

TABLE 3. List of calculated and observed squared structure factors for the Cr-bearing perovskite (to be deposited)

<i>h</i>	<i>k</i>	<i>l</i>	F_c^2	F_o^2					
2	0	0	2562.43	2856.82	1	7	0	212.82	223.85
4	0	0	1131.99	1043.43	2	7	0	22.98	21.14
6	0	0	515.11	504.49	3	7	0	124.02	135.99
1	1	0	418.7	491.51	4	7	0	5.14	4.61
2	1	0	794.93	788.75	0	8	0	14.31	12.46
3	1	0	104.23	131.81	1	8	0	0.17	0.14
4	1	0	241.63	235.35	2	8	0	7.32	7.43
5	1	0	13.33	18.01	1	0	1	5.34	5.81
6	1	0	2.3	1.98	3	0	1	74.67	74.29
0	2	0	2293.98	2558.8	5	0	1	16.7	16.31
1	2	0	235.63	239	1	1	1	318.96	318.83
2	2	0	4333.01	4441.23	2	1	1	556.21	556.6
3	2	0	217.56	204.96	3	1	1	254.64	239.77
4	2	0	659.42	598.77	4	1	1	52.27	49.56
5	2	0	38.74	38.02	5	1	1	1.36	1.65
6	2	0	93.55	95.33	6	1	1	3.35	4.98
1	3	0	1464.41	1504.72	0	2	1	45.92	48.34
2	3	0	0.75	1.01	1	2	1	203.67	203.83
3	3	0	9.44	6.18	2	2	1	564.43	537.33
4	3	0	5.65	5.62	3	2	1	7.48	7.81
5	3	0	215.95	189.33	4	2	1	265.56	244.39
6	3	0	38.07	37.53	5	2	1	15.56	15.1
0	4	0	417.18	416.4	6	2	1	41.21	43.39
1	4	0	445.04	431.92	1	3	1	1233.23	1125.34
2	4	0	263.66	247.37	2	3	1	4.33	4.23
3	4	0	21.35	18.41	3	3	1	195.22	171.52
4	4	0	97.13	84.99	4	3	1	28.89	29.95
5	4	0	0	0.16	5	3	1	46.09	52.41
6	4	0	31.73	31.13	6	3	1	2.21	1.45
1	5	0	491.63	421.33	0	4	1	281.24	258.54
2	5	0	0.45	0.25	1	4	1	2.84	2.8
3	5	0	707.87	654.54	2	4	1	144.77	128.68
4	5	0	4.11	3.5	3	4	1	4.57	4.8
5	5	0	68.03	70.76	4	4	1	190.22	183.17
6	5	0	15.36	14.77	5	4	1	0.3	0.51
0	6	0	38.3	36.58	6	4	1	64.14	70.45
1	6	0	4.48	5.17	1	5	1	251.36	230.66
2	6	0	1.22	1.8	2	5	1	0.11	0.34
3	6	0	21.25	20.45	3	5	1	32.52	36.42
4	6	0	6.47	4.57	4	5	1	13.52	12.67
5	6	0	2.22	3.36	5	5	1	6.15	11.03
					6	5	1	0.58	0.88

0	6	1	1.35	0.71	3	5	2	116.06	111.09
1	6	1	2.34	2.13	4	5	2	3.26	4.96
2	6	1	13.39	15.91	5	5	2	0.32	0.38
3	6	1	0.76	1.52	6	5	2	4.15	5.52
4	6	1	19.82	21.5	0	6	2	687.62	674.74
5	6	1	3.75	5.43	1	6	2	34.42	34.69
1	7	1	0.59	0.66	2	6	2	267.97	268.64
2	7	1	8.73	7.85	3	6	2	5.16	4.29
3	7	1	0.01	0.11	4	6	2	136.34	159.46
