

Exploring the structure-composition phase space of lithium borocarbide, Li_xBC for $x \leq 1$

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Abstract

The following Supplementary Information contains detailed lists of the calculated reflections of the Li_xBC structures reported in the X-ray diffraction peaks, Figure.7 and corresponding to those listed in Table.1. Miller indices ($h k l$), interplanar spacing (d_{hkl} in Å), diffraction angles ($2\theta^\circ$) and the relative intensity of the diffraction peaks (I/I_{max}) are reported.

1 X-ray diffraction peaks

The X-ray calculations were performed by using *Reflex Power Diffraction* module implemented in Materials Studio6.0. In particular, the following settings were used:

Cu radiation with $\lambda_1 = 1.540562$ Å

anomalous dispersion included

monochromator single $d_{hkl} = 1.00$ Å and angle = 50.370129 degrees

Profile: Pseudo-Voigt peak shape function

Temperature factor atomic and anisotropic for all three species, Li, B, C.

1.1 $x = 1$, LiBC

The calculated reflections of LiBC hexagonal structure, symmetry space group $P6_3/mmc$ (No 194) and lattice parameters a , c equal to 2.730 Å, 6.957 Å.

h	k	l	d_{hkl}	2θ	I/I_{max}
0	0	2	3.478	25.588	100
1	-1	0	2.364	38.026	2.38
0	1	0	2.364	38.026	2.38
1	0	0	2.364	38.026	2.38

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1	-1	1	2.239	40.252	0.56
1	-1	-1	2.239	40.252	0.56
0	1	1	2.239	40.252	0.56
0	1	-1	2.239	40.252	0.56
1	0	1	2.239	40.252	0.56
1	0	-1	2.239	40.252	0.56
1	-1	-2	1.955	46.397	15.72
1	-1	2	1.955	46.397	15.72
0	1	2	1.955	46.397	15.72
0	1	-2	1.955	46.397	15.72
1	0	2	1.955	46.397	15.72
1	0	-2	1.955	46.397	15.72
0	0	4	1.739	52.576	27.25
1	-1	-3	1.656	55.454	0.13
1	-1	3	1.656	55.454	0.13
0	1	3	1.656	55.454	0.13
0	1	-3	1.656	55.454	0.13
1	0	3	1.656	55.454	0.13
1	0	-3	1.656	55.454	0.13
1	-1	4	1.401	66.707	0.21
1	-1	-4	1.401	66.707	0.21
0	1	-4	1.401	66.707	0.21
0	1	4	1.401	66.707	0.21
1	0	4	1.401	66.707	0.21
1	0	-4	1.401	66.707	0.21
1	-2	0	1.365	68.704	12.53
2	-1	0	1.365	68.704	12.53
1	1	0	1.365	68.704	12.53
1	-2	-2	1.271	74.627	2.62
1	-2	2	1.271	74.627	2.62
2	-1	2	1.271	74.627	2.62
2	-1	-2	1.271	74.627	2.62
1	1	2	1.271	74.627	2.62
1	1	-2	1.271	74.627	2.62
1	-1	-5	1.199	79.935	0.02
1	-1	5	1.199	79.935	0.02
0	1	-5	1.199	79.935	0.02
0	1	5	1.199	79.935	0.02
1	0	5	1.199	79.935	0.02
1	0	-5	1.199	79.935	0.02
2	-2	0	1.182	81.321	0.16
0	2	0	1.182	81.321	0.16
2	0	0	1.182	81.321	0.16
2	-2	-1	1.165	82.739	0.02
2	-2	1	1.165	82.739	0.02
0	2	-1	1.165	82.739	0.02
0	2	1	1.165	82.739	0.02
2	0	-1	1.165	82.739	0.02
2	0	1	1.165	82.739	0.02

0	0	6	1.159	83.261	1.93
2	-2	-2	1.119	86.972	2.64
2	-2	2	1.119	86.972	2.64
0	2	2	1.119	86.972	2.64
0	2	-2	1.119	86.972	2.64
2	0	2	1.119	86.972	2.64
2	0	-2	1.119	86.972	2.64

1.2 $x = 0.875$

The calculated reflections of trigonal $\text{Li}_{0.875}\text{BC}$, symmetry space group $P\bar{3}_1$ (No 164) and lattice parameters a , c equal to 5.437 Å, 6.987 Å.

