

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= 5.4663 Å
Atom coordinates	

Element	Oxid.	x	y	z	Bi	Focc
Li		0.250	0.250	0.250	6.548458	1.000000
Li		0.500	0.500	0.500	28.206944	0.450000
S		0.000	0.000	0.000	0.199027	0.550000
N		0.000	0.000	0.000	0.199027	0.450000
Cl		0.000	0.000	0.000	0.199027	0.000000
Br		0.000	0.000	0.000	0.199027	0.000000

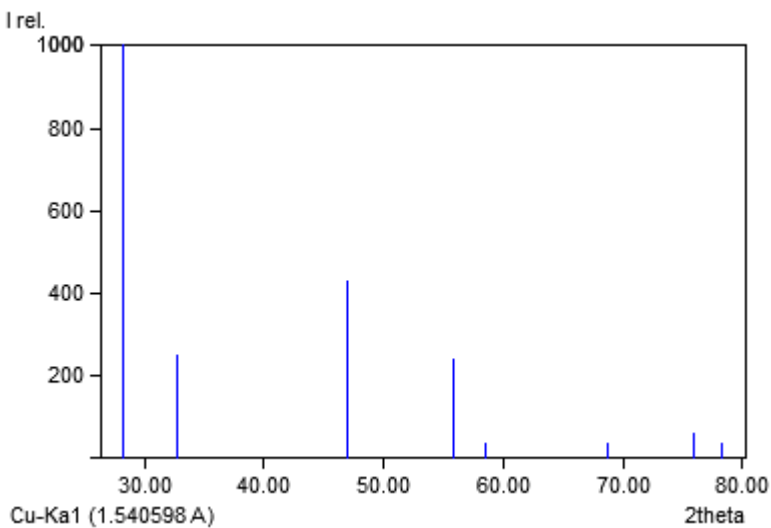
Refined diffraction data

Diffraction lines



d [Å]	Int.	h	k	l	Mult.
3.1560	1000.0	1	1	1	8
3.1560	497.3	1	1	1	8
2.7332	249.1	2	0	0	6
2.7332	123.9	2	0	0	6
1.9326	430.9	2	2	0	12
1.9326	214.2	2	2	0	12
1.6482	241.1	3	1	1	24
1.6482	119.8	3	1	1	24
1.5780	38.6	2	2	2	8
1.5780	19.2	2	2	2	8
1.3666	34.8	4	0	0	6
1.3666	17.3	4	0	0	6
1.2541	60.5	3	3	1	24
1.2541	30.1	3	3	1	24
1.2223	35.9	4	2	0	24
1.2223	17.6	4	2	0	24

Diffraction pattern graphics



Rietveld refinement using FullProf

Refinement results

Automatic refinement	No
Final weighted average Bragg R-factor	5.1
Final reduced chi ²	3.0
FullProf comment	Your refinement could still be improved! => Your refinement could still be improved!

Refined parameters

Parameter	Final value
Biso_S3_ph1	0.199027
Biso_N4_ph1	0.199027
Biso_Cl5_ph1	0.199027
Biso_Br6_ph1	0.199027

Fixed parameters

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Parameter	Final value
Zero_pat1	-0.28444
SyCos_pat1	-0.335879
SySin_pat1	0
Lambda_pat1	1.54187
P0_mabs_pat1	0
Cp_mabs_pat1	0
Tau_mabs_pat1	0.1
Bck_0_pat1	0.998435
Bck_1_pat1	0
Bck_2_pat1	0
Bck_3_pat1	0
Scale_ph1_pat1	0.0458372
Bover_ph1_pat1	3.02937
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	2.58382
V-Cagl_ph1_pat1	0
W-Cagl_ph1_pat1	0.469938
EtaPV_ph1_pat1	0.759577
Cell_A_ph1_pat1	5.46633
Cell_B_ph1_pat1	5.46633
Cell_C_ph1_pat1	5.46633
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	6.54846
Occ_Li1_ph1	1
X_Li2_ph1	0.5
Y_Li2_ph1	0.5
Z_Li2_ph1	0.5
Biso_Li2_ph1	28.2069
Occ_Li2_ph1	0.45
X_S3_ph1	0
Y_S3_ph1	0
Z_S3_ph1	0
Occ_S3_ph1	0.55
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
X_Br6_ph1	0
Y_Br6_ph1	0
Z_Br6_ph1	0
Occ_Br6_ph1	0