Structure and superconductivity of LiFeAs

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Table S1. Summary of joint refinement for LiFeAs Sample 2 against Powder Neutron Diffraction (PND) and Synchrotron X-ray diffraction data at 295 K and individual comparative refinements against PND data at 295 K and 6.5 K.

Instrument	Joint HRPD + ID31	HRPD	
Temperature / K	295	295	6.5
Space group		*P*4/*nmm* (No. 129)	
a / Å	3.776360(4)	3.77543(3)	3.76982(4)
c / Å	6.35679(1)	6.35345(6)	6.30693(7)
V / Å^3	90.6536(2)	90.561(1)	89.631(2)
R_{wp}	0.0521	0.0389	0.0304
χ^2	10.07	7.035	8.115

Table S2. Refined atomic parameters for LiFeAs Sample 2 at 295 K from joint refinement against PND and Synchrotron X-ray diffraction data.

Atom	Site	*x*	*y*	*z*	U_{equiv} / Å^2 × 100	Refined fractional occupancy
Fe	2*a*	0.75	0.25	0	0.68(1)	1
Li	2*c*	0.25	0.25	0.6536(2)	1.78(5)	0.997(4)
As	2*c*	0.25	0.25	0.23715(3)	0.74(1)	0.995(1)

Table S3. Refined atomic parameters for LiFeAs Sample 2 at 295 K (upper) and 6.5 K (lower) obtained by refinement against PND data.

Atom	Site	*x*	*y*	*z*	U_{equiv} / Å^2 × 100	Refined fractional occupancy
Fe	2*a*	0.75	0.25	0	0.66(1) 0.18(1)	1 1
Li	2*c*	0.25	0.25	0.6538(1) 0.6554(2)	1.61(5) 0.77(6)	0.963(4) 0.950(4)
As	2*c*	0.25	0.25	0.23685(4) 0.23646(5)	0.62(2) 0.12(1)	0.972(1) 0.976(1)

Table S4. Refined anisotropic displacement parameters for LiFeAs Sample 2 at 295 K from joint refinement against PND and Synchrotron X-ray diffraction data.

Atom	$U_{11} = U_{22}$ /Å^2 × 100	U_{33} / /Å^2 × 100
Fe	0.609(6)	0.835(8)
Li	2.03(4)	1.29(6)
As	0.769(5)	0.673(8)

Table S5. Refined anisotropic displacement parameters for LiFeAs Sample 2 at 295 K (upper) and 6.5 K (lower) obtained by refinement against PND data.

Atom	$U_{11} = U_{22}$ /Å^2 × 100	U_{33} / /Å^2 × 100
Fe	0.580(8) 0.184(7)	0.82(1) 0.177(9)
Li	1.95(4) 0.90(4)	0.94(6) 0.50(6)
As	0.535(9) 0.089(9)	0.80(2) 0.18(1)

Table S6. Summary of refinement for LiFeAs Sample 1 against Powder Neutron Diffraction (NPD) at 295 K on POLARIS

Instrument	POLARIS
Temperature / K	295
Space group	*P*4/*nmm*
a / Å	3.7773(7)
c / Å	6.3565(1)
V / Å^3	90.696(5)
R_{wp}	0.0264
χ^2	0.7325

Table S7. Refined atomic parameters for LiFeAs Sample 1 at 295 K from POLARIS NPD data.

Atom	Site	*x*	*y*	*z*	U_{equiv} / Å^2 × 100	Refined fractional occupancy
Fe	2*a*	0.75	0.25	0	0.65(2)	1
Li	2*c*	0.25	0.25	0.6551(4)	1.77(9)	0.99(1)
As	2*c*	0.25	0.25	0.23654(9)	0.65(2)	0.977(3)

Table S8. Refined anisotropic displacement parameters for LiFeAs Sample 1 at 295 K from POLARIS NPD data.

