

Supporting information

Comments on *A new method for quantitative phase analysis using X-ray powder diffraction: direct derivation of weight fractions from observed integrated intensities and chemical compositions of individual phases* by Toraya (2016)

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S1. Calculation of the proportionality constant C

The proportionality constant C is defined by Toraya (2016) as

$$C = \frac{\sum_{j=1}^{N_k} m_{jk} |F_{jk}|^2}{U_k Z_k \sum_{i=1}^{A_k} n_i^2}$$

where m_{jk} is the multiplicity of the j th reflection of k th phase in the sample, F_{jk} is the structure factor, N_k is the number of observed diffraction lines in the range $2\theta \leq 2\theta^{UL}$ and $2\theta^{UL}$ defines the upper limit of 2θ of the observed diffraction pattern, Z_k and U_k are the number of chemical formula units in the unit cell and the volume of unit cell, respectively. A_k is the total number of atoms in the chemical formula of the k th component phase, n_i is the number of electrons belonging to the i th atom in the chemical formula unit.

S1.1. Li₂CO₃**Table S1** Crystallographic data for Li₂CO₃.

Space group	a (Å)	b (Å)	c (Å)	β (°)	U_k (Å ³)	Z_k	$\sum_{i=1}^{A_k} n_i^2$
<i>C2/c</i>	8.3593	4.9725	6.1975	114.83	233.8	4	246

Table S2 Atomic coordinates of Li₂CO₃.

atoms	Wyck	x	y	z	SOF	B
Li	8f	0.1965	0.4484	0.8344	1.0	0.0
C	4e	0	0.0657	0.25	1.0	0.0
O1	4e	0	0.3213	0.25	1.0	0.0
O2	8f	0.1459	-0.0635	0.3127	1.0	0.0

Table S3 The proportionality constant C of Li₂CO₃ at various $2\theta^{UL}$ (Cu K α 1 radiation).

2θ	hkl	F(hkl)	Multiplicity	$2\theta^{UL}$	$m_{jk} F_{jk} ^2$	$\sum_{j=1}^{N_k} m_{jk} F_{jk} ^2$	$C = \frac{\sum_{j=1}^{N_k} m_{jk} F_{jk} ^2}{U_k Z_k \sum_{i=1}^{A_k} n_i^2}$
21.348	1 1 0	31.52	4		3974.0416		
23.433	2 0 0	18.96	2		718.9632		
23.475	-1 1 1	9.69	4		375.5844		
29.481	1 1 1	24.88	4	30	2476.0576	7544.6468	0.032794371
30.581	-2 0 2	67.25	2		9045.125		
31.793	0 0 2	80.43	2		12937.9698		
34.101	-1 1 2	32.62	4		4256.2576		
36.097	0 2 0	38	2		2888		
36.966	-3 1 1	42.05	4		7072.81		
39.601	0 2 1	27.75	4		3080.25		
39.965	3 1 0	22.11	4	40	1955.4084	48780.4084	0.212034156
40.841	-3 1 2	0.59	4		1.3924		
42.714	-2 2 1	13.22	4		699.0736		

42.724	1	1	2	6.04	4		145.9264		
43.486	2	2	0	19.51	4		1522.5604		
45.016	-4	0	2	15.79	2		498.6482		
47.62	2	0	2	14.13	2		399.3138		
47.925	4	0	0	0.66	2		0.8712		
48.016	-2	2	2	10.64	4		452.8384		
48.406	-1	1	3	3.44	4		47.3344		
48.787	3	1	1	36.74	4		5399.3104		
48.855	0	2	2	18.95	4	50	1436.41	59384.1468	0.258125503
50.11	2	2	1	2.1	4		17.64		
50.279	-3	1	3	22.3	4		1989.16		
56.81	1	3	0	23.51	4		2210.8804		
57.721	-4	2	1	14.91	4		889.2324		
57.773	-1	3	1	27.18	4		2955.0096		
58.124	-2	2	3	18.33	4		1343.9556		
58.419	1	1	3	27.41	4		3005.2324		
58.664	-5	1	2	24.95	4		2490.01		
58.948	-5	1	1	20.6	4		1697.44		
59.007	-4	2	2	30.84	4		3804.4224		
59.722	-2	0	4	64.82	2	60	8403.2648	88190.3944	0.38333783
60.886	1	3	1	0.02	4		0.0016		
61.179	2	2	2	29.56	4		3495.1744		
61.437	4	2	0	18.87	4		1424.3076		
61.559	3	1	2	23.72	4		2250.5536		
61.939	0	2	3	12.91	4		666.6724		
63.302	-5	1	3	27.78	4		3086.9136		
63.479	-3	1	4	12.25	4		600.25		
63.635	-1	3	2	20.92	4		1750.5856		
63.665	-4	0	4	1.77	2		6.2658		

64.117	5	1	0	12.04	4		579.8464		
64.873	-1	1	4	15.66	4		980.9424		
65.115	-4	2	3	4.74	4		89.8704		
65.479	-3	3	1	32.56	4		4240.6144		
66.434	0	0	4	16.38	2		536.6088		
67.172	-6	0	2	33.01	2		2179.3202		
67.513	3	3	0	12.01	4		576.9604		
68.126	-3	3	2	17.44	4		1216.6144		
69.472	1	3	2	18.24	4		1330.7904		
69.685	4	2	1	11.68	4	70	545.6896	113748.3764	0.494430896
70.537	4	0	2	24.78	2		1228.0968		
71.807	-2	2	4	22.62	4		2046.6576		
72.333	-5	1	4	15.05	4		906.01		
73.606	5	1	1	8.84	4		312.5824		
73.746	-1	3	3	25.58	4		2617.3456		
74.044	3	3	1	31.64	4		4004.3584		
75.065	6	0	0	41.74	2		3484.4552		
75.222	-3	3	3	9	4		324		
75.425	-4	2	4	18.41	4		1355.7124		
75.653	2	2	3	9.74	4		379.4704		
76.245	1	1	4	6.28	4		157.7536		
76.581	0	4	0	1.11	2		2.4642		
77.372	3	1	3	18.46	4		1363.0864		
77.402	-6	0	4	8.23	2		135.4658		
78.005	0	2	4	6.39	4		163.3284		
78.698	-6	2	2	5.81	4		135.0244		
78.781	0	4	1	5.73	4		131.3316		
79.689	-3	1	5	5.5	4	80	121	132616.5196	0.576445191
80.306	-6	2	1	4.74	4		89.8704		

80.863	-2	4	1	12.2	4		595.36		
81.396	2	4	0	4.98	4		99.2016		
81.456	-6	2	3	8.13	4		264.3876		
81.882	4	2	2	1.47	4		8.6436		
81.967	1	3	3	22.62	4		2046.6576		
82.178	-5	3	2	4.72	4		89.1136		
82.424	-5	3	1	8.48	4		287.6416		
82.503	2	0	4	4.09	2		33.4562		
83.186	-7	1	2	15.7	4		985.96		
83.663	-1	1	5	8.17	4		266.9956		
84.573	-7	1	3	6.35	4		161.29		
84.665	-2	4	2	2.83	4		32.0356		
84.705	3	3	2	5.37	4		115.3476		
85.258	-5	1	5	22.68	4		2057.5296		
85.295	0	4	2	2.09	4		17.4724		
86.119	-7	1	1	5.28	4		111.5136		
86.23	6	2	0	12.02	4		577.9216		
86.252	2	4	1	21.79	4		1899.2164		
86.254	-5	3	3	24.66	4		2432.4624		
86.413	-3	3	4	15.82	4		1001.0896		
86.966	5	1	2	8.87	4		314.7076		
86.986	5	3	0	6.5	4		169		
87.669	-1	3	4	15.39	4		947.4084		
88.503	-6	2	4	8.04	4		258.5664		
88.778	-2	2	5	12.22	4		597.3136		
89.572	-4	2	5	4.57	4	90	83.5396	148160.2218	0.644009115
90.258	-7	1	4	3.84	4		58.9824		
92.402	-4	4	1	34.14	4		4662.1584		
92.743	-2	4	3	6.25	4		156.25		