h	k	l	d_{hkl}	2θ	I/I_{max}
0	0	1	6.987	12.659	1.05
1	0	0	4.708	18.832	0.86
1	0	1	3.904	22.756	0.74
1	0	-1	3.904	22.756	0.56
0	0	2	3.493	25.476	100.00
1	0	2	2.806	31.872	0.09
1	0	-2	2.806	31.872	0.64
1	1	0	2.718	32.923	0.23
1	1	1	2.533	35.403	0.37
2	0	0	2.354	38.199	7.87
0	0	3	2.329	38.627	0.05
2	0	1	2.231	40.398	2.49
2	0	-1	2.231	40.398	0.70
1	1	2	2.145	42.083	0.25
1	0	3	2.088	43.307	0.10
1	0	-3	2.088	43.307	0.12
2	0	2	1.952	46.478	38.38
2	0	-2	1.952	46.478	36.46
2	1	0	1.780	51.298	0.19
1	1	3	1.769	51.638	0.16
0	0	4	1.747	52.333	22.57
2	1	-1	1.724	53.061	0.17
2	1	1	1.724	53.061	0.11
2	0	3	1.656	55.452	0.11
2	0	-3	1.656	55.452	0.68
1	0	4	1.638	56.115	0.16
2	1	2	1.586	58.127	0.02
2	1	-2	1.586	58.127	0.16
3	0	0	1.569	58.788	0.05
3	0	1	1.531	60.403	0.02
3	0	-1	1.531	60.403	0.08
1	1	4	1.469	63.226	0.08
3	0	2	1.432	65.104	0.04
3	0	-2	1.432	65.104	0.04
2	1	3	1.414	66.015	0.08
2	1	-3	1.414	66.015	0.05
2	0	4	1.403	66.613	0.83
2	0	-4	1.403	66.613	0.55
0	0	5	1.397	66.903	0.01
2	2	0	1.359	69.046	27.90
1	0	5	1.340	70.199	0.03
1	0	-5	1.340	70.199	0.03
2	2	1	1.334	70.530	0.06

3	1	0	1.306	72.297	0.05
3	0	3	1.301	72.576	0.05
3	0	-3	1.301	72.576	0.01
3	1	-1	1.284	73.753	0.06
3	1	1	1.284	73.753	0.05
2	2	2	1.267	74.907	12.40
2	1	4	1.247	76.329	0.17
2	1	-4	1.247	76.329	0.01
1	1	5	1.243	76.603	0.04
3	1	2	1.223	78.062	0.09
3	1	-2	1.223	78.062	0.02
2	0	5	1.202	79.737	0.12
4	0	0	1.177	81.750	0.40
2	2	3	1.174	82.019	0.04
3	0	4	1.167	82.572	0.02
3	0	-4	1.167	82.572	0.02
0	0	6	1.164	82.825	1.58
4	0	-1	1.161	83.155	0.10
3	1	3	1.139	85.106	0.04
3	1	-3	1.139	85.106	0.03
1	0	-6	1.130	85.908	0.08
4	0	2	1.115	87.349	5.32
4	0	-2	1.115	87.349	5.59
2	1	5	1.099	88.994	0.02
2	1	-5	1.099	88.994	0.04

1.3 $x = 0.750$

The calculated reflections of orthorhombic $\text{Li}_{0.750}\text{BC}$, symmetry space group $Cmcm$ (No 63) and lattice parameters a , b , c equal to 5.424 Å, 9.393 Å, 6.981 Å.

