

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= 5.4744 Å |

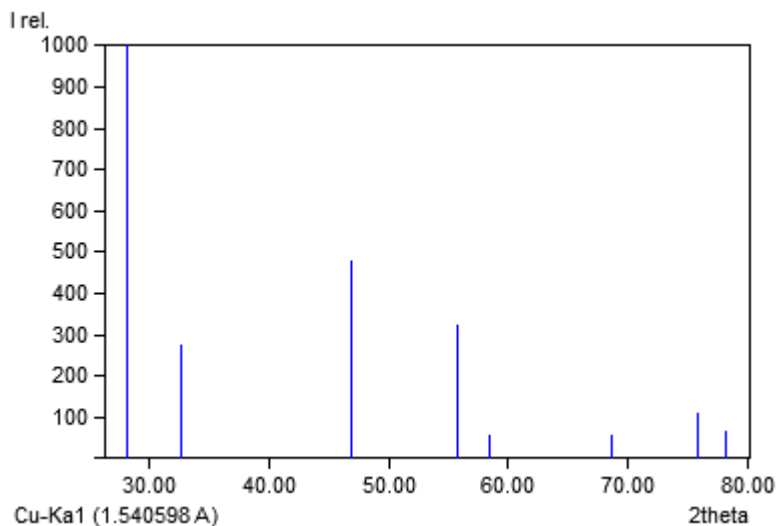
| Atom coordinates | Element | Oxid. | x | y | z | Bi | Focc |
|-------------------------|----------------|--------------|----------|----------|----------|-----------|-------------|
| | Li | | 0.250 | 0.250 | 0.250 | 5.722794 | 1.000000 |
| | Li | | 0.500 | 0.500 | 0.500 | 14.799024 | 0.174900 |
| | S | | 0.000 | 0.000 | 0.000 | 1.000000 | 0.275000 |
| | N | | 0.000 | 0.000 | 0.000 | 1.000000 | 0.450000 |
| | Cl | | 0.000 | 0.000 | 0.000 | 1.000000 | 0.137500 |
| | Br | | 0.000 | 0.000 | 0.000 | 1.000000 | 0.137500 |

Refined diffraction data

Diffraction lines

| d [Å] | Int. | h | k | l | Mult. |
|--------------|-------------|----------|----------|----------|--------------|
| 3.1607 | 1000.0 | 1 | 1 | 1 | 8 |
| 3.1607 | 497.3 | 1 | 1 | 1 | 8 |
| 2.7372 | 274.9 | 2 | 0 | 0 | 6 |
| 2.7372 | 136.7 | 2 | 0 | 0 | 6 |
| 1.9355 | 480.5 | 2 | 2 | 0 | 12 |
| 1.9355 | 238.8 | 2 | 2 | 0 | 12 |
| 1.6506 | 322.3 | 3 | 1 | 1 | 24 |
| 1.6506 | 160.3 | 3 | 1 | 1 | 24 |
| 1.5803 | 57.2 | 2 | 2 | 2 | 8 |
| 1.5803 | 28.4 | 2 | 2 | 2 | 8 |
| 1.3686 | 55.3 | 4 | 0 | 0 | 6 |
| 1.3686 | 27.5 | 4 | 0 | 0 | 6 |
| 1.2559 | 107.6 | 3 | 3 | 1 | 24 |
| 1.2559 | 53.4 | 3 | 3 | 1 | 24 |
| 1.2241 | 67.2 | 4 | 2 | 0 | 24 |
| 1.2241 | 33.1 | 4 | 2 | 0 | 24 |

Diffraction pattern graphics



Rietveld refinement using FullProf

Refinement results

| | |
|--|--|
| Automatic refinement | Yes |
| Final weighted average Bragg R-factor | 6.2 |
| Final reduced χ^2 | 1.7 |
| FullProf comment | Your refinement could still be improved! => Your refinement could still be improved! |

Refined parameters

| Parameter | Final value |
|------------------|--------------------|
| Bck_0_pat1 | 1.00037 |
| Scale_ph1_pat1 | 0.0135299 |
| Bover_ph1_pat1 | 0.172943 |
| U-Cagl_ph1_pat1 | 1.93066 |
| Cell_A_ph1_pat1 | 5.47444 |

Fixed parameters

| Parameter | Final value |
|-------------------|-------------|
| Zero_pat1 | -0.492188 |
| SyCos_pat1 | -0.586278 |
| SySin_pat1 | 0 |
| Lambda_pat1 | 1.54187 |
| P0_mabs_pat1 | 0 |
| Cp_mabs_pat1 | 0 |
| Tau_mabs_pat1 | 0.1 |
| Bck_1_pat1 | 0 |
| Bck_2_pat1 | 0 |
| Bck_3_pat1 | 0 |
| 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 |
| V-Cagl_ph1_pat1 | 0 |
| W-Cagl_ph1_pat1 | 0.516903 |
| EtaPV_ph1_pat1 | 0.726632 |
| Cell_B_ph1_pat1 | 5.47452 |
| Cell_C_ph1_pat1 | 5.47452 |
| 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 | 5.72279 |
| Occ_Li1_ph1 | 1 |
| X_Li2_ph1 | 0.5 |
| Y_Li2_ph1 | 0.5 |
| Z_Li2_ph1 | 0.5 |
| Biso_Li2_ph1 | 14.799 |
| Occ_Li2_ph1 | 0.1749 |
| X_S3_ph1 | 0 |
| Y_S3_ph1 | 0 |
| Z_S3_ph1 | 0 |
| Biso_S3_ph1 | 1 |
| Occ_S3_ph1 | 0.275 |
| X_N4_ph1 | 0 |
| Y_N4_ph1 | 0 |
| Z_N4_ph1 | 0 |
| Biso_N4_ph1 | 1 |
| Occ_N4_ph1 | 0.45 |
| X_CI5_ph1 | 0 |
| Y_CI5_ph1 | 0 |
| Z_CI5_ph1 | 0 |
| Biso_CI5_ph1 | 1 |
| Occ_CI5_ph1 | 0.1375 |
| X_Br6_ph1 | 0 |
| Y_Br6_ph1 | 0 |
| Z_Br6_ph1 | 0 |
| Biso_Br6_ph1 | 1 |
| Occ_Br6_ph1 | 0.1375 |