4	7	1	3.12	3.13	5	6	2	0.05	0.02
0	8	1	11.5	11.95	1	7	2	9.31	6.57
1	8	1	0.05	0.2	2	7	2	0.14	0.41
2	8	1	5.51	6.45	3	7	2	0.26	0.55
0	0	2	416.03	520.5	4	7	2	9.45	8.81
2	0	2	423.46	360.36	0	8	2	75.4	88.1
4	0	2	86.13	84.36	1	8	2	0.19	0.1
6	0	2	94.25	77.97	2	8	2	111.35	134.02
1	1	2	2447.24	2945.52	1	0	3	1179.83	1273.67
2	1	2	195.55	213.08	3	0	3	1.95	1.58
3	1	2	3250.95	3369.37	5	0	3	63.28	67.21
4	1	2	90.84	93.58	1	1	3	748.13	782.76
5	1	2	761.04	765.9	2	1	3	90.58	96.25
6	1	2	29.15	32.22	3	1	3	20.27	25.99
0	2	2	338.56	294.6	4	1	3	129.55	134.63
1	2	2	576.89	616.61	5	1	3	81.25	86.47
2	2	2	385.2	460.38	6	1	3	0	0.27
3	2	2	31.84	28.47	0	2	3	894.38	912.63
4	2	2	193.98	180.86	1	2	3	74.17	78.52
5	2	2	1.33	1.32	2	2	3	73.31	64.18
6	2	2	21.79	17.68	3	2	3	38.18	41.26
1	3	2	1106.72	1190.56	4	2	3	181.45	180.47
2	3	2	67.88	70.42	5	2	3	0.56	0.62
3	3	2	239.8	224.52	6	2	3	80.1	88.72
4	3	2	19.75	24.15	1	3	3	655.18	625.11
5	3	2	420.94	427.87	2	3	3	175.23	187.68
6	3	2	11	14.2	3	3	3	286.3	284.05
0	4	2	606.63	575.78	4	3	3	21.83	21.11
1	4	2	24.12	29.88	5	3	3	11.67	17.44
2	4	2	516.88	477.22	6	3	3	3.35	4.25
3	4	2	115.24	112.49	0	4	3	0.22	2.31
4	4	2	266.51	255.14	1	4	3	2.1	2.2
5	4	2	23.8	25.65	2	4	3	364.9	364.65
6	4	2	73.74	86.37	3	4	3	3.17	3.7
1	5	2	19.26	14.83	4	4	3	156.06	163.79
2	5	2	26.51	23.81	5	4	3	0.24	0.43

6	4	3	15.02	20.36	2	4	4	156.94	145.65
1	5	3	146.86	146.85	3	4	4	28.23	27.63
2	5	3	31.9	31.76	4	4	4	59.13	55.69
3	5	3	57.85	66.25	5	4	4	2.04	3.42
4	5	3	5.17	5.98	6	4	4	19.83	21.93
5	5	3	0.42	2.28	1	5	4	362.57	337.36
6	5	3	7.73	8.58	2	5	4	2.98	2.7
0	6	3	16.71	20.87	3	5	4	290.77	288.25
1	6	3	9.33	10.57	4	5	4	0.12	0.04
2	6	3	0.06	0.28	5	5	4	75.83	86.47
3	6	3	0.26	0.05	6	5	4	7.32	7.57
4	6	3	14.92	16.18	0	6	4	4.6	3.94
5	6	3	0.43	1.08	1	6	4	0.68	0.53
1	7	3	5.47	6.14	2	6	4	0.63	0.42
2	7	3	2.01	1.62	3	6	4	8.24	8.54
3	7	3	10.49	9.2	4	6	4	4.21	3.4
4	7	3	7.99	8.21	5	6	4	0.37	0.84
0	8	3	9.31	10.17	1	7	4	125.67	152.17
1	8	3	7.42	6.64	2	7	4	4.93	4.42
