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Single-crystal X-ray structure study of synthetic pyrope almandine garnets at  
100 and 293 K

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For deposit: Table 3

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Armbruster et al.

Single crystal X-ray structure study of synthetic  
pyrope-almandine garnets at 100 and 293 K.

Table 3 (24 pages)

Observed and calculated structure factors for pyrope-  
almandine end- and solid solution members (100 and  
293 K). R = rejected, L =  $F_{\text{obs}} < 6\sigma (F_{\text{obs}})$

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	4	0	31.56	28.89	11	11	2	14.97	14.46	4	4	4	279.76	271.60
4	4	0	84.68	81.03	0	12	2	154.04	155.17	4	6	4	288.68	279.04
6	6	0	107.99	108.66	0	16	2	38.77	39.03	6	6	4	266.96	260.20
8	8	0	324.70	317.78	0	18	2	7.98	6.58	4	8	4	196.12	196.14
10	10	0	107.99	108.66	19	19	2	112.42	112.61	4	8	4	185.49	185.12
1	2	1	36.40	35.00	0	20	2	112.42	112.61	8	8	4	154.69	154.73
1	2	1	39.86	38.34	0	22	2	14.97	14.35	8	8	4	196.36	195.67
3	4	1	116.29	108.67	0	24	2	3.48	2.16	10	10	4	193.86	192.71
4	5	1	86.65	81.90	10	24	2	5.75	4.97	10	10	4	193.86	192.71
4	5	1	20.70	20.01	0	26	2	30.44	30.44	10	10	4	149.26	150.30
6	6	1	137.82	131.67	0	26	2	59.93	60.10	10	10	4	32.08	31.11
6	6	1	43.53	42.22	4	26	2	8.89	8.79	10	10	4	5.79	4.76
6	6	1	2.60	1.32	1	27	2	10.48	10.27	10	10	4	115.37	115.88
6	7	1	14.51	13.28	5	27	2	76.84	72.61	10	10	4	163.94	164.34
6	7	1	64.38	62.83	2	5	3	23.27	21.96	10	10	4	97.68	98.01
6	7	1	80.82	82.07	4	3	3	3.76	1.84	10	10	4	128.76	128.77
6	8	1	64.34	65.96	3	5	3	71.18	69.47	10	10	4	46.05	45.55
6	8	1	19.06	18.40	5	6	3	59.84	58.96	10	10	4	87.13	87.45
7	2	9	10.81	11.31	2	4	3	35.94	37.75	10	10	4	21.35	20.45
7	2	9	80.71	81.77	4	6	3	11.74	11.45	10	10	4	6.34	6.34
7	2	9	3.16	2.07	6	7	3	91.07	92.64	10	10	4	36.92	36.38
6	8	9	48.47	47.96	5	8	3	33.59	34.48	10	10	4	44.48	44.16
6	9	1	70.58	70.82	7	8	3	11.39	10.17	10	10	4	64.75	64.49
1	10	1	13.31	14.51	2	9	3	47.01	47.01	10	10	4	53.12	53.25
3	10	1	11.49	11.63	9	9	3	2.75	0.83	10	10	4	49.17	49.32
7	10	1	20.41	20.22	6	9	3	18.06	18.31	10	10	4	56.93	57.08
9	10	1	10.30	9.62	8	9	3	1.09	1.11	10	10	4	30.16	30.17
9	10	1	3.69	2.43	5	10	3	3.29	2.65	10	10	4	22.43	23.02
4	11	1	41.68	42.32	10	10	3	4.11	2.69	10	10	4	54.32	54.07
4	11	1	22.70	22.18	7	10	3	16.43	16.47	10	10	4	69.82	72.19
6	11	1	26.07	26.51	9	10	3	17.94	17.85	10	10	4	31.77	32.13
8	11	1	15.42	14.91	4	11	3	51.00	51.26	10	10	4	18.42	19.11
10	11	1	39.93	39.87	6	11	3	23.28	23.93	10	10	4	19.05	18.95
5	12	1	5.62	5.62	8	11	3	32.68	32.93	10	10	4	8.72	10.14
7	12	1	4.69	4.69	10	11	3	35.80	35.29	10	10	4	2.92	1.36
9	12	1	19.85	18.85	5	12	3	45.82	46.28	10	10	4	28.91	28.88
9	12	1	45.36	45.36	7	12	3	23.80	23.87	10	10	4	19.54	18.56
2	13	1	2.27	1.16	9	12	3	6.37	5.91	10	10	4	26.34	25.96
4	13	1	26.88	26.70	2	13	3	24.44	24.34	10	10	4	30.41	30.23
