TABLE 3. List of observed and calculated structure factors for the structure of ingersonite

h	k	l	F_o	F_c
0	1	0	38.00	-41.86
-1	2	0	113.86	-53.00
0	2	0	18.64	9.84
-1	3	0	26.22	-7.30
0	3	0	74.01	73.43
-2	4	0	662.68	-334.17
-1	4	0	53.54	52.54
0	4	0	30.86	12.79
-2	5	0	24.09	-7.50
-1	5	0	73.53	-39.67
0	5	0	35.40	-35.34
-3	6	0	86.62	87.88
-2	6	0	33.37	-5.41
-1	6	0	61.05	-44.24
0	6	0	380.39	377.18
-3	7	0	54.47	46.35
-2	7	0	52.51	-25.27
-1	7	0	40.47	-10.41
0	7	0	5.81	-2.37
-4	8	0	325.02	-159.00
-3	8	0	59.84	-25.60
-2	8	0	17.08	-10.17
-1	8	0	61.21	-28.45
0	8	0	0.00	-7.77
-4	9	0	23.06	18.48
-3	9	0	49.80	49.71
-2	9	0	49.11	14.24
-1	9	0	58.95	-4.23
0	9	0	38.64	40.35
-5	10	0	66.58	-35.15
-4	10	0	18.84	13.33
-3	10	0	55.38	53.36
-2	10	0	219.89	-110.12
-1	10	0	36.75	37.34
0	10	0	6.23	15.67
-5	11	0	53.90	-49.43
-4	11	0	40.35	-20.51
-3	11	0	23.98	-20.11
-2	11	0	6.42	-8.70
-1	1	1	75.61	73.64
0	1	1	39.03	-20.88
-2	2	1	9.07	-9.39
-1	2	1	56.77	-19.36
0	2	1	219.57	111.82
-3	3	1	56.68	60.92
-2	3	1	22.17	-3.26
-1	3	1	32.60	-27.76
0	3	1	82.56	-41.73
-4	4	1	187.23	-192.19
-3	4	1	51.94	44.01
-2	4	1	43.35	-15.56
-1	4	1	32.86	30.36
0	4	1	25.89	0.52
-5	5	1	45.28	44.60
-4	5	1	56.66	56.44
-3	5	1	62.35	-36.92
-2	5	1	25.60	0.61
-1	5	1	40.66	3.32
0	5	1	43.02	-22.19
-6	6	1	19.90	19.59
-5	6	1	14.56	-11.25
-4	6	1	25.15	-8.54
-3	6	1	31.11	-27.66
-2	6	1	122.17	61.44
-1	6	1	51.55	-43.48
0	6	1	19.96	0.64
-7	7	1	40.93	40.17
-6	7	1	36.04	-35.05
-5	7	1	30.21	-23.68
-4	7	1	29.27	26.80
-3	7	1	53.72	-10.70
-2	7	1	59.82	-29.51
-1	7	1	28.16	27.25
0	7	1	18.30	-9.22
-8	8	1	27.78	21.10
-7	8	1	42.33	-0.89
-6	8	1	125.08	61.25
-5	8	1	47.12	9.22
-4	8	1	25.99	-3.79
-3	8	1	13.27	8.81
-2	8	1	9.37	1.90
-1	8	1	25.36	6.98
0	8	1	77.53	37.18
-9	9	1	12.46	12.58
-8	9	1	19.95	1.09
-7	9	1	56.47	-33.24
-6	9	1	54.12	-36.00
-5	9	1	34.04	-8.74
-4	9	1	23.59	11.00
-3	9	1	29.47	24.05
-2	9	1	28.38	-9.93
-1	9	1	48.70	-34.34
0	9	1	48.30	-24.66
-10	10	1	100.13	-99.36
-9	10	1	28.57	18.92
-8	10	1	22.00	-9.58
-7	10	1	8.13	2.87
-6	10	1	11.78	-11.53
-5	10	1	26.49	17.21
