



AM-76-014

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Table 3a. <sup>4 3b.</sup> Observed and calculated structure factors for  
synthetic titanite at 25°C

Table 3a. Observed and Calculated Structure Factors for Synthetic Titanite at 25°C

H	K	L	F <sub>O</sub>	F <sub>C</sub>	σ	H	K	L	F <sub>O</sub>	F <sub>C</sub>	σ
-8	1	2	12.46	12.32	1.22	-6	7	1	43.34	41.62	1.04
-8	1	1	9.80	5.45	1.31	-5	8	2	9.46	2.99	1.30
-8	2	2	13.58	13.73	1.16	-5	6	4	11.07	11.53	1.27
-8	2	3	12.51	12.52	1.22	-5	6	0	28.56	27.69	0.80
-8	3	3	60.74	60.89	1.38	-5	5	0	11.65	9.24	0.93
-7	5	1	17.85	14.61	0.84	-5	5	1	9.65	10.90	1.28
-7	4	5	11.11	7.95	1.14	-5	5	2	8.96	10.07	1.27
-7	4	4	17.58	16.43	0.91	-5	5	4	8.73	10.95	1.43
-7	4	3	9.87	9.07	1.28	-5	5	5	10.63	10.56	1.23
-7	4	2	11.34	9.30	1.14	-5	4	4	36.47	37.52	0.89
-7	4	0	17.79	18.69	1.03	-5	3	1	35.46	35.43	0.84
-7	3	1	12.53	9.62	1.03	-5	3	3	33.39	35.04	0.82
-7	3	3	24.52	26.06	0.80	-5	3	5	12.41	10.57	0.87
-7	2	6	21.64	21.95	0.82	-5	3	7	18.39	16.94	0.94
-7	1	1	20.00	20.09	0.87	-5	2	6	8.63	3.44	1.30
-7	1	5	9.59	9.89	1.49	-5	2	4	11.50	11.04	1.10
-6	0	0	46.51	46.95	1.05	-5	2	2	16.95	17.63	0.75
-6	0	1	8.91	9.89	1.21	-5	2	0	15.05	15.51	0.90
-6	0	2	31.50	31.96	0.80	-5	1	1	11.42	12.24	0.99
-6	0	3	10.43	10.50	1.03	-5	1	3	17.03	17.39	0.75
-6	0	4	33.28	34.44	0.81	-5	1	5	11.53	11.59	0.98
-6	0	5	9.76	9.31	1.18	-5	1	7	17.95	17.30	0.85
-6	0	6	16.07	17.19	1.01	-4	0	0	82.33	85.05	1.83
-6	0	7	9.80	9.14	1.40	-4	0	1	19.96	21.61	0.58
-6	1	7	30.84	32.92	0.95	-4	0	2	129.27	131.25	3.19
-6	1	6	17.76	15.82	0.85	-4	0	3	21.15	22.17	0.61
-6	1	5	56.76	57.61	1.26	-4	0	4	169.48	164.97	4.73
-6	1	4	18.26	18.76	0.82	-4	0	5	17.71	17.92	0.80
-6	1	3	28.26	27.27	0.77	-4	0	6	84.15	84.97	1.89
-6	1	2	20.42	19.87	0.72	-4	0	7	14.67	14.99	0.98
-6	1	1	45.02	45.22	1.02	-4	1	7	22.22	22.04	0.88
-6	1	0	19.22	19.67	0.80	-4	1	6	10.46	8.22	1.08
-6	2	0	45.50	44.03	1.05	-4	1	5	30.20	30.05	0.79
-6	2	1	19.69	18.97	0.76	-4	1	4	9.41	11.05	1.09
-6	2	2	82.37	81.88	1.84	-4	1	3	7.78	10.26	1.12
-6	2	3	21.09	20.98	0.72	-4	1	2	10.00	12.25	0.80
-6	2	4	54.33	55.51	1.21	-4	1	1	51.89	53.19	1.12
-6	2	5	16.83	17.75	0.91	-4	1	0	10.58	12.38	0.83
-6	2	6	28.17	28.28	0.87	-4	2	0	24.84	26.81	0.70
-6	2	7	16.47	15.11	0.96	-4	2	1	9.24	10.83	0.94
-6	3	6	9.74	8.96	1.32	-4	2	2	14.66	15.59	0.68
-6	3	5	16.30	15.42	0.86	-4	2	3	9.87	10.77	0.92
-6	3	4	9.28	11.07	1.23	-4	2	6	11.72	12.68	1.09
-6	3	3	14.23	12.60	0.83	-4	3	7	71.56	71.57	1.61
-6	3	2	10.32	9.50	1.05	-4	3	6	15.26	14.14	0.93
-6	3	0	9.89	8.36	1.30	-4	3	5	79.79	76.99	1.78
-6	4	0	40.46	40.51	0.97	-4	3	4	18.72	17.47	0.73
-6	4	1	17.60	18.14	0.84	-4	3	3	94.01	91.44	2.13
-6	4	2	34.48	34.13	0.86	-4	3	2	19.61	20.72	0.64
-6	4	3	18.93	18.17	0.72	-4	3	1	143.00	133.61	3.67
-6	4	4	38.63	39.71	0.95	-4	3	0	20.33	19.78	0.66
-6	4	5	17.16	16.45	0.93	-4	4	0	8.98	8.07	1.21
-6	4	6	41.54	43.48	1.05	-4	4	1	9.30	10.54	1.15
-6	5	5	54.57	55.64	1.26	-4	4	2	17.76	18.34	0.75
-6	5	4	18.33	17.50	0.85	-4	4	3	9.89	11.17	1.11
-6	5	3	57.56	57.00	1.29	-4	4	4	25.22	26.27	0.77
-6	5	2	17.55	17.57	0.87	-4	4	5	9.78	7.75	1.13
-6	5	1	49.50	49.40	1.15	-4	4	6	20.06	21.16	0.88
-6	5	0	17.32	16.69	0.90	-4	5	5	10.73	6.21	0.95
-6	6	0	11.79	5.69	1.08	-4	5	4	8.56	6.67	1.40
-6	6	1	9.27	9.07	1.51	-4	5	3	11.96	9.32	0.90
-6	6	2	13.32	12.59	1.08	-4	5	2	8.57	6.10	1.22