6	13	1	23.39	19.92	4	13	3	34.50	34.30	10	10	4	3.38	2.02
8	13	1	20.34	16.63	6	13	3	33.69	34.00	10	10	4	6.65	5.62
1	14	1	16.77	15.37	8	13	3	12.39	11.71	10	10	4	44.12	44.37
5	14	1	52.91	53.27	10	13	3	1.75	0.89	10	10	4	30.30	29.92
7	14	1	7.14	6.95	3	14	3	6.93	6.44	10	10	4	6.87	6.87
15	14	1	13.87	13.94	7	14	3	28.96	28.91	10	10	4	15.47	15.44
2	15	1	4.66	4.16	2	15	3	14.59	13.88	10	10	4	67.63	67.60
10	19	1	10.29	10.28	4	15	3	13.73	13.43	10	10	4	23.24	23.03
18	21	1	4.23	5.13	1	16	3	3.44	0.36	10	10	4	6.61	6.51
18	21	1	2.30	0.66	1	18	3	20.49	20.36	10	10	4	35.11	35.11
13	22	1	18.64	19.08	1	20	3	10.03	9.78	10	10	4	36.89	36.67
3	25	1	169.24	157.82	15	22	3	12.13	12.10	10	10	4	19.02	18.86
3	4	0	243.41	233.49	12	23	3	8.77	8.62	10	10	4	12.84	12.73
5	5	0	42.16	41.97	14	23	3	7.78	7.65	10	10	4	11.44	10.96
0	5	0	106.20	101.86	1	24	3	6.76	7.08	10	10	4	39.60	39.54
7	7	0	18.16	16.50	3	24	3	20.78	20.79	10	10	4	32.59	32.77
7	8	0	50.99	51.81	3	27	3	10.25	11.79	10	10	4	2.58	1.71
9	9	0	25.78	25.66	2	27	3	130.82	137.35	10	10	4	3.90	1.48
0	10	2	95.03	97.02	2	2	4	130.82	137.35	10	10	4	11.70	11.90

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	13	7	9.68	9.61	6	20	8	78.31	78.50	3	26	9	7.57	7.72	9	20	11	4.35	3.82
4	13	7	17.21	16.63	14	20	8	41.35	41.26	11	11	10	23.90	23.90	10	21	11	14.89	14.88
6	13	7	11.09	11.44	15	21	8	14.78	14.90	10	12	10	98.79	99.32	11	21	11	14.89	14.73
8	13	7	31.92	31.70	0	22	8	5.35	5.35	2	12	10	123.03	123.25	10	21	11	20.05	20.12
5	14	7	16.18	16.12	0	22	8	64.11	64.11	8	12	10	179.02	179.40	10	21	11	3.14	3.19
7	14	7	35.59	35.28	6	22	8	8.31	6.80	11	15	10	20.66	20.72	11	22	11	14.93	14.96
2	15	7	2.80	0.62	5	23	8	22.98	23.06	1	16	10	101.50	9.06	3	22	11	17.39	17.29
4	15	7	6.54	6.54	8	23	8	8.81	8.62	12	16	10	4.09	101.56	5	22	11	17.41	17.40
1	16	7	20.36	20.30	0	24	8	109.74	109.48	1	17	10	4.09	4.26	9	22	11	21.17	21.00
5	16	7	21.94	22.19	4	24	8	6.22	5.77	3	17	10	3.02	4.26	6	23	11	4.30	3.72
2	17	7	4.52	4.50	4	24	8	60.76	60.82	13	17	10	13.43	13.35	7	23	11	7.82	7.68
6	17	7	8.18	7.74	6	24	8	7.18	6.14	33	18	10	33.93	34.13	6	23	11	25.86	26.06
8	18	7	16.72	16.69	3	25	8	14.49	14.45	6	18	10	60.17	60.19	8	24	11	19.78	20.05
5	18	7	10.93	10.56	4	25	8	5.91	5.65	4	18	10	9.63	8.52	1	24	11	6.04	5.65
7	18	7	15.46	15.12	5	25	8	3.24	1.98	5	19	10	9.83	9.78	4	25	11	12.80	12.77
2	19	7	10.62	10.33	7	26	8	4.09	0.29	3	20	10	36.53	36.44	0	0	12	94.75	94.99
6	19	7	22.99	22.90	9	26	8	14.68	14.47	2	20	10	43.11	42.72	2	0	12	212.31	211.66
1	20	7	20.89	21.19	4	27	9	47.81	47.95	4	20	10	75.65	76.00	4	2	12	102.93	102.93
10	19	7	2.98	1.42	20	27	9	6.11	5.42	6	22	10	22.50	22.08	6	4	12	126.66	126.66
5	20	7	4.12	4.33	6	27	9	22.05	21.98	4	22	10	60.48	60.23	8	6	12	114.96	115.14
9	20	7	12.85	12.43	8	27	9	14.90	14.64	3	22	10	3.26	2.03	4	10	12	7.08	5.39
13	20	7	19.16	18.85	10	28	9	18.02	17.83	7	23	10	5.43	4.54	6	10	12	126.07	127.22