93.343	7	1	0	26.17	4		2739.4756		
93.498	-4	4	2	4.02	4		64.6416		
93.526	2	2	4	15.73	4		989.7316		
94.616	-5	3	4	7.73	4		239.0116		
95.387	2	4	2	4.44	4		78.8544		
95.505	-8	0	2	28.44	2		1617.6672		
95.614	4	4	0	1.75	4		12.25		
95.838	5	3	1	6.93	4		192.0996		
96.058	0	4	3	8.8	4		309.76		
96.425	6	2	1	15.79	4		997.2964		
96.548	3	1	4	11.91	4		567.3924		
96.878	-4	0	6	20.03	2		802.4018		
97.076	1	1	5	20.67	4		1708.9956		
97.457	0	2	5	1.66	4		11.0224		
98.035	4	2	3	0.64	4		1.6384		
98.406	1	3	4	10.6	4		449.44		
98.778	-2	0	6	39.05	2		3049.805		
98.925	-4	4	3	23.14	4		2141.8384		
99.414	-3	1	6	11.37	4		517.1076		
99.517	3	3	3	12.85	4		660.49		
99.865	-6	2	5	10.32	4		426.0096		
99.925	-8	0	4	33.28	2		2215.1168		
99.939	6	0	2	30.19	2	100	1822.8722	174652.5308	0.759163428
100.289	-7	1	5	10.54	4		444.3664		
101.827	-3	3	5	11.37	4		517.1076		
102.308	-5	1	6	0.49	4		0.9604		
102.739	1	5	0	14.87	4		884.4676		
103.224	4	4	1	32.1	4		4121.64		
103.571	-1	5	1	20.42	4		1667.9056		

104.562	5	1	3	4.49	4		80.6404		
104.586	-6	0	6	6.19	2		76.6322		
105.03	7	1	1	7.22	4		208.5136		
105.292	-2	4	4	0.92	4		3.3856		
105.386	-7	3	2	14.99	4		898.8004		
105.878	-1	3	5	5.07	4		102.8196		
106.194	-1	1	6	6.97	4		194.3236		
106.342	1	5	1	2.43	4		23.6196		
106.733	-8	2	2	5.78	4		133.6336		
106.775	-8	2	3	16.84	4		1134.3424		
106.821	-7	3	3	8.78	4		308.3536		
107.535	-5	3	5	24.56	4		2412.7744		
107.686	4	0	4	30.06	2		1807.2072		
108.164	-4	2	6	1.04	4		4.3264		
108.438	-7	3	1	10.06	4		404.8144		
108.638	8	0	0	17.17	2		589.6178		
108.895	-1	5	2	16.83	4		1132.9956		
108.923	-4	4	4	4.23	4		71.5716		
109.156	2	4	3	28.04	4		3144.9664		
109.332	5	3	2	12.1	4	110	585.64	195607.9568	0.85025053
110.157	-2	2	6	14.14	4		799.7584		
110.513	0	0	6	4.87	2		47.4338		
110.664	-3	5	1	19.23	4		1479.1716		
111.237	-8	2	1	16.47	4		1085.0436		
111.367	-8	2	4	10.07	4		405.6196		
111.382	6	2	2	7.6	4		231.04		
111.599	0	4	4	3.5	4		49		
112.331	-6	4	2	0.37	4		0.5476		
112.672	3	5	0	3.59	4		51.5524		

112.859	-7	3	4	7.17	4		205.6356		
113.288	-3	5	2	7.43	4		220.8196		
114.052	-6	4	1	14.18	4		804.2896		
114.662	1	5	2	9.04	4		326.8864		
115.155	-9	1	3	7.93	4		251.5396		
115.301	-6	4	3	27.58	4		3042.6256		
115.324	-7	1	6	12.16	4		591.4624		
115.768	4	4	2	0.34	4		0.4624		
116.249	7	3	0	19.38	4		1502.3376		
116.348	-6	2	6	15.46	4		956.0464		
116.476	2	2	5	9.42	4		354.9456		
116.598	-9	1	2	13.79	4		760.6564		
118.518	-9	1	4	22.68	4		2057.5296		
119.212	-1	5	3	20.95	4		1755.61		
119.54	3	5	1	18.89	4		1427.3284		
119.721	4	2	4	9.08	4		329.7856		
119.868	3	3	4	4.23	4	120	71.5716	214416.6562	0.932006441
120.475	1	3	5	23.38	4		2186.4976		
120.677	6	4	0	1.78	4		12.6736		
120.769	8	2	0	0.26	4		0.2704		
120.853	-3	5	3	4.11	4		67.5684		
121.003	-8	2	5	6.4	4		163.84		
121.447	3	1	5	7.63	4		232.8676		
122.368	7	1	2	17.81	4		1268.7844		
122.847	0	2	6	14.58	4		850.3056		
123.052	-9	1	1	10.8	4		466.56		
123.197	-3	3	6	12.08	4		583.7056		
123.29	-8	0	6	25.06	2		1256.0072		
123.354	-6	4	4	0.97	4		3.7636		

123.685	-2	4	5	4.75	4	90.25			
123.999	1	1	6	10.65	4	453.69			
124.234	-7	3	5	2.53	4	25.6036			
124.644	-4	4	5	11.79	4	556.0164			
125.531	-3	1	7	1.3	4	6.76			
125.735	-5	1	7	13.08	4	684.3456			
126.665	-5	3	6	10.16	4	412.9024			
127.217	-9	1	5	4.75	4	90.25			
128.916	1	5	3	14.32	4	820.2496			
129.108	5	1	4	19.55	4	1528.81			
129.185	-5	5	2	3.85	4	59.29			
129.449	5	3	3	9.27	4	343.7316			
129.5	-5	5	1	2.34	4	21.9024			
129.602	2	4	4	2.08	4	130	17.3056	226620.6074	0.985053445

S1.2. β -Ga₂O₃

Table S4 Crystallographic data for β -Ga₂O₃.

Space group	a (Å)	b (Å)	c (Å)	β (°)	U_k (Å ³)	Z_k	$\sum_{i=1}^{A_k} n_i^2$
<i>C2/m</i>	12.214	3.0371	5.7981	103.83	208.85	4	2114

Table S5 Atomic coordinates of β -Ga₂O₃.

atoms	Wyck	x	y	z	SOF	B
Ga1	4i	0.09050	0	0.79460	1.0	0.0
Ga2	4i	0.15866	0.5	0.31402	1.0	0.0
O1	4i	0.1645	0	0.1098	1.0	0.0
O2	4i	0.1733	0	0.5632	1.0	0.0
O3	4i	-0.0041	0.5	0.2566	1.0	0.0

Table S6 The proportionality constant C of β -Ga₂O₃ at various $2\theta^{\text{UL}}$ (Cu K α 1 radiation).

