

Phase classification

Formula	LiSCIN
I/Ic	3.530000

Refined crystal structure

Crystallographic data

Space group	F m -3 m (225)
Crystal system	cubic
Cell parameters	a= 5.4632 Å
Atom coordinates	

Element	Oxid.	x	y	z	Bi	Focc
Li		0.250	0.250	0.250	7.315914	1.000000
Li		0.500	0.500	0.500	1.000000	0.030000
S		0.000	0.000	0.000	0.813529	0.137500
N		0.000	0.000	0.000	0.813529	0.450000
Cl		0.000	0.000	0.000	0.813529	0.210000
Br		0.000	0.000	0.000	0.813529	0.210000

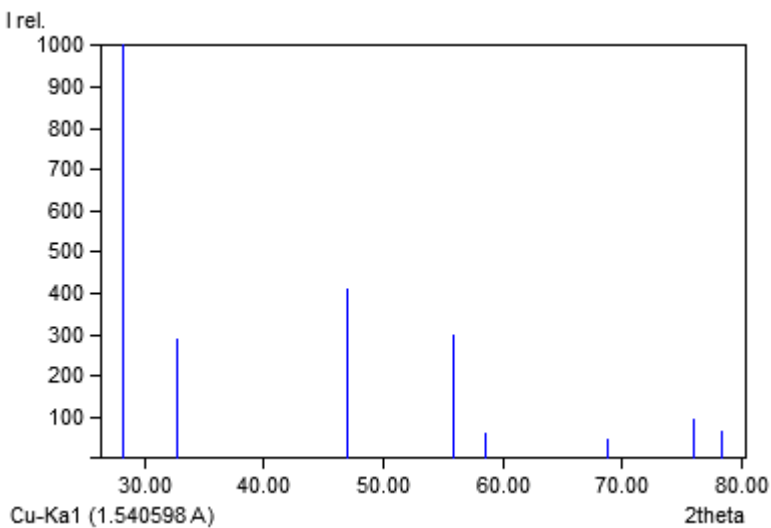
Refined diffraction data

Diffraction lines



d [Å]	Int.	h	k	l	Mult.
3.1542	1000.0	1	1	1	8
3.1542	497.4	1	1	1	8
2.7316	287.5	2	0	0	6
2.7316	143.0	2	0	0	6
1.9315	411.1	2	2	0	12
1.9315	204.4	2	2	0	12
1.6472	300.4	3	1	1	24
1.6472	149.3	3	1	1	24
1.5771	59.9	2	2	2	8
1.5771	29.8	2	2	2	8
1.3658	44.4	4	0	0	6
1.3658	22.1	4	0	0	6
1.2533	92.6	3	3	1	24
1.2533	46.0	3	3	1	24
1.2216	65.0	4	2	0	24
1.2216	32.0	4	2	0	24

Diffraction pattern graphics



Rietveld refinement using FullProf

Refinement results

Automatic refinement	No
Final weighted average Bragg R-factor	7.1
Final reduced chi²	2.7
FullProf comment	Your refinement could still be improved! => Your refinement could still be improved!

Refined parameters

Parameter	Final value
Biso_S3_ph1	0.813529
Biso_N4_ph1	0.813529
Biso_Cl5_ph1	0.813529
Biso_Br6_ph1	0.813529

Fixed parameters

--	--

--	--

Parameter	Final value
Zero_pat1	-0.196581
SyCos_pat1	-0.321912
SySin_pat1	0
Lambda_pat1	1.54187
P0_mabs_pat1	0
Cp_mabs_pat1	0
Tau_mabs_pat1	0.1
Bck_0_pat1	0.999792
Bck_1_pat1	0
Bck_2_pat1	0
Bck_3_pat1	0
Scale_ph1_pat1	0.0273073
Bover_ph1_pat1	0.886898
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	2.38317
V-Cagl_ph1_pat1	0
W-Cagl_ph1_pat1	0.447293
EtaPV_ph1_pat1	0.695858
Cell_A_ph1_pat1	5.46319
Cell_B_ph1_pat1	5.46319
Cell_C_ph1_pat1	5.46319
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
Biso_Li1_ph1	7.31591
Occ_Li1_ph1	1
X_Li2_ph1	0.5
Y_Li2_ph1	0.5
Z_Li2_ph1	0.5
Biso_Li2_ph1	1
Occ_Li2_ph1	0.03
X_S3_ph1	0
Y_S3_ph1	0
Z_S3_ph1	0
Occ_S3_ph1	0.1375
X_N4_ph1	0
Y_N4_ph1	0
Z_N4_ph1	0
Occ_N4_ph1	0.45
X_CI5_ph1	0
Y_CI5_ph1	0
Z_CI5_ph1	0
Occ_CI5_ph1	0.21
X_Br6_ph1	0
Y_Br6_ph1	0
Z_Br6_ph1	0
Occ_Br6_ph1	0.21