14	21	7	15.40	15.27	11	28	9	18.02	17.83	8	23	10	10.75	10.81	10	10	12	52.81	53.11
1	22	7	14.65	14.35	2	29	9	15.91	15.59	1	23	10	2.75	2.40	0	10	12	10.86	10.81
3	22	7	9.47	9.46	6	29	9	18.87	18.80	0	24	10	4.14	2.68	4	4	12	134.69	135.40
5	22	7	5.28	4.71	8	29	9	3.84	4.00	8	24	10	4.20	4.11	8	12	12	23.90	19.94
13	22	7	19.09	19.17	10	30	9	27.87	27.78	1	25	10	3.29	8.85	12	14	12	36.32	36.22
2	25	7	3.16	1.84	1	31	9	4.97	5.06	5	25	10	8.88	8.78	7	14	12	103.15	103.38
4	25	7	5.27	5.68	3	31	9	9.10	8.52	1	25	10	41.55	41.51	6	16	12	1.88	0.17
10	26	7	13.38	13.68	5	31	9	45.80	46.24	8	26	11	8.57	8.26	6	16	12	67.62	67.69
1	26	7	9.10	8.99	7	32	9	16.29	16.05	3	26	11	3.97	1.61	16	16	12	66.81	66.64
3	26	7	22.36	22.49	2	33	9	28.04	27.69	2	26	11	35.46	35.40	16	16	12	32.98	33.05
0	26	7	341.58	326.48	4	33	9	22.04	22.14	3	27	11	36.18	36.41	1	17	12	23.04	23.19
2	4	6	40.22	43.04	6	33	9	3.26	1.81	8	27	11	3.77	1.42	9	18	12	2.97	1.91
4	6	6	13.53	13.03	1	34	9	22.51	22.49	10	27	11	3.59	1.98	2	18	12	68.54	68.39
8	8	8	43.53	43.04	3	34	9	26.52	26.49	1	28	11	3.38	1.58	8	18	12	56.95	57.12
8	8	8	13.53	13.03	5	34	9	12.83	12.30	10	28	11	38.77	38.85	10	19	12	63.88	63.71
0	10	10	273.59	269.25	7	34	9	15.12	15.04	2	28	11	12.43	12.39	2	20	12	2.97	1.25
2	10	10	16.40	15.49	13	34	9	27.88	27.89	5	34	11	13.41	13.01	8	20	12	8.52	7.69
4	10	10	164.88	165.23	10	34	9	7.69	7.55	9	14	11	16.63	16.54	6	20	12	14.50	13.91
6	10	10	18.02	19.41	14	34	9	3.99	0.24	2	15	11	40.87	41.01	10	20	12	19.63	19.40
8	10	10	129.47	130.11	17	34	9	3.86	1.87	4	15	11	3.62	3.79	1	21	12	21.62	21.95
2	12	12	133.50	133.68	8	35	9	4.10	4.35	6	15	11	18.22	18.25	2	22	12	74.38	74.37
4	12	12	24.81	23.76	3	35	9	13.81	13.69	1	16	11	3.26	1.64	8	22	12	48.47	48.80
7	15	15	23.74	23.39	14	35	9	15.66	15.74	5	16	11	7.79	7.55	6	22	12	40.67	40.52
8	16	16	93.08	93.24	24	35	9	2.58	1.87	1	18	11	6.06	6.78	1	23	12	18.89	19.05
8	16	16	163.49	163.49	5	36	9	24.32	24.32	3	18	11	21.68	21.71	8	23	12	44.77	44.77
8	16	16	15.49	14.86	20	36	9	20.71	20.90	7	18	11	13.71	13.63	8	24	12	4.54	4.01
8	18	18	13.35	12.63	10	37	9	10.72	10.54	3	19	11	13.19	13.30	3	10	13	13.64	13.53
8	18	18	5.98	2.26	7	37	9	8.79	8.79	8	19	11	21.19	21.30	5	10	13	13.52	13.47
17	19	19	21.88	21.95	6	38	9	19.45	19.44	15	19	11	15.09	15.31	7	10	13	19.53	19.66
8	20	20	59.76	59.69	1	38	9	18.71	18.63	3	20	11	3.30	2.93	1	12	13	4.96	4.95
8	20	20			8	38	9	11.13	11.36	1	20	11	16.05	15.92	1	13	13	30.52	30.05

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
6	21	17	3.04	2.88	9	10	19	8.11	7.95	2	1	21	10.48	9.79	6	1	23	15.56	15.43
1	22	17	2.99	3.57	2	11	19	6.87	6.64	1	3	21	3.11	1.31	1	2	23	16.89	16.98
1	1	18	3.63	1.74	4	11	19	10.60	10.96	3	4	21	29.44	29.31	1	3	23	0.50	0.92
5	3	18	28.37	28.37	10	11	19	12.96	12.97	2	4	21	6.52	5.76	2	8	23	2.64	2.00
0	6	18	26.49	1.52	5	5	21	2.78	1.52	3	3	21	13.54	13.57	2	9	23	11.45	11.54
2	1	18	13.64	27.18	7	12	19	28.08	28.25	3	3	21	15.87	15.68	4	9	23	2.60	2.27