h	k	l	d_{hkl}	2θ	I/I_{max}
1	1	0	4.697	18.876	2.15
0	2	0	4.697	18.878	1.08
1	1	1	3.897	22.800	0.01
0	2	1	3.897	22.801	0.01
0	0	2	3.490	25.500	100.00
1	1	2	2.802	31.918	1.48
0	2	2	2.801	31.919	0.74
2	0	0	2.712	33.001	0.29
1	3	0	2.712	33.004	0.57
2	2	0	2.349	38.291	6.27
0	4	0	2.348	38.294	3.15
2	2	1	2.226	40.490	1.81
0	4	1	2.226	40.493	0.88
2	0	2	2.142	42.162	0.31
1	3	2	2.141	42.164	0.62
2	2	2	1.949	46.571	41.40
0	4	2	1.948	46.573	20.75
3	1	0	1.775	51.425	0.23
2	4	0	1.775	51.428	0.23
1	5	0	1.775	51.430	0.23
0	0	4	1.745	52.385	19.62
2	2	3	1.653	55.549	0.42
0	4	3	1.653	55.552	0.20
1	1	4	1.636	56.181	0.25
0	2	4	1.636	56.182	0.12
3	1	2	1.582	58.255	0.19
2	4	2	1.582	58.258	0.19
1	5	2	1.582	58.260	0.19
3	3	0	1.566	58.938	0.12
0	6	0	1.566	58.943	0.06
3	3	1	1.528	60.554	0.02
0	6	1	1.528	60.559	0.01
2	0	4	1.468	63.319	0.10
1	3	4	1.468	63.321	0.20
3	3	2	1.429	65.257	0.18
0	6	2	1.428	65.262	0.09
2	2	4	1.401	66.720	1.26
0	4	4	1.401	66.722	0.64
4	0	0	1.356	69.228	7.98
2	6	0	1.356	69.234	15.96
4	2	0	1.303	72.491	0.06
3	5	0	1.303	72.494	0.06
1	7	0	1.303	72.499	0.06

3	3	3	1.299	72.735	0.01
0	6	3	1.299	72.740	0.01
4	0	2	1.264	75.094	4.30
2	6	2	1.264	75.100	8.59
3	1	4	1.245	76.473	0.15
2	4	4	1.245	76.476	0.15
1	5	4	1.245	76.477	0.15
4	2	2	1.221	78.261	0.12
3	5	2	1.221	78.265	0.12
1	7	2	1.220	78.269	0.12
2	2	5	1.200	79.860	0.05
0	4	5	1.200	79.862	0.02
4	4	0	1.174	81.982	0.37
0	8	0	1.174	81.990	0.18
3	3	4	1.165	82.743	0.09
0	6	4	1.165	82.748	0.05
0	0	6	1.163	82.918	1.67
4	4	1	1.158	83.388	0.04
0	8	1	1.158	83.397	0.02
1	1	6	1.129	86.014	0.09
0	2	6	1.129	86.014	0.05
4	4	2	1.113	87.588	6.01
0	8	2	1.113	87.596	2.99

1.4 $x = 0.625$

The calculated reflections of the monoclinic $\text{Li}_{0.625}\text{BC}$ structure, symmetry space group $C2/m$ (No 12) and lattice parameters a, b, c, β equal to 9.349 Å, 5.418 Å, 6.972 Å, 90.848°.

h	k	l	d_{hkl}	2θ	I/I_{max}
0	0	1	6.972	12.687	0.83
1	1	-1	4.688	18.915	0.50
2	0	-2	4.674	18.972	2.28
2	0	-1	3.909	22.729	0.26
1	1	0	3.904	22.762	0.41
1	1	-2	3.877	22.921	0.32
2	0	-3	3.856	23.047	0.12
0	0	2	3.486	25.533	100.00
2	0	0	2.814	31.770	0.39
1	1	1	2.807	31.852	0.05
1	1	-3	2.787	32.086	0.36
2	0	-4	2.775	32.236	1.23
0	2	0	2.709	33.037	0.61
3	1	-3	2.701	33.138	0.13
3	1	-2	2.530	35.456	0.11
0	2	1	2.525	35.521	0.11
3	1	-4	2.508	35.775	0.11
2	2	-2	2.344	38.372	7.09
4	0	-4	2.337	38.490	3.92
0	0	3	2.324	38.716	0.05
2	2	-1	2.227	40.478	0.46
4	0	-3	2.226	40.496	0.59
2	2	-3	2.217	40.668	1.55
4	0	-5	2.206	40.875	0.13
3	1	-1	2.149	42.019	0.07
0	2	2	2.139	42.213	0.65
3	1	-5	2.122	42.570	0.07
2	0	1	2.093	43.183	0.02
1	1	2	2.088	43.292	0.06
1	1	-4	2.076	43.561	0.07
2	0	-5	2.069	43.722	0.04
4	0	-2	1.955	46.420	9.33
2	2	0	1.952	46.489	16.63
2	2	-4	1.938	46.829	17.21
4	0	-6	1.928	47.099	8.37
1	3	-1	1.773	51.491	0.05
3	1	0	1.773	51.504	0.05
4	2	-4	1.770	51.609	0.47
5	1	-5	1.767	51.679	0.06
0	2	3	1.764	51.788	0.05
3	1	-6	1.751	52.211	0.04
0	0	4	1.743	52.458	16.94