Table 3a - Continued

H	K	L	F <sub>O</sub>	F <sub>C</sub>	σ	H	K	L	F <sub>O</sub>	F <sub>C</sub>	σ
-4	6	2	77.65	76.44	1.73	-2	4	4	69.03	67.80	1.51
-4	6	3	16.71	15.01	0.80	-2	4	5	9.63	7.74	1.15
-4	6	4	57.69	56.28	1.29	-2	4	6	40.81	41.28	1.01
-4	6	5	13.96	12.25	1.13	-2	5	6	8.97	7.17	1.49
-4	6	6	66.96	65.90	1.52	-2	5	5	79.41	77.66	1.78
-4	7	3	18.84	19.74	0.91	-2	5	4	8.52	8.40	1.34
-4	7	2	10.59	8.40	1.13	-2	5	3	118.48	113.31	2.85
-4	7	1	13.38	10.70	0.94	-2	5	2	10.77	10.71	0.84
-4	8	2	13.11	10.79	1.00	-2	5	1	120.17	114.93	2.89
-4	8	4	27.13	27.56	0.87	-2	5	0	10.80	9.82	0.85
-4	9	1	39.82	38.45	0.99	-2	6	0	17.45	15.72	0.75
-3	9	3	11.30	11.38	1.34	-2	6	4	20.90	20.96	0.76
-3	8	4	14.74	14.64	1.10	-2	7	5	55.11	55.23	1.26
-3	8	2	34.05	34.07	0.89	-2	7	3	35.41	34.28	0.85
-3	8	0	31.40	28.95	0.82	-2	7	2	8.81	6.70	1.22
-3	7	0	9.21	10.33	1.27	-2	7	1	31.57	31.58	0.79
-3	7	1	7.91	4.59	1.32	-2	7	0	10.42	8.69	1.03
-3	7	2	10.45	10.98	1.05	-2	8	0	73.56	72.58	1.63
-3	6	2	41.60	42.45	0.96	-2	8	2	87.95	87.28	1.99
-3	6	0	19.64	19.99	0.80	-2	8	4	55.41	55.76	1.27
-3	5	1	8.29	7.75	1.18	-2	10	0	26.71	26.04	0.89
-3	5	3	20.24	20.83	0.75	-1	10	0	14.53	11.32	0.92
-3	4	7	9.14	9.01	1.50	-1	9	0	8.76	10.61	1.45
-3	4	4	17.01	16.81	0.74	-1	9	1	19.10	18.53	0.82
-3	4	3	10.51	9.79	0.89	-1	8	4	27.95	27.82	0.86
-3	4	2	18.00	18.94	0.68	-1	8	2	29.21	29.97	0.82
-3	4	0	30.53	28.76	0.73	-1	8	1	10.12	10.81	1.09
-3	3	1	10.84	9.33	0.61	-1	8	0	16.37	14.05	0.68
-3	3	2	6.73	5.08	0.98	-1	7	0	8.27	11.05	1.26
-3	3	3	11.29	9.41	0.75	-1	7	3	10.74	10.27	1.10
-3	3	5	45.34	46.49	1.02	-1	6	6	18.66	19.79	1.04
-3	3	7	14.10	13.82	1.06	-1	6	4	23.97	24.17	0.75
-3	2	6	15.19	16.60	0.96	-1	6	2	34.94	35.41	0.82
-3	2	2	37.58	34.80	0.82	-1	6	0	12.65	11.89	0.82
-3	2	0	13.06	13.27	0.65	-1	5	1	34.54	35.23	0.78
-3	1	1	64.15	63.10	1.38	-1	5	2	8.74	9.64	1.01
-3	1	2	6.90	8.76	0.85	-1	5	3	18.22	17.20	0.68
-3	1	3	11.80	11.26	0.65	-1	5	4	9.53	10.45	1.08
-3	1	4	8.73	6.72	0.91	-1	5	6	10.23	9.65	1.14
-3	1	7	10.98	10.54	1.23	-1	4	6	22.95	23.40	0.87
-2	0	0	34.26	32.55	0.73	-1	4	4	22.52	23.77	0.72
-2	0	1	5.58	5.81	0.91	-1	4	2	18.35	18.43	0.56
-2	0	2	56.26	53.40	1.19	-1	4	0	71.81	70.35	1.56
-2	0	6	44.12	45.46	1.01	-1	3	1	8.66	6.60	0.61
-2	1	7	54.91	53.93	1.26	-1	3	2	6.21	7.17	0.84
-2	1	5	43.63	42.09	0.98	-1	3	3	26.59	25.98	0.65
-2	1	4	11.70	10.38	0.69	-1	3	4	7.39	6.80	1.17
-2	1	3	91.52	91.41	2.06	-1	2	6	11.39	10.65	1.12
-2	1	2	11.11	12.67	0.53	-1	2	4	7.96	6.39	1.06
-2	1	1	132.21	131.51	3.28	-1	2	2	20.72	18.93	0.52
-2	1	0	10.10	12.18	0.59	-1	1	3	70.61	67.94	1.53
-2	2	0	115.79	114.29	2.75	-1	1	5	22.25	21.84	0.74
-2	2	1	11.23	12.49	0.53	-1	0	3	5.96	0.00	0.82
-2	2	2	31.60	36.95	0.70	0	0	4	105.42	105.69	2.45
-2	2	3	11.44	11.95	0.59	0	0	6	89.94	90.17	2.05
-2	2	4	87.81	85.35	1.97	0	1	7	16.81	16.34	1.00
-2	2	6	70.19	68.64	1.56	0	1	3	60.41	61.42	1.30
-2	2	7	11.63	7.71	1.02	0	1	1	38.53	40.42	0.80
-2	3	5	23.54	23.12	0.76	0	2	0	14.95	15.98	0.43
-2	3	3	48.38	45.77	1.04	0	2	2	10.28	8.18	0.59
-2	3	2	6.84	5.64	0.83	0	2	4	29.29	21.79	0.75

Table 3a - Continued

H	K	L	F <sub>O</sub>	F <sub>C</sub>	σ	H	K	L	F <sub>O</sub>	F <sub>C</sub>	σ
0	4	2	29.99	30.92	0.70	2	4	1	10.77	9.49	0.72
0	4	4	9.21	9.25	1.25	2	4	2	51.53	54.72	1.12
0	5	5	15.24	15.40	0.94	2	4	3	8.78	8.26	1.21
0	5	4	7.94	1.19	1.26	2	4	4	45.43	47.08	1.03
0	5	3	26.58	28.17	0.74	2	5	5	59.23	61.14	1.35
0	5	1	18.37	18.07	0.58	2	5	4	9.25	4.76	1.22
0	6	0	73.67	76.44	1.62	2	5	3	54.53	56.71	1.21
0	6	2	102.34	103.18	2.37	2	5	1	94.62	98.16	2.15
0	6	4	76.41	77.28	1.71	2	5	0	9.85	9.82	0.91
0	7	5	37.64	38.66	0.97	2	6	0	15.94	15.72	0.78
0	7	3	9.86	7.53	1.14	2	6	2	12.14	12.46	0.98
0	7	1	9.32	10.59	1.26	2	7	3	46.18	47.91	1.09
0	8	0	37.16	40.24	0.90	2	7	1	78.45	80.40	1.75
0	8	2	8.40	5.11	1.38	2	8	0	69.92	72.58	1.55
0	8	4	9.88	6.29	1.35	2	8	2	71.26	73.04	1.60
0	9	3	45.90	47.65	1.10	2	8	3	9.71	6.10	1.39
0	9	1	80.17	80.42	1.81	2	10	0	27.20	26.04	0.82
0	10	0	27.92	28.20	0.86	3	8	2	18.06	16.28	0.92
0	10	1	8.99	1.81	1.37	3	8	0	28.71	28.95	0.84
1	10	1	9.66	8.08	1.46	3	7	0	10.05	10.33	1.09
1	10	0	12.94	11.32	1.10	3	7	2	11.86	9.90	0.94
1	9	0	9.16	10.61	1.39	3	6	2	13.64	14.19	0.95
1	9	1	14.20	13.51	0.99	3	6	0	19.32	19.99	0.78
1	9	3	12.18	9.52	1.30	3	5	3	22.66	23.78	0.83
1	8	4	21.09	21.21	0.94	3	4	4	21.50	22.01	0.83
1	8	1	9.08	8.34	1.24	3	4	2	29.26	31.40	0.78
1	8	0	13.72	14.05	0.91	3	4	0	28.49	28.76	0.70
1	6	5	10.56	6.86	1.16	3	3	0	7.55	5.39	0.85
1	6	4	24.62	25.73	0.81	3	3	1	27.10	28.18	0.69
1	6	2	13.76	12.67	0.82	3	3	5	27.33	27.57	0.87
1	6	0	11.75	11.89	0.90	3	2	4	11.04	7.11	1.00
1	5	0	7.77	9.73	1.01	3	2	0	13.51	13.27	0.56
1	5	5	14.11	13.82	1.00	3	1	0	6.34	7.06	0.91
1	4	4	25.13	24.48	0.71	3	1	1	29.55	29.77	0.69
1	4	2	14.22	14.79	0.69	3	1	3	18.04	17.23	0.74
1	4	1	7.03	7.22	0.88	3	0	5	10.21	0.00	1.14
1	4	0	68.00	70.35	1.47	4	0	0	82.61	85.05	1.83
1	3	0	5.78	7.77	0.85	4	0	1	19.00	20.35	0.67
1	3	1	80.85	81.18	1.78	4	0	2	117.85	117.50	2.83
1	3	3	33.86	34.65	0.79	4	0	3	15.99	15.65	0.88
1	3	5	9.31	9.44	1.24	4	0	4	80.13	78.79	1.81
1	2	4	15.01	14.47	0.78	4	1	3	15.61	13.22	0.76
1	2	2	45.22	46.50	0.96	4	1	2	10.56	8.28	0.96
1	2	1	6.04	6.84	0.85	4	1	1	10.73	8.31	0.85
1	1	1	12.79	10.93	0.49	4	1	0	10.33	12.38	0.84
1	1	3	6.90	5.90	1.07	4	2	0	25.13	26.81	0.67
1	1	5	16.52	15.37	0.75	4	2	1	10.14	9.69	1.03
2	0	0	34.87	32.55	0.74	4	2	2	29.66	30.69	0.78
2	0	1	6.07	7.57	0.84	4	2	3	8.34	9.34	1.37
2	0	2	64.66	63.09	1.39	4	2	4	12.21	9.98	1.07
2	0	4	62.03	60.47	1.37	4	3	4	14.93	11.93	0.96
2	1	6	9.16	4.47	1.50	4	3	3	76.31	75.15	1.71
2	1	5	49.11	48.60	1.12	4	3	2	15.27	15.23	0.88
2	1	3	74.51	76.26	1.64	4	3	1	106.69	109.00	2.49
2	1	2	8.35	8.66	0.91	4	3	0	19.56	19.78	0.68
2	1	1	35.31	40.00	0.76	4	4	0	10.28	8.07	0.97
2	1	0	9.69	12.18	0.61	4	4	1	9.16	8.53	1.25
2	2	0	103.71	114.29	2.39	4	4	2	11.67	9.53	0.97
2	2	1	10.98	11.54	0.60	4	4	3	8.97	7.26	1.42
2	2	2	114.12	119.09	2.70	4	4	4	19.26	17.67	0.87
2	2	3	8.14	7.53	1.28	4	5	1	19.03	19.15	0.78
2	2	4	62.74	62.52	1.38	4	5	0	8.12	8.73	1.33