1	3	18	28.45	27.18	6	7	21	20.94	21.04	4	6	21	17.31	17.27	6	10	23	11.76	11.42
0	2	18	6.78	6.78	4	13	19	5.88	5.40	1	3	21	38.41	38.41	1	10	23	5.35	5.38
0	8	18	10.94	10.56	6	13	19	6.36	6.84	1	3	21	10.52	10.27	5	10	23	2.24	0.89
0	2	18	21.07	21.07	7	8	21	7.72	7.87	5	5	21	4.65	4.43	9	10	23	18.74	18.74
4	4	18	84.76	84.76	8	8	21	12.81	12.39	7	4	21	6.36	5.54	9	11	23	9.24	1.95
1	3	18	9.45	9.32	5	14	19	3.52	4.62	4	6	21	12.39	12.19	7	12	23	2.45	3.15
7	9	18	14.51	14.51	15	14	19	15.17	15.17	6	4	21	3.09	1.70	9	12	23	2.72	1.55
0	9	18	1.90	32.63	13	14	19	25.68	26.12	8	9	21	21.86	21.84	2	13	23	2.95	4.86
0	9	18	32.63	9.09	2	15	19	13.01	13.01	1	3	21	34.55	34.70	6	13	23	4.94	1.12
1	11	18	1.04	21.04	6	15	19	30.09	30.54	1	3	21	14.45	14.41	1	14	23	2.77	7.45
1	11	18	13.61	13.61	10	15	19	8.81	8.38	5	10	21	8.11	7.88	4	15	23	7.58	114.45
1	11	18	19.69	19.69	5	16	19	3.90	3.22	7	9	21	4.24	4.34	0	2	24	114.45	115.16
1	12	18	107.99	108.43	7	16	19	17.18	17.22	9	10	21	7.87	8.00	2	4	24	16.32	3.10
4	12	18	9.61	8.67	10	17	19	3.19	3.19	6	11	21	14.10	14.20	4	6	24	4.81	0.87
0	14	18	10.20	8.86	5	17	19	3.56	0.62	3	13	21	2.84	1.12	8	6	24	92.89	92.79
8	14	18	6.84	6.62	7	18	19	21.65	21.88	5	12	21	18.49	18.72	1	5	24	5.83	6.57
12	14	18	27.54	46.82	6	19	19	2.48	2.85	9	12	21	20.95	20.77	1	5	24	30.01	30.40
11	15	18	19.36	19.61	2	20	19	2.61	1.08	9	12	21	4.27	4.31	4	10	24	46.62	46.55
15	15	18	3.25	4.13	3	20	19	4.28	4.99	2	4	21	26.80	26.95	3	0	24	3.03	1.26
0	16	18	21.90	22.37	0	2	20	101.25	129.54	6	13	21	29.60	29.56	5	13	24	3.66	57.87
0	16	18	20.84	20.81	2	4	20	78.90	79.01	10	13	21	2.96	2.93	0	1	24	7.93	3.11
12	16	18	7.24	5.67	4	4	20	9.05	8.74	12	15	21	3.69	3.38	1	2	25	18.25	18.26
1	17	18	7.02	6.96	6	6	20	39.39	39.39	6	15	21	17.10	17.18	1	2	25	4.52	3.10
5	17	18	6.50	5.90	3	7	20	82.22	82.57	1	16	21	4.67	4.40	2	2	25	10.42	10.24
7	17	18	4.24	4.26	2	8	20	12.10	12.01	1	3	22	39.30	39.70	1	3	25	21.95	22.05
0	18	18	11.52	11.56	4	8	20	80.75	80.70	5	5	22	28.88	29.15	2	1	25	3.92	2.62
4	18	18	21.18	19.54	8	8	20	13.08	13.08	0	7	22	18.66	18.37	1	5	25	17.89	17.98
3	19	18	66.40	66.71	8	8	20	63.85	64.06	7	8	22	16.18	15.22	6	6	25	5.34	6.57
9	19	18	25.61	25.65	1	9	20	24.10	24.15	2	7	22	31.74	32.01	5	6	25	17.71	17.60
2	19	18	2.64	2.63	0	10	20	64.53	65.05	3	7	22	13.22	12.90	2	9	25	23.66	23.70
3	19	18	55.54	55.54	6	10	20	21.00	20.40	3	7	22	27.93	28.12	2	10	25	3.07	0.85
3	19	18	4.61	5.18	10	10	20	54.41	54.48	7	9	22	6.88	6.93	3	2	25	14.94	14.84
2	19	18	27.90	18.35	9	10	20	69.77	69.49	2	1	22	3.20	3.69	2	1	26	9.54	9.61
1	2	19	18.74	18.35	5	11	20	27.17	27.26	0	7	22	3.20	3.69	1	1	26	5.47	5.87
1	3	19	7.46	6.79	0	12	20	27.75	27.54	10	11	22	12.28	12.19	1	1	26	70.07	69.94
2	4	19	0.66	0.66	4	12	20	59.95	60.15	11	11	22	29.89	30.16	0	1	26	23.23	23.49
5	5	19	22.75	22.71	12	12	20	33.93	34.02	4	12	22	7.56	6.31	4	5	26	7.61	6.70
6	6	19	10.97	10.97	5	13	20	3.93	3.40	10	12	22	41.40	41.55	5	7	26	5.99	6.01