-4	10	1	81.81	-81.41
-3	10	1	38.52	33.31
-2	10	1	0.00	-6.34
-1	10	1	0.00	1.63
0	10	1	19.71	-8.15
-9	11	1	16.14	-14.89
-8	11	1	21.42	13.97
-7	11	1	17.37	-0.94
-6	11	1	27.80	-22.75
-5	11	1	53.57	53.86
-4	11	1	49.65	51.62
-3	11	1	10.19	-15.89
-2	11	1	18.54	-0.02
-1	1	2	53.46	-56.79
0	1	2	125.50	-60.77
-2	2	2	665.17	668.11
-1	2	2	64.52	-65.65
0	2	2	12.78	-7.24
-3	3	2	53.90	-57.63
-2	3	2	45.16	29.99
-1	3	2	37.77	-18.68
0	3	2	87.34	45.60
-4	4	2	9.05	-8.41
-3	4	2	110.23	-52.78
-2	4	2	6.99	-6.51
-1	4	2	66.10	-14.70
0	4	2	516.94	-261.20
-5	5	2	19.44	19.52
-4	5	2	65.20	9.58
-3	5	2	78.45	25.03
-2	5	2	132.66	134.08
-1	5	2	39.41	37.54
0	5	2	34.14	-17.07
-6	6	2	9.55	11.99
-5	6	2	43.18	43.39
-4	6	2	423.60	-211.03
-3	6	2	43.96	43.62
-2	6	2	12.35	7.34
-1	6	2	71.49	-36.64
0	6	2	37.84	-6.04
-7	7	2	66.85	-67.27
-6	7	2	76.00	-40.74
-5	7	2	21.92	4.09
-4	7	2	26.91	-26.10
-3	7	2	39.08	-17.90
-2	7	2	61.65	-60.51
-1	7	2	61.85	-52.01
0	7	2	81.49	-39.78
-8	8	2	287.56	280.71
-7	8	2	61.59	-42.51
-6	8	2	6.72	0.20
-5	8	2	65.76	65.77
-4	8	2	10.58	-9.77
-3	8	2	55.95	-42.70
-2	8	2	308.02	303.33
-1	8	2	30.69	-17.56
0	8	2	16.54	-8.29
-9	9	2	2.88	1.89
-8	9	2	33.94	-9.30
-7	9	2	30.74	-16.18
-6	9	2	62.97	53.90
-5	9	2	58.84	40.56
-4	9	2	54.63	-26.37
-3	9	2	22.28	-16.70
-2	9	2	21.85	20.01
-1	9	2	44.39	-22.09
0	9	2	46.54	23.09
-10	10	2	0.00	-2.76
-9	10	2	46.80	-19.53
-8	10	2	15.24	-1.03
-7	10	2	40.89	-19.12
-6	10	2	246.52	-120.81
-5	10	2	45.17	-21.52
-4	10	2	16.83	-3.33
-3	10	2	43.57	-18.40
-2	10	2	16.81	13.81
-1	10	2	55.50	-9.75
0	10	2	198.81	-98.78
-8	11	2	29.31	31.80
-7	11	2	2.07	5.19
-6	11	2	21.61	13.89
-5	11	2	31.68	33.48
-4	11	2	52.73	9.02
-3	11	2	51.28	-6.37
0	0	3	209.31	-215.63
-1	1	3	56.87	56.53
0	1	3	59.85	59.61
-2	2	3	11.77	9.92
-1	2	3	70.59	-40.54
0	2	3	6.73	-7.59
-3	3	3	101.74	102.71
-2	3	3	31.64	-17.52
-1	3	3	16.23	0.27
0	3	3	4.82	-1.03
-4	4	3	6.93	7.48
-3	4	3	62.12	-22.78
-2	4	3	154.52	78.26
-1	4	3	59.94	1.42
0	4	3	20.98	-20.95
-5	5	3	4.88	2.99
-4	5	3	44.50	-13.11
-3	5	3	79.82	-46.15
-2	5	3	64.73	-40.03
-1	5	3	66.05	-26.11