Table 3a - Continued

H	K	L	F <sub>O</sub>	F <sub>C</sub>	$\sigma$
-8	0	1	21.18	21.16	1.02
-8	0	2	72.61	73.64	1.63
-8	0	3	22.75	22.36	0.87
-8	0	4	38.27	38.14	0.96
-8	0	5	20.23	19.40	0.96
-8	1	5	15.83	16.96	1.13
-8	1	4	13.29	13.36	1.15
-8	1	3	12.22	12.24	1.22
4	7	2	11.71	7.40	1.06
4	7	1	32.45	32.80	0.88
5	6	2	28.12	28.36	0.91
5	6	0	26.29	27.69	0.82
5	5	0	9.81	9.24	1.17
5	4	0	9.05	7.27	1.23
5	3	1	12.67	12.20	0.96
5	3	3	17.07	14.60	0.88
5	2	2	14.86	15.19	0.98
5	2	0	16.09	15.51	0.78
5	1	1	15.76	15.05	0.84
5	1	3	15.26	15.68	1.08
5	0	2	8.39	0.00	1.23
6	0	0	46.95	46.95	1.07
6	1	2	18.45	15.07	0.83
6	1	1	49.44	49.97	1.13
6	1	0	19.40	19.67	0.79
6	2	0	44.11	44.03	1.02
6	2	1	15.64	16.21	1.00
6	2	2	39.65	38.67	0.98
6	3	1	18.32	17.09	0.84
6	4	0	38.19	40.51	0.94
6	4	1	16.18	15.04	0.95
6	5	1	55.94	55.53	1.28
6	5	0	16.00	16.69	1.00
7	4	0	19.02	18.69	0.93

-6 6 1 9.27 9.07 1.51  
-6 6 2 13.32 12.59 1.08

-4 5 3 11.96 9.32 0.90  
-4 5 2 8.57 6.10 1.33

-7 4 5 11.11 7.95 1.14  
-7 4 4 17.58 16.43 0.91  
-7 4 3 9.87 9.07 1.28  
-7 4 2 11.34 9.30 1.14  
-7 4 0 17.79 18.69 1.03  
-7 3 1 12.53 9.62 1.03  
-7 3 3 24.52 26.06 0.80  
-7 2 6 21.64 21.95 0.82  
-7 1 1 20.00 20.09 0.87  
-7 1 5 9.59 9.89 1.49  
-6 0 0 46.51 46.95 1.05  
-6 0 1 8.91 9.89 1.21  
-6 0 2 31.50 31.96 0.80  
-6 0 3 10.43 10.50 1.03  
-6 0 4 33.28 34.44 0.81  
-6 0 5 9.76 9.31 1.18  
-6 0 6 16.07 17.19 1.01  
-6 0 7 9.80 9.14 1.40  
-6 1 7 30.84 32.92 0.95  
-6 1 6 17.76 15.82 0.85  
-6 1 5 56.76 57.61 1.26  
-6 1 4 18.26 18.76 0.82  
-6 1 3 28.26 27.27 0.77  
-6 1 2 20.42 19.87 0.72  
-6 1 1 45.02 45.22 1.02  
-6 1 0 19.22 19.67 0.80  
-6 2 0 45.50 44.03 1.05  
-6 2 1 19.69 18.97 0.76  
-6 2 2 82.37 81.88 1.84  
-6 2 3 21.09 20.98 0.72  
-6 2 4 54.33 55.51 1.21  
-6 2 5 16.83 17.75 0.91  
-6 2 6 28.17 28.28 0.87  
-6 2 7 16.47 15.11 0.96  
-6 3 6 9.74 8.96 1.32  
-6 3 5 16.30 15.42 0.86  
-6 3 4 9.28 11.07 1.23  
-6 3 3 14.23 12.60 0.83  
-6 3 2 10.32 9.50 1.05  
-6 3 0 9.89 8.36 1.30  
-6 4 0 40.46 40.51 0.97  
-6 4 1 17.60 18.14 0.84  
-6 4 2 34.48 34.13 0.86  
-6 4 3 18.93 18.17 0.72  
-6 4 4 38.63 39.71 0.95  
-6 4 5 17.16 16.45 0.93  
-6 4 6 41.54 43.48 1.05  
-6 5 5 54.57 55.64 1.26  
-6 5 4 18.33 17.50 0.85  
-6 5 3 57.56 57.00 1.29  
-6 5 2 17.55 17.57 0.87  
-6 5 1 49.50 49.40 1.15  
-6 5 0 17.32 16.69 0.90  
-6 6 0 11.79 5.69 1.08  
-6 6 1 9.27 9.07 1.51  
-6 6 2 13.32 12.59 1.08  
-6 6 3 9.43 7.46 1.46  
-6 6 5 9.47 6.18 1.49  
-6 7 3 55.02 54.92 1.26  
-6 7 2 15.76 14.08 1.04

