

AM-88-374

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Crystal chemistry of double-ring silicates: Structures of sugilite and bran-
nockite

Thomas Armbruster, Roland Oberhänsli

For deposit: Table 4

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Table 4 (for deposit)

observed and calculated structure factors for
sugilite (Wessels Mine S.A.R.),
brannockite (large domain),
brannockite (small domain).

Reflections with $F_{\text{obs}} > 6 \sigma(F_{\text{obs}})$ are marked "L"
and were rejected (marked "R").

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
0	0	2	87.27	84.12	3	3	6	51.39	50.57	3	4	7	38.38	40.43
0	0	4	235.47	235.47	3	3	8	4.87	3.81	3	4	8	19.70	19.17
0	0	6	84.76	72.38	3	3	10	72.06	71.26	3	4	9	90.30	91.52
0	0	8	325.43	328.49	3	3	12	77.08	75.94	3	4	10	5.97	5.89
0	0	10	24.47	25.11	3	3	14	3.05	3.96	3	4	11	17.57	18.05
0	0	12	23.88	25.64	3	3	16	15.10	15.00	3	4	12	4.23	4.56
0	0	14	136.52	135.75	0	0	0	32.96	35.54	3	4	13	37.47	37.66
0	0	16	113.23	114.12	0	0	2	46.89	46.71	3	4	14	4.12	3.43
0	0	18	80.01	79.85	0	0	4	20.06	17.07	3	4	15	15.99	16.60
0	1	0	26.73	24.03	0	0	6	20.06	20.47	3	4	16	7.63	7.55
0	1	2	15.24	13.12	0	0	8	27.11	27.47	3	4	17	23.10	23.11
0	1	4	71.39	70.03	0	0	10	64.07	65.42	4	4	0	4.51	3.02
0	1	6	39.16	36.86	0	0	12	1.20	2.68	4	4	2	49.45	48.57
0	1	8	32.06	31.23	0	0	14	48.14	48.50	4	4	4	119.57	120.16
0	1	10	3.02	1.56	0	0	16	15.93	15.86	4	4	6	61.48	61.01
0	1	12	50.15	50.03	0	0	18	44.48	44.01	4	4	8	39.16	38.22
0	1	14	19.65	20.23	1	1	0	115.38	114.33	4	4	10	67.33	66.56
0	1	16	4.17	2.03	1	1	2	102.61	100.67	4	4	12	43.98	44.32
0	1	18	4.43	5.91	1	1	4	55.52	55.43	4	4	14	6.40	5.86
1	1	0	6.83	5.38	1	1	6	32.21	32.28	4	4	16	22.42	22.64
1	1	2	115.54	114.12	1	1	8	107.23	107.96	0	5	0	57.99	56.91
1	1	4	221.98	222.12	1	1	10	42.27	42.47	0	5	2	15.15	14.74
1	1	6	36.86	36.39	1	1	12	17.93	18.20	0	5	4	8.66	7.30
1	1	8	15.74	14.66	1	1	14	64.44	64.34	0	5	6	6.00	4.83
1	1	10	89.04	88.96	1	1	16	63.91	63.10	0	5	8	13.79	12.85
1	1	12	106.03	105.90	1	1	18	68.65	69.07	0	5	10	3.07	2.85
1	1	14	23.91	24.26	1	1	0	59.13	57.94	0	5	12	10.86	10.97
1	1	16	15.09	14.69	1	1	2	9.44	8.81	0	5	14	20.62	20.57
1	1	18	58.68	58.07	1	1	4	66.88	65.92	0	5	16	7.63	8.34
0	2	0	194.82	200.38	1	1	6	18.41	18.33	1	5	0	1.32	1.60
0	2	2	55.84	54.09	1	1	8	17.97	18.44	1	5	1	100.73	101.22
0	2	4	101.64	101.13	1	1	10	17.68	17.97	1	5	2	31.39	30.87
0	2	6	11.18	10.20	1	1	12	35.83	35.77	1	5	3	50.67	52.04
0	2	8	110.72	109.36	1	1	14	24.87	24.53	1	5	4	44.12	45.29
0	2	10	42.25	42.43	1	1	16	39.78	41.03	1	5	5	83.08	83.14
0	2	12	35.15	34.91	1	1	18	12.82	12.93	1	5	6	44.44	44.74
0	2	14	23.94	23.29	2	2	0	14.23	15.16	1	5	7	36.80	38.00
0	2	16	29.92	30.05	2	2	2	37.43	38.74	1	5	8	31.85	33.02
0	2	18	28.92	27.94	2	2	4	5.61	4.45	1	5	9	94.91	95.25
1	2	0	44.19	45.04	2	2	6	29.18	30.25	1	5	10	53.09	52.55
1	2	2	130.10	129.72	2	2	8	10.43	11.29	1	5	11	10.73	10.20
1	2	4	31.71	30.26	2	2	10	3.25	3.20	1	5	12	40.52	40.69
1	2	6	58.82	58.76	2	2	12	13.08	13.30	1	5	13	64.87	64.62
1	2	8	23.40	26.53	2	2	14	27.64	27.32	1	5	14	23.39	23.39
1	2	10	6.37	9.88	2	2	16	2.74	2.82	1	5	15	15.63	15.72
1	2	12	1.18	1.54	2	2	18	4.21	3.67	1	5	16	5.25	6.58
1	2	14	42.82	41.83	2	2	0	9.08	9.92	2	5	0	194.08	196.57
1	2	16	13.30	13.68	2	2	2	22.09	22.29	2	5	1	83.68	84.29
1	2	18	54.27	55.00	2	2	4	15.44	15.28	2	5	2	39.15	39.15
1	2	0	55.75	56.56	2	2	6	5.51	5.44	2	5	3	57.98	59.28
1	2	2	46.22	47.65	2	2	8	11.23	10.32	2	5	4	17.10	18.05
1	2	4	11.81	11.34	2	2	10	4.45	4.23	2	5	5	40.63	41.04
1	2	6	39.97	40.64	2	2	12	70.72	72.01	2	5	6	58.96	57.68
1	2	8	23.87	24.37	2	2	14	4.42	4.23	2	5	7	51.60	52.51
1	2	10	27.79	28.18	2	2	16	11.59	12.69	2	5	8	121.19	121.54
1	2	12	6.83	7.84	2	2	18	26.81	26.22	2	5	9	44.47	44.76
1	2	14	61.47	61.71	2	2	0	74.41	75.46	2	5	10	3.62	2.48
1	2	16	45.60	46.21	2	2	2	9.79	10.05	2	5	11	0.00	4.54
1	2	18	33.74	33.18	2	2	4	191.81	192.09	2	5	12	12.83	12.31
1	2	0	182.57	190.70	3	3	6			3	3	0		

