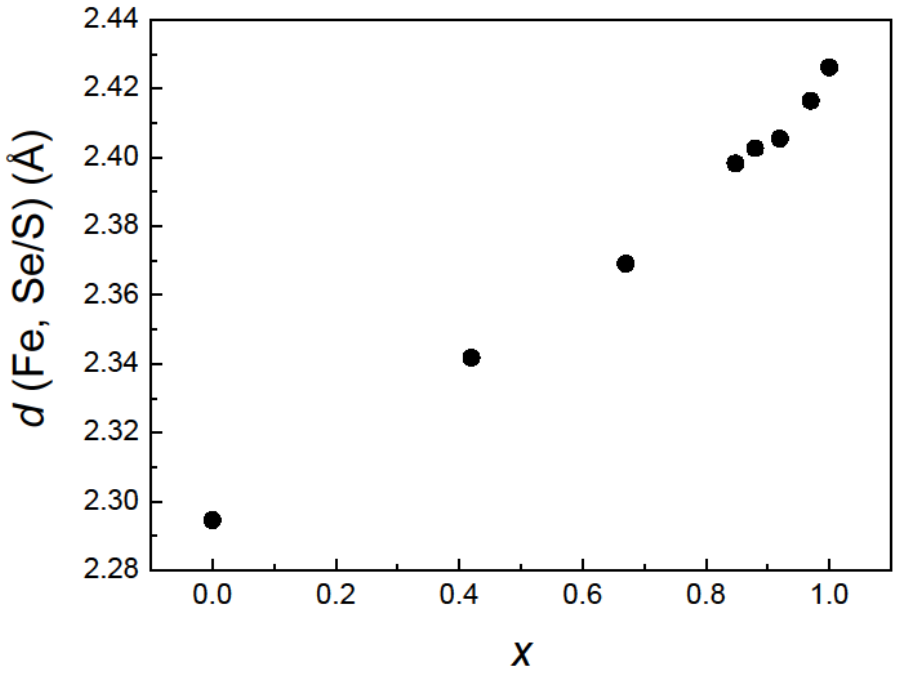


III. Curie-Weiss fit for $[(Li_{0.8}Fe_{0.2})OH]FeS$



IV. Evolution of Fe-*Ch* distances (a) and *Ch*-Fe-*Ch* bond angles (b) in $[(Li_{0.8}Fe_{0.2})OH]Fe(S_{1-x}Se_x)]$ ($0 \leq x \leq 1$)

(a)



(b)