2θ	hkl	$ F(\text{hkl}) $	Multiplicity	$2\theta^{\text{UL}}$	$m_{jk} F_{jk} ^2$	$\sum_{j=1}^{N_k} m_{jk} F_{jk} ^2$	$C = \frac{\sum_{j=1}^{N_k} m_{jk} F_{jk} ^2}{U_k Z_k \sum_{i=1}^{A_k} n_i^2}$
14.928	2 0 0	0.3	2		0.18		
15.728	0 0 1	19.07	2		727.3298		
18.949	-2 0 1	36.54	2		2670.3432		
24.242	2 0 1	31.87	2	30	2031.3938	5429.2468	0.003074257
30.116	4 0 0	134.13	2		35981.7138		
30.355	1 1 0	30.59	4		3742.9924		
30.508	-4 0 1	149.5	2		44700.5		
31.736	-2 0 2	125.37	2		31435.2738		
31.762	0 0 2	161.08	2		51893.5328		
33.492	-1 1 1	80.18	4		25715.3296		
35.217	1 1 1	168.89	4		114095.3284		
37.306	3 1 0	18.52	4		1371.9616		
37.479	4 0 1	150.82	2		45493.3448		
38.421	-3 1 1	140.81	4		79309.8244		
38.443	-4 0 2	50.74	2		5149.0952		
38.509	2 0 2	41.03	2		3366.9218	447685.0654	0.253497192
42.905	3 1 1	63.62	4		16190.0176		
43.102	-1 1 2	55.97	4		12530.5636		
44.78	-6 0 1	70.27	2		9875.7458		
45.842	-3 1 2	90.41	4		32695.8724		
45.872	6 0 0	55.44	2		6147.1872		
45.881	1 1 2	61.62	4		15188.0976		
47.135	-2 0 3	26.42	2		1396.0328		
48.282	-5 1 1	33.14	4		4393.0384		
48.468	0 0 3	3.92	2		30.7328		
48.668	5 1 0	108.53	4		47115.0436		
49.573	-6 0 2	45.66	2		4169.6712		
49.664	4 0 2	80.9	2		13089.62	610506.6884	0.345693308
50.949	-4 0 3	69.76	2		9732.9152		
52.566	6 0 1	52.34	2		5478.9512		
53.442	-5 1 2	14.65	4		858.49		
53.511	3 1 2	10.58	4		447.7456		
54.515	5 1 1	67.21	4		18068.7364		
54.668	2 0 3	76.01	2		11555.0402		
56.534	-1 1 3	50.69	4		10277.9044		
57.661	-3 1 3	159.01	4		101136.7204		
59.186	-6 0 3	114.89	2		26399.4242		

59.97	1	1	3	155.17	4	60	96310.9156	890773.5316	0.504391605
60.622	-8	0	1	160.53	2		51539.7618		
60.963	0	2	0	208.93	2		87303.4898		
61.316	-7	1	1	28.62	4		3276.4176		
62.611	8	0	0	25.6	2		1310.72		
62.746	7	1	0	118.85	4		56501.29		
63.152	2	2	0	0.08	4		0.0256		
63.197	-5	1	3	13.75	4		756.25		
63.389	0	2	1	12.02	4		577.9216		
63.498	-8	0	2	0.37	2		0.2738		
63.606	6	0	2	19.47	2		758.1618		
64.202	-2	0	4	190.82	2		72824.5448		
64.457	-2	2	1	23.84	4		2273.3824		
64.714	-7	1	2	194.38	4		151134.3376		
64.78	4	0	3	68.84	2		9477.8912		
64.806	5	1	2	188.77	4		142536.4516		
66.301	-4	0	4	21.88	2		957.4688		
66.361	0	0	4	31.79	2		2021.2082		
66.597	2	2	1	23.35	4		2180.89		
67.543	3	1	3	32.9	4		4329.64		
68.837	7	1	1	1.34	4		7.1824		
69.23	8	0	1	140.27	2		39351.3458		
69.489	4	2	0	99.38	4		39505.5376		
69.7	-4	2	1	108.31	4	70	46924.2244	1606321.948	0.909563742
70.375	-2	2	2	92.81	4		34454.7844		
70.39	0	2	2	118.94	4		56586.8944		
70.913	-8	0	3	63.48	2		8059.4208		
72.473	-6	0	4	71.75	2		10296.125		
72.578	-7	1	3	47.33	4		8960.5156		
72.588	2	0	4	111.09	2		24681.9762		
72.642	-3	1	4	46.73	4		8734.7716		
72.671	-1	1	4	0.78	4		2.4336		
73.802	4	2	1	113.34	4		51383.8224		
74.419	-4	2	2	49.84	4		9936.1024		
74.462	2	2	2	42.94	4		7375.3744		
76.625	-5	1	4	30.5	4		3721		
76.71	1	1	4	21.96	4		1928.9664		
76.88	-9	1	1	24.19	4		2340.6244		
78.09	6	0	3	114.5	2		26220.5		
78.239	-10	0	1	35.91	2		2579.0562		

78.696	5	1	3	39.42	4		6215.7456		
78.744	-6	2	1	52.53	4		11037.6036		
78.981	-9	1	2	11.36	4		516.1984		
79.093	7	1	2	14.65	4		858.49		
79.167	9	1	0	58.85	4		13853.29		
79.534	6	2	0	33.4	4		4462.24		
79.835	-10	0	2	10.05	2		202.005		
79.961	8	0	2	4.72	2	80	44.5568	1900774.446	1.076294524
80.465	-2	2	3	22.32	4		1992.7296		
81.008	10	0	0	0.79	2		1.2482		
81.465	0	2	3	5.13	4		105.2676		
82.308	-6	2	2	35.53	4		5049.5236		
82.363	-8	0	4	28.41	2		1614.2562		
82.377	4	2	2	62.53	4		15640.0036		
82.529	4	0	4	17.16	2		588.9312		
83.374	-4	2	3	52.44	4		10999.8144		
83.383	-2	0	5	5.28	2		55.7568		
84.321	-4	0	5	23.42	2		1096.9928		
84.444	-7	1	4	110.21	4		48584.9764		
84.582	3	1	4	56.92	4		12959.5456		
84.651	6	2	1	41.29	4		6819.4564		
85.388	-9	1	3	16	4		1024		
85.742	-10	0	3	99.32	2		19728.9248		
85.754	9	1	1	52.66	4		11092.3024		
86.33	0	0	5	2.57	2		13.2098		
86.348	2	2	3	60.88	4		14825.4976		
88.058	10	0	1	33.05	2		2184.605		
89.13	-6	0	5	120.72	2	90	29146.6368	2084298.124	1.180212972
90.136	-6	2	3	92.71	4		34380.5764		
90.752	-3	1	5	64.77	4		16780.6116		
91.378	-8	2	1	126.81	4		64323.1044		
91.753	-1	1	5	92.22	4		34018.1136		
93.129	8	2	0	20.14	4		1622.4784		
93.136	2	0	5	96.72	2		18709.5168		
93.294	7	1	3	1.95	4		15.21		
93.62	-5	1	5	63.51	4		16134.0804		
93.922	-8	2	2	0.01	4		0.0004		
94.018	6	2	2	15.22	4		926.5936		
94.556	-2	2	4	148.87	4		88649.1076		
94.637	8	0	3	67.25	2		9045.125		

95.079	4	2	3	55.56	4		12347.6544		
95.365	-11	1	1	71.93	4		20695.6996		
95.903	-10	0	4	38.21	2		2920.0082		
96.038	-9	1	4	74.54	4		22224.8464		
96.125	6	0	4	3.65	2		26.645		
96.232	5	1	4	106.81	4		45633.5044		
96.451	-11	1	2	96.87	4		37535.1876		
96.471	-4	2	4	17.89	4		1280.2084		
96.526	0	2	4	25.49	4		2598.9604		
96.589	9	1	2	108.59	4		47167.1524		
96.636	1	1	5	75.87	4		23025.0276		
97.821	-8	0	5	30.78	2		1894.8168		
98.6	11	1	0	66.52	4		17699.6416		
98.65	-12	0	1	75.25	2		11325.125		
99.207	8	2	1	113.55	4		51574.41		
99.251	-12	0	2	71.66	2		10270.3112		
99.404	10	0	2	45.47	2		4135.0418		
99.575	1	3	0	18.37	4	100	1349.8276	2682606.711	1.518999227
100.408	-7	1	5	15.39	4		947.4084		
100.814	-8	2	3	52.5	4		11025		
101.261	-1	3	1	49.64	4		9856.5184		
101.893	-11	1	3	77.73	4		24167.8116		
102.256	1	3	1	103.9	4		43180.84		
102.325	-6	2	4	58.51	4		13693.6804		
102.411	12	0	0	128.49	2		33019.3602		
102.438	2	2	4	90.55	4		32797.21		
103.523	3	3	0	24.36	4		2373.6384		
103.941	4	0	5	21.43	2		918.4898		
104.228	-3	3	1	88.3	4		31187.56		
104.24	-12	0	3	31.95	2		2041.605		
105.547	3	1	5	50.05	4		10020.01		
106.194	-4	0	6	52.21	2		5451.7682		
106.237	-2	0	6	109.53	2		23993.6418		
106.286	11	1	1	43.76	4		7659.7504		
107.264	3	3	1	39.79	4		6332.9764		
107.404	-1	3	2	24.67	4		2434.4356		
107.954	6	2	3	94.29	4		35562.4164		
108.107	-10	2	1	30.02	4		3604.8016		
109.428	-3	3	2	57.47	4		13211.2036		
109.457	1	3	2	38.88	4		6046.6176		