1	3	19	25.32	22.46	9	13	20	10.35	10.47	7	13	22	21.21	21.18	2	8	26	7.38	7.70
5	6	19	16.74	16.63	4	15	20	5.95	8.70	11	15	22	19.80	19.87	1	3	27	8.20	8.98
1	3	19	10.80	15.55	15	15	20	11.35	11.35	0	16	22	11.10	10.51	5	5	27	9.10	9.10
5	7	19	15.68	6.04	2	16	20	20.03	18.98	1	2	23	27.68	27.72	5	5	27	23.23	23.49
7	8	19	6.62	6.04	0	16	20	12.49	11.28	1	2	23	15.33	15.36	2	2	27	7.61	6.70
2	4	19	26.98	27.17	10	16	20	63.21	63.21	1	2	23	3.41	0.89	5	5	27	7.61	6.70
2	4	19	17.94	17.94	5	17	20	9.65	9.72	1	3	23	29.86	29.95	2	1	27	5.99	6.01
6	9	19	38.06	38.04	9	17	20	2.30	2.66	2	4	23	16.62	16.50	1	3	27	8.20	8.98
6	9	19	2.55	2.82	0	18	20	60.35	60.70	4	5	23	28.59	28.60	1	3	27	9.10	9.10
1	10	19	27.52	27.51	4	1	21	14.94	14.78	2	4	23	25.57	25.68	1	3	27	9.10	9.10
1	10	19	14.84	14.67	1	2	21	12.19	11.80	2	4	23	2.90	1.44	1	3	27	9.10	9.10

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
5	12	13	13.17	13.07	0	14	14	18.78	18.86	5	16	15	13.14	12.96	1	19	16	5.19	4.28
7	12	13	35.17	35.46	4	14	14	59.79	59.79	9	16	15	6.83	7.23	3	19	16	2.81	1.11
11	12	13	14.21	14.20	8	14	14	23.69	22.00	11	16	15	6.59	6.42	9	19	16	21.67	21.61
6	13	13	8.15	8.15	12	14	14	85.56	85.71	13	16	15	3.91	LR	11	19	16	2.42	LR
10	13	13	23.01	22.82	6	16	14	25.54	25.24	13	16	15	5.29	5.12	6	20	16	59.25	59.94
10	13	13	14.03	13.77	6	16	14	3.13	0.31	14	17	15	26.71	26.81	6	20	16	49.79	49.83
1	14	13	3.10	1.31	8	16	14	20.71	20.31	14	17	15	6.89	6.06	8	21	16	15.19	15.11
1	14	13	10.26	10.16	1	18	15	41.30	41.11	1	18	15	26.89	26.06	3	21	16	3.30	LR
5	14	13	4.85	3.30	3	18	15	13.24	13.23	3	18	15	38.05	38.07	5	21	16	9.31	9.17
7	14	13	4.73	4.09	5	18	15	16.94	11.92	7	18	15	3.41	LR	7	22	16	3.36	LR
9	14	13	21.95	21.60	13	17	14	11.94	11.92	13	17	14	13.26	13.32	2	22	16	27.64	27.42
11	14	13	3.56	4.09	9	18	15	10.19	8.30	9	18	15	10.31	10.09	1	2	3	14.47	14.19
13	14	13	42.67	43.58	4	18	14	71.52	71.52	4	19	15	14.34	14.75	1	2	3	25.80	26.19
4	15	13	12.92	12.44	6	18	14	15.84	15.52	8	19	15	7.45	7.10	1	3	4	25.42	25.51
6	15	13	11.92	11.92	7	19	14	14.32	14.37	12	19	15	15.35	15.60	3	4	4	32.02	32.95
8	15	13	3.53	4.25	9	19	14	34.85	34.31	3	20	15	5.67	5.46	2	4	5	32.49	32.39
1	16	13	3.48	1.11	0	20	14	50.72	50.76	7	20	15	10.11	10.02	1	4	5	30.20	30.16
1	16	13	7.81	7.28	2	20	14	51.76	51.89	9	20	15	9.76	9.88	1	4	6	24.79	24.66
3	16	13	12.27	12.31	6	20	14	4.89	4.76	11	20	15	15.25	15.25	1	4	7	15.39	15.19
5	16	13	19.47	19.40	12	20	14	24.18	24.51	4	21	15	13.12	13.14	3	8	17	22.78	22.70
7	16	13	17.76	17.79	5	21	14	9.14	9.13	4	21	15	5.62	5.97	5	8	17	10.43	10.31
10	17	13	4.10	4.33	11	21	14	5.68	5.53	10	21	15	2.89	LR	2	8	17	13.71	13.57
1	18	13	11.77	11.59	0	22	14	12.68	12.10	5	22	15	0.74	LR	8	9	17	5.62	5.11
3	18	13	16.95	16.56	2	22	14	19.16	8.50	2	23	16	10.08	10.18	5	10	17	7.34	6.86
7	18	13	20.95	20.95	2	22	14	7.44	7.27	2	23	16	147.37	148.11	2	10	17	24.38	24.39