0	5	3	16.25	-15.85
-6	6	3	126.47	-127.47
-5	6	3	35.30	27.32
-4	6	3	25.56	-3.30
-3	6	3	64.19	64.93
-2	6	3	13.70	-7.74
-1	6	3	35.69	33.37
0	6	3	106.63	-107.55
-7	7	3	72.67	71.73
-6	7	3	48.86	47.67
-5	7	3	47.19	-26.00
-4	7	3	19.32	11.14
-3	7	3	12.70	-3.56
-2	7	3	12.93	-6.19
-1	7	3	57.96	54.39
0	7	3	65.82	64.61
-8	8	3	28.13	27.68
-7	8	3	41.72	-30.35
-6	8	3	5.81	6.83
-5	8	3	47.50	-34.96
-4	8	3	111.76	55.80
-3	8	3	50.40	-37.62
-2	8	3	7.97	9.22
-1	8	3	34.62	-24.12
0	8	3	0.00	6.90
-9	9	3	16.34	17.97
-8	9	3	28.89	-28.18
-7	9	3	10.11	-6.69
-6	9	3	22.20	19.77
-5	9	3	60.68	-28.89
-4	9	3	53.64	-22.52
-3	9	3	18.83	16.05
-2	9	3	7.85	-0.65
-1	9	3	29.06	-28.72
0	9	3	12.23	11.15
-10	10	3	14.98	7.34

-9	10	3	33.19	-10.42	-7	9	4	7.81	-3.86	-6	8	5	8.75	-9.17	-7	7	6	9.08	6.47
-8	10	3	107.88	53.62	-6	9	4	16.60	-14.80	-5	8	5	50.92	48.76	-6	7	6	29.02	-8.61
-7	10	3	34.40	1.16	-5	9	4	48.75	-22.98	-4	8	5	5.47	-6.34	-5	7	6	80.45	-39.49
-6	10	3	16.24	-8.07	-4	9	4	67.52	-61.98	-3	8	5	49.37	39.55	-4	7	6	74.64	54.71
-5	10	3	30.82	-7.84	-3	9	4	66.52	-54.14	-2	8	5	120.49	-119.58	-3	7	6	45.97	44.96
-4	10	3	0.00	2.29	-2	9	4	46.46	-21.44	-1	8	5	47.18	41.57	-2	7	6	54.05	-27.93
-3	10	3	36.45	8.40	-1	9	4	28.34	-12.57	0	8	5	5.18	-2.50	-1	7	6	39.38	-22.65
-2	10	3	73.14	37.16	0	9	4	20.26	-9.42	-9	9	5	58.49	58.77	0	7	6	11.02	-9.30
-1	10	3	46.05	-10.69	-10	10	4	219.19	222.72	-8	9	5	49.87	48.69	-8	8	6	9.53	8.54
0	10	3	0.00	2.20	-9	10	4	54.84	-43.86	-7	9	5	11.69	-6.77	-7	8	6	29.92	-14.19
-8	11	3	36.24	-21.89	-8	10	4	12.63	-13.99	-6	9	5	15.74	-0.08	-6	8	6	23.10	-16.72
-7	11	3	7.61	1.64	-7	10	4	32.84	32.19	-5	9	5	20.37	11.41	-5	8	6	47.01	-23.26
-6	11	3	16.43	6.07	-6	10	4	14.54	-14.61	-4	9	5	24.40	-17.03	-4	8	6	314.94	-154.87
-5	11	3	16.72	12.84	-5	10	4	46.06	-20.68	-3	9	5	62.53	59.49	-3	8	6	58.53	-10.96
-4	11	3	11.89	0.13	-4	10	4	249.66	247.75	-2	9	5	49.34	49.14	-2	8	6	16.39	1.19
-3	11	3	42.72	-30.27	-3	10	4	44.48	-30.72	-1	9	5	24.44	-19.49	-1	8	6	47.90	-19.16
-1	1	4	131.26	130.53	-2	10	4	23.26	-14.17	0	9	5	4.67	-2.66	0	8	6	2.15	-0.27