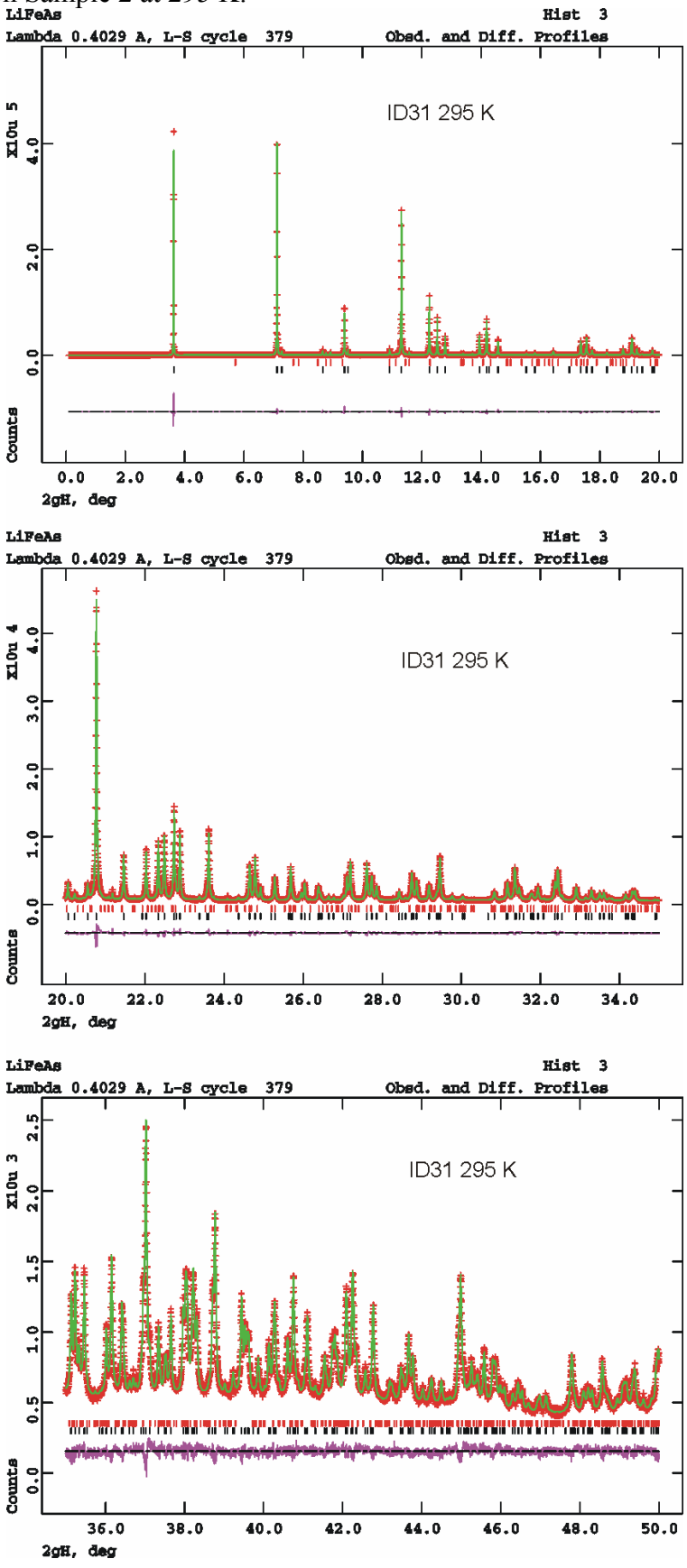
Atom	$U_{11} = U_{22}$ /Å^2 × 100	U_{33} / /Å^2 × 100
Fe	0.66(1)	0.64(2)
Li	2.13(8)	1.1(1)
As	0.63(2)	0.70(3)

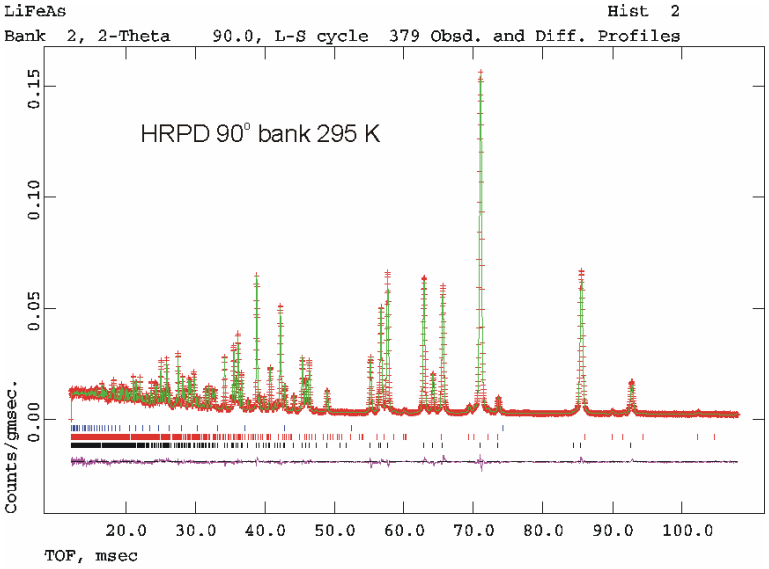
Table S9. Refined bond lengths (Å) and angles (degrees) for LiFeAs: Sample 2 at 295 K and 6.5 K obtained by joint refinement against Powder Neutron Diffraction (PND) and Synchrotron X-ray diffraction data at 295 K from individual comparative refinements against PND data at 295 K and 6.5 K; Sample 1 at 295 K from POLARIS NPD data