2	8	3	4.26	5.33	3	7	4	94.82	113.66
0	0	4	6859.59	7535.86	0	8	4	1.67	1.1
2	0	4	2349.62	2437.34	1	0	5	192.68	189.89
4	0	4	683.53	671.13	3	0	5	41.76	44.18
6	0	4	221.69	253.28	5	0	5	0.4	0.83
1	1	4	167.52	229.71	1	1	5	26.84	22.54
2	1	4	32.13	34.75	2	1	5	189.48	194.16
3	1	4	16.74	16.23	3	1	5	271.67	264.76
4	1	4	15.78	16.52	4	1	5	4.38	4.96
5	1	4	0.34	1.85	5	1	5	8.19	6.63
6	1	4	1.09	1.33	6	1	5	4.48	6.37
0	2	4	2049.46	2167.25	0	2	5	0.41	2.49
1	2	4	0.87	0.94	1	2	5	164.49	170.46
2	2	4	1564	1592.22	2	2	5	344.5	331.38
3	2	4	57.49	59.16	3	2	5	0.38	0.29
4	2	4	380.53	372.18	4	2	5	112.23	114.95
5	2	4	10.74	11.56	5	2	5	15.57	16.36
6	2	4	88.74	101.43	6	2	5	8.14	11.63
1	3	4	518.71	498.27	1	3	5	469.36	443.1
2	3	4	2.51	2.63	2	3	5	14.57	13.91
3	3	4	93.59	79.48	3	3	5	49.74	48.56
4	3	4	0.25	0.34	4	3	5	60.95	62.47
5	3	4	65.58	60.33	5	3	5	35.76	44.36
6	3	4	17.06	18.9	6	3	5	6.76	5.53
0	4	4	234.78	226.32	0	4	5	303.49	301.87
1	4	4	54.95	54.6	1	4	5	0.97	0.95

2	4	5	16.7	17.85	4	4	6	99.13	95.27
3	4	5	1.92	2.16	5	4	6	1.73	2.08
4	4	5	82.64	90.89	6	4	6	30.31	36.32
5	4	5	0.15	0.3	1	5	6	25.94	20.94
6	4	5	55.42	63.8	2	5	6	1.98	1.24
1	5	5	124	124.61	3	5	6	5.28	4.37
2	5	5	9.16	9.73	4	5	6	0.13	0.01
3	5	5	7.21	10.06	5	5	6	8.65	8.85
4	5	5	28.16	27.28	0	6	6	165.94	162.38
5	5	5	7.02	11.04	1	6	6	0.35	0.28
0	6	5	10.28	7.7	2	6	6	150.4	153.97
1	6	5	10.29	9.57	3	6	6	5.5	4.64
2	6	5	16.17	19.29	4	6	6	58.85	71.06
3	6	5	1.65	2.46	1	7	6	1.73	1.09
4	6	5	10.54	12.14	2	7	6	3.06	2.41
1	7	5	0.09	0.08	1	0	7	96.09	91.91
2	7	5	7.37	6.97	3	0	7	1.05	0.86
3	7	5	3.09	3.48	5	0	7	18.3	18.68
0	0	6	89.26	95.12	1	1	7	104.22	95.08
2	0	6	13.26	10.21	2	1	7	12.46	13.33
4	0	6	34.09	26.87	3	1	7	1.72	1.33
6	0	6	6.04	3.83	4	1	7	30.32	30.11
1	1	6	959.53	888.93	5	1	7	23.37	24.09
2	1	6	10.02	10.51	0	2	7	163.34	143.75
3	1	6	719.35	690.21	1	2	7	10.44	9.09
4	1	6	7.43	7.97	2	2	7	23.17	22.11
5	1	6	344.21	367.32	3	2	7	6.11	5.92
6	1	6	0.43	0.83	4	2	7	46.57	49.02
0	2	6	43.89	34.64	5	2	7	0.14	0.32
1	2	6	0.51	0.48	1	3	7	138.08	132.03