4	2	-3	1.720	53.218	0.06
1	3	0	1.720	53.219	0.03
5	1	-4	1.719	53.248	0.05
1	3	-2	1.717	53.296	0.04
4	2	-5	1.711	53.526	0.02
5	1	-6	1.707	53.633	0.03
4	0	-1	1.660	55.289	0.02
2	2	1	1.656	55.425	0.42
2	2	-5	1.644	55.874	0.08
2	0	2	1.641	55.990	0.31
1	1	3	1.638	56.117	0.10
4	0	-7	1.636	56.186	0.15
2	0	-6	1.625	56.584	0.03
5	1	-3	1.585	58.143	0.04
4	2	-2	1.585	58.151	0.34
1	3	1	1.582	58.261	0.01
1	3	-3	1.579	58.406	0.05
4	2	-6	1.571	58.731	0.11
5	1	-7	1.567	58.868	0.01
3	3	-3	1.563	59.070	0.03
6	0	-6	1.558	59.262	0.13
3	3	-2	1.527	60.581	0.01
3	3	-4	1.522	60.794	0.04
6	0	-7	1.516	61.089	0.04
3	1	1	1.473	63.053	0.02
0	2	4	1.466	63.406	0.21
3	1	-7	1.456	63.882	0.02
6	0	-4	1.430	65.171	0.10
3	3	-1	1.430	65.193	0.02
3	3	-5	1.422	65.601	0.02
5	1	-2	1.416	65.895	0.02
4	2	-1	1.416	65.936	0.01
6	0	-8	1.415	65.985	0.09
1	3	2	1.412	66.140	0.02
1	3	-4	1.408	66.342	0.02
4	0	0	1.407	66.379	0.52
2	2	2	1.404	66.568	0.68
4	2	-7	1.400	66.746	0.03
5	1	-8	1.397	66.906	0.02
0	0	5	1.394	67.070	0.01
2	2	-6	1.394	67.106	0.89
4	0	-8	1.387	67.454	0.37
0	4	0	1.355	69.313	6.94
6	2	-6	1.351	69.548	13.69
2	0	3	1.342	70.082	0.01
1	1	4	1.339	70.227	0.02
1	1	-6	1.334	70.555	0.02
2	0	-7	1.331	70.738	0.01
0	4	1	1.330	70.801	0.02
6	2	-5	1.329	70.838	0.06

6	0	-3	1.303	72.478	0.03
3	3	0	1.301	72.596	0.02
2	4	-2	1.301	72.606	0.12
5	3	-5	1.299	72.740	0.02
7	1	-7	1.297	72.894	0.01
3	3	-6	1.292	73.178	0.01
2	4	-1	1.280	74.002	0.02
5	3	-4	1.279	74.039	0.01
7	1	-6	1.278	74.127	0.02
2	4	-3	1.278	74.130	0.01
5	3	-6	1.275	74.360	0.02
7	1	-8	1.271	74.577	0.01
6	2	-4	1.265	75.035	4.51
0	4	2	1.263	75.191	4.49
6	2	-8	1.254	75.801	4.35
4	2	0	1.249	76.172	0.05
3	1	2	1.246	76.406	0.01
1	3	3	1.245	76.459	0.05
0	2	5	1.240	76.825	0.01
4	2	-8	1.235	77.188	0.29
3	1	-8	1.233	77.358	0.01
5	1	-9	1.232	77.372	0.05
5	3	-3	1.221	78.204	0.02
7	1	-5	1.221	78.227	0.01
2	4	0	1.221	78.262	0.08
2	4	-4	1.217	78.514	0.19
7	1	-9	1.210	79.110	0.03
4	0	1	1.205	79.449	0.03
2	2	-7	1.194	80.317	0.08
4	4	-4	1.172	82.185	0.51
0	4	3	1.170	82.327	0.01
6	0	-2	1.170	82.334	0.05
8	0	-8	1.168	82.481	0.20
3	3	1	1.168	82.542	0.01
0	0	6	1.162	83.049	1.70
6	2	-9	1.161	83.110	0.04
3	3	-7	1.159	83.289	0.01
4	4	-3	1.157	83.470	0.04
6	0	-10	1.153	83.828	0.05
8	0	-9	1.150	84.138	0.04
7	1	-4	1.139	85.082	0.01
5	3	-2	1.139	85.121	0.01
2	4	1	1.137	85.271	0.01
2	4	-5	1.133	85.643	0.01
5	3	-8	1.129	86.051	0.01
1	1	-7	1.126	86.343	0.04
7	1	-10	1.125	86.384	0.01
2	0	-8	1.124	86.547	0.13
4	4	-2	1.113	87.557	2.65
8	0	-6	1.113	87.603	1.14