-5 5 2 8.96 10.07 1.27  
-5 5 4 8.73 10.95 1.43  
-5 5 5 10.63 10.56 1.23  
-5 4 4 36.47 37.52 0.89  
-5 3 1 35.46 35.43 0.84  
-5 3 3 33.39 35.04 0.82  
-5 3 5 12.41 10.57 0.87  
-5 3 7 18.39 16.94 0.94  
-5 2 6 8.63 3.44 1.30  
-5 2 4 11.50 11.04 1.10  
-5 2 2 16.95 17.63 0.75  
-5 2 0 15.05 15.51 0.90  
-5 1 1 11.42 12.24 0.99  
-5 1 3 17.03 17.39 0.75  
-5 1 5 11.53 11.59 0.98  
-5 1 7 17.95 17.30 0.85  
-4 0 0 82.33 85.05 1.83  
-4 0 1 19.96 21.61 0.58  
-4 0 2 129.27 131.25 3.19  
-4 0 3 21.15 22.17 0.61  
-4 0 4 169.48 164.97 4.73  
-4 0 5 17.71 17.92 0.80  
-4 0 6 84.15 84.97 1.89  
-4 0 7 14.67 14.99 0.98  
-4 1 7 22.22 22.04 0.88  
-4 1 6 10.46 8.22 1.08  
-4 1 5 30.20 30.05 0.79  
-4 1 4 9.41 11.05 1.09  
-4 1 3 7.78 10.26 1.12  
-4 1 2 10.00 12.25 0.80  
-4 1 1 51.89 53.19 1.12  
-4 1 0 10.58 12.38 0.83  
-4 2 0 24.84 26.81 0.70  
-4 2 1 9.24 10.83 0.94  
-4 2 2 14.66 15.59 0.68  
-4 2 3 9.87 10.77 0.92  
-4 2 6 11.72 12.68 1.09  
-4 3 7 71.56 71.57 1.61  
-4 3 6 15.26 14.14 0.93  
-4 3 5 79.79 76.99 1.78  
-4 3 4 18.72 17.47 0.73  
-4 3 3 94.01 91.44 2.13  
-4 3 2 19.61 20.72 0.64  
-4 3 1 143.00 133.61 3.67  
-4 3 0 20.33 19.78 0.66  
-4 4 0 8.98 8.07 1.21  
-4 4 1 9.30 10.54 1.15  
-4 4 2 17.76 18.34 0.75  
-4 4 3 9.89 11.17 1.11  
-4 4 4 25.22 26.27 0.77  
-4 4 5 9.78 7.75 1.13  
-4 4 6 20.06 21.16 0.88  
-4 5 5 10.73 6.21 0.95  
-4 5 4 8.56 6.67 1.40  
-4 5 3 11.96 9.32 0.90  
-4 5 2 8.57 6.10 1.33  
-4 5 1 32.72 32.75 0.82  
-4 5 0 8.89 8.73 1.30  
-4 6 0 85.73 81.89 1.93  
-4 6 1 17.77 15.99 0.75

-2	5	3	48.38	45.77	1.04	0	2	2	10.28	8.18	0.59
-2	3	2	6.84	5.64	0.83	0	2	4	29.39	21.78	0.75
-4	7	2	10.59	8.40	1.13	-2	5	3	118.48	113.31	2.85
-4	7	1	13.38	10.70	0.94	-2	5	2	10.77	10.71	0.84
-4	8	2	13.11	10.79	1.00	-2	5	1	120.17	114.93	2.89
-4	8	4	27.13	27.56	0.87	-2	5	0	10.80	9.82	0.85
-4	9	1	39.82	38.45	0.99	-2	6	0	17.45	15.72	0.75
-3	9	3	11.30	11.38	1.34	-2	6	4	20.90	20.96	0.76
-3	8	4	14.74	14.64	1.10	-2	7	5	55.11	55.23	1.26
-3	8	2	34.05	34.07	0.89	-2	7	3	35.41	34.28	0.85
-3	8	0	31.40	28.95	0.82	-2	7	2	8.81	6.70	1.22
-3	7	0	9.21	10.33	1.27	-2	7	1	31.57	31.58	0.79
-3	7	1	7.91	4.59	1.32	-2	7	0	10.42	8.69	1.03
-3	7	2	10.45	10.98	1.05	-2	8	0	73.56	72.58	1.63
-3	6	2	41.60	42.45	0.96	-2	8	2	87.95	87.28	1.99
-3	6	0	19.64	19.99	0.80	-2	8	4	55.41	55.76	1.27
-3	5	1	8.29	7.75	1.18	-2	10	0	26.71	26.04	0.89
-3	5	3	20.24	20.83	0.75	-1	10	0	14.53	11.32	0.92
-3	4	7	9.14	9.01	1.50	-1	9	0	8.76	10.61	1.45
-3	4	4	17.01	16.81	0.74	-1	9	1	19.10	18.53	0.82
-3	4	3	10.51	9.79	0.89	-1	8	4	27.95	27.82	0.86
-3	4	2	18.00	18.94	0.68	-1	8	2	29.21	29.97	0.82
-3	4	0	30.53	28.76	0.73	-1	8	1	10.12	10.81	1.09
-3	3	1	10.84	9.33	0.61	-1	8	0	16.37	14.05	0.68
-3	3	2	6.73	5.08	0.98	-1	7	0	8.27	11.05	1.26
-3	3	3	11.29	9.41	0.75	-1	7	3	10.74	10.27	1.10
-3	3	5	45.34	46.49	1.02	-1	6	6	18.66	19.79	1.04
-3	3	7	14.10	13.82	1.06	-1	6	4	23.97	24.17	0.76
-3	2	6	15.19	16.60	0.96	-1	6	2	34.94	35.41	0.82
-3	2	2	37.58	34.80	0.82	-1	6	0	12.65	11.89	0.82
-3	2	0	13.06	13.27	0.65	-1	5	1	34.54	35.23	0.78
-3	1	1	64.15	63.10	1.38	-1	5	2	8.74	9.64	1.01
-3	1	2	6.90	8.76	0.85	-1	5	3	18.22	17.20	0.68
-3	1	3	11.80	11.26	0.65	-1	5	4	9.53	10.45	1.08
-3	1	4	8.73	6.72	0.91	-1	5	6	10.23	9.65	1.14
-3	1	7	10.98	10.54	1.23	-1	4	6	22.95	23.40	0.87
-2	0	0	34.26	32.55	0.73	-1	4	4	22.52	23.77	0.72
-2	0	1	5.58	5.81	0.91	-1	4	2	18.35	18.43	0.56
-2	0	2	56.26	53.40	1.19	-1	4	0	71.81	70.35	1.56
-2	0	6	44.12	45.46	1.01	-1	3	1	8.66	6.60	0.61
-2	1	7	54.91	53.93	1.26	-1	3	2	6.21	7.17	0.84
-2	1	5	43.63	42.09	0.98	-1	3	3	26.59	25.98	0.65
-2	1	4	11.70	10.38	0.69	-1	3	4	7.39	6.80	1.17
-2	1	3	91.52	91.41	2.06	-1	2	6	11.39	10.65	1.12
-2	1	2	11.11	12.67	0.53	-1	2	4	7.96	6.39	1.06
-2	1	1	132.21	131.51	3.28	-1	2	2	20.72	18.93	0.52
-2	1	0	10.10	12.18	0.59	-1	1	3	70.61	67.94	1.53
-2	2	0	115.79	114.29	2.75	-1	1	5	22.25	21.84	0.74
-2	2	1	11.23	12.49	0.53	-1	0	3	5.96	0.00	0.82
-2	2	2	31.60	36.95	0.70	0	0	4	105.42	105.69	2.45
-2	2	3	11.44	11.95	0.59	0	0	6	89.94	90.17	2.05
-2	2	4	87.81	85.35	1.97	0	1	7	16.81	16.34	1.00
-2	2	6	70.19	68.64	1.50	0	1	3	60.41	61.42	1.30
-2	2	7	11.63	7.71	1.02	0	1	1	38.53	40.42	0.80
-2	3	5	23.54	23.12	0.76	0	2	0	14.95	15.98	0.43
-2	3	3	48.38	45.77	1.04	0	2	2	10.28	8.18	0.59
-2	3	2	6.84	5.64	0.83	0	2	4	29.39	31.78	0.75
-2	3	1	44.45	41.94	0.95	0	2	6	24.65	25.67	0.79
-2	4	0	82.01	82.31	1.81	0	3	5	101.08	100.26	2.34
-2	4	1	9.53	10.51	0.76	0	3	3	149.09	145.80	3.89
-2	4	2	103.12	99.22	2.38	0	3	1	133.38	135.19	3.32
-2	4	3	9.63	11.19	0.94	0	4	0	42.01	44.00	0.90