9	18	13	2.89	3.96	8	22	14	8.68	8.10	4	24	16	28.06	3.18	4	11	17	3.17	2.05
11	18	13	20.70	20.60	5	23	14	31.54	32.13	4	24	16	19.41	19.56	8	11	17	18.70	18.55
13	18	13	19.38	19.57	7	23	14	30.62	30.62	0	24	16	12.63	11.76	10	11	17	24.96	24.94
8	19	13	11.08	10.89	4	24	16	26.29	26.21	0	26	16	23.06	21.33	5	12	17	8.95	8.57
10	19	13	10.32	10.05	6	24	16	16.13	16.07	2	26	16	25.41	25.39	7	12	17	7.11	7.03
10	19	13	3.91	3.40	1	6	7	50.38	50.38	3	26	16	218.55	219.79	11	12	17	16.41	16.42
12	19	13	16.13	16.19	1	8	15	14.55	14.10	0	28	16	12.92	12.39	4	13	17	4.45	3.22
1	20	13	2.25	2.10	5	8	15	28.93	28.68	2	28	16	21.09	21.79	6	13	17	3.24	2.47
3	20	13	13.55	13.55	8	9	15	4.93	4.40	0	28	16	30.83	30.26	8	13	17	9.17	8.88
11	20	13	9.89	9.89	1	10	15	4.93	4.40	4	10	16	44.69	44.26	3	14	17	27.47	27.44
3	21	13	17.80	17.88	3	10	15	7.60	7.29	4	10	16	44.48	45.02	5	14	17	20.79	20.82
5	22	13	9.16	9.50	5	10	15	22.37	22.24	7	10	16	25.90	25.85	7	14	17	22.44	22.45
9	22	13	3.90	5.05	9	10	15	24.10	23.94	0	12	16	111.54	111.61	2	15	17	6.91	6.82
4	23	13	26.34	26.63	1	12	15	11.13	10.57	2	12	16	74.85	75.28	6	15	17	18.06	18.05
8	23	13	13.08	12.92	3	12	15	6.41	6.01	12	12	16	10.34	9.75	8	15	17	18.05	18.05
1	24	13	13.09	13.45	9	12	15	6.53	6.51	12	12	16	10.64	8.99	10	15	17	3.25	2.60
0	8	14	32.66	32.07	0	14	16	7.05	7.09	0	14	16	41.84	41.34	12	15	17	24.38	24.60
2	8	14	21.54	21.08	4	14	16	16.80	16.79	2	14	16	14.96	14.55	12	15	17	17.55	17.54
6	8	14	111.29	111.59	10	13	15	21.01	21.16	4	14	16	67.56	67.58	9	16	17	16.44	16.41
6	8	14	17.36	15.87	14	13	15	38.93	39.19	14	14	16	7.41	6.62	11	16	17	3.35	3.32
0	10	14	32.86	32.92	0	14	16	5.15	5.36	0	16	16	136.02	135.45	13	16	17	3.00	0.67
2	10	14	77.73	78.55	4	14	15	8.30	7.94	4	16	16	88.21	88.40	6	17	17	13.27	12.78
4	10	14	31.44	31.48	9	14	15	5.43	5.88	8	16	16	9.01	9.04	6	17	17	3.64	0.44
6	10	14	6.44	4.72	13	14	15	2.69	0.34	16	16	16	14.15	13.98	10	17	17	30.93	31.64
11	11	14	108.92	108.93	5	14	15	42.65	42.85	16	16	16	4.97	5.04	11	18	17	8.01	7.63
0	12	14	18.92	18.76	2	15	15	2.65	2.67	3	17	16	9.92	9.77	6	19	17	20.79	20.61
2	12	14	54.65	54.90	6	15	15	3.88	1.72	5	17	16	74.31	74.33	6	20	17	15.25	15.22
4	12	14	4.21	3.24	10	15	15	16.02	15.80	15	18	16	21.58	21.75	3	20	17	12.11	11.85
8	12	14	78.05	77.89	14	15	15	3.07	2.99	6	18	16	13.91	12.81	7	20	17	5.00	5.08
10	12	14	80.44	80.64	1	16	15	3.32	2.90	8	18	16	12.27	12.19	4	21	17	17.71	18.05

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	4	0	18.60	8.58	16	16	4	82.72	83.38	8	11	7	24.91	28.49					
0	0	0	102.03	98.87	18	18	4	60.60	60.28	1	12	7	0.00	5.59					
0	0	0	0.00	0.00	18	18	4	72.59	73.55	7	12	7	14.40	0.00					
0	6	0	18.52	21.49	2	24	4	58.25	57.59	2	13	7	10.75	18.26					
0	6	0	374.92	373.99	0	24	4	69.26	70.37	6	13	7	0.00	4.14					
0	8	0	0.00	0.00	0	26	4	78.05	80.47	1	14	7	19.32	16.00					
0	10	0	10.45	16.26	5	6	5	36.73	34.40	7	14	7	44.63	43.88					
0	10	0	103.82	105.74	2	7	6	41.93	41.11	0	0	8	395.21	408.36					