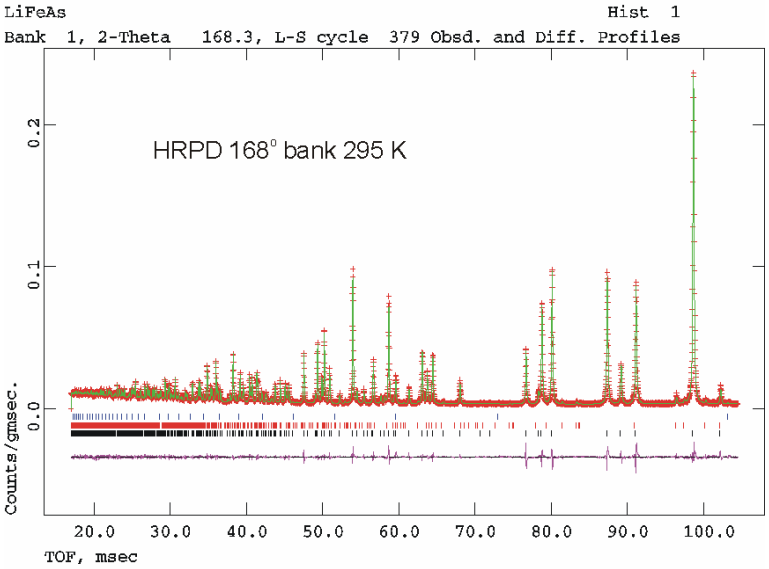
	Sample 2			Sample 1
	Joint 295 K	HRPD 295 K	HRPD 6.5 K	POLARIS 295 K
Fe−As [4][a]	2.4162(1)	2.4141(2)	2.4035(2)	2.4141(3)(
Li−As [4]	2.7592(3)	2.7585(3)	2.7515(3)	2.7584(6)
Li−As [1]	2.647(1)	2.6493(9)	2.642(1)	2.661(2)
Fe−Fe [4]	2.67029(1)	2.66963(2)	2.66566(3)	2.67098(5)
Li–Fe [4]	2.9008(8)	2.8984(7)	2.8767(8)	2.894(2)
Li−Li [4]	3.308(1)	3.309(1)	3.309(1)	3.320(3)
As−Fe−As [4]	112.910(3)	112.865(5)	112.643(6)	112.83(1)
As−Fe−As [2]	102.793(6)	102.88(1)	103.30(1)	102.95(2)
As−Li−As [4]	104.58(2)	104.58(2)	104.35(2)	104.46(5)
As−Li−As[4]	86.37(1)	86.37(1)	86.48(1)	86.43(3)

[a] The number in square brackets indicates the number of symmetry equivalent bond lengths and angles

Figure S1. Rietveld refinements for the joint PND and Synchrotron X-ray refinements on Sample 2 at 295 K.




LiFeAs
Hist 2
Bank 2, 2-Theta 90.0, L-S cycle 379 Obsd. and Diff. Profiles
HRPD 90° bank 295 K
Counts/gmsec.
0.15
0.10
0.05
0.00
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
TOF, msec


LiFeAs
Hist 1
Bank 1, 2-Theta 168.3, L-S cycle 379 Obsd. and Diff. Profiles
HRPD 168° bank 295 K
Counts/gmsec.
0.2
0.1
0.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
TOF, msec

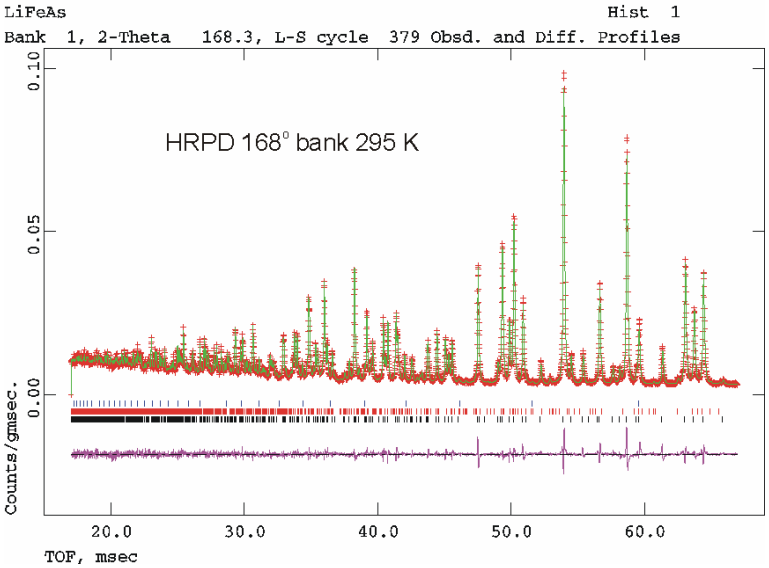

LiFeAs
Hist 1
Bank 1, 2-Theta 168.3, L-S cycle 379 Obsd. and Diff. Profiles
HRPD 168° bank 295 K
Counts/gmsec.
0.10
0.05
0.00
20.0
30.0
40.0
50.0
60.0
TOF, msec

Figure S2. Rietveld refinements for the POLARIS NPD refinement on Sample 1 at 295 K.