109.764	-10	2	2	10.01	4		400.8004		
109.895	8	2	2	1.91	4	110	14.5924	3002548.848	1.700163263
110.222	-6	0	6	45.49	2		4138.6802		
110.354	0	0	6	30.34	2		1841.0312		
110.752	12	0	1	58.54	2		6853.8632		
110.784	-10	0	5	121.48	2		29514.7808		
110.997	10	2	0	0.5	4		1		
111.333	-5	3	1	22.35	4		1998.09		
111.449	-9	1	5	6.42	4		164.8656		
111.643	5	3	0	69.79	4		19482.5764		
112.006	-11	1	4	62.54	4		15645.0064		
112.236	9	1	3	61.99	4		15371.0404		
112.273	7	1	4	36.07	4		5204.1796		
112.44	-8	2	4	22.12	4		1957.1776		
112.619	4	2	4	12.6	4		635.04		
113.54	-2	2	5	4.93	4		97.2196		
113.545	-3	1	6	8.65	4		299.29		
113.96	-12	0	4	16.79	2		563.8082		
114.261	8	0	4	6.33	2		80.1378		
114.561	-4	2	5	18.78	4		1410.7536		
115.626	-5	1	6	66.37	4		17619.9076		
115.697	-5	3	2	9.24	4		341.5104		
115.718	-1	1	6	14.33	4		821.3956		
115.758	3	3	2	7.28	4		211.9936		
115.821	10	0	3	69.56	2		9677.1872		
116.127	-10	2	3	82.82	4		27436.6096		
116.664	5	3	1	43.65	4		7621.29		
116.783	0	2	5	1.8	4		12.96		
118.542	-1	3	3	31.92	4		4075.5456		
118.681	-8	0	6	8.07	2		130.2498		
118.733	10	2	1	27.52	4		3029.4016		
118.782	-13	1	1	32.4	4		4199.04		
118.904	-13	1	2	24.24	4		2350.3104		
118.917	2	0	6	68.43	2		9365.3298		
119.092	11	1	2	15.45	4		954.81		
119.209	5	1	5	21.79	4		1899.2164		
119.625	-3	3	3	103.12	4		42534.9376		
119.645	6	0	5	113.6	2		25809.92		
119.963	-6	2	5	100.22	4	120	40176.1936	3306075.197	1.872032023
121.924	1	3	3	102.14	4		41730.3184		

122.21	-7	1	6	31.82	4	4050.0496			
122.405	1	1	6	14.53	4	844.4836			
123.317	-7	3	1	18.04	4	1301.7664			
123.676	13	1	0	28.63	4	3278.7076			
124.061	-13	1	3	33.25	4	4422.25			
124.436	-14	0	2	71.84	2	10321.9712			
124.653	12	0	2	80.59	2	12989.4962			
124.704	2	2	5	80.78	4	26101.6336			
124.842	7	3	0	79.25	4	25122.25			
124.899	-14	0	1	3.2	2	20.48			
125.333	-5	3	3	10.48	4	439.3216			
126.546	8	2	3	56.43	4	12737.3796			
127.022	-7	3	2	126.89	4	64404.2884			
127.125	5	3	2	122.83	4	60348.8356			
128.132	-10	2	4	32.18	4	4142.2096			
128.184	-11	1	5	38.66	4	5978.3824			
128.412	6	2	4	3.1	4	38.44			
129.326	-14	0	3	40.67	2	3308.0978			
129.874	-12	0	5	1.91	2	130	7.2962	3587662.855	2.031478219

S1.3. Ag₂Te-III

Table S7 Crystallographic data for Ag₂Te-III.

Space group	a (Å)	b (Å)	c (Å)	β (°)	U_k (Å ³)	Z_k	$\sum_{i=1}^{A_k} n_i^2$
<i>P2₁/c</i>	8.164	4.468	8.977	124.16	270.96	4	7122

Table S8 Atomic coordinates of Ag₂Te-III.

atoms	Wyck	x	y	z	SOF	B
Ag1	4e	0.01880	0.1507	0.37099	1.0	0.0
Ag2	4e	0.3327	0.8383	0.99566	1.0	0.0
Te	4e	0.27179	0.1584	0.24247	1.0	0.0

Table S9 The proportionality constant C of Ag₂Te-III at various $2\theta^{UL}$ (Cu K α 1 radiation).

2θ	hkl	$ F(hkl) $	Multiplicity	$2\theta^{UL}$	$m_{jk} F_{jk} ^2$	$\sum_{j=1}^{N_k} m_{jk} F_{jk} ^2$	$C = \frac{\sum_{j=1}^{N_k} m_{jk} F_{jk} ^2}{U_k Z_k \sum_{i=1}^{A_k} n_i^2}$
13.095	1 0 0	62.64	2		7847.5392		

19.766	-1	0	2	79.74	2		12716.9352		
23.132	-1	1	1	6.74	4		181.7104		
23.213	0	1	1	25.73	4		2648.1316		
23.625	-2	0	2	46.55	2		4333.805		
23.858	1	1	0	44.52	4		7928.1216		
23.94	0	0	2	23.2	2		1076.48		
26.365	2	0	0	96.39	2		18582.0642		
28.159	-1	1	2	130.69	4		68319.5044		
29.756	-2	1	1	117.91	4		55611.0724		
29.947	1	1	1	206.78	4	30	171031.8736	350277.2376	0.04537794
31.047	-2	1	2	296.1	4		350700.84		
31.293	0	1	2	107.54	4		46259.4064		
32.935	-3	0	2	12.18	2		296.7048		
33.224	2	1	0	105.45	4		44478.81		
33.399	1	0	2	52.18	2		5445.5048		
36.647	-2	1	3	80.5	4		25921		
36.807	-1	1	3	58.2	4		13548.96		
38.754	-3	1	2	225.2	4		202860.16		
39.158	1	1	2	368.94	4	40	544466.8944	1584255.518	0.205238147
40.007	3	0	0	349.87	2		244818.0338		
40.121	-3	1	1	35.05	4		4914.01		
40.152	-2	0	4	343.28	2		235682.3168		
40.34	0	2	0	177.53	2		63033.8018		
40.367	2	1	1	93.42	4		34909.1856		
41.238	-3	1	3	230.43	4		212391.9396		
41.67	0	1	3	128.36	4		65905.1584		
42.161	-1	2	1	193.94	4		150450.8944		
42.208	0	2	1	247.46	4		244945.8064		
42.222	-3	0	4	103.52	2		21432.7808		
42.59	1	2	0	4.78	4		91.3936		
42.598	-1	0	4	276.01	2		152363.0402		
44.735	-4	0	2	270.56	2		146405.4272		
45.047	3	1	0	78.16	4		24435.9424		
45.179	-2	1	4	13.35	4		712.89		
45.273	2	0	2	100.53	2		20212.5618		
45.308	-1	2	2	27.04	4		2924.6464		
46.385	-2	2	1	127.93	4		65464.3396		
46.516	1	2	1	38.13	4		5815.5876		
47.07	-3	1	4	166.71	4		111168.8964		
47.281	-2	2	2	17.31	4		1198.5444		
47.416	-1	1	4	1.73	4		11.9716		
47.453	0	2	2	2.62	4		27.4576		
48.337	-4	0	4	82.44	2		13592.7072		
48.837	2	2	0	47.85	4		9158.49		
49.013	0	0	4	147.85	2		43719.245		
49.388	-4	1	2	77.68	4		24136.7296		