0	12	0	21.45	21.63	2	4	5	70.17	72.30	2	4	8	29.30	28.48					
0	12	0	135.15	137.56	7	7	5	42.62	42.82	4	6	8	33.45	32.67					
0	12	0	139.88	140.52	6	5	5	0.00	0.00	4	4	8	24.06	23.03					
0	12	0	115.45	116.60	7	7	5	20.36	19.38	8	8	8	307.88	308.67					
0	14	0	0.00	0.00	2	4	9	9.03	8.03	2	10	8	4.48	7.25					
0	16	0	156.12	157.08	6	6	9	13.62	9.49	4	10	8	186.90	186.49					
0	16	0	45.95	46.39	5	9	5	30.39	9.39	6	10	8	14.73	11.48					
0	20	0	82.49	81.60	8	8	5	0.00	0.00	1	11	8	22.70	25.87					
1	2	2	10.05	13.88	5	10	5	4.53	9.36	2	12	8	151.90	152.89					
1	2	2	12.27	19.07	7	10	5	22.50	25.39	6	12	8	149.73	149.85					
1	3	1	0.00	0.00	4	11	5	19.04	20.14	1	13	8	18.69	24.54					
1	3	1	118.18	111.07	2	11	5	0.00	2.44	3	13	8	33.33	33.64					
1	3	1	104.03	100.04	2	11	5	0.00	2.44	0	16	8	249.68	249.58					
1	3	1	17.78	150.71	8	11	5	9.99	3.80	2	24	8	126.82	129.32					
1	3	1	156.11	150.71	10	11	5	45.01	43.71	0	24	8	0.00	0.95					
1	3	1	28.85	26.96	1	12	9	16.26	20.97	1	10	9	0.00	0.00					
1	3	1	14.22	12.94	5	12	9	8.99	4.45	2	11	9	11.09	3.59					
1	3	1	0.00	0.00	7	12	9	7.86	0.00	4	11	9	15.95	19.96					
1	3	1	64.75	63.61	4	13	5	1.85	7.05	6	11	9	40.02	39.45					
1	3	1	69.56	69.77	6	13	5	23.79	23.83	1	12	9	16.64	19.57					
1	3	1	8.74	13.31	8	13	5	36.23	35.40	5	12	9	24.36	23.81					
1	3	1	65.77	65.44	10	13	5	45.43	44.81	1	12	9	17.98	16.24					
1	3	1	16.25	17.71	1	14	5	11.69	8.40	8	10	10	9.35	6.74					
1	3	1	83.40	82.73	2	15	5	45.86	45.15	6	11	10	138.00	137.95					
1	3	1	9.51	17.88	7	13	7	0.00	9.77	0	20	10	80.06	78.65					
1	3	1	48.08	48.61	0	2	6	34.03	35.53	4	22	10	66.72	67.36					
1	3	1	57.85	58.72	4	14	6	181.79	179.59	2	2	12	224.35	228.96					
1	3	1	8.47	8.39	9	9	6	78.47	76.79	4	4	10	130.11	130.98					
1	3	1	22.49	22.49	0	2	6	56.89	56.12	2	4	12	138.36	137.78					
1	3	1	3.39	3.39	2	4	6	41.17	40.41	6	6	12	32.54	31.60					
1	3	1	22.49	22.49	2	4	6	156.44	156.40	8	8	12	123.12	124.81					
1	3	1	42.21	42.21	4	4	6	120.50	121.19	10	10	12	61.22	61.89					
1	3	1	11.98	11.32	4	4	6	12.54	15.24	10	10	12	160.06	159.19					
1	3	1	11.32	11.32	4	4	6	16.50	18.56	12	12	12	55.17	55.79					
1	3	1	22.93	22.93	6	6	6	20.86	25.17	12	14	12	123.27	124.16					
1	3	1	147.01	147.01	2	2	8	26.91	26.38	6	6	14	113.34	112.57					
1	3	1	298.21	298.21	2	2	8	11.28	17.81	8	14	12	93.32	92.40					
1	3	1	56.43	56.43	2	2	8	85.15	87.81	10	14	12	89.80	88.94					
1	3	1	87.78	87.78	2	2	8	91.61	91.52	14	14	12	96.88	94.15					
1	3	1	28.12	28.12	6	6	6	16.35	0.00	14	14	12	121.15	121.15					
1	3	1	54.91	54.91	10	10	4	21.98	25.64	0	16	12	83.12	82.24					
1	3	1	108.78	108.78	2	2	8	21.98	20.31	6	16	12	116.46	114.71					
1	3	1	5.37	5.37	4	4	4	19.43	20.31	10	18	12	117.93	121.39					
1	3	1	177.51	177.51	6	6	8	29.40	16.03	2	18	12	77.20	77.23					
1	3	1	134.00	134.00	10	10	4	18.63	29.65	6	18	12	78.49	77.90					
1	3	1	35.71	35.71	10	10	4	15.85	15.85	8	18	12	70.96	69.98					