1	8	11	20.81	20.89	17.07	17.40	2	10	7	6.15	7.75
1	8	12	27.07	27.23	14.06	13.88	3	10	0	4.46	1.31
1	8	13	3.97	3.86	33.89	33.16	3	10	1	37.40	36.80
1	8	14	17.19	16.51	3.58	5.85	3	10	2	4.20	5.96
2	8	0	9.64	10.42	40.91	41.61	3	10	3	36.70	36.69
2	8	1	3.66	2.88	16.77	16.30	3	10	4	18.57	18.53
2	8	2	37.46	36.72	16.90	16.28	0	11	0	39.65	39.57
2	8	3	10.37	11.27	18.52	18.91	0	11	2	3.56	0.92
2	8	4	107.68	107.73	22.27	21.43	0	11	4	6.40	7.60
2	8	5	14.26	14.84	5.18	5.83	0	11	6	3.33	3.25
2	8	6	34.18	33.88	6.00	7.28	0	11	8	25.90	25.60
2	8	7	0.00	2.18	3.38	4.72	1	11	0	7.73	9.09
2	8	8	22.22	22.08	20.47	20.74	1	11	1	40.69	39.49
2	8	9	4.93	4.49	3.70	4.83	1	11	2	9.71	9.36
2	8	10	59.97	59.46	29.59	29.01	1	11	3	29.13	28.29
2	8	11	2.36	4.12	26.29	26.12	1	11	4	33.87	33.68
2	8	12	46.60	46.81	11.61	11.07	1	11	5	54.58	52.97
3	8	0	16.56	17.02	4.06	4.09	1	11	6	17.12	16.79
3	8	1	22.83	22.75	45.49	44.77	1	11	0	52.54	51.69
3	8	2	3.69	1.18	3.08	2.09	2	11	1	9.82	9.78
3	8	3	12.87	13.16	42.12	41.96	2	11	1	35.03	35.30
3	8	4	11.16	11.23	36.92	36.48	0	12	0	40.80	41.03
3	8	5	51.32	51.39	26.49	27.13	0	12	2		
3	8	6	5.35	4.79	25.82	25.22					
3	8	7	6.43	6.40	31.56	31.56					
3	8	8	14.80	14.64	40.46	40.46					
3	8	9	46.03	45.19	41.11	41.41					
3	8	10	10.29	9.77	37.30	37.92					
3	8	11	15.61	16.56	11.54	11.41					
3	8	12	42.78	41.38	44.85	44.85					
4	8	0	26.75	26.93	39.02	38.71					
4	8	1	4.92	4.81	37.76	37.39					
4	8	2	20.76	20.62	10.83	10.82					
4	8	3	24.01	23.34	4.14	1.95					
4	8	4	13.95	14.06	7.78	7.63					
4	8	5	3.30	2.35	6.77	6.26					
4	8	6	13.29	13.11	15.51	15.56					
4	8	7	31.37	31.51	73.51	72.47					
4	8	8	14.64	14.80	6.23	6.84					
4	8	9	30.74	31.79	47.91	46.21					
5	8	0	22.35	21.86	4.83	5.89					
5	8	1	28.90	29.14	43.61	44.53					
5	8	2	30.33	29.86	18.86	19.11					
5	8	3	54.05	54.74	47.90	48.57					
5	8	4	26.43	25.68	32.77	32.25					
5	8	5	16.95	17.36	25.58	26.03					
5	8	6	6.98	6.23	21.03	20.54					
5	8	7	6.29	8.30	47.06	47.22					
6	8	0	20.19	19.43	10.60	11.18					
6	8	1	97.20	97.29	22.31	22.36					
0	9	0	19.53	19.70	24.50	24.49					
0	9	1	7.69	9.56	39.73	39.98					
0	9	2	90.11	89.19	16.72	16.38					
0	9	3	93.68	93.16	68.84	66.66					
0	9	4	15.47	14.96	20.57	20.27					
0	9	5	11.72	11.36	3.87	4.04					
0	9	6	29.90	30.72	22.06	22.08					
1	9	0	1.31	0.77	77.86	77.08					
1	9	1	0	0	1.8	1.8					

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
0	1	0	57.51	58.03	5	11	0	85.43	87.34	2	12	1	6.53	7.89
1	1	0	41.01	48.76	6	11	0	33.22	33.20	4	10	1	3.39	12.54
0	1	0	209.52	222.47	0	12	0	78.06	77.46	5	10	1	11.70	12.32
1	2	0	23.40	16.53	1	13	0	54.85	53.01	6	10	2	25.53	23.68
2	2	0	234.36	240.85	2	12	0	31.57	31.02	7	10	2	4.24	67.28
0	3	0	161.76	168.83	4	12	0	48.48	48.81	7	10	2	23.84	52.15
1	3	0	44.22	34.96	5	12	0	38.90	39.36	2	11	2	16.55	76.98
2	3	0	116.13	115.36	0	13	0	58.85	60.08	0	11	2	17.26	31.63
3	3	0	15.25	7.60	1	14	1	86.20	85.93	3	11	2	18.17	76.85
0	4	0	71.77	73.55	2	14	1	15.23	16.90	4	11	2	19.92	19.30
2	4	0	2.68	6.20	1	15	1	0.00	6.03	5	11	2	0.00	19.60
3	4	0	32.32	33.75	0	1	2	51.97	50.21	6	11	2	84.98	58.18
4	4	0	35.33	37.30	1	2	2	14.11	12.73	0	12	2	239.01	27.66
0	5	0	110.38	107.03	1	2	2	56.02	53.63	6	12	2	90.92	94.77
1	5	0	20.63	22.11	2	2	2	39.68	38.58	4	12	2	119.52	33.45
2	5	0	253.69	256.65	0	3	0	144.31	135.70	5	12	2	154.68	22.02
4	5	0	54.12	54.92	1	3	1	35.94	38.39	0	13	2	25.30	24.91
5	5	0	62.48	65.46	2	3	1	8.18	6.38	1	13	2	11.88	64.26
0	6	0	136.40	135.27	2	3	1	16.17	14.66	2	13	2	150.31	28.64
1	6	0	109.77	109.15	3	4	1	69.15	66.93	1	13	2	10.69	20.72
2	6	0	29.62	29.44	2	4	1	102.84	98.16	3	13	2	65.84	20.72
3	6	0	129.59	129.22	2	4	1	58.23	55.43	4	14	2	32.48	61.22
4	6	0	0.00	1.71	4	4	1	58.16	55.43	2	14	2	129.11	25.58
6	6	0	150.75	151.36	0	5	1	16.10	15.91	1	14	2	60.38	52.71
1	7	0	99.41	99.85	1	5	1	19.94	18.62	1	15	2	84.11	51.03
2	7	0	81.40	81.28	2	5	1	34.30	38.50	1	15	2	118.19	12.35
3	7	0	17.30	14.66	4	5	1	59.58	54.15	1	15	2	29.02	55.29
4	7	0	121.85	121.67	5	5	1	15.62	17.41	1	15	2	119.38	74.95
5	7	0	51.50	50.68	0	6	1	36.66	36.74	2	16	2	199.52	26.11
6	7	0	8.96	10.42	1	6	1	30.81	29.84	3	16	2	38.99	29.04
0	8	0	113.60	105.85	2	6	1	44.42	44.47	1	16	2	6.88	1.24
1	8	0	32.14	32.00	3	6	1	11.53	10.62	1	16	2	85.22	49.88
3	8	0	64.45	66.08	4	6	1	42.68	41.81	2	16	2	47.62	58.88
4	8	0	55.03	55.30	6	6	1	4.88	3.94	4	16	2	47.62	31.27
5	8	0	25.47	26.01	1	7	1	26.11	26.43	6	6	2	110.09	16.02
6	8	0	58.34	59.76	2	7	1	26.30	25.40	1	7	2	122.53	15.35
7	8	0	88.85	89.70	4	7	1	21.19	21.79	2	7	2	13.80	31.11
8	8	0	140.64	140.56	5	7	1	22.83	22.57	3	7	2	39.69	32.98
0	9	0	54.93	55.49	6	7	1	9.02	3.73	4	7	2	91.50	16.99
1	9	0	14.18	15.27	7	7	1	0.00	2.00	1	7	2	33.58	33.68
2	9	0	88.76	88.88	6	7	1	13.28	13.14	2	7	2	41.28	40.83
3	9	0	24.98	24.38	0	8	1	46.41	46.62	3	7	2	62.68	62.51
5	9	0	40.68	41.02	5	8	1	33.45	33.94	4	7	2	35.85	36.10
6	9	0	22.84	22.52	6	8	1	12.36	11.46	5	7	2	34.15	34.15
7	9	0	16.43	17.54	7	8	1	14.84	15.54	6	7	2	21.12	21.26
8	9	0	52.42	50.16	8	8	1	0.00	1.36	1	8	2	81.77	81.77
9	9	0	96.49	93.76	1	10	1	44.37	43.47	3	8	2	13.59	14.40
0	10	0	95.49	95.74	2	10	1	22.22	23.14	4	8	2	25.68	25.51
1	10	0	39.03	39.07	3	10	1	44.57	44.86	5	8	2	52.40	50.85
2	10	0	16.78	16.40	4	10	1	23.80	24.41	6	8	2	79.85	80.45
3	10	0	72.68	72.90	5	10	1	22.11	22.38	7	8	2	17.79	18.29
4	10	0	39.05	40.82	6	10	1	8.81	10.72	8	8	2	78.84	78.62
5	10	0	41.60	40.12	7	10	1	5.16	1.51	9	8	2	34.17	33.85
6	10	0	44.22	44.57	8	10	1	0.00	1.17	5	9	2	69.03	69.69
7	10	0	56.32	57.21	3	11	1	0.00	8.99	6	9	2	13.46	12.28
8	10	0	83.65	81.81	4	11	1	0.00	1.22	8	9	2	30.68	28.95
9	10	0	73.61	74.37	5	11	1	13.65	12.75	9	9	2	50.26	48.55
0	11	0	9.33	10.64	6	11	1	0.00	22.39	0	10	2	24.80	24.18
1	11	0	7.33	7.43	1	12	1	0.00	3.88	1	10	2	89.26	86.67
2	11	0	9.33	10.64	2	12	1	0.00	3.88	2	10	2	33.87	33.60