49.487	-4	1	3	14.64	4		857.3184		
49.888	2	1	2	10.27	4	50	421.8916	3485458.526	0.451536409
50.11	1	1	3	104.57	4		43739.5396		
51.392	-2	2	3	73.73	4		21744.4516		
51.514	-1	2	3	206.41	4		170420.3524		
52.467	-4	1	1	12.7	4		645.16		
52.747	3	1	1	74.87	4		22422.0676		
52.749	-4	1	4	67.12	4		18020.3776		
53.022	-3	2	2	13.26	4		703.3104		
53.34	1	2	2	20.91	4		1748.9124		
53.384	0	1	4	0.14	4		0.0784		
54.102	-3	2	1	174.31	4		121535.9044		
54.272	4	0	0	176.63	2		62396.3138		
54.297	2	2	1	37.18	4		5529.4096		
54.996	-3	2	3	18.29	4		1338.0964		
55.344	0	2	3	40.79	4		6655.2964		
55.444	-3	1	5	27.75	4		3080.25		
55.636	-2	1	5	33.43	4		4470.2596		
57.524	-5	0	4	260.14	2		135345.6392		
58.031	-5	0	2	35.8	2		2563.28		
58.117	3	2	0	116.91	4		54671.7924		
58.227	-2	2	4	112.37	4		50508.0676		
58.366	4	1	0	14.47	4		837.5236		
58.422	1	0	4	169.12	2		57203.1488		
58.628	3	0	2	119.62	2		28617.8888		
58.803	-4	1	5	27.92	4		3118.1056		
59.358	-1	1	5	68.45	4		18741.61		
59.817	-3	2	4	51.82	4	60	10741.2496	4332256.612	0.561237949
60.11	-1	2	4	89.34	4		31926.5424		
60.313	-5	1	3	8.39	4		281.5684		
61.077	2	1	3	5.16	4		106.5024		
61.477	-5	1	4	105.58	4		44588.5456		
61.797	-4	2	2	93.57	4		35021.3796		
61.882	-4	2	3	21.74	4		1890.5104		
61.965	-5	1	2	89.73	4		32205.8916		
61.982	-3	0	6	92.59	2		17145.8162		
62.229	2	2	2	32.13	4		4129.3476		
62.341	1	1	4	17.94	4		1287.3744		
62.421	1	2	3	14.4	4		829.44		
62.539	3	1	2	21.62	4		1869.6976		
63.444	-4	0	6	96.42	2		18593.6328		
63.638	-1	3	1	0.19	4		0.1444		
63.674	0	3	1	47.18	4		8903.8096		
63.869	-2	0	6	117.49	2		27607.8002		
63.961	1	3	0	15.3	4		936.36		
64.477	-4	2	1	304.52	4		370929.7216		

64.723	3	2	1	98.27	4	38627.9716			
64.725	-4	2	4	22.17	4	1966.0356			
65.285	0	2	4	69.03	4	19060.5636			
65.372	-5	1	5	24.17	4	2336.7556			
65.776	-3	1	6	13.44	4	722.5344			
66.042	-1	3	2	5.19	4	107.7444			
66.242	0	1	5	121.56	4	59107.3344			
66.313	-5	1	1	11.58	4	536.3856			
66.624	4	1	1	128.95	4	66512.41			
66.885	-2	3	1	154.89	4	95963.6484			
66.988	1	3	1	273.41	4	299012.1124			
67.115	-3	2	5	20.37	4	1659.7476			
67.193	-4	1	6	238.62	4	227758.0176			
67.288	-2	2	5	305.2	4	372588.16			
67.594	-2	3	2	50.62	4	10249.5376			
67.605	-2	1	6	63.77	4	16266.4516			
67.731	0	3	2	32.24	4	4157.6704			
68.137	-5	0	6	144.59	2	41812.5362			
68.84	2	3	0	11.96	4	572.1664			
68.956	-1	0	6	11.17	2	249.5378			
69.075	-6	0	4	34.12	2	2328.3488			
69.518	5	0	0	46.47	2	4318.9218			
69.748	4	2	0	53.17	4	70	11308.1956	6207733.484	0.804203426
70.145	-4	2	5	59.45	4	14137.21			
70.159	2	0	4	313.36	2	196388.9792			
70.651	-1	2	5	55.18	4	12179.3296			
70.928	-2	3	3	99.68	4	39744.4096			
71.029	-1	3	3	96.89	4	37550.6884			
71.523	-5	2	3	8.09	4	261.7924			
71.763	-5	1	6	39.57	4	6263.1396			
72.224	2	2	3	287.39	4	330372.0484			
72.286	-3	3	2	48.02	4	9223.6816			
72.552	1	3	2	62.98	4	15865.9216			
72.564	-1	1	6	262.02	4	274617.9216			
72.592	-5	2	4	89.14	4	31783.7584			
72.681	-6	1	4	166.09	4	110343.5524			
72.751	-6	0	2	113.43	2	25732.7298			
73.042	-5	2	2	8.44	4	284.9344			
73.114	5	1	0	216.59	4	187644.9124			
73.195	-3	3	1	43.49	4	7565.5204			
73.208	-6	1	3	182.65	4	133444.09			
73.36	2	3	1	121.75	4	59292.25			
73.389	1	2	4	53.14	4	11295.4384			
73.414	4	0	2	118.08	2	27885.7728			
73.572	3	2	2	44.59	4	7953.0724			
73.742	2	1	4	55.35	4	12254.49			

73.954	-3	3	3	319.44	4	408167.6544			
74.101	3	1	3	23.98	4	2300.1616			
74.251	0	3	3	174.87	4	122318.0676			
74.723	-6	1	5	4.79	4	91.7764			
75.777	-6	0	6	250.69	2	125690.9522			
75.872	1	1	5	44.54	4	7935.2464			
76.208	-5	2	5	287.2	4	329935.36			
76.285	-6	1	2	145.84	4	85077.2224			
76.587	-3	2	6	32.89	4	4327.0084			
76.647	3	3	0	6.34	4	160.7824			
76.743	-2	3	4	10.09	4	407.2324			
76.938	4	1	2	211.76	4	179369.1904			
76.953	0	0	6	5.3	2	56.18			
77.024	0	2	5	41.81	4	6992.3044			
77.091	-5	2	1	59.08	4	13961.7856			
77.384	4	2	1	47.22	4	8918.9136			
77.627	-4	1	7	152.88	4	93489.1776			
77.855	-3	1	7	44.75	4	8010.25			
77.919	-4	2	6	44.15	4	7796.89			
78.139	-3	3	4	31.15	4	3881.29			
78.308	-2	2	6	38.5	4	5929			
78.399	-1	3	4	2.94	4	34.5744			
79.266	-6	1	6	22.08	4	1950.1056			
79.9	-4	3	2	7.8	4	243.36			
79.976	-4	3	3	36.66	4	80	5375.8224	9182239.436	1.189546624
80.287	2	3	2	19.64	4	1542.9184			
80.427	0	1	6	130.2	4	67808.16			
80.436	-5	1	7	117.71	4	55422.5764			
80.459	1	3	3	145.1	4	84216.04			
81.112	-2	1	7	39.54	4	6253.6464			
81.821	-6	1	1	2.61	4	27.2484			
82.174	5	1	1	144.2	4	83174.56			
82.264	-5	2	6	45.95	4	8445.61			
82.319	-4	3	1	15.9	4	1011.24			
82.544	3	3	1	126.33	4	63837.0756			
82.545	-4	3	4	12.61	4	636.0484			
82.801	-7	0	4	14.01	2	392.5602			
83.032	-1	2	6	0.77	4	2.3716			
83.057	0	3	4	0.72	4	2.0736			
83.145	-6	2	4	2.3	4	21.16			
83.562	5	2	0	27.45	4	3014.01			
83.652	-6	2	3	68.23	4	18621.3316			
84.079	3	0	4	28.94	2	1675.0472			
84.167	2	2	4	109.83	4	48250.5156			
84.514	3	2	3	67.02	4	17966.7216			
84.742	-3	3	5	39.77	4	6326.6116			