0	1	4	74.86	37.27	-1	10	4	36.81	36.11	-10	10	5	0.00	4.92	-9	9	6	47.19	46.76
-2	2	4	4.88	-5.11	0	10	4	0.00	-5.30	-9	10	5	14.77	-17.34	-8	9	6	68.28	-0.09
-1	2	4	45.54	26.37	-8	11	4	53.12	46.42	-8	10	5	3.38	0.67	-7	9	6	36.02	6.37
0	2	4	484.51	-243.36	-7	11	4	50.69	43.52	-7	10	5	47.56	-40.78	-6	9	6	45.50	45.15
-3	3	4	77.23	-81.36	-6	11	4	40.47	-23.34	-6	10	5	91.52	46.19	-5	9	6	23.05	17.68
-2	3	4	120.81	-58.90	-5	11	4	11.81	-0.99	-5	10	5	35.77	-33.26	-4	9	6	10.39	9.12
-1	3	4	19.43	16.37	-4	11	4	16.29	12.64	-4	10	5	2.46	1.78	-3	9	6	55.61	54.62
0	3	4	26.09	14.11	-3	11	4	40.34	-21.02	-3	10	5	39.44	-27.76	-2	9	6	59.33	19.22
-4	4	4	452.16	459.03	-1	1	5	45.10	31.65	-2	10	5	6.19	10.96	-1	9	6	50.25	-16.06
-3	4	4	75.48	-74.48	0	1	5	97.66	-48.71	-1	10	5	33.42	-33.04	0	9	6	40.98	41.58
-2	4	4	13.14	-0.70	-2	2	5	39.45	-35.45	0	10	5	115.01	55.48	-9	10	6	32.10	32.03
-1	4	4	65.00	65.38	-1	2	5	52.73	52.18	-8	11	5	0.00	11.91	-8	10	6	219.17	-110.18
0	4	4	26.27	-13.44	0	2	5	3.91	1.38	-7	11	5	53.11	-17.87	-7	10	6	61.70	56.44
-5	5	4	6.99	3.32	-3	3	5	74.14	74.88	-6	11	5	44.59	-18.70	-6	10	6	10.70	4.74
-4	5	4	22.72	-13.88	-2	3	5	32.52	30.68	-5	11	5	13.96	14.97	-5	10	6	28.12	-18.85
-3	5	4	75.10	-38.27	-1	3	5	60.80	-34.43	-4	11	5	0.00	-9.81	-4	10	6	11.91	13.33
-2	5	4	85.62	61.44	0	3	5	44.01	-23.25	-3	11	5	19.84	-19.45	-3	10	6	50.22	50.01
-1	5	4	66.57	57.15	-4	4	5	11.65	8.84	0	0	6	645.35	662.06	-2	10	6	229.35	-116.52
0	5	4	77.70	-39.14	-3	4	5	68.03	-41.63	-1	1	6	35.62	-34.39	-1	10	6	39.35	38.74
-6	6	4	10.96	11.31	-2	4	5	24.18	23.25	0	1	6	25.14	-26.34	-8	11	6	20.59	-20.50
-5	6	4	61.54	-28.70	-1	4	5	41.56	-36.09	-2	2	6	3.31	-1.57	-7	11	6	38.08	-17.09
-4	6	4	16.80	11.75	0	4	5	113.02	58.43	-1	2	6	78.07	-37.44	-6	11	6	58.69	-54.25
-3	6	4	44.22	-20.75	-5	5	5	14.55	12.92	0	2	6	2.40	0.35	-5	11	6	45.20	-33.83
-2	6	4	379.77	-188.92	-4	5	5	27.66	-17.47	-3	3	6	125.92	128.16	-4	11	6	45.43	-20.73
-1	6	4	40.67	-0.03	-3	5	5	31.21	-27.64	-2	3	6	55.57	16.65	-3	11	6	21.21	-17.86
0	6	4	15.38	-7.75	-2	5	5	39.24	36.68	-1	3	6	42.58	-19.00	-1	1	7	24.45	-20.15