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
5	10	3	27.64	29.11	6	9	5	11.85	12.95	7	8	6	44.41	45.11
6	10	3	7.85	10.34	8	9	5	6.30	5.50	8	8	6	89.48	89.04
2	11	3	0.00	7.21	1	10	5	17.75	15.36	0	9	6	153.64	159.85
3	11	3	11.88	10.87	1	9	5	16.59	15.98	1	9	6	68.37	67.91
3	11	3	0.00	0.56	2	10	5	24.48	24.26	2	9	6	50.99	51.13
4	11	3	10.55	8.81	3	10	5	23.38	22.83	3	9	6	93.00	91.28
5	11	3	17.52	18.72	4	10	5	39.57	40.27	5	9	6	18.07	16.10
6	11	3	0.00	2.87	5	10	5	6.64	10.99	6	9	6	65.14	66.25
1	12	3	0.00	10.29	6	10	5	14.92	16.20	7	9	6	41.20	40.72
2	12	3	16.76	15.11	7	10	5	0.00	6.42	8	9	6	4.99	5.55
4	12	3	8.85	4.52	8	10	5	0.00	12.09	9	10	6	39.68	41.14
5	12	3	10.91	10.91	9	10	5	13.09	12.04	10	10	6	66.95	67.26
1	13	3	5.07	6.38	3	11	5	8.38	9.38	1	10	6	8.08	7.80
2	13	3	2.83	2.73	4	11	5	36.48	37.35	2	10	6	38.83	37.85
3	13	3	27.99	27.93	5	11	5	0.00	11.25	3	10	6	87.05	85.54
4	13	3	22.27	21.96	6	11	5	16.93	18.23	4	10	6	14.42	13.60
1	14	3	9.62	10.00	1	12	5	15.79	14.60	5	10	6	30.70	24.99
2	14	3	10.26	11.86	2	12	5	9.44	12.04	6	10	6	37.96	36.08
1	15	3	0.00	5.75	4	12	5	6.81	6.86	7	10	6	14.98	15.16
0	0	4	108.40	104.28	5	12	5	39.04	40.99	8	11	6	63.68	61.87
1	1	4	277.54	288.28	1	13	5	17.75	17.05	9	11	6	42.17	40.71
0	1	4	81.51	70.18	2	13	5	23.74	22.71	0	11	6	25.99	23.80
1	2	4	50.55	55.75	3	13	5	16.89	17.96	4	11	6	64.08	63.80
2	2	4	111.99	113.49	4	13	5	24.93	24.21	5	11	6	21.89	22.29
3	2	4	152.60	156.63	5	13	5	10.86	12.83	6	11	6	46.47	47.09
4	2	4	126.56	121.74	6	13	5	133.17	136.76	0	12	6	26.92	26.44
3	3	4	12.62	15.21	0	14	6	63.40	62.64	2	12	6	36.64	35.85
3	3	4	241.68	242.41	1	14	6	48.72	47.79	4	12	6	23.28	20.94
0	3	4	45.94	45.95	2	14	6	252.50	252.99	5	12	6	19.85	17.47
4	3	4	28.54	30.82	1	15	6	191.81	189.51	0	13	6	24.18	24.76
4	4	4	51.07	50.35	0	15	6	65.16	66.68	1	13	6	68.24	69.70
4	4	4	177.52	178.51	1	15	6	70.16	70.05	2	13	6	10.19	1.65
4	4	4	9.91	13.25	2	15	6	123.50	126.32	3	13	6	31.04	30.58
1	5	4	70.26	70.45	3	15	6	62.29	62.44	1	14	6	15.49	14.40
2	5	4	24.38	26.35	0	16	6	25.38	26.56	2	14	6	69.10	69.57
4	5	4	9.81	12.10	3	16	6	50.06	50.72	0	15	6	42.40	42.40
4	5	4	121.11	119.51	4	16	6	125.71	126.84	1	15	6	29.43	27.84
4	5	4	152.97	161.40	4	16	6	28.15	29.79	1	16	6	34.35	33.50
6	6	4	14.65	17.73	0	17	6	15.31	10.50	2	16	6	18.26	16.65
4	6	4	44.14	45.86	1	17	6	151.65	150.50	4	16	6	4.05	5.44
4	6	4	101.39	102.51	2	17	6	53.63	54.80	3	16	6	28.56	28.94
6	6	4	59.31	58.12	4	17	6	88.09	87.85	1	17	6	19.12	18.13
4	6	4	66.77	68.08	5	17	6	74.15	76.55	2	17	6	46.92	46.32
4	6	4	136.67	132.58	6	17	6	23.07	24.61	4	17	6	10.64	9.65
7	7	4	4.56	5.89	1	18	6	61.88	59.67	1	18	6	5.72	3.56
4	7	4	66.02	64.67	2	18	6	113.93	113.33	2	18	6	6.17	4.58
4	7	4	62.60	61.70	3	18	6	14.70	12.86	3	18	6	6.71	7.33
4	7	4	15.88	15.23	4	18	6	27.59	26.27	4	18	6	6.45	7.79
7	7	4	76.71	76.30	6	18	6	79.07	78.52	6	18	6	20.18	20.98
6	7	4	110.99	114.99	1	19	6	68.76	67.39	1	19	6	23.06	24.25
4	7	4	32.44	33.48	2	19	6	33.73	34.47	2	19	6	0.00	9.19
4	7	4	0.00	6.99	3	19	6	6.62	10.24	3	19	6	0.00	2.21
4	7	4	99.94	97.09	4	19	6	8.49	9.16	4	19	6	7.55	6.43
4	7	4	21.70	17.09	5	19	6	9.59	9.20	5	19	6	8.74	8.45
4	7	4	16.44	39.18	6	19	6	20.05	20.57	6	19	6	5.19	8.85
4	7	4	39.92	35.51	7	19	6	31.35	30.95	7	19	6	5.06	1.11
4	7	4	6.60	2.65	8	19	6	67.46	66.71	8	19	6	5.56	2.65
4	7	4	20.06	28.77	9	19	6	29.33	28.35	9	19	6	6.00	5.39