84.901	-2	3	5	56.66	4	12841.4224			
85.116	-6	2	5	142.14	4	80815.1184			
86.159	-7	0	6	89.57	2	16045.5698			
86.215	-6	1	7	52.48	4	11016.6016			
86.223	-7	1	4	181.26	4	131420.7504			
86.23	1	2	5	146.11	4	85392.5284			
86.338	6	0	0	102.42	2	20979.7128			
86.632	-6	2	2	52.84	4	11168.2624			
86.662	-7	1	5	66.05	4	17450.41			
86.713	-4	0	8	83.19	2	13841.1522			
87.196	4	3	0	15.03	4	903.6036			
87.199	0	4	0	223.93	2	100289.2898			
87.268	4	2	2	49.86	4	9944.0784			
87.328	-1	1	7	146.06	4	85334.0944			
87.494	3	1	4	106.7	4	45539.56			
87.569	-4	3	5	38.59	4	5956.7524			
87.685	1	0	6	49.79	2	4958.0882			
87.941	-4	2	7	10.95	4	479.61			
87.95	-5	0	8	63.06	2	7953.1272			
88.046	-1	3	5	95.98	4	36848.6416			
88.092	2	1	5	15.75	4	992.25			
88.163	-3	2	7	80.5	4	25921			
88.251	-7	1	3	59.03	4	13938.1636			
88.401	-1	4	1	103.67	4	42989.8756			
88.432	0	4	1	134.09	4	71920.5124			
88.458	-3	0	8	271.06	2	146947.0472			
88.69	1	4	0	40	4	6400			
88.871	-5	3	3	26.33	4	2773.0756			
89.299	4	1	3	25.39	4	2578.6084			
89.335	-7	0	2	233.4	2	108951.12			
89.538	2	3	3	16.59	4	1100.9124			
89.547	-6	2	6	90.91	4	33058.5124			
89.568	-7	1	6	83.54	4	27915.7264			
89.747	6	1	0	15.34	4	941.2624			
89.889	-5	3	4	0.93	4	3.4596	10836496.86	1.403853423	
90.097	5	0	2	59.54	2	7090.0232			
90.12	-4	1	8	64.58	4	16682.3056			
90.318	-5	3	2	19.8	4	1568.16			
90.576	-1	4	2	29.24	4	3419.9104			
90.651	1	3	4	8.68	4	301.3696			
90.69	0	2	6	4.25	4	72.25			
90.699	-5	2	7	2.54	4	25.8064			
90.826	3	3	2	11.05	4	488.41			
91.091	1	1	6	94.25	4	35532.25			
91.349	-2	4	1	99.23	4	39386.3716			
91.357	-5	1	8	187.02	4	139905.9216			

91.366	-2	2	7	33.92	4	4602.2656			
91.444	1	4	1	39.86	4	6355.2784			
91.865	-3	1	8	42.2	4	7123.36			
92.003	-2	4	2	20.75	4	1722.25			
92.068	-6	2	1	28.17	4	3174.1956			
92.13	0	4	2	19.51	4	1522.5604			
92.167	-6	0	8	119.22	2	28426.8168			
92.417	5	2	1	34.48	4	4755.4816			
92.742	-7	1	2	26.8	4	2872.96			
93.161	2	4	0	26.19	4	2743.6644			
93.184	-2	0	8	30.74	2	1889.8952			
93.373	-5	3	5	35.18	4	4950.5296			
93.505	5	1	2	78.74	4	24799.9504			
93.742	-3	3	6	13.79	4	760.6564			
94.168	0	3	5	183.1	4	134102.44			
94.234	-5	3	1	18.27	4	1335.1716			
94.52	4	3	1	189.27	4	143292.5316			
94.941	-7	1	7	72.82	4	21211.0096			
95.045	-4	3	6	44.14	4	7793.3584			
95.127	-2	4	3	32.87	4	4321.7476			
95.223	-1	4	3	121.69	4	59233.8244			
95.427	-2	3	6	9.31	4	346.7044			
95.581	-6	1	8	40.85	4	6674.89			
96.422	-3	4	2	7.76	4	240.8704			
96.45	-6	2	7	65.6	4	17213.44			
96.457	-7	2	4	2.07	4	17.1396			
96.505	0	1	7	16.1	4	1036.84			
96.603	-2	1	8	56.58	4	12805.1856			
96.678	1	4	2	18.21	4	1326.4164			
96.899	-7	2	5	74.15	4	21992.89			
97.296	-3	4	1	92.31	4	34084.5444			
97.456	2	4	1	17.53	4	1229.2036			
97.569	-1	2	7	68.71	4	18884.2564			
97.737	3	2	4	23.17	4	2147.3956			
98.031	-3	4	3	17.52	4	1227.8016			
98.32	0	4	3	37.15	4	5520.49			
98.34	2	2	5	90.62	4	32847.9376			
98.5	-7	2	3	27.89	4	3111.4084			
99.12	-8	0	4	59.64	2	7113.8592			
99.359	-5	3	6	22.54	4	2032.2064			
99.404	-7	0	8	94.05	2	17690.805			
99.423	-8	0	6	28.33	2	1605.1778			
99.561	4	2	3	86.65	4	30032.89			
99.743	-7	1	1	53.95	4	11642.41			
99.834	-7	2	6	43.46	4	100	7555.0864	11786339.44	1.526904236
100.016	6	2	0	35.95	4	5169.61			

100.132	-1	3	6	50.35	4	10140.49
100.162	6	1	1	36.57	4	5349.4596
100.246	-6	3	4	36.05	4	5198.41
100.395	-4	2	8	22.35	4	1998.09
100.667	4	0	4	24.79	2	1229.0882
100.667	5	3	0	36.92	4	5452.3456
100.671	3	4	0	160.19	4	102643.3444
100.759	-6	3	3	277.59	4	308224.8324
100.766	-2	4	4	162.46	4	105573.0064
100.952	-1	0	8	27.35	2	1496.045
101.28	2	3	4	1.93	4	14.8996
101.359	2	0	6	39.54	2	3126.8232
101.384	1	2	6	20.48	4	1677.7216
101.481	-8	1	5	21.36	4	1824.9984
101.632	3	3	3	35.95	4	5169.61
101.655	-5	2	8	31.18	4	3888.7696
102.157	-3	4	4	29.98	4	3595.2016
102.174	-3	2	8	99.33	4	39465.7956
102.245	-6	3	5	3.37	4	45.4276
102.417	-1	4	4	132.25	4	69960.25
102.588	-8	1	4	93.82	4	35208.7696
102.876	-7	1	8	16.1	4	1036.84
102.895	-8	1	6	49.83	4	9932.1156
103.073	-7	2	2	84.11	4	28297.9684
103.269	3	1	5	155.46	4	96671.2464
103.384	1	3	5	78.19	4	24454.7044
103.797	-6	3	2	33.58	4	4510.4656
103.856	5	2	2	16.21	4	1051.0564
103.931	-4	4	2	126.62	4	64130.4976
104.008	-4	4	3	14.54	4	845.6464
104.155	4	1	4	70.92	4	20118.5856
104.324	2	4	2	53.24	4	11337.9904
104.444	-1	1	8	43.22	4	7471.8736
104.452	4	3	2	41.07	4	6746.9796
104.5	1	4	3	26.9	4	2894.44
104.857	2	1	6	137.94	4	76109.7744
104.863	-5	1	9	13.14	4	690.6384
105.147	-4	3	7	232.41	4	216057.6324
105.158	-4	1	9	9.48	4	359.4816
105.336	-7	2	7	9.25	4	342.25
105.377	-3	3	7	83.56	4	27929.0944
105.913	7	0	0	106.83	2	22825.2978
105.997	-6	2	8	43.87	4	7698.3076
106.252	-8	1	3	24.11	4	2325.1684
106.408	-4	4	1	185.19	4	137181.3444
106.639	3	4	1	56.24	4	12651.7504