4	4	-6	1.108	88.051	2.46
8	0	-10	1.103	88.593	1.17
5	1	0	1.102	88.673	0.01
4	2	1	1.101	88.773	0.01
1	3	4	1.098	89.145	0.01
1	3	-6	1.095	89.454	0.01

1.5 $x = 0.500$

The calculated reflections of the orthorhombic $\text{Li}_{0.5}\text{BC}$ structure, symmetry space group $Pnmm$ (No 58) and lattice parameters a , b , c equal to 4.582 Å, 6.969 Å, 2.711 Å.

h	k	l	d_{hkl}	2θ	I/I_{max}
1	1	0	3.829	23.212	3.22
2	0	0	3.484	25.544	100.00
2	1	0	2.774	32.248	6.13
1	0	1	2.527	35.499	1.45
0	1	1	2.333	38.552	6.48
0	2	0	2.291	39.291	4.11
1	1	1	2.213	40.746	8.21
1	2	0	2.177	41.452	2.11
3	1	0	2.072	43.650	2.47
2	1	1	1.939	46.819	24.91
2	2	0	1.914	47.453	13.85
3	0	1	1.764	51.783	0.97
4	0	0	1.742	52.481	13.27
1	2	1	1.697	53.980	2.42
3	1	1	1.646	55.797	2.19
3	2	0	1.631	56.357	0.73
4	1	0	1.628	56.460	3.37
2	2	1	1.564	59.019	1.07
1	3	0	1.492	62.165	0.39
3	2	1	1.398	66.885	0.02
4	1	1	1.396	66.979	1.17
4	2	0	1.387	67.482	0.68
0	0	2	1.356	69.254	7.51
5	1	0	1.333	70.574	0.01
0	3	1	1.331	70.736	6.33
1	3	1	1.307	72.212	12.24
1	1	2	1.278	74.140	0.32
3	3	0	1.276	74.250	0.26
2	0	2	1.263	75.138	5.80
2	3	1	1.243	76.574	3.19
5	0	1	1.240	76.840	0.15
4	2	1	1.235	77.201	1.92
2	1	2	1.218	78.465	0.73
5	1	1	1.197	80.145	0.46
5	2	0	1.191	80.616	0.24
0	2	2	1.167	82.636	0.63
6	0	0	1.161	83.090	1.03
3	3	1	1.155	83.684	7.45
1	2	2	1.151	84.046	0.82
0	4	0	1.146	84.505	0.01
3	1	2	1.134	85.538	0.81
1	4	0	1.130	85.910	1.46

6	1	0	1.126	86.342	2.09
2	2	2	1.106	88.256	4.34
5	2	1	1.090	89.908	2.42

1.6 $x = 0.375$

The calculated reflections of the monoclinic $\text{Li}_{0.375}\text{BC}$ structure, symmetry space group $C2/m$ (No 12) and lattice parameters a , b , c , β equal to 9.545 Å, 5.514 Å, 5.202 Å, 97.846°.