2 2 4 62.74 62.52 1.38

4 5 1 19.03 19.15 0.78  
4 5 0 8.12 8.73 1.33

0	6	0	73.67	76.44	1.62
0	6	2	102.34	103.18	2.37
0	6	4	76.41	77.28	1.71
0	7	5	37.64	38.66	0.97
0	7	3	9.86	7.53	1.14
0	7	1	9.32	10.59	1.26
0	8	0	37.16	40.24	0.90
0	8	2	8.40	5.11	1.38
0	8	4	9.88	6.29	1.35
0	9	3	45.90	47.65	1.10
0	9	1	80.17	80.42	1.81
0	10	0	27.92	28.20	0.86
0	10	1	8.99	1.81	1.37
1	10	1	9.66	8.08	1.46
1	10	0	12.94	11.32	1.10
1	9	0	9.16	10.61	1.39
1	9	1	14.20	13.51	0.99
1	9	3	12.18	9.52	1.30
1	8	4	21.09	21.21	0.94
1	8	1	9.08	8.34	1.24
1	8	0	13.72	14.05	0.91
1	6	5	10.56	6.86	1.16
1	6	4	24.62	25.73	0.81
1	6	2	13.76	12.67	0.82
1	6	0	11.75	11.89	0.90
1	5	0	7.77	9.73	1.01
1	5	5	14.11	13.82	1.00
1	4	4	25.13	24.48	0.71
1	4	2	14.22	14.79	0.69
1	4	1	7.03	7.22	0.88
1	4	0	68.00	70.35	1.47
1	3	0	5.78	7.77	0.85
1	3	1	80.85	81.18	1.78
1	3	3	33.86	34.65	0.79
1	3	5	9.31	9.44	1.24
1	2	4	15.01	14.47	0.78
1	2	2	45.22	46.50	0.96
1	2	1	6.04	6.84	0.85
1	1	1	12.79	10.93	0.49
1	1	3	6.90	5.90	1.07
1	1	5	16.52	15.37	0.75
2	0	0	34.87	32.55	0.74
2	0	1	6.07	7.57	0.84
2	0	2	64.66	63.09	1.39
2	0	4	62.03	60.47	1.37
2	1	6	9.16	4.47	1.50
2	1	5	49.11	48.60	1.12
2	1	3	74.51	76.26	1.64
2	1	2	8.35	8.66	0.91
2	1	1	35.31	40.00	0.76
2	1	0	9.69	12.18	0.61
2	2	0	103.71	114.29	2.39
2	2	1	10.98	11.54	0.60
2	2	2	114.12	119.09	2.70
2	2	3	8.14	7.53	1.28
2	2	4	62.74	62.52	1.38
2	2	6	49.45	49.06	1.16
2	3	5	17.44	18.41	0.96
2	3	1	27.93	27.30	0.65
2	4	0	76.32	82.31	1.67

2	5	3	54.53	56.71	1.21
2	5	1	94.62	98.16	2.15
2	5	0	9.85	9.82	0.91
2	6	0	15.94	15.72	0.78
2	6	2	12.14	12.46	0.98
2	7	3	46.18	47.91	1.09
2	7	1	78.45	80.40	1.75
2	8	0	69.92	72.58	1.55
2	8	2	71.26	73.04	1.60
2	8	3	9.71	6.10	1.39
2	10	0	27.20	26.04	0.82
3	8	2	18.06	16.28	0.92
3	8	0	28.71	28.95	0.84
3	7	0	10.05	10.33	1.09
3	7	2	11.86	9.90	0.94
3	6	2	13.64	14.19	0.95
3	6	0	19.32	19.99	0.78
3	5	3	22.66	23.78	0.83
3	4	4	21.50	22.01	0.83
3	4	2	29.26	31.40	0.78
3	4	0	28.49	28.76	0.70
3	3	0	7.55	5.39	0.85
3	3	1	27.10	28.18	0.69
3	3	5	27.33	27.57	0.87
3	2	4	11.04	7.11	1.00
3	2	0	13.51	13.27	0.56
3	1	0	6.34	7.06	0.91
3	1	1	29.55	29.77	0.69
3	1	3	18.04	17.23	0.74
3	0	5	10.21	0.00	1.14
4	0	0	82.61	85.05	1.83
4	0	1	19.00	20.35	0.67
4	0	2	117.85	117.50	2.83
4	0	3	15.99	15.65	0.88
4	0	4	80.13	78.79	1.81
4	1	3	15.61	13.22	0.76
4	1	2	10.56	8.28	0.96
4	1	1	10.73	8.31	0.85
4	1	0	10.33	12.38	0.84
4	2	0	25.13	26.81	0.67
4	2	1	10.14	9.69	1.03
4	2	2	29.66	30.69	0.78
4	2	3	8.34	9.34	1.37
4	2	4	12.21	9.98	1.07
4	3	4	14.93	11.93	0.96
4	3	3	76.31	75.15	1.71
4	3	2	15.27	15.23	0.88
4	3	1	106.69	109.00	2.49
4	3	0	19.56	19.78	0.68
4	4	0	10.28	8.07	0.97
4	4	1	9.16	8.53	1.25
4	4	2	11.67	9.53	0.97
4	4	3	8.97	7.26	1.42
4	4	4	19.26	17.67	0.87
4	5	1	19.03	19.15	0.78
4	5	0	8.12	8.73	1.33
4	6	0	79.11	81.89	1.77
4	6	1	14.52	14.12	0.94
4	6	2	51.04	53.08	1.19
4	6	3	12.03	12.86	1.28



-8	1	4	13.29	13.36	1.15
-8	1	3	12.22	12.24	1.22
4	7	2	11.71	7.40	1.06
4	7	1	32.45	32.80	0.88
5	6	2	28.12	28.36	0.91
5	6	0	26.29	27.69	0.82
5	5	0	9.81	9.24	1.17
5	4	0	9.05	7.27	1.23
5	3	1	12.67	12.20	0.96
5	3	3	17.07	14.60	0.88
5	2	2	14.86	15.19	0.98
5	2	0	16.09	15.51	0.78
5	1	1	15.76	15.05	0.84
5	1	3	15.26	15.68	1.08
5	0	2	8.39	0.00	1.23
6	0	0	46.95	46.95	1.07
6	1	2	18.45	15.07	0.83
6	1	1	49.44	49.97	1.13
6	1	0	19.40	19.67	0.79
6	2	0	44.11	44.03	1.02
6	2	1	15.64	16.21	1.00
6	2	2	39.65	38.67	0.98
6	3	1	18.32	17.09	0.84
6	4	0	38.19	40.51	0.94
6	4	1	16.18	15.04	0.95
6	5	1	55.94	55.53	1.28
6	5	0	16.00	16.69	1.00
7	4	0	19.02	18.69	0.93

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Table 3b. Observed and Calculated Structure Factors for Synthetic Titanite at 270°C