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
1	9	7	11.36	11.99	5	8	8	50.69	50.81	2	9	10	19.64	20.09
2	9	7	11.76	12.27	6	8	8	42.03	41.65	3	9	10	66.01	69.17
3	9	7	6.24	5.83	7	8	8	44.29	43.90	4	9	10	38.83	37.78
5	9	7	0.00	8.86	8	9	9	91.76	88.52	6	9	10	79.36	77.78
6	9	7	0.00	0.81	0	9	8	130.19	131.93	7	9	10	0.00	5.02
7	9	7	6.04	16.91	1	10	9	58.03	62.63	0	10	10	7.12	4.75
8	9	7	4.39	26.32	2	10	9	22.49	23.27	1	10	10	70.33	74.78
1	10	7	0.00	3.32	3	9	8	90.11	90.45	2	10	10	47.66	51.24
2	10	7	24.90	26.75	4	10	9	20.65	19.12	3	10	10	15.52	13.16
3	10	7	4.14	0.87	5	10	9	61.13	58.68	4	10	10	54.98	55.27
4	10	7	16.23	20.92	6	10	9	36.70	36.24	5	10	10	48.66	48.79
5	10	7	7.92	17.66	7	10	9	0.00	3.69	6	10	10	0.00	7.93
6	10	7	5.73	0.02	8	10	8	54.50	55.34	0	11	10	24.59	25.01
7	10	7	8.37	6.10	9	10	8	71.37	74.88	1	11	10	65.96	68.85
8	10	7	0.00	3.53	1	10	9	24.94	25.73	2	11	10	0.00	3.95
9	10	7	0.00	4.56	2	10	8	30.40	30.74	3	11	10	25.90	26.47
1	11	7	0.00	9.76	3	10	8	87.54	86.00	4	11	10	40.09	39.00
2	11	7	9.93	1.80	4	10	8	5.00	5.26	5	11	10	72.83	74.17
3	11	7	8.24	0.90	5	10	8	18.06	14.19	6	11	10	22.74	21.69
4	12	7	9.17	1.11	6	10	8	37.41	35.94	7	11	10	17.95	18.49
5	11	7	6.70	4.76	7	10	8	33.31	34.89	8	11	10	8.23	5.35
6	11	7	0.00	9.61	8	11	8	65.50	67.18	9	11	10	50.36	51.32
7	11	7	8.10	4.49	9	11	8	52.20	51.00	1	12	10	50.39	52.02
8	11	7	0.00	6.08	0	11	8	26.73	25.89	2	12	10	78.01	74.88
9	11	7	10.74	10.11	1	12	8	68.51	69.65	3	11	10	42.69	41.52
1	12	7	14.52	6.00	2	12	8	27.54	28.82	4	11	10	37.51	38.72
2	12	7	41.85	47.85	3	12	8	35.45	34.83	5	11	10	5.96	3.16
3	12	7	145.17	135.33	4	12	8	29.51	28.92	6	11	10	12.01	13.17
4	12	7	21.64	23.48	5	12	8	31.88	31.42	7	11	10	35.25	34.07
5	12	7	235.62	240.07	6	12	8	69.97	72.28	8	11	10	9.57	9.36
6	12	7	182.14	176.08	7	12	8	0.00	1.56	9	11	10	38.86	4.04
7	12	7	26.41	29.28	8	12	8	22.13	22.07	1	13	10	0.00	4.43
8	12	7	96.45	97.84	9	12	8	2.64	9.34	2	13	10	16.82	17.04
9	12	7	56.30	59.01	0	13	8	57.38	55.93	3	13	10	0.00	6.95
1	13	7	44.00	43.49	1	13	8	137.27	134.56	4	13	10	21.53	20.89
2	13	7	8.63	7.65	2	13	8	21.32	21.33	5	13	10	8.02	8.21
3	13	7	50.36	52.96	3	13	8	17.00	15.57	6	13	10	34.03	35.08
4	13	7	90.86	89.49	4	13	8	103.22	100.09	7	13	10	3.18	6.60
5	13	7	45.22	44.50	5	13	8	90.35	91.49	8	13	10	7.50	5.84
6	13	7	9.01	5.35	6	13	8	51.85	53.54	9	13	10	13.40	13.68
7	13	7	169.82	173.97	7	13	8	35.14	33.92	1	14	10	22.15	21.85
8	13	7	64.59	63.58	8	13	8	10.07	10.49	2	14	10	0.00	8.83
9	13	7	53.71	52.28	9	13	8	30.10	30.00	3	14	10	10.99	11.05
1	14	7	23.74	24.95	0	14	8	57.21	55.85	4	14	10	4.24	9.48
2	14	7	49.66	51.26	1	14	8	46.79	47.42	5	14	10	9.04	3.34
3	14	7	38.14	37.91	2	14	8	9.34	10.37	6	14	10	14.71	14.63
4	14	7	130.58	131.55	3	14	8	0.00	5.89	7	14	10	23.19	24.26
5	14	7	6.09	2.40	4	14	8	0.00	1.41	8	14	10	17.96	19.14
6	14	7	84.04	81.51	5	14	8	69.21	68.22	9	14	10	10.48	9.81
7	14	7	77.69	83.71	6	14	8	20.09	19.70	0	15	10	0.00	4.43
8	14	7	67.89	67.50	7	14	8	46.61	46.98	1	16	10	0.00	7.10
9	14	7	19.99	20.72	8	14	8	21.74	23.69	2	16	10	0.00	2.44
1	15	7	88.13	87.79	9	14	8	44.42	47.36	3	16	10	0.00	6.25
2	15	7	25.84	25.82	0	15	8	21.49	20.29	4	16	10	4.12	4.65
3	15	7	14.75	14.75	1	15	8	7.66	11.35	5	16	10	8.19	6.76
4	15	7	41.17	39.22	2	15	8	29.37	29.24	6	16	10	0.00	0.49
5	15	7	19.13	20.26	3	15	8	15.55	15.48	7	16	10	0.00	6.05
6	15	7	30.99	31.01	4	15	8	18.14	19.79	8	16	10	8.72	8.18
7	15	7	51.77	51.77	5	15	8	39.94	41.50	9	16	10	19.64	21.54