h	k	l	d_{hkl}	2θ	I/I_{max}
0	0	1	5.154	17.192	100.00
1	1	0	4.763	18.613	0.79
2	0	0	4.728	18.754	0.05
2	0	1	3.748	23.719	0.01
1	1	1	3.624	24.541	0.52
1	1	-1	3.384	26.315	0.44
2	0	-1	3.269	27.260	7.01
0	2	0	2.757	32.449	0.11
3	1	0	2.736	32.699	0.24
0	0	2	2.577	34.786	12.99
3	1	1	2.545	35.236	0.17
0	2	1	2.431	36.947	0.01
2	0	2	2.405	37.365	2.47
2	2	0	2.382	37.741	20.64
4	0	0	2.364	38.034	5.29
1	1	2	2.335	38.530	0.29
3	1	-1	2.306	39.023	0.15
4	0	1	2.269	39.686	0.01
2	2	1	2.221	40.589	13.45
1	1	-2	2.204	40.915	0.11
2	0	-2	2.143	42.132	0.68
2	2	-1	2.107	42.878	7.97
4	0	-1	2.045	44.244	12.59
3	1	2	1.998	45.357	0.07
0	2	2	1.883	48.306	0.36
4	0	2	1.874	48.539	6.12
2	2	2	1.812	50.308	9.08
1	3	0	1.804	50.547	0.13
4	2	0	1.795	50.838	0.43
5	1	0	1.789	51.012	0.09
3	1	-2	1.774	51.471	0.05
5	1	1	1.762	51.850	0.05
4	2	1	1.752	52.162	0.06
0	0	3	1.718	53.281	15.60
1	3	1	1.717	53.315	0.08
2	2	-2	1.692	54.163	3.39
2	0	3	1.690	54.219	3.14
1	3	-1	1.689	54.260	0.02
1	1	3	1.653	55.561	0.01
4	2	-1	1.643	55.928	0.28
4	0	-2	1.634	56.238	0.34
5	1	-1	1.626	56.548	0.07

3	3	0	1.588	58.045	0.04
1	1	-3	1.582	58.288	0.05
6	0	0	1.576	58.521	0.01
6	0	1	1.568	58.842	0.15
5	1	2	1.567	58.874	0.03
4	2	2	1.550	59.603	2.34
2	0	-3	1.548	59.674	3.14
3	3	1	1.548	59.700	0.09
3	1	3	1.539	60.050	0.08
1	3	2	1.496	61.964	0.03
4	0	3	1.490	62.270	0.06
3	3	-1	1.489	62.313	0.02
1	3	-2	1.460	63.677	0.03
0	2	3	1.458	63.784	0.48
6	0	-1	1.453	64.048	0.01
2	2	3	1.441	64.624	3.15
4	2	-2	1.406	66.446	0.11
3	3	2	1.395	67.019	0.01
5	1	-2	1.388	67.421	0.03
3	1	-3	1.383	67.693	0.06
0	4	0	1.378	67.946	10.40
6	2	0	1.368	68.527	13.42
6	2	1	1.363	68.822	1.26
2	2	-3	1.350	69.587	0.27
0	4	1	1.332	70.682	1.63
5	1	3	1.328	70.927	0.05
2	4	0	1.323	71.192	0.01
5	3	0	1.318	71.524	0.01
7	1	1	1.314	71.792	0.03
3	3	-2	1.312	71.901	0.04
7	1	0	1.312	71.904	0.03
4	2	3	1.311	71.990	2.18
4	0	-3	1.307	72.196	0.80
5	3	1	1.307	72.214	0.03
0	0	4	1.288	73.433	0.15
6	2	-1	1.285	73.651	6.98
6	2	2	1.272	74.507	7.03
2	4	-1	1.270	74.667	0.49
6	0	-2	1.270	74.710	0.24
1	1	4	1.266	74.964	0.03
1	3	3	1.261	75.329	0.01
6	0	3	1.249	76.128	0.08
5	3	-1	1.249	76.174	0.04
7	1	2	1.237	76.999	0.03
7	1	-1	1.233	77.326	0.01
1	3	-3	1.228	77.679	0.05
3	1	4	1.223	78.086	0.02
1	1	-4	1.223	78.098	0.02
5	3	2	1.221	78.190	0.03
0	4	2	1.215	78.652	1.40