H	K	L	F <sub>o</sub>	F <sub>c</sub>	σ	H	K	L	F <sub>o</sub>	F <sub>c</sub>	σ
-7	5	3	25.40	22.51	2.62	-4	6	6	120.20	120.09	2.75
-7	4	4	32.29	32.70	2.20	-4	7	5	19.21	5.02	2.85
-7	4	0	30.11	31.13	2.50	-4	7	3	41.68	41.00	1.70
-7	3	3	43.88	47.42	1.80	-4	7	1	27.68	25.09	2.10
-7	2	6	46.13	44.28	1.65	-4	8	4	45.11	46.07	1.89
-7	1	1	39.78	40.07	1.92	-4	9	1	73.35	70.18	1.95
-6	0	0	82.07	83.00	1.93	-3	9	3	20.30	21.12	3.24
-6	0	2	54.84	54.52	1.53	-3	8	2	62.07	59.13	1.71
-6	0	4	57.13	56.97	1.53	-3	8	0	54.31	51.79	1.73
-6	0	6	24.03	25.14	2.59	-3	6	2	81.39	81.96	1.88
-6	1	7	59.96	60.59	1.82	-3	6	0	42.03	39.82	1.59
-6	1	5	104.04	107.76	2.35	-3	5	1	22.35	16.04	2.09
-6	1	3	53.56	52.95	1.65	-3	5	3	37.84	37.79	1.56
-6	1	1	88.08	84.93	2.02	-3	5	5	17.59	11.40	2.83
-6	2	0	86.74	85.55	2.03	-3	4	4	29.41	28.49	1.82
-6	2	2	156.31	155.07	3.47	-3	4	2	35.09	34.59	1.39
-6	2	4	102.77	104.27	2.31	-3	4	0	56.66	54.93	1.49
-6	2	6	57.04	54.04	1.76	-3	3	1	19.93	18.21	1.59
-6	3	5	21.74	20.82	2.72	-3	3	3	17.38	18.37	2.34
-6	4	0	74.83	74.79	1.91	-3	3	5	83.63	87.55	1.97
-6	4	2	63.78	64.59	1.73	-3	3	7	26.94	24.87	2.41
-6	4	4	71.86	72.68	1.86	-3	2	6	28.41	29.26	1.95
-6	4	6	77.63	78.80	1.99	-3	2	2	75.15	70.47	1.66
-6	5	5	100.33	102.18	2.37	-3	2	0	25.20	23.36	1.32
-6	5	3	106.86	106.69	2.44	-3	1	1	124.20	121.55	2.66
-6	5	1	91.17	93.15	2.18	-3	1	3	17.85	17.88	1.92
-6	7	3	96.97	97.30	2.30	-3	1	7	24.75	23.34	2.43
-6	7	1	76.25	75.67	2.04	-2	0	0	67.28	64.38	1.46
-5	6	0	50.50	49.53	1.71	-2	0	6	78.95	82.24	1.92
-5	5	1	25.41	22.40	2.07	-2	1	7	104.49	101.95	2.40
-5	4	4	62.35	64.90	1.69	-2	1	5	82.92	80.57	1.93
-5	3	1	65.18	67.49	1.67	-2	1	3	182.50	180.38	4.08
-5	3	3	64.72	66.09	1.62	-2	1	1	265.67	260.73	6.54
-5	3	7	29.96	31.17	2.33	-2	2	0	228.02	225.24	5.35
-5	2	4	29.13	24.89	1.79	-2	2	2	63.86	73.40	1.41
-5	2	2	30.45	28.77	1.67	-2	2	4	168.16	167.17	3.73
-5	2	0	29.83	32.18	2.10	-2	2	6	131.65	130.41	2.92
-5	1	1	22.05	18.88	2.10	-2	3	5	45.76	42.91	1.57
-5	1	3	37.72	37.91	1.57	-2	3	3	90.85	88.06	1.98
-5	1	5	21.23	27.63	2.76	-2	3	1	85.73	80.78	1.83
-5	1	7	31.82	25.19	1.84	-2	4	0	157.23	159.38	3.45
-4	0	0	161.38	166.68	3.56	-2	4	2	196.43	191.35	4.52
-4	0	2	249.55	255.72	6.03	-2	4	4	129.82	128.59	2.84
-4	0	4	316.94	315.50	8.44	-2	4	6	80.13	75.26	1.93
-4	0	6	157.51	156.49	3.52	-2	5	5	146.82	147.35	3.28
-4	1	7	43.05	43.92	1.94	-2	5	3	226.39	216.90	5.33
-4	1	5	59.82	60.29	1.64	-2	5	1	230.05	224.13	5.43
-4	1	3	22.90	24.14	1.78	-2	6	0	31.73	29.24	1.80
-4	1	1	104.54	106.95	2.25	-2	6	2	21.71	17.37	2.18
-4	2	0	52.34	54.21	1.46	-2	6	4	34.98	37.11	1.87
-4	2	2	33.89	34.66	1.40	-2	7	5	98.70	99.61	2.31
-4	2	6	21.35	21.42	2.55	-2	7	3	65.08	62.71	1.66
-4	3	7	128.35	129.46	2.92	-2	7	1	58.80	59.59	1.64
-4	3	5	146.27	145.26	3.24	-2	8	0	139.73	138.37	3.11
-4	3	3	179.65	175.14	4.03	-2	8	2	164.25	163.14	3.70
-4	3	1	268.37	258.59	6.66	-2	8	4	99.92	103.19	2.37
-4	4	0	20.90	19.50	2.52	-2	8	4	99.92	103.19	2.37
-4	4	2	41.51	42.36	1.51	-2	10	0	49.86	48.23	1.88
-4	4	4	53.35	54.63	1.59	-1	9	1	31.79	33.98	2.24
-4	4	6	41.16	43.06	1.91	-1	8	4	50.52	48.81	1.81
-4	5	5	20.46	15.74	2.58	-1	8	2	54.37	54.96	1.62
-4	5	3	20.74	20.04	2.64	-1	8	0	28.52	25.55	1.91
-4	5	1	57.48	58.87	2.64	-1	7	3	20.15	20.93	2.53