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
3	11	11	17.30	16.74	1	12	12	19.50	19.50	5	5	14	72.01	74.86
4	11	11	15.42	18.17	0	12	12	5.02	5.02	0	6	14	123.65	122.76
2	12	11	8.95	8.14	1	13	12	25.41	26.41	1	6	14	54.10	52.40
1	13	11	0.00	1.68	1	13	12	49.76	47.76	2	6	14	51.90	50.82
2	13	11	18.72	20.24	1	2	13	39.18	39.18	3	6	14	66.70	68.41
1	13	11	9.48	11.11	2	3	13	65.64	65.64	4	6	14	2.28	13.51
0	1	12	82.64	79.59	1	2	3	10.11	10.11	2	10	15	0.00	0.00
1	1	12	160.29	152.11	2	4	13	24.81	24.81	3	10	15	11.84	13.23
0	2	12	0.00	2.93	3	4	13	35.52	35.52	4	10	15	11.84	13.23
1	2	12	27.10	26.68	1	5	13	62.05	62.05	3	10	15	15.07	12.95
2	2	12	67.98	68.28	2	5	13	26.59	26.59	4	10	15	16.72	18.92
0	3	12	84.94	83.92	4	5	13	26.86	26.86	2	11	15	24.67	25.68
1	3	12	47.29	46.80	3	6	13	11.26	11.26	1	12	15	0.00	4.20
2	3	12	21.32	22.63	0	6	13	27.65	27.65	0	1	16	30.09	28.84
3	3	12	114.14	116.18	6	6	13	41.05	41.05	1	1	16	78.76	76.67
0	4	12	46.94	46.29	4	6	13	44.37	44.37	0	2	16	42.26	41.11
2	4	12	22.05	22.50	1	7	13	0.87	0.87	1	2	16	27.97	28.14
3	4	12	25.45	25.64	3	7	13	12.14	12.14	1	2	16	95.19	93.79
4	4	12	85.58	88.01	4	7	13	1.27	1.27	0	3	16	90.65	89.74
0	5	12	39.13	38.93	5	7	13	43.19	43.19	1	3	16	28.49	27.22
1	5	12	54.44	53.54	6	7	13	0.20	0.20	2	3	16	37.28	37.27
2	5	12	67.17	67.35	7	7	13	31.84	31.84	3	3	16	71.91	69.18
4	5	12	9.84	7.23	1	8	13	2.47	2.47	0	4	16	22.43	21.88
5	5	12	86.97	88.30	2	8	13	35.98	35.98	3	4	16	32.18	31.12
0	6	12	155.30	152.39	3	8	13	10.94	10.94	4	4	16	71.18	71.75
1	6	12	46.40	45.32	4	8	13	18.60	18.60	0	5	16	35.10	34.52
2	6	12	31.87	33.86	5	8	13	20.57	20.57	1	5	16	31.50	31.77
3	6	12	69.28	73.56	6	8	13	23.11	23.11	2	5	16	82.57	82.76
4	6	12	37.31	38.17	7	8	13	2.76	2.76	4	5	16	32.01	31.15
6	6	12	90.71	90.71	1	9	13	4.42	4.42	5	5	16	59.39	60.90
1	7	12	96.82	97.96	2	9	13	19.34	19.34	0	6	16	69.86	69.39
2	7	12	22.00	21.85	3	9	13	36.93	36.93	1	6	16	34.38	33.80
3	7	12	21.16	21.78	4	9	13	32.78	32.78	2	6	16	21.03	18.50
4	7	12	70.27	71.04	5	9	13	12.11	12.11	3	6	16	77.84	78.53
5	7	12	30.81	31.34	6	10	13	8.13	8.13	4	6	16	27.27	27.41
6	7	12	54.04	55.76	1	10	13	16.71	16.71	6	6	16	78.59	82.55
0	8	12	33.39	31.88	3	10	13	21.44	21.44	1	7	16	73.29	73.82
1	8	12	44.40	43.93	4	10	13	29.22	29.22	2	7	16	25.60	25.00
3	8	12	25.87	26.74	5	10	13	8.39	8.39	3	7	16	27.89	28.04
4	8	12	3.37	10.52	6	11	13	8.92	8.92	4	7	16	59.75	58.29
5	8	12	78.52	80.77	7	11	13	1.62	1.62	5	7	16	20.28	19.71
6	8	12	9.61	11.30	8	11	13	11.64	11.64	6	7	16	22.18	22.59
7	8	12	5.76	5.43	9	12	13	12.46	12.46	0	8	16	19.26	18.64
0	9	12	42.88	42.13	2	12	13	10.51	10.51	1	8	16	29.99	29.71
1	9	12	0.00	4.34	0	1	14	50.16	50.16	3	8	16	27.64	27.24
2	9	12	20.75	19.68	1	1	14	75.56	75.56	4	8	16	28.47	27.65
3	9	12	52.88	53.37	0	2	14	60.85	60.85	5	8	16	50.43	51.41
5	9	12	25.19	24.84	1	2	14	1.87	1.87	6	8	16	24.90	25.29
6	9	12	48.52	48.48	2	2	14	141.24	141.24	0	9	16	58.27	58.75
0	10	12	12.24	12.05	0	3	14	84.77	84.77	1	9	16	25.12	24.40
2	10	12	72.81	75.92	1	3	14	18.70	18.70	2	9	16	17.00	15.24
3	10	12	55.74	56.64	3	3	14	52.81	52.81	3	9	16	58.00	58.32
4	10	12	25.20	25.26	4	4	14	38.72	38.72	0	10	16	25.51	23.66
5	10	12	49.93	50.68	0	4	14	80.53	80.53	1	10	16	65.35	65.72
0	11	12	31.24	32.13	2	4	14	13.16	13.16	2	10	16	19.63	18.04
2	11	12	25.83	25.78	3	4	14	19.52	19.52	3	10	16	21.88	19.69
3	11	12	61.83	63.96	4	4	14	43.00	43.00	0	11	16	32.91	32.46
4	11	12	13.49	13.85	6	5	14	53.35	53.35	2	11	16	57.97	57.29
0	12	12	19.94	19.49	1	5	14	2.38	2.38	0	12	16	60.87	53.69
1	12	12	92.68	94.12	2	5	14	143.46	143.46	1	12	16	60.87	53.69
					4	5	14	27.10	27.10	5	5	15	21.84	23.48

11.81	13.31
4.58	5.13
18.32	15.66
11.80	11.54
10.75	10.01
12.02	13.09
0.00	1.94
11.58	11.08
6.35	3.92
0.00	5.51
0.00	7.50
10.30	12.34
8.47	6.51
7.91	7.08
9.41	5.24
2.49	7.75
23.09	22.97
51.55	50.19
38.85	37.54
11.88	12.01
97.70	98.12
63.98	65.60
24.26	23.02
36.07	35.89
43.17	44.35
45.87	46.62
16.41	14.70
22.04	22.38
48.79	48.76
26.13	25.46
0.00	2.51
83.67	84.70
26.14	25.34
57.20	57.64
26.05	25.01
38.33	38.39
52.47	53.86
43.33	40.16
13.37	15.46
12.52	14.06
57.15	59.58
4.86	1.98
15.69	15.07
28.05	28.74
32.36	35.02
8.21	5.13
4.31	4.99

17.65	17.48
57.02	54.90
8.04	7.35
57.31	57.31
38.04	38.36
18.65	18.36
48.78	48.24
71.35	69.04
12.32	11.12
11.19	11.83
31.42	31.95
50.10	48.69
21.38	22.45
31.96	31.60
5.73	8.29
12.29	0.00
29.76	28.53
22.91	21.02
10.01	3.33
10.82	10.37
14.02	12.41
31.25	29.77
11.58	8.89
0.04	0.00
15.93	17.56
4.93	6.52
29.76	28.16
9.32	0.00
19.97	19.61
53.12	51.99
40.18	41.38
12.21	13.55
104.46	103.92
78.88	81.20
35.17	34.31
43.84	44.85
60.70	61.48
40.62	41.74
6.73	0.00
31.28	31.57
64.59	63.67
19.17	20.33
2.32	74.03
74.33	29.71
43.87	44.71
33.67	35.21
26.59	26.73
41.12	40.45
76.03	75.51
3.52	0.00
53.70	55.59
41.87	40.53
17.76	17.65
55.93	55.08
5.48	6.40
20.79	21.84
19.16	21.18
74.95	72.51
36.85	36.12

20.84	20.92
8.91	10.30
11.37	10.12
45.91	45.67
29.76	29.21
36.16	35.05
7.72	9.82
10.42	10.66
25.30	24.33
18.88	20.37
4.63	0.00
13.35	11.50
26.71	25.39
16.76	15.62
3.68	4.82
21.28	21.33
10.37	12.28
5.16	4.90
15.92	10.07
13.83	0.00
13.36	12.48
11.05	12.04
20.72	21.50
18.79	17.93
11.59	12.69
18.38	19.26
112.43	113.40
9.62	8.18
71.74	72.26
45.83	46.58
90.06	92.54
37.16	37.17
2.49	2.15
118.86	119.46
27.73	27.70
50.44	52.09
32.51	32.49
111.17	112.43
13.56	9.11
60.81	61.16
22.61	23.42
28.92	28.99
74.68	74.08
64.28	65.55
2.13	0.00
7.27	7.61
58.49	58.80
53.92	53.16
62.71	64.36
81.42	82.13
14.01	12.43
62.25	61.69
31.04	31.71
3.09	0.00
104.97	103.04
37.84	37.84
33.04	33.04
13.46	13.46
24.13	26.26
11.54	13.14