2	2	6	26.36	19.68	2	3	7	33.88	32.04
3	2	6	27.22	26.5	3	3	7	72.61	75.04
4	2	6	62.68	53.31	4	3	7	6.3	4.78
5	2	6	6.06	6.86	5	3	7	3.9	7.3
6	2	6	25.61	24.71	0	4	7	0.29	0.92
1	3	6	220.02	198.88	1	4	7	0.39	0.46
2	3	6	0.9	0.84	2	4	7	95.68	95.76
3	3	6	270.73	263.28	3	4	7	0.86	0.97
4	3	6	0.03	0.32	4	4	7	47.76	51.67
5	3	6	72.89	81.87	5	4	7	0.09	0.16
6	3	6	9.3	11.77	1	5	7	39.75	43.19
0	4	6	208.22	188.84	2	5	7	9.4	8.43
1	4	6	26.2	25.96	3	5	7	18.41	21.87
2	4	6	181.62	168	4	5	7	1.74	1.5
3	4	6	15.16	14	0	6	7	5.66	6.85

1	6	7	3.19	3.06	2	2	9	30.65	34.16
2	6	7	0.04	0.23	3	2	9	0.16	0.12
3	6	7	0.08	0.01	4	2	9	20.24	24.47
0	0	8	467.74	437.19	5	2	9	1.56	1.85
2	0	8	688.73	642.98	1	3	9	63.82	69.7
4	0	8	159.47	168.81	2	3	9	0.12	0.25
1	1	8	45.2	36.93	3	3	9	16.21	20.34
2	1	8	11.49	10.27	4	3	9	2.46	2.55
3	1	8	0	0.34	0	4	9	21.91	26.53
4	1	8	9.76	8.11	1	4	9	0.2	0.18
5	1	8	1.37	0.63	2	4	9	12.07	16.76
0	2	8	606.19	566.1	3	4	9	0.35	0.44
1	2	8	28.99	27.61	1	5	9	22.1	25.38
2	2	8	189.19	183.52	2	5	9	0.01	0.01
3	2	8	2.91	3.39	0	0	10	31.05	35.52
4	2	8	84.08	90.8	2	0	10	12.24	8.36
5	2	8	0.18	0.46	4	0	10	5.13	4.27
1	3	8	59.02	52.74	1	1	10	138.24	149.27
2	3	8	4.71	4.32	2	1	10	8.69	7.71
3	3	8	85.33	78.76	3	1	10	84.62	104.43
4	3	8	3.78	4.14	4	1	10	9.06	8.65
5	3	8	1.54	2.56	0	2	10	22.55	18.24
0	4	8	50.81	49.7	1	2	10	2.67	2.04
1	4	8	3.05	2.4	2	2	10	0.57	0.51
2	4	8	35.69	35.7	3	2	10	6.27	6.59
3	4	8	15.89	16.08	4	2	10	8.59	9.08
4	4	8	14.26	16.22	1	3	10	22.51	27.45
1	5	8	116.63	124.1	2	3	10	0.12	0.15
2	5	8	3.47	2.99	3	3	10	67.83	75.26
3	5	8	31.44	40.36	0	4	10	31.92	36.8
0	6	8	1.79	1.47	1	4	10	15.17	14.35
1	6	8	6.12	5.6	2	4	10	28.44	34.1
2	6	8	2.82	2.81	1	0	11	0.18	0.11
1	0	9	0.45	0.28	3	0	11	0.4	0.27
3	0	9	1.16	1.09	1	1	11	4	5.42
5	0	9	1.36	2.31	2	1	11	4.27	5.21
1	1	9	12.59	13.59	3	1	11	4.69	5.8
2	1	9	13.8	14.66	0	2	11	3.73	5.65
3	1	9	13.84	14.51	1	2	11	1.21	1.16
4	1	9	3.36	4.34	2	2	11	10.82	14.02
5	1	9	0.2	0.59	1	3	11	21.38	28.14
0	2	9	10.02	12.06					
1	2	9	3.6	3.62					