106.641	-4	4	4	43.33	4	7509.9556			
106.817	-6	3	6	4.64	4	86.1184			
106.875	-8	1	7	127.2	4	64719.36			
106.955	0	2	7	127.3	4	64821.16			
107.057	-2	2	8	20.42	4	1667.9056			
107.172	0	4	4	51.7	4	10691.56			
107.546	5	1	3	35.33	4	4992.8356			
107.669	-6	1	9	1.54	4	9.4864			
108.015	0	3	6	33.54	4	4499.7264			
108.025	-5	3	7	177.14	4	125514.3184			
108.571	-3	1	9	1.8	4	12.96			
108.727	-2	3	7	54.78	4	12003.3936			
108.934	-3	4	5	3.1	4	38.44			
108.977	1	1	7	0.15	4	0.09			
108.986	-8	0	2	162.61	2	52884.0242			
109.102	-2	4	5	188.67	4	142385.4756			
109.47	-6	3	1	8.6	4	295.84			
109.489	7	1	0	64.97	4	16884.4036			
109.84	5	3	1	220.65	4	194745.69			
109.929	6	0	2	228.57	2	104488.4898			
109.937	-8	0	8	17.73	2	110	628.7058	14095343.51	1.826032572
110.339	-7	2	1	241.25	4	232806.25			
110.779	6	2	1	55.4	4	12276.64			
111.543	4	4	0	98.35	4	38690.89			
111.945	-4	4	5	59.34	4	14084.9424			
112.114	0	0	8	277.74	2	154279.0152			
112.172	-8	2	5	136.97	4	75043.1236			
112.459	-1	4	5	17.66	4	1247.5024			
112.631	-8	1	2	28.24	4	3189.9904			
113.346	-8	2	4	20.33	4	1653.2356			
113.355	-5	4	3	2.11	4	17.8084			
113.597	6	1	2	5.05	4	102.01			
113.605	-8	1	8	228.35	4	208574.89			
113.652	-7	2	8	29.45	4	3469.21			
113.672	-8	2	6	2.26	4	20.4304			
113.738	-7	1	9	28.92	4	3345.4656			
114.07	3	2	5	17.43	4	1215.2196			
114.083	2	4	3	181.03	4	131087.4436			
114.177	-6	3	7	96.44	4	37202.6944			
114.185	-7	3	4	35.4	4	5012.64			
114.468	-5	4	4	132.63	4	70362.8676			
114.667	-7	3	5	105.91	4	44867.7124			
114.941	-5	4	2	21.1	4	1780.84			
115.016	4	2	4	3.4	4	46.24			
115.308	1	4	4	91.32	4	33357.3696			
115.308	-2	1	9	66.64	4	17763.5584			

115.326	-1	2	8	20.54	4	1687.5664			
115.401	-1	3	7	227.1	4	206297.64			
115.502	3	4	2	55.4	4	12276.64			
115.585	3	3	4	21.36	4	1824.9984			
115.769	2	2	6	13.52	4	731.1616			
115.775	-5	2	9	75.9	4	23043.24			
115.842	0	1	8	29.96	4	3590.4064			
116.093	-4	2	9	198.39	4	157434.3684			
116.249	2	3	5	15.52	4	963.4816			
116.426	-7	3	3	82.85	4	27456.49			
116.515	-9	0	6	277.99	2	154556.8802			
117.271	-8	2	3	122.97	4	60486.4836			
117.602	4	3	3	35.4	4	5012.64			
117.906	-7	3	6	16.56	4	1096.9344			
117.945	-8	2	7	60.85	4	14810.89			
118.109	6	3	0	6.06	4	146.8944			
118.223	-5	0	10	1.79	2	6.4082			
118.357	-5	4	5	180.9	4	130899.24			
118.533	-4	3	8	23.05	4	2125.21			
118.673	5	2	3	196.15	4	153899.29			
118.776	-3	4	6	45.26	4	8193.8704			
118.807	-6	2	9	72.83	4	21216.8356			
119.099	3	0	6	57.73	2	6665.5058			
119.262	0	4	5	40.46	4	6548.0464			
119.337	-5	4	1	59.56	4	14189.5744			
119.562	-6	0	10	41.17	2	3389.9378			
119.626	-9	0	4	46.26	2	4279.9752			
119.644	1	3	6	3.2	4	40.96			
119.665	4	4	1	20.65	4	1705.69			
119.79	-3	2	9	171.01	4	116977.6804			
119.95	-5	3	8	34.6	4	4788.64	120	16333185.08	2.115941902
120.234	1	2	7	150.68	4	90817.8496			
120.269	-4	4	6	37.44	4	5607.0144			
120.294	-4	0	10	175.71	2	61748.0082			
120.39	-9	1	6	39.82	4	6342.5296			
120.471	-1	5	1	8	4	256			
120.508	0	5	1	32.14	4	4131.9184			
120.538	-3	3	8	1.26	4	6.3504			
120.552	-9	1	5	32.06	4	4111.3744			
120.711	-2	4	6	64.91	4	16853.2324			
120.795	7	2	0	34.01	4	4626.7204			
120.807	1	5	0	34.63	4	4796.9476			
121.562	-7	3	2	17.58	4	1236.2256			
121.692	5	0	4	181.19	2	65659.6322			
122.164	-5	1	10	87.52	4	30639.0016			
122.19	-8	1	1	35.71	4	5100.8164			

122.46	5	3	2	28.77	4	3310.8516			
122.754	7	1	1	39.79	4	6332.9764			
122.979	4	1	5	13.37	4	715.0276			
123.029	-1	5	2	76.31	4	23292.8644			
123.077	3	1	6	167.57	4	112318.8196			
123.124	-9	1	7	0.81	4	2.6244			
123.56	-6	1	10	103.62	4	42948.4176			
123.614	-8	1	9	59.75	4	14280.25			
123.627	-9	1	4	59.33	4	14080.1956			
123.956	-2	5	1	24.65	4	2430.49			
124.071	1	5	1	42.58	4	7252.2256			
124.174	-7	3	7	111.46	4	49693.3264			
124.272	-8	2	2	57.76	4	13344.8704			
124.325	-4	1	10	71.15	4	20249.29			
124.46	-7	0	10	238.84	2	114089.0912			
124.747	-2	5	2	193.26	4	149397.7104			
124.791	-9	0	8	14.19	2	402.7122			
124.902	0	5	2	74.89	4	22434.0484			
124.947	-6	3	8	4.72	4	89.1136			
125.355	6	2	2	86.8	4	30136.96			
125.362	-5	4	6	82.76	4	27396.8704			
125.364	-8	2	8	2.46	4	24.2064			
125.513	-7	2	9	228.72	4	209251.3536			
125.789	5	1	4	99.38	4	39505.5376			
126.015	-3	0	10	41.84	2	3501.1712			
126.05	-1	1	9	8.48	4	287.6416			
126.076	0	3	7	14.77	4	872.6116			
126.094	2	1	7	61.92	4	15336.3456			
126.169	2	5	0	65.78	4	17308.0336			
126.196	-2	3	8	9.59	4	367.8724			
126.302	-1	4	6	12.19	4	594.3844			
126.441	-6	4	4	30.74	4	3779.7904			
126.958	5	4	0	10.93	4	477.8596			
127.07	-6	4	3	46.21	4	8541.4564			
127.288	-2	2	9	65.63	4	17229.1876			
127.714	2	4	4	167.17	4	111783.2356			
127.896	0	2	8	102.96	4	42403.0464			
127.945	1	0	8	85.15	2	14501.045			
128.152	3	4	3	33.28	4	4430.2336			
128.637	-2	5	3	1.6	4	10.24			
128.703	-7	1	10	8.5	4	289			
128.759	-1	5	3	40.96	4	6710.8864			
128.918	-6	4	5	80.85	4	26146.89			
129.053	-9	1	8	51.03	4	10416.2436			
129.96	-9	1	3	83.51	4	130	27895.6804	17850981.39	2.312570349