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
0	1	0	54.64	57.39	0	12	0	77.64	77.50	1	13	1	13.80	25.35
1	0	0	41.35	48.40	1	12	0	55.56	55.58	1	11	1	0.00	5.86
1	0	0	226.83	222.14	1	12	0	0.00	32.67	1	11	1	21.90	17.76
2	0	0	238.62	241.51	3	12	0	36.49	34.77	4	11	1	0.00	2.64
2	0	0	163.15	168.18	4	12	0	54.17	50.53	1	14	1	0.00	19.01
0	3	0	44.57	35.96	5	12	0	38.48	41.04	6	11	2	0.00	0.12
1	2	3	114.91	116.63	5	10	0	60.03	60.40	0	12	2	85.36	86.68
3	0	0	10.99	6.58	1	13	0	84.48	86.43	1	12	2	253.23	252.87
0	4	0	70.28	74.04	1	0	0	0.00	16.09	2	12	2	3.36	4.89
1	3	4	180.74	178.68	2	13	0	49.15	52.34	2	12	2	118.18	124.93
1	3	4	31.66	34.28	2	14	0	17.29	12.41	3	12	2	157.43	160.56
4	0	0	43.40	38.96	2	14	0	56.47	56.07	4	12	2	23.05	28.53
4	0	0	106.79	105.66	1	15	0	34.55	39.35	5	12	2	8.05	17.27
1	2	5	21.61	22.46	2	3	1	36.72	39.40	0	13	2	151.47	152.73
1	2	5	258.20	256.94	1	3	1	9.10	5.71	1	13	2	9.75	10.75
3	5	0	4.63	13.94	1	4	1	110.79	103.02	4	4	2	13.34	10.75
4	5	0	53.77	55.46	1	4	1	69.34	67.32	2	14	2	164.50	164.76
5	0	0	63.36	64.95	1	5	1	101.61	99.19	1	14	2	26.71	32.95
5	0	0	131.65	135.22	1	5	1	94.01	93.12	2	15	2	128.52	129.94
1	6	0	110.48	110.92	3	5	1	71.02	71.55	0	15	2	61.51	62.45
2	6	0	28.48	29.14	4	5	1	54.37	54.85	1	15	3	84.29	84.06
4	6	0	0.00	2.63	1	6	1	0.00	15.70	2	3	3	119.93	120.42
4	6	0	68.91	68.33	1	6	1	21.50	18.33	1	4	4	42.54	43.79
6	6	0	148.79	153.84	4	6	1	39.87	39.03	3	4	4	26.11	30.81
1	7	0	98.69	100.39	4	6	1	8.05	0.18	1	5	5	119.05	120.42
2	7	0	82.54	81.45	5	6	1	9.75	17.34	2	6	5	205.87	204.55
3	7	0	8.57	14.74	1	7	1	36.94	37.20	0	6	6	40.74	40.98
4	7	0	120.60	123.46	1	7	1	33.92	29.70	2	6	6	0.00	8.31
5	7	0	55.24	51.19	3	7	1	46.11	44.41	4	6	6	49.52	49.65
6	0	0	12.02	10.92	4	7	1	12.01	10.76	2	6	6	37.30	30.15
6	0	0	107.06	107.23	5	7	1	41.84	42.44	6	6	6	108.31	109.74
1	8	0	17.12	15.57	6	7	1	8.37	4.34	1	7	7	119.54	121.29
2	8	0	30.03	32.00	1	8	1	0.00	6.31	2	7	7	17.49	15.74
3	8	0	34.82	34.37	1	8	1	28.01	27.00	3	7	7	40.36	39.85
5	8	0	56.72	56.42	3	8	1	10.23	22.35	4	7	7	92.29	93.75
6	8	0	0.00	26.42	6	8	1	32.18	22.28	5	7	7	39.06	34.92
7	8	0	55.69	61.66	7	8	1	0.00	3.92	6	7	7	41.16	41.16
8	0	0	89.39	90.70	8	8	1	12.66	12.77	6	8	8	62.16	62.67
8	0	0	141.16	139.65	2	9	1	48.21	46.22	0	8	8	35.57	36.66
2	9	0	0.00	16.88	3	9	1	11.34	15.24	1	8	8	101.35	102.13
3	9	0	87.53	91.83	4	9	1	31.14	34.16	2	8	8	34.75	35.88
4	9	0	46.85	51.33	5	9	1	16.85	11.99	3	8	8	80.01	82.87
5	9	0	11.88	25.63	6	9	1	25.77	16.28	5	8	8	0.00	15.13
6	9	0	40.21	41.63	7	9	1	46.32	43.63	6	8	8	16.06	27.17
7	9	0	0.00	22.52	8	9	1	25.62	22.32	7	8	8	47.90	52.36
9	0	0	58.19	54.54	3	10	1	42.87	46.18	2	9	9	82.14	80.28
10	0	0	96.66	96.31	4	10	1	14.10	24.30	0	9	9	37.84	33.05
1	10	0	96.07	97.80	6	10	1	0.00	9.66	2	9	9	79.43	80.82
2	10	0	40.47	39.83	7	10	1	0.00	2.79	4	9	9	26.89	26.92
3	10	0	14.88	17.41	8	10	1	0.00	1.47	5	9	9	34.34	35.21
4	10	0	73.14	74.08	1	11	1	44.82	45.92	6	9	9	67.91	69.95
6	10	0	28.08	30.86	3	11	1	0.00	0.43	7	9	9	15.98	12.43
7	10	0	46.65	43.16	4	11	1	0.00	12.14	7	9	9	47.48	51.35
8	10	0	38.95	46.97	5	11	1	13.18	22.10	9	10	10	19.13	26.32
0	11	0	57.50	59.30	6	11	1	0.00	3.04	10	10	10	84.46	87.77
1	11	0	0.00	11.00	1	12	1	15.59	3.98	6	10	10	30.70	34.21
3	11	0	73.45	75.76	2	12	1	0.00	8.13	7	10	10	11.99	17.69
4	11	0	0.00	12.18	3	12	1	0.00	7.52	4	10	10	61.44	63.00
5	11	0	87.97	90.08	4	12	1	0.00	13.46	6	10	10	0.00	23.59
6	11	0	42.94	34.82	5	12	1	14.83	12.72	7	10	10	64.95	68.21