Table 3b - Continued

H	K	L	F <sub>O</sub>	F <sub>C</sub>	σ	H	K	L	F <sub>O</sub>	F <sub>C</sub>	σ
-1	5	1	64.01	67.69	1.53	2	1	1	70.61	79.26	1.54
-1	5	3	34.82	33.39	1.62	2	2	2	227.11	234.94	5.34
-1	4	6	39.19	40.70	1.89	2	2	4	120.72	120.98	2.67
-1	4	4	46.50	47.84	1.53	2	2	6	92.32	92.77	2.26
-1	4	2	34.29	36.33	1.27	2	3	5	34.18	35.78	1.97
-1	4	0	139.34	138.89	3.01	2	3	1	54.44	53.69	1.33
-1	3	1	18.28	13.66	1.37	2	4	0	151.68	159.38	3.31
-1	3	3	49.88	50.26	1.32	2	4	2	102.49	105.72	2.25
-1	2	6	25.21	22.05	2.23	2	4	4	87.41	88.59	2.02
-1	2	4	16.84	12.68	2.27	2	5	5	113.44	113.51	2.59
-1	2	2	40.98	38.07	1.08	2	5	3	106.73	109.86	2.38
-1	1	1	10.28	2.14	1.65	2	5	1	187.16	190.21	4.23
-1	1	3	138.30	131.43	2.98	2	6	0	25.95	29.24	2.21
-1	1	5	39.67	39.75	1.67	2	6	2	22.80	24.00	2.33
-1	1	7	21.64	16.73	2.70	2	7	3	87.48	88.88	2.11
0	0	4	204.01	205.67	4.68	2	7	1	148.76	149.69	3.30
0	0	6	169.82	172.90	3.84	2	8	0	136.30	138.37	3.03
0	1	7	32.32	27.91	2.23	2	8	2	130.88	136.58	2.95
0	1	3	121.09	121.89	2.59	2	10	0	50.49	48.23	1.81
0	1	1	77.83	80.72	1.62	3	8	2	27.89	28.71	2.66
0	2	0	29.61	32.19	0.94	3	8	0	53.41	51.79	1.69
0	2	2	21.59	16.28	1.30	3	7	1	17.42	6.78	2.70
0	2	4	57.32	59.38	1.50	3	6	2	28.01	27.34	2.02
0	2	6	45.58	47.03	1.79	3	6	0	39.72	39.82	1.62
0	3	5	191.95	191.88	4.38	3	5	1	17.96	12.06	2.68
0	3	3	291.38	286.27	7.46	3	5	3	41.11	42.43	1.80
0	3	1	262.73	268.78	6.44	3	4	4	41.13	41.55	1.71
0	4	0	84.42	89.94	1.81	3	4	2	56.52	58.76	1.59
0	4	2	61.20	62.89	1.43	3	4	0	55.87	54.93	1.46
0	4	4	22.49	20.49	2.24	3	3	1	53.03	55.29	1.44
0	5	5	31.60	28.71	1.76	3	3	3	23.15	17.18	2.10
0	5	3	52.12	53.42	1.51	3	3	5	49.85	50.22	1.90
0	5	1	34.76	36.22	1.31	3	2	0	22.32	23.36	1.52
0	6	0	145.64	150.18	3.19	3	1	1	56.12	57.43	1.37
0	6	2	196.12	198.84	4.48	3	1	3	32.30	33.50	1.95
0	6	4	145.74	147.88	3.24	4	0	0	163.82	166.68	3.62
0	7	5	70.37	71.99	1.93	4	0	2	225.84	226.89	5.32
0	7	1	24.54	22.83	2.11	4	0	4	151.13	150.74	3.40
0	8	0	73.82	74.61	1.78	4	1	3	31.07	25.37	1.75
0	9	3	85.48	87.66	2.13	4	1	1	25.75	20.76	1.73
0	9	1	150.61	147.99	3.38	4	2	0	53.07	54.21	1.38
0	10	0	52.39	52.33	1.86	4	2	2	59.51	59.67	1.60
1	9	1	28.61	25.22	2.14	4	2	4	20.19	17.04	3.01
1	9	3	22.17	17.21	3.09	4	3	3	143.68	143.19	3.20
1	8	4	36.97	38.06	2.16	4	3	1	209.24	211.69	4.84
1	8	0	26.92	25.55	2.00	4	4	0	19.69	19.51	2.56
1	6	4	47.20	47.22	1.70	4	4	2	23.68	20.92	2.23
1	6	2	21.08	23.95	2.54	4	4	4	29.68	33.90	2.77
1	6	0	23.51	23.71	1.98	4	5	1	32.55	34.55	1.92
1	5	3	20.90	12.24	2.31	4	6	0	152.13	153.39	3.38
1	5	5	28.69	26.90	2.16	4	6	2	99.84	101.00	2.30
1	4	4	45.11	44.93	1.55	4	7	1	63.83	62.93	1.76
1	4	2	29.83	28.73	1.42	5	6	2	50.98	51.96	1.93
1	4	0	135.68	138.89	2.93	5	6	0	50.11	49.53	1.66
1	3	1	161.11	158.42	3.53	5	4	0	17.62	9.80	2.75
1	3	3	66.70	67.98	1.60	5	3	1	24.28	21.15	2.26
1	2	4	24.55	27.07	2.27	5	3	3	24.24	25.55	2.99
1	2	2	90.21	92.55	1.93	5	2	2	30.97	30.74	2.02
1	1	1	25.00	22.61	1.14	5	2	0	32.99	32.18	1.84
1	1	3	14.77	11.10	2.25	5	1	1	22.00	25.84	2.67
1	1	5	25.64	26.34	2.23	5	1	3	30.97	26.27	2.07

Table 3b - Continued

H	K	L	F <sub>O</sub>	F <sub>C</sub>	$\sigma$
6	4	0	76.13	74.79	1.87
6	5	1	109.22	104.55	2.50
7	4	0	30.51	31.13	2.33
7	2	0	21.93	14.99	2.63
-8	0	2	127.88	133.64	2.91
-8	0	4	73.97	71.25	1.87
-8	1	5	35.58	36.20	2.00
-8	1	3	28.76	29.57	2.61
-8	2	2	26.37	29.68	2.92
-8	2	4	28.43	22.38	2.29
-8	3	3	108.24	110.78	2.53
-7	5	1	26.69	19.51	2.42

-4 5 3 20.74 20.04 2.64

-1 7 3 20.15 20.93 2.53

-6 0 0 82.07 83.00 1.93  
-6 0 2 54.84 54.52 1.53  
-6 0 4 57.13 56.97 1.53  
-6 0 6 24.03 25.14 2.59  
-6 1 7 59.96 60.59 1.82  
-6 1 5 104.04 107.76 2.35  
-6 1 3 53.56 52.95 1.65  
-6 1 1 88.08 84.93 2.02  
-6 2 0 86.74 85.55 2.03  
-6 2 2 156.31 155.07 3.47  
-6 2 4 102.77 104.27 2.31  
-6 2 6 57.04 54.04 1.76  
-6 3 5 21.74 20.82 2.72  
-6 4 0 74.83 74.79 1.91  
-6 4 2 63.78 64.59 1.73  
-6 4 4 71.86 72.68 1.86  
-6 4 6 77.63 78.80 1.99  
-6 5 5 100.33 102.18 2.37  
-6 5 3 106.86 106.69 2.44  
-6 5 1 91.17 93.15 2.18  
-6 7 3 96.97 97.30 2.30  
-6 7 1 76.25 75.67 2.04  
-5 6 0 50.50 49.53 1.71  
-5 5 1 25.41 22.40 2.07  
-5 4 4 62.35 64.90 1.69  
-5 3 1 65.18 67.49 1.67  
-5 3 3 64.72 66.09 1.62  
-5 3 7 29.96 31.17 2.33  
-5 2 4 29.13 24.89 1.79  
-5 2 2 30.45 28.77 1.67  
-5 2 0 29.83 32.18 2.10  
-5 1 1 22.05 18.88 2.10  
-5 1 3 37.72 37.91 1.57  
-5 1 5 21.23 27.63 2.76  
-5 1 7 31.82 25.19 1.84  
-4 0 0 161.38 166.68 3.56  
-4 0 2 249.55 255.72 6.03  
-4 0 4 316.94 315.50 8.44  
-4 0 6 157.51 156.49 3.52  
-4 1 7 43.05 43.92 1.94  
-4 1 5 59.82 60.29 1.64  
-4 1 3 22.90 24.14 1.78  
-4 1 1 104.54 106.95 2.25  
-4 2 0 52.34 54.21 1.46  
-4 2 2 33.89 34.66 1.40  
-4 2 6 21.35 21.42 2.55  
-4 3 7 128.35 129.46 2.92  
-4 3 5 146.27 145.26 3.24  
-4 3 3 179.65 175.14 4.03  
-4 3 1 268.37 258.59 6.66  
-4 4 0 20.90 19.50 2.52  
-4 4 2 41.51 42.36 1.51  
-4 4 4 53.35 54.63 1.59  
-4 4 6 41.16 43.06 1.91  
-4 5 5 20.46 15.74 2.58  
-4 5 3 20.74 20.04 2.64  
-4 5 1 57.43 58.87 1.67  
-4 6 0 157.48 153.39 3.51  
-4 6 2 143.54 143.49 3.19  
-4 6 4 105.58 104.32 2.38

