

Phase classification

Formula	LiSCIN
I/Ic	3.210000

Refined crystal structure

Crystallographic data

Space group
Crystal system
Cell parameters
Atom coordinates

F m -3 m (225)
cubic
a= 5.4444 Å

Element	Oxid.	x	y	z	Bi	Focc
Li		0.250	0.250	0.250	6.786028	1.000000
Li		0.500	0.500	0.500	25.561359	0.312500
S		0.000	0.000	0.000	0.789798	0.412500
N		0.000	0.000	0.000	0.789798	0.450000
Cl		0.000	0.000	0.000	0.789798	0.137500

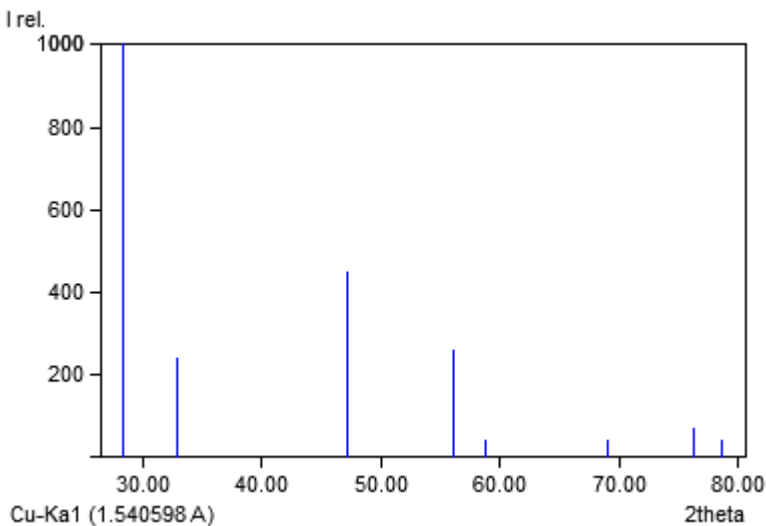
Refined diffraction data

Diffraction lines



d [Å]	Int.	h	k	l	Mult.
3.1433	1000.0	1	1	1	8
3.1433	497.3	1	1	1	8
2.7222	241.3	2	0	0	6
2.7222	120.0	2	0	0	6
1.9249	448.0	2	2	0	12
1.9249	222.7	2	2	0	12
1.6416	260.8	3	1	1	24
1.6416	129.6	3	1	1	24
1.5717	41.7	2	2	2	8
1.5717	20.7	2	2	2	8
1.3611	40.5	4	0	0	6
1.3611	20.2	4	0	0	6
1.2490	72.1	3	3	1	24
1.2490	35.7	3	3	1	24
1.2174	41.0	4	2	0	24
1.2174	19.8	4	2	0	24

Diffraction pattern graphics



Rietveld refinement using FullProf

Refinement results

Automatic refinement	No
Final weighted average Bragg R-factor	3.9
Final reduced chi²	2.5
FullProf comment	Your refinement seems to be very good! => Your refinement seems to be very good!

Refined parameters

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Parameter	Final value
Biso_Li1_ph1	6.78603

Fixed parameters

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Parameter	Final value
Zero_pat1	-0.548269
SyCos_pat1	-0.48618
SySin_pat1	0

Lambda_pat1	1.54187
P0_mabs_pat1	0
Cp_mabs_pat1	0
Tau_mabs_pat1	0.1
Bck_0_pat1	1.00087
Bck_1_pat1	0
Bck_2_pat1	0
Bck_3_pat1	0
Scale_ph1_pat1	0.0289198
Bover_ph1_pat1	1.59503
Strain1_ph1_pat1	0
Strain2_ph1_pat1	0
Strain3_ph1_pat1	0
G-Size_ph1_pat1	0
L-Size_ph1_pat1	0
Y-cos_ph1_pat1	0
EtaRght0_ph1_pat1	0
X-tan_ph1_pat1	0
U-Cagl_ph1_pat1	2.66037
V-Cagl_ph1_pat1	0
W-Cagl_ph1_pat1	0.304439
EtaPV_ph1_pat1	0.85362
Cell_A_ph1_pat1	5.44444
Cell_B_ph1_pat1	5.44444
Cell_C_ph1_pat1	5.44444
Cell_D_ph1_pat1	90
Cell_E_ph1_pat1	90
Cell_F_ph1_pat1	90
Or1_ph1_pat1	0
Or2_ph1_pat1	0
Asym1_ph1_pat1	0
Asym2_ph1_pat1	0
Asym3_ph1_pat1	0
Asym4_ph1_pat1	0
X_Li1_ph1	0.25
Y_Li1_ph1	0.25
Z_Li1_ph1	0.25
Occ_Li1_ph1	1
X_Li2_ph1	0.5
Y_Li2_ph1	0.5
Z_Li2_ph1	0.5
Biso_Li2_ph1	25.5614
Occ_Li2_ph1	0.3125
X_S3_ph1	0
Y_S3_ph1	0
Z_S3_ph1	0
Biso_S3_ph1	0.789798
Occ_S3_ph1	0.4125
X_N4_ph1	0
Y_N4_ph1	0
Z_N4_ph1	0
Biso_N4_ph1	0.789798
Occ_N4_ph1	0.45
X_CI5_ph1	0
Y_CI5_ph1	0
Z_CI5_ph1	0
Biso_CI5_ph1	0.789798
Occ_CI5_ph1	0.1375