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
6	11	3	17.70	1.98	3	10	4	36.81	40.14	3	4	5	16.69	11.83
1	12	3	0.00	10.74	4	10	4	70.90	71.70	4	5	5	21.19	10.13
2	12	3	0.00	16.47	6	10	4	14.12	20.41	4	10	6	41.93	38.59
3	12	3	0.00	0.08	7	10	4	73.83	77.76	6	10	6	17.16	12.35
4	12	3	21.21	6.08	0	11	4	18.68	14.79	5	10	6	0.00	18.39
5	12	3	5.64	13.05	1	11	4	50.36	53.85	5	10	6	0.00	13.46
1	13	3	0.00	6.54	3	11	4	8.77	13.96	5	11	6	20.81	9.89
2	13	3	12.06	1.59	4	11	4	46.40	38.12	5	11	6	14.66	11.14
4	13	3	17.97	23.10	5	11	4	42.13	42.61	5	11	6	0.00	5.53
1	14	3	13.06	11.02	6	11	4	0.00	9.99	5	12	5	40.21	16.23
2	14	3	0.00	11.14	0	12	4	89.65	2.58	5	12	5	7.72	18.21
1	15	3	0.00	3.94	1	12	4	0.00	4.00	5	14	5	21.23	25.59
0	1	4	105.58	104.60	2	12	4	83.23	85.64	5	14	5	8.12	13.76
1	1	4	289.74	286.82	3	12	4	19.08	2.72	6	1	6	134.65	136.08
0	2	4	79.79	70.02	4	12	4	13.87	11.34	6	2	6	59.02	61.16
2	2	4	109.46	111.62	5	12	4	17.00	4.82	6	2	6	254.48	250.08
0	3	4	155.54	156.09	0	13	4	43.40	42.99	6	2	6	190.14	186.66
1	3	4	122.34	120.87	1	13	4	62.49	63.48	6	3	6	64.15	67.20
1	3	4	0.00	15.22	2	13	4	64.93	64.86	6	3	6	69.49	68.60
4	3	4	243.21	241.46	4	13	4	36.92	38.05	6	3	6	124.75	124.75
0	4	4	44.82	44.56	1	14	4	54.23	52.18	6	4	6	62.80	62.91
4	4	4	158.95	160.55	2	14	4	87.53	92.31	6	4	6	94.69	97.37
4	4	4	49.62	50.79	0	15	4	109.10	104.81	6	4	6	48.53	49.83
4	4	4	177.11	177.06	1	3	5	25.60	22.42	6	4	6	30.95	30.49
0	5	4	0.00	14.71	2	3	5	56.07	52.18	6	5	6	14.38	10.64
1	5	4	68.17	70.07	1	3	5	89.94	89.02	6	5	6	150.87	148.64
4	5	4	26.82	27.07	3	4	5	26.97	23.46	6	5	6	42.44	42.04
3	5	4	60.19	62.21	1	5	5	89.61	85.27	6	5	6	54.59	55.71
5	5	4	0.00	11.36	2	5	5	68.47	66.96	6	5	6	88.87	88.88
5	5	4	118.63	120.68	3	5	5	26.94	23.46	6	5	6	76.41	77.38
5	5	4	158.97	161.19	4	5	5	13.83	14.56	6	5	6	20.27	23.51
0	6	4	7.32	17.93	1	6	5	37.79	38.34	6	6	6	62.63	60.67
1	6	4	43.14	46.43	2	6	5	62.85	61.11	6	6	6	0.00	13.54
4	6	4	61.73	58.72	4	6	5	8.37	1.40	6	6	6	47.48	47.39
4	6	4	32.33	9.95	5	6	5	16.54	14.55	6	6	6	31.35	23.74
6	6	4	67.97	69.35	1	7	5	19.80	11.44	6	6	6	77.03	77.92
7	7	4	134.16	133.77	2	7	5	67.66	69.94	6	7	6	66.56	68.40
1	7	4	14.43	7.19	3	7	5	9.93	5.62	6	7	6	18.44	23.92
3	7	4	66.87	64.76	4	7	5	45.26	45.87	6	7	6	108.72	107.63
4	7	4	62.15	61.41	5	7	5	26.05	22.47	6	7	6	35.37	35.04
5	7	4	75.78	78.69	6	7	5	19.64	19.70	6	7	6	0.00	7.80
0	8	4	116.90	115.44	1	8	5	57.55	60.42	6	8	6	17.45	7.07
0	8	4	68.96	69.00	2	8	5	21.15	23.96	6	8	6	0.00	9.23
1	8	4	153.20	152.39	3	8	5	31.88	31.28	6	8	6	84.55	86.59
2	8	4	27.88	33.09	5	8	5	17.20	16.41	6	8	6	18.95	20.24
5	8	4	100.88	102.06	6	8	5	31.57	26.73	6	8	6	65.40	67.41
6	8	4	28.91	23.32	2	9	5	56.14	54.68	6	8	6	41.15	46.48
7	8	4	0.00	17.58	3	9	5	0.00	13.64	6	8	6	87.95	89.79
8	8	4	37.97	40.55	4	9	5	16.27	14.23	6	9	6	165.07	161.38
4	9	4	35.17	35.14	5	9	5	12.59	14.76	6	9	6	53.66	51.70
4	9	4	25.66	29.02	6	9	5	22.02	24.98	6	9	6	91.85	89.85
4	9	4	63.79	66.40	7	9	5	17.67	17.92	6	9	6	44.39	47.86
4	9	4	0.00	5.20	8	9	5	12.59	14.76	6	9	6	0.00	16.38
5	9	4	9.85	27.18	9	9	5	25.02	22.28	6	9	6	64.28	67.43
6	9	4	79.49	79.12	3	10	5	31.03	40.12	6	9	6	37.66	42.29
6	9	4	18.64	25.56	4	10	5	0.00	17.90	6	9	6	71.08	71.08
7	9	4	31.91	30.02	5	10	5	0.00	6.52	6	9	6	39.67	41.08
0	10	4	84.68	85.08	6	10	5	66.85	69.32	6	10	6	71.08	66.28
1	10	4	92.68	96.90	1	11	5			6	10	6		

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
3	11	7	6.04	4.86	1	13	9	44.53	43.36	1	2	10	18.62	21.76
4	11	7	0.00	5.17	1	13	9	0.00	16.32	1	2	10	12.35	18.55
5	11	7	0.00	11.13	1	14	9	0.00	23.06	1	3	10	59.49	61.68
6	11	7	0.00	1.70	1	1	10	37.59	39.69	0	13	10	16.44	6.60
1	12	7	12.60	1.41	1	1	10	163.09	175.79	1	2	10	49.99	50.22
2	12	7	15.03	1.70	0	2	10	19.33	15.28	1	2	10	48.78	51.02
3	12	7	0.00	0.95	2	3	10	56.92	57.09	1	2	11	41.62	38.67
4	12	7	0.00	4.93	0	2	10	124.80	121.44	1	2	11	35.20	38.80
1	13	7	0.00	10.08	1	3	10	38.79	37.16	1	2	11	13.87	1.61
2	13	7	0.00	5.39	1	3	10	0.00	3.13	1	3	11	18.46	15.07
1	14	1	23.92	11.27	3	4	10	157.00	152.20	1	2	11	31.24	32.79
0	1	8	0.00	7.28	0	4	10	37.27	35.64	1	2	11	16.35	9.60
1	0	1	41.39	45.55	4	4	10	34.08	34.63	3	4	11	0.00	2.95
1	0	2	140.15	133.05	1	3	4	136.01	134.38	4	1	11	35.66	37.82
2	0	2	244.53	236.31	4	4	10	28.50	29.17	1	2	4	0.00	3.90
0	1	2	174.41	172.61	0	1	10	90.99	90.85	2	4	4	0.00	3.66
1	2	3	26.72	30.00	4	5	10	42.42	43.60	2	4	6	0.00	7.24
1	2	3	97.22	96.03	1	2	3	33.41	32.85	5	5	11	0.00	0.43
3	3	3	55.18	57.42	2	3	4	15.88	25.85	4	5	11	11.34	21.20
3	3	3	41.50	42.25	5	5	10	99.43	99.32	1	2	7	0.00	3.31
0	1	4	115.54	112.62	4	5	10	136.46	128.61	3	4	7	33.02	35.41
1	3	4	51.57	51.87	0	6	10	0.00	11.66	4	7	11	14.41	4.60
4	4	4	90.12	88.33	1	2	3	10.00	15.17	5	6	11	0.00	4.53
8	8	8	41.60	42.66	6	6	10	72.02	70.55	6	7	11	10.45	13.09
0	1	2	12.42	6.33	4	5	6	0.00	5.08	1	2	8	28.48	22.01
1	2	3	169.37	169.37	6	6	10	101.02	99.93	2	3	3	18.04	2.88
1	2	3	16.29	16.65	6	6	10	114.09	112.58	3	5	5	0.00	9.43
5	5	5	64.41	63.75	7	7	10	18.73	18.27	5	6	11	5.24	10.04
5	5	5	51.59	51.00	1	2	3	64.82	64.48	6	7	11	0.00	2.34
8	8	8	24.01	22.46	3	3	7	48.76	48.01	7	8	11	5.46	13.95
8	8	8	52.47	49.98	4	4	7	0.00	0.00	2	2	9	0.00	18.74
8	8	8	36.29	38.60	5	5	10	0.00	11.86	3	4	9	0.00	9.95
1	2	4	169.12	169.37	6	6	10	56.02	51.53	4	5	11	21.79	23.66
5	5	5	30.83	35.35	0	8	10	121.09	120.22	5	6	11	0.00	5.24
6	6	6	79.54	80.44	8	8	10	48.76	47.78	6	7	11	0.00	5.91
6	6	6	82.23	82.60	1	2	3	115.49	116.58	7	8	11	12.98	3.15
7	7	7	68.27	66.45	2	3	8	36.34	39.32	8	9	11	0.00	5.44
1	2	3	0.00	21.01	3	5	8	76.81	72.45	1	10	11	18.62	4.61
3	3	3	85.67	86.03	5	8	8	16.02	22.53	2	3	4	0.00	7.22
4	4	4	0.00	14.20	6	7	8	0.00	8.54	3	4	10	0.00	1.40
5	5	5	13.90	14.24	8	8	10	33.63	29.98	6	10	11	13.00	0.84
8	8	8	39.69	38.07	0	9	10	28.13	25.60	1	11	11	21.77	6.02
8	8	8	13.09	19.67	2	3	4	20.85	19.65	3	3	11	5.53	17.03
8	8	8	69.69	70.78	4	5	9	68.62	67.52	4	4	11	18.88	17.18
8	8	8	33.69	30.56	9	9	10	0.00	16.75	1	12	11	0.00	6.91
8	8	8	52.24	42.77	5	9	10	40.41	37.39	2	3	5	0.00	3.02
8	8	8	41.19	44.73	6	7	9	77.01	76.16	3	1	13	24.36	5.15
8	8	8	87.40	88.40	7	9	10	0.00	5.54	1	2	12	0.00	19.29
0	2	3	131.00	130.70	0	10	10	0.00	3.91	2	0	12	20.88	11.91
2	3	4	24.68	22.74	1	1	10	75.53	73.58	0	1	12	66.63	74.73
3	4	5	91.96	88.24	3	3	10	48.42	49.04	1	0	12	131.04	3.36
4	5	6	48.24	48.36	4	4	10	59.49	54.25	2	0	12	63.23	62.31
5	6	7	0.00	18.70	6	6	10	14.07	6.33	0	2	12	78.84	78.97
6	7	8	59.05	60.01	6	10	10	18.64	25.48	1	2	3	41.53	43.37
7	8	9	37.88	37.22	0	11	10	47.19	46.16	1	2	3	115.12	20.88
8	8	8	54.34	54.56	3	3	11	7.70	4.04	3	0	4	115.12	110.47
8	8	8	76.21	74.64	4	5	11	31.88	27.48	0	4	12	46.88	43.01
1	10	10	25.33	26.63	5	5	11	40.94	39.81	1	3	4	116.55	111.85
2	10	10	0.00	0.00	6	6	11	70.63	70.40	3	3	4	26.71	24.78