-3 9 3 20.30 21.12 3.24  
-3 8 2 62.07 59.13 1.71  
-3 8 0 54.31 51.79 1.73  
-3 6 2 81.39 81.96 1.88  
-3 6 0 42.03 39.82 1.59  
-3 5 1 22.35 16.04 2.09  
-3 5 3 37.84 37.79 1.56  
-3 5 5 17.59 11.40 2.83  
-3 4 4 29.41 28.49 1.82  
-3 4 2 35.09 34.59 1.39  
-3 4 0 56.66 54.93 1.49  
-3 3 1 19.93 18.21 1.59  
-3 3 3 17.38 18.37 2.34  
-3 3 5 83.63 87.55 1.97  
-3 3 7 26.94 24.87 2.41  
-3 2 6 28.41 29.26 1.95  
-3 2 2 75.15 70.47 1.66  
-3 2 0 25.20 23.36 1.32  
-3 1 1 124.20 121.55 2.66  
-3 1 3 17.85 17.88 1.92  
-3 1 7 24.75 23.34 2.43  
-2 0 0 67.28 64.38 1.46  
-2 0 6 78.95 82.24 1.92  
-2 1 7 104.49 101.95 2.40  
-2 1 5 82.92 80.57 1.93  
-2 1 3 182.50 180.38 4.08  
-2 1 1 265.67 260.73 6.54  
-2 2 0 228.02 225.24 5.35  
-2 2 2 63.86 73.40 1.41  
-2 2 4 168.16 167.17 3.73  
-2 2 6 131.65 130.41 2.92  
-2 3 5 45.76 42.91 1.57  
-2 3 3 90.86 88.06 1.98  
-2 3 1 85.73 80.78 1.83  
-2 4 0 157.23 159.38 3.45  
-2 4 2 198.43 191.35 4.52  
-2 4 4 129.82 128.59 2.84  
-2 4 6 80.13 75.26 1.93  
-2 5 5 146.82 147.35 3.28  
-2 5 3 226.39 216.90 5.33  
-2 5 1 230.05 224.13 5.43  
-2 6 0 31.73 29.24 1.80  
-2 6 2 21.71 17.37 2.18  
-2 6 4 34.98 37.11 1.87  
-2 7 5 98.70 99.61 2.31  
-2 7 3 65.08 62.71 1.66  
-2 7 1 58.80 59.59 1.64  
-2 8 0 139.73 138.37 3.11  
-2 8 2 164.25 163.14 3.70  
-2 8 4 99.92 103.19 2.37  
-2 10 0 49.86 48.23 1.88  
-1 9 1 31.79 33.98 2.24  
-1 8 4 50.52 48.81 1.81  
-1 8 2 54.37 54.96 1.62  
-1 8 0 28.52 25.55 1.91  
-1 7 3 20.15 20.93 2.53  
-1 6 6 38.80 37.48 1.87  
-1 6 4 44.57 46.05 1.63  
-1 6 2 68.24 68.22 1.65  
-1 6 0 27.60 23.71 1.63

1	1	5	25.64	26.34	2.23	5	1	1	22.00	25.84	2.67
2	0	0	67.92	64.38	1.46	5	1	3	30.97	26.27	2.07
-1	3	1	18.28	13.66	1.37	2	4	0	151.68	159.38	3.31
-1	3	3	49.88	50.26	1.32	2	4	2	102.49	105.72	2.25
-1	2	6	25.21	22.05	2.23	2	4	4	87.41	88.59	2.02
-1	2	4	16.84	12.68	2.27	2	5	5	113.44	113.51	2.59
-1	2	2	40.98	38.07	1.08	2	5	3	106.73	109.86	2.38
-1	1	1	10.28	2.14	1.65	2	5	1	187.16	190.21	4.23
-1	1	3	138.30	131.43	2.98	2	6	0	25.95	29.24	2.21
-1	1	5	39.67	39.75	1.67	2	6	2	22.80	24.00	2.33
-1	1	7	21.64	16.73	2.70	2	7	3	87.48	88.88	2.11
0	0	4	204.01	205.67	4.68	2	7	1	148.76	149.69	3.30
0	0	6	169.82	172.90	3.84	2	8	0	136.30	138.37	3.03
0	1	7	32.32	27.91	2.23	2	8	2	130.88	136.58	2.95
0	1	3	121.09	121.89	2.59	2	10	0	50.49	48.23	1.81
0	1	1	77.83	80.72	1.62	3	8	2	27.89	28.71	2.66
0	2	0	29.61	32.19	0.94	3	8	0	53.41	51.79	1.69
0	2	2	21.59	16.28	1.30	3	7	1	17.42	6.78	2.70
0	2	4	57.32	59.38	1.50	3	6	2	28.01	27.34	2.02
0	2	6	45.58	47.03	1.79	3	6	0	39.72	39.82	1.62
0	3	5	191.95	191.88	4.38	3	5	1	17.96	12.06	2.68
0	3	3	291.38	286.27	7.46	3	5	3	41.11	42.43	1.80
0	3	1	262.73	268.78	6.44	3	4	4	41.13	41.55	1.71
0	4	0	84.42	89.94	1.81	3	4	2	56.52	58.76	1.59
0	4	2	61.20	62.89	1.43	3	4	0	55.87	54.93	1.46
0	4	4	22.49	20.49	2.24	3	3	1	53.03	55.29	1.44
0	5	5	31.60	28.71	1.76	3	3	3	23.15	17.18	2.10
0	5	3	52.12	53.42	1.51	3	3	5	49.85	50.22	1.90
0	5	1	34.76	36.22	1.31	3	2	0	22.32	23.36	1.52
0	6	0	145.64	150.18	3.19	3	1	1	56.12	57.43	1.37
0	6	2	196.12	198.84	4.48	3	1	3	32.30	33.50	1.95
0	6	4	145.74	147.88	3.24	4	0	0	163.82	166.68	3.62
0	7	5	70.37	71.99	1.93	4	0	2	225.84	226.89	5.32
0	7	1	24.54	22.83	2.11	4	0	4	151.13	150.74	3.40
0	8	0	73.82	74.61	1.78	4	1	0	31.07	25.37	1.75
0	9	3	85.48	87.66	2.13	4	1	1	25.75	20.76	1.73
0	9	1	150.61	147.99	3.38	4	2	0	53.07	54.21	1.38
0	10	0	52.39	52.33	1.86	4	2	2	59.51	59.67	1.60
1	9	1	28.61	25.22	2.14	4	2	4	20.19	17.04	3.01
1	9	3	22.17	17.21	3.09	4	3	3	143.68	143.19	3.20
1	8	4	36.97	38.06	2.16	4	3	1	209.24	211.69	4.84
1	8	0	26.92	25.55	2.00	4	4	0	19.69	19.51	2.56
1	6	4	47.20	47.22	1.70	4	4	2	23.68	20.92	2.23
1	6	2	21.08	23.95	2.54	4	4	4	29.68	33.90	2.77
1	6	0	23.51	23.71	1.98	4	5	1	32.55	34.55	1.92
1	5	3	20.90	12.24	2.31	4	6	0	152.13	153.39	3.38
1	5	5	28.69	26.90	2.16	4	6	2	99.84	101.00	2.30
1	4	4	45.11	44.93	1.55	4	7	1	63.83	62.93	1.76
1	4	2	29.83	28.73	1.42	5	6	2	50.98	51.96	1.93
1	4	0	135.68	138.89	2.93	5	6	0	50.11	49.53	1.66
1	3	1	161.11	158.42	3.53	5	4	0	17.62	9.80	2.75
1	3	3	66.70	67.98	1.60	5	3	1	24.28	21.15	2.26
1	2	4	24.55	27.07	2.27	5	3	3	24.24	25.55	2.99
1	2	2	90.21	92.55	1.93	5	2	2	30.97	30.74	2.02
1	1	1	25.00	22.61	1.14	5	2	0	32.99	32.18	1.84
1	1	3	14.77	11.10	2.25	5	1	1	22.00	25.84	2.67
1	1	5	25.64	26.34	2.23	5	1	3	30.97	26.27	2.07
2	0	0	67.92	64.38	1.46	6	0	0	84.14	83.00	1.98
2	0	2	123.24	122.75	2.65	6	1	1	95.30	94.18	2.22
2	0	4	119.50	118.05	2.64	6	2	0	86.00	85.55	2.03
2	1	5	96.16	94.35	2.20	6	2	2	74.66	72.48	1.95
2	1	3	149.04	148.03	3.27	6	3	1	29.27	28.01	2.23

			73.97	71.25	1.87
-8	1	5	35.58	36.20	2.00
-8	1	3	28.76	29.57	2.61
-8	2	2	26.37	29.68	2.92
-8	2	4	28.43	22.38	2.29
-8	3	3	108.24	110.78	2.53
-7	5	1	26.69	19.51	2.42

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