3	3	3	1.208	79.223	0.02
4	0	4	1.202	79.680	0.04
2	0	-4	1.202	79.696	1.32
2	4	2	1.196	80.196	0.32
4	4	0	1.191	80.612	0.88
8	0	0	1.182	81.340	0.25
4	2	-3	1.181	81.395	2.50
4	4	1	1.178	81.660	0.08
2	2	4	1.167	82.582	0.60
0	2	4	1.167	82.587	0.13
5	1	-3	1.166	82.685	0.01
2	4	-2	1.159	83.276	0.19
6	2	-2	1.153	83.825	0.38
4	4	-1	1.143	84.730	2.94
6	2	3	1.138	85.203	5.01
8	0	2	1.135	85.514	2.03
5	3	-2	1.131	85.888	0.03
3	3	-3	1.128	86.140	0.03
8	0	-1	1.119	86.979	1.19
7	1	3	1.117	87.242	0.01
5	1	4	1.116	87.291	0.01
3	1	-4	1.116	87.313	0.01
7	1	-2	1.111	87.775	0.01
4	4	2	1.110	87.845	1.75
4	2	4	1.102	88.681	0.03
2	2	-4	1.102	88.697	0.55
5	3	3	1.097	89.168	0.01
6	0	-3	1.090	89.976	0.01

1.7 $x = 0.250$

The calculated reflections of the monoclinic $\text{Li}_{0.250}\text{BC}$ structure, symmetry space group $P2/m$ (No 10) and lattice parameters a , b , c , β equal to 4.752 Å, 2.749 Å, 5.202 Å, 101.580°.

h	k	l	d_{hkl}	2θ	I/I_{max}
1	0	0	5.096	17.389	100.00
0	0	1	4.655	19.048	0.19
1	0	-1	3.843	23.128	0.17
1	0	1	3.138	28.422	7.69
0	1	0	2.749	32.544	0.44
2	0	0	2.548	35.194	16.26
2	0	-1	2.452	36.620	1.58
1	1	0	2.419	37.129	0.16
0	1	1	2.367	37.980	23.02
0	0	2	2.328	38.649	6.89
1	0	-2	2.299	39.154	0.02
1	1	-1	2.236	40.305	11.31
1	1	1	2.068	43.743	5.02
2	0	1	2.067	43.757	1.57
1	0	2	1.973	45.963	7.49
2	0	-2	1.921	47.272	6.30
2	1	0	1.869	48.686	0.69
2	1	-1	1.830	49.790	6.25
0	1	2	1.776	51.393	1.20
1	1	-2	1.764	51.798	0.29
3	0	-1	1.710	53.545	4.13
3	0	0	1.699	53.935	13.15
2	1	1	1.652	55.579	3.22
1	1	2	1.603	57.445	0.15
1	0	-3	1.575	58.549	0.22
2	1	-2	1.575	58.567	2.36
2	0	2	1.569	58.811	0.33
0	0	3	1.552	59.521	0.03
3	0	-2	1.526	60.647	0.41
3	0	1	1.502	61.725	2.39
2	0	-3	1.462	63.582	0.04
3	1	-1	1.452	64.076	3.03
3	1	0	1.445	64.425	0.42
1	0	3	1.408	66.342	0.01
0	2	0	1.375	68.165	9.15
1	1	-3	1.367	68.607	0.18
2	1	2	1.363	68.848	0.08
0	1	3	1.351	69.500	13.27
3	1	-2	1.334	70.539	1.45
1	2	0	1.327	70.960	1.80
0	2	1	1.318	71.508	0.03
3	1	1	1.318	71.537	0.78

1	2	-1	1.294	73.049	0.03
2	1	-3	1.291	73.268	7.54
3	0	-3	1.281	73.939	0.10
4	0	0	1.274	74.407	0.12
1	2	1	1.259	75.440	0.66
3	0	2	1.257	75.570	0.63
1	1	3	1.253	75.862	5.36
4	0	-2	1.226	77.851	0.01
2	0	3	1.221	78.233	0.18
2	2	0	1.210	79.098	1.96
2	2	-1	1.199	79.948	0.16
1	0	-4	1.188	80.875	0.01
0	2	2	1.184	81.204	1.22
1	2	-2	1.180	81.525	0.08
4	1	-1	1.173	82.105	0.35
4	0	1	1.170	82.315	0.97
0	0	4	1.164	82.879	0.50
3	1	-3	1.161	83.128	5.64
2	0	-4	1.149	84.156	1.52
2	2	1	1.145	84.594	0.46
3	1	2	1.143	84.711	3.27
1	2	2	1.128	86.155	1.81
4	1	-2	1.120	86.937	0.09
2	2	-2	1.118	87.108	1.65
4	0	-3	1.099	89.025	0.02
1	1	-4	1.090	89.910	0.02