-7	7	4	52.90	52.13	-1	5	5	64.05	-22.19	0	3	6	49.35	48.13	0	1	7	42.30	-21.39
-6	7	4	68.14	3.36	0	5	5	50.81	-25.16	-4	4	6	5.51	1.64	-2	2	7	10.00	10.04
-5	7	4	72.16	19.25	-6	6	5	6.42	-6.94	-3	4	6	44.61	44.77	-1	2	7	66.30	7.80
-4	7	4	69.58	68.85	-5	6	5	52.50	-1.91	-2	4	6	513.07	-255.92	0	2	7	131.84	67.91
-3	7	4	6.18	4.67	-4	6	5	113.01	57.16	-1	4	6	52.59	50.68	-3	3	7	27.53	27.08
-2	7	4	14.69	5.04	-3	6	5	38.91	-1.03	0	4	6	20.79	20.73	-2	3	7	69.95	-30.97
-1	7	4	43.61	43.20	-2	6	5	12.40	10.61	-5	5	6	25.03	-24.91	-1	3	7	47.83	-38.59
0	7	4	78.71	38.89	-1	6	5	53.32	-17.72	-4	5	6	34.02	-15.36	0	3	7	76.65	-38.26
-8	8	4	9.16	10.01	0	6	5	14.70	-6.73	-3	5	6	29.08	-11.47	-4	4	7	112.85	-118.55
-7	8	4	31.40	32.41	-7	7	5	10.23	9.69	-2	5	6	16.54	4.10	-3	4	7	46.76	43.75
-6	8	4	324.65	-158.38	-6	7	5	31.35	-6.69	-1	5	6	95.67	-50.36	-2	4	7	19.57	0.23
-5	8	4	61.85	54.34	-5	7	5	76.06	-44.62	0	5	6	68.84	-68.28	-1	4	7	26.38	22.51
-4	8	4	13.81	12.03	-4	7	5	56.71	-35.46	-6	6	6	337.95	338.93	0	4	7	4.43	2.57
-3	8	4	37.90	-22.83	-3	7	5	25.97	-8.08	-5	6	6	69.61	-58.44	-5	5	7	40.65	40.31
-2	8	4	15.67	-1.17	-2	7	5	17.18	15.23	-4	6	6	15.57	-14.14	-4	5	7	63.41	54.64
-1	8	4	58.97	57.58	-1	7	5	33.21	23.16	-3	6	6	44.51	44.29	-3	5	7	10.01	-6.96
0	8	4	265.83	-130.75	0	7	5	24.84	-10.69	-2	6	6	12.21	5.05	-2	5	7	35.58	-17.05
-9	9	4	47.03	-48.05	-8	8	5	94.33	-93.94	-1	6	6	56.68	-35.06	-1	5	7	38.46	10.98
-8	9	4	37.99	-20.84	-7	8	5	28.87	22.89	0	6	6	372.96	371.11	0	5	7	91.21	-45.96

-6	6	7	4.44	-5.04	0	4	8	492.67	-245.20	-1	3	9	29.20	-12.78	-2	2	10	11.85	-11.08
-5	6	7	36.83	-25.95	-5	5	8	85.96	86.36	0	3	9	72.56	72.75	-1	2	10	16.84	13.99
-4	6	7	1.60	-0.14	-4	5	8	76.09	0.04	-4	4	9	8.72	8.12	0	2	10	559.30	-281.41
-3	6	7	46.27	-42.97	-3	5	8	29.09	12.80	-3	4	9	44.99	-18.03	-3	3	10	37.49	-38.23
-2	6	7	115.85	59.13	-2	5	8	55.06	53.82	-2	4	9	193.45	98.72	-2	3	10	114.08	-59.10
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-7	7	7	11.29	11.20	-6	6	8	23.69	23.57	-5	5	9	7.28	7.89	-4	4	10	434.03	431.73
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