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
4	4	12	87.57	83.20	6	8	14	24.52	3.76	3	3	16	60.90	61.86
0	1	5	37.45	37.23	7	0	14	46.94	46.52	0	4	16	22.67	21.50
1	5	12	53.83	51.38	0	9	14	125.69	120.00	1	4	16	76.68	81.18
2	5	12	66.63	63.34	2	9	14	37.63	39.59	3	4	16	4.90	27.15
3	5	12	37.37	39.79	3	9	14	66.12	59.99	4	4	16	61.89	63.29
4	5	12	0.00	6.18	4	9	14	34.48	34.10	0	5	16	25.95	31.11
5	5	12	83.66	84.86	5	9	14	14.30	15.45	1	5	16	17.32	28.39
0	6	12	148.54	144.02	6	9	14	30.83	29.88	2	5	16	73.79	75.24
1	6	12	44.05	42.73	0	10	14	56.18	57.44	3	5	16	22.58	19.07
2	6	12	33.25	31.26	0	10	14	61.53	56.60	4	5	16	18.75	27.09
4	6	12	39.00	37.72	1	10	14	0.00	5.73	5	5	16	60.01	54.41
5	6	12	15.60	30.38	2	10	14	13.83	21.32	4	5	16	67.12	64.60
6	6	12	88.96	87.23	3	10	14	51.68	48.95	0	6	16	30.10	31.70
1	7	12	95.78	92.65	4	11	14	22.46	24.56	1	6	16	19.73	17.03
2	7	12	19.31	20.19	0	11	14	0.00	3.29	2	6	16	0.00	25.21
3	7	12	17.12	21.15	1	11	14	52.92	50.26	4	6	16	0.00	19.63
4	7	12	70.63	67.45	3	11	14	76.12	75.35	5	6	16	80.26	76.00
5	7	12	23.54	30.35	0	12	14	36.25	39.10	6	6	16	70.32	67.41
6	7	12	58.04	53.35	1	12	14	26.20	24.73	1	7	16	18.51	23.38
0	8	12	36.56	31.30	2	12	14	44.77	42.83	3	7	16	23.49	23.79
1	8	12	45.13	41.95	0	13	15	36.16	33.19	4	7	16	53.50	53.47
2	8	12	79.30	77.01	1	3	15	33.87	33.19	5	7	16	23.47	18.51
3	8	12	14.05	25.56	2	4	15	19.04	10.23	6	7	16	0.00	22.07
4	8	12	78.80	76.66	3	4	15	0.00	7.68	0	8	16	19.84	14.99
5	8	12	5.39	10.80	1	5	15	39.18	39.73	2	8	16	31.73	27.67
6	8	12	8.46	8.24	3	5	15	0.00	7.99	4	8	16	65.02	59.46
7	8	12	42.82	38.29	2	5	15	20.32	25.62	1	8	16	27.61	25.41
0	9	12	22.48	19.71	3	5	15	10.09	31.49	2	8	16	54.44	47.74
2	9	12	55.69	52.15	4	5	15	4.77	7.68	5	8	16	0.00	22.51
3	9	12	0.00	4.09	1	6	15	0.00	13.39	6	8	16	58.51	51.99
4	9	12	22.71	24.29	2	6	15	22.95	26.21	0	9	16	17.59	13.64
5	9	12	42.35	45.89	4	6	15	0.00	6.44	3	9	16	58.96	53.23
6	9	12	19.87	11.20	1	7	15	0.00	17.11	4	9	16	0.00	18.81
0	10	12	76.47	72.62	2	7	15	11.34	5.19	0	10	16	18.43	22.40
1	10	12	55.38	56.39	3	7	15	20.45	18.40	1	10	16	63.14	60.05
2	10	12	21.54	24.50	2	7	15	22.22	17.14	2	10	16	0.00	16.92
3	10	12	46.78	48.88	4	7	15	0.00	3.84	3	10	16	31.91	18.19
4	10	12	0.00	48.88	5	7	15	16.71	19.78	0	11	16	19.27	24.06
0	11	12	37.09	38.70	6	7	15	11.05	16.77	1	11	16	48.66	49.35
1	11	12	0.00	12.59	1	8	15	0.00	7.61	0	12	16	28.75	31.30
3	11	12	0.00	20.15	2	8	15	0.00	10.61	1	3	17	17.32	21.07
4	11	12	93.25	91.11	3	8	15	0.00	22.32	2	3	17	14.47	19.43
0	12	12	0.00	18.79	6	8	15	0.00	8.51	1	4	17	14.36	8.75
1	12	12	9.85	4.39	2	9	15	14.41	14.72	3	5	17	42.06	43.07
2	12	12	55.31	55.75	3	9	15	0.00	20.96	1	2	17	24.61	28.01
3	12	12	24.62	24.47	4	9	15	0.00	13.13	3	3	17	0.00	23.34
0	13	12	52.45	62.85	5	9	15	0.00	10.68	4	5	17	27.12	34.69
1	13	12	66.96	62.85	4	9	15	17.39	1.98	3	5	17	21.15	7.43
2	13	12	8.21	12.17	1	10	15	13.80	11.92	1	6	17	0.00	7.90
3	13	12	21.41	18.71	2	10	15	0.43	12.76	2	6	17	0.00	17.69
4	13	12	37.48	32.90	3	10	15	20.43	18.61	4	6	17	0.00	1.30
1	2	3	62.78	60.19	4	10	15	0.00	22.85	5	6	17	19.08	6.17
2	3	4	23.52	25.73	1	11	15	18.86	4.72	1	7	17	0.00	11.95
3	4	5	47.48	45.21	0	12	16	24.83	27.14	2	7	17	0.00	26.33
4	4	5	24.10	27.20	1	1	16	66.43	69.34	3	7	17	19.96	14.93
5	5	6	10.81	11.31	0	1	16	34.07	36.56	4	7	17	12.69	14.93
1	2	4	29.54	25.03	2	0	16	78.60	83.31	5	7	17	0.00	20.36
2	4	6	44.84	42.03	0	2	16	76.79	79.34	6	7	17	0.00	12.01
3	5	7	0.00	3.72	1	2	16	23.48	23.50	1	8	17	0.00	1.43
4	5	7	12.98	1.34	2	3	16	26.18	33.50	2	8	17	0.00	1.43

H K L F(OBS) F(CALC) H K L F(OBS) F(CALC) H K L F(OBS) F(CALC)

Table with 12 columns: H, K, L, F(OBS), F(CALC), H, K, L, F(OBS), F(CALC), H, K, L, F(OBS), F(CALC). Rows contain numerical data for structure factors across different levels (H, K, L).