S2. Derivation of weight fractions from simulated X-ray powder diffraction data sets of two-phase samples with the direct derivation method

S2.1. The method

According to Eq. (7) presented in Toraya's original paper [J. Appl. Cryst. (2016). 49, 1508–1516], the weight fraction of a component of a mixture can be calculated by

$$w_k = M_k \left(\sum_{j=1}^{N_k} I_{jk} G_{jk} \right) \left(\sum_{i=1}^{A_k} n_i^2 \right)^{-1} / \sum_{k'=1}^K M_{k'} \left(\sum_{j=1}^{N_{k'}} I_{jk'} G_{jk'} \right) \left(\sum_{i=1}^{A_{k'}} n_i^2 \right)^{-1}.$$

Since

$$\sum_{j=1}^{N_k} I_{jk} G_{jk} = I_0 \frac{Q}{\mu} \frac{v_k}{U_k^2} \sum_{j=1}^{N_k} m_{jk} |F_{jk}|^2 \quad [\text{Eq. (2) in the above-mentioned paper}],$$

We have

$$w_k = M_k \left(\frac{v_k}{U_k^2} \sum_{j=1}^{N_k} m_{jk} |F_{jk}|^2 \right) \left(\sum_{i=1}^{A_k} n_i^2 \right)^{-1} / \sum_{k'=1}^K M_{k'} \left(\frac{v_{k'}}{U_{k'}^2} \sum_{j=1}^{N_{k'}} m_{jk'} |F_{jk'}|^2 \right) \left(\sum_{i=1}^{A_{k'}} n_i^2 \right)^{-1}.$$

The volume fraction of the k th component, v_k , can be calculated by

$$v_k = \frac{\frac{w_k}{\rho_k}}{\sum_{k'=1}^K \frac{w_{k'}}{\rho_{k'}}} = \frac{\frac{w_k U_k}{M_k Z_k}}{\sum_{k'=1}^K \frac{w_{k'} U_{k'}}{M_{k'} Z_{k'}}}$$

For a sample consisting of two phases, A and B, in the weight ratio of 1:1, we have

$$v_A = \frac{\frac{U_A}{M_A Z_A}}{\frac{U_A}{M_A Z_A} + \frac{U_B}{M_B Z_B}}.$$

Then the weight fraction of component A derived with the direct derivation method can be calculated by

$$w_A = \frac{\frac{\sum_{j=1}^{N_A} m_{jA} |F_{jA}|^2}{\left(\frac{U_A}{M_A Z_A} + \frac{U_B}{M_B Z_B} \right) U_A Z_A \sum_{i=1}^{A_A} n_i^2}}{\frac{\sum_{j=1}^{N_A} m_{jA} |F_{jA}|^2}{\left(\frac{U_A}{M_A Z_A} + \frac{U_B}{M_B Z_B} \right) U_A Z_A \sum_{i=1}^{A_A} n_i^2} + \frac{\sum_{j=1}^{N_B} m_{jB} |F_{jB}|^2}{\left(\frac{U_A}{M_A Z_A} + \frac{U_B}{M_B Z_B} \right) U_B Z_B \sum_{i=1}^{A_B} n_i^2}}.$$

S2.2. Mixture of Li₂CO₃ and Ag₂Te-III

Table S10 U , M , Z , and $\sum_{i=1}^{A_k} n_i^2$ of Li₂CO₃ and Ag₂Te-III.

phase	U (Å ³)	M	Z	$\sum_{i=1}^{A_k} n_i^2$
Li ₂ CO ₃	233.80	73.892	4	246

Ag ₂ Te-III	270.96	343.4	4	7122
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Table S11 Weight fraction of Li₂CO₃ and Ag₂Te-III derived with the direct derivation method.

2θ ^{UL} (°)	Li ₂ CO ₃		Ag ₂ Te-III	
	$\sum_{j=1}^{N_A} m_j F_j ^2$	wt%	$\sum_{j=1}^{N_A} m_j F_j ^2$	wt%
30	7544.6468	41.95	350277.2376	58.05
40	48780.4084	50.81	1584255.518	49.19
50	59384.1468	36.37	3485458.526	63.63
60	88190.3944	40.58	4332256.612	59.42
70	113748.3764	38.07	6207733.484	61.93
80	132616.5196	32.64	9182239.436	67.36
90	148160.2218	31.45	10836496.86	68.55
100	174652.5308	33.21	11786339.44	66.79
110	195607.9568	31.77	14095343.51	68.23
120	214416.6562	30.58	16333185.08	69.42
130	226620.6074	29.87	17850981.39	70.13

S2.3. Mixture of Li₂CO₃ and β-Ga₂O₃**Table S12** U , M , Z , and $\sum_{i=1}^{A_k} n_i^2$ of Li₂CO₃ and β-Ga₂O₃.

phase	U (Å ³)	M	Z	$\sum_{i=1}^{A_k} n_i^2$
Li ₂ CO ₃	233.80	73.892	4	246
β-Ga ₂ O ₃	208.85	187.44	4	2114

Table S13 Weight fraction of Li₂CO₃ and β-Ga₂O₃ derived with the direct derivation method.

2θ ^{UL} (°)	Li ₂ CO ₃		β-Ga ₂ O ₃	
	$\sum_{j=1}^{N_A} m_j F_j ^2$	wt%	$\sum_{j=1}^{N_A} m_j F_j ^2$	wt%
30	7544.6468	91.43	5429.2468	8.57
40	48780.4084	45.55	447685.0654	54.45
50	59384.1468	42.75	610506.6884	57.25
60	88190.3944	43.18	890773.5316	56.82

70	113748.3764	35.22	1606321.948	64.78
80	132616.5196	34.88	1900774.446	65.12
90	148160.2218	35.30	2084298.124	64.70
100	174652.5308	33.32	2682606.711	66.68
110	195607.9568	33.34	3002548.848	66.66
120	214416.6562	33.24	3306075.197	66.76
130	226620.6074	32.66	3587662.855	67.34

S2.4. Mixture of β -Ga₂O₃ and Ag₂Te-III

Table S14 U , M , Z , and $\sum_{i=1}^{A_k} n_i^2$ of β -Ga₂O₃ and Ag₂Te-III.

phase	U (Å ³)	M	Z	$\sum_{i=1}^{A_k} n_i^2$
β -Ga ₂ O ₃	208.85	187.44	4	2114
Ag ₂ Te-III	270.96	343.4	4	7122

Table S15 Weight fraction of β -Ga₂O₃ and Ag₂Te-III derived with the direct derivation method.

$2\theta^{\text{UL}}$ (°)	β -Ga ₂ O ₃		Ag ₂ Te-III	
	$\sum_{j=1}^{N_A} m_j F_j ^2$	wt%	$\sum_{j=1}^{N_A} m_j F_j ^2$	wt%
30	5429.2468	6.34	350277.2376	93.66
40	447685.0654	55.26	1584255.518	44.74
50	610506.6884	43.36	3485458.526	56.64
60	890773.5316	47.33	4332256.612	52.67
70	1606321.948	53.07	6207733.484	46.93
80	1900774.446	47.50	9182239.436	52.50
90	2084298.124	45.67	10836496.86	54.33
100	2682606.711	49.87	11786339.44	50.13
110	3002548.848	48.21	14095343.51	51.78
120	3306075.197	46.94	16333185.08	53.06

130	3587662.855	46.76	17850981.39	53.24
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