1	3	1	14.52	14.52	1	1	15	9.29	2.86	8	18	12	77.99	77.65					
1	3	1	59.04	59.04	2	2	16	15.88	19.46	4	20	12	81.68	82.35					
1	3	1	10.86	10.86	4	4	4	59.08	58.95	6	22	12	56.06	55.12					
1	3	1	9.89	9.89	4	4	4	6.81	7.33	6	22	12	28.47	26.78					

PYROPE 80		- ALMANDINE 20		100 K		STRUCTURE FACTORS		PAGE . 2	
H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
4	6	14	109.92	110.09					
4	8	14	129.34	127.73					
9	9	14	25.43	23.02					
4	16	14	80.65	81.43					
12	16	14	56.68	53.66					
4	18	14	80.14	79.39					
0	0	16	171.54	176.79					
2	2	16	33.97	35.20					
4	6	16	115.26	114.45					
4	8	16	103.46	103.24					
8	8	16	188.34	188.93					
4	10	16	58.99	59.60					
10	10	16	50.48	51.08					
2	12	16	90.01	90.46					
12	12	16	21.92	14.20					
8	16	16	110.84	108.94					
4	18	16	87.60	86.39					
2	20	16	18.31	23.73					
6	20	16	71.24	71.47					
2	4	18	94.81	95.42					
4	6	18	89.43	89.35					
4	8	18	98.91	98.66					
0	0	20	137.57	139.69					
2	2	20	111.61	110.74					
4	4	20	99.93	99.73					
6	8	20	92.64	92.32					
8	10	20	56.43	55.66					
10	10	20	79.44	78.47					
2	14	20	56.99	59.13					
4	8	22	76.20	76.20					
0	0	24	133.64	135.03					
4	4	24	66.81	66.79					
4	8	24	66.93	69.24					



H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	4	0	15.68	10.89	1	13	6	9.33	12.70	5	9	8	31.13	30.14
4	0	0	117.81	116.09	13	13	6	37.56	37.41	7	9	8	14.88	15.94
6	0	0	33.63	32.71	13	14	6	35.12	36.10	0	10	8	15.35	15.82
8	0	0	402.13	404.51	4	14	6	119.11	118.40	2	10	8	9.74	13.82
10	0	0	96.65	97.87	1	15	6	10.73	11.48	4	10	8	208.38	205.44
12	12	0	17.31	24.56	1	15	6	14.78	13.59	6	10	8	4.24	3.97
14	14	0	32.29	32.08	5	15	6	13.46	8.82	10	10	8	33.75	33.24
1	1	2	6.54	6.76	0	16	6	19.65	22.37	1	11	8	26.70	26.93
3	3	2	7.60	2.43	2	16	6	27.93	28.40	3	11	8	21.96	24.18
5	5	2	119.88	116.73	4	16	6	28.95	130.97	5	11	8	44.53	44.35
7	7	2	71.15	71.16	1	17	6	16.56	17.84	7	11	8	147.78	150.19
9	9	2	78.83	71.90	3	17	6	37.70	38.12	4	12	8	41.21	171.30
1	1	7	7.47	13.92	0	18	6	16.78	2.12	2	12	8	171.55	40.86
3	3	7	41.79	40.58	2	18	6	28.44	26.65	6	12	8	8.63	167.59
5	5	5	10.92	13.06	2	18	6	101.73	97.37	12	12	8	22.11	6.50
7	7	5	44.30	43.41	4	19	6	11.24	10.72	3	13	8	33.77	33.78
9	9	5	116.51	121.03	1	19	6	0.00	5.35	5	13	8	39.16	37.53
11	11	2	13.03	12.12	3	19	6	18.74	17.72	7	13	8	32.80	32.36
13	13	2	192.29	199.16	5	19	6	37.07	36.96	0	14	8	31.28	32.46
0	0	2	20.51	22.48	1	20	6	20.99	20.36	2	14	8	147.44	149.62
2	2	2	37.07	36.18	3	20	6	14.13	15.30	4	14	8	8.12	3.41
4	4	2	14.60	14.05	5	20	6	20.34	20.03	6	14	8	49.01	51.20
6	6	2	8.42	8.31	9	20	6	57.28	56.57	1	15	8	6.49	14.56
8	8	2	0.00	14.53	1	21	6	16.78	16.08	3	15	8	31.16	30.54
10	10	2	149.69	144.53	6	21	6	59.58	59.93	7	15	8	16.63	24.41
12	12	3	109.55	105.59	4	21	6	0.00	2.50	0	16	8	262.85	274.25
14	14	3	33.53	31.79	6	21	6	11.37	5.94	2	16	8	14.75	20.02
16	16	3	33.53	31.79	1	22	6	46.01	46.54	4	16	8	5.84	6.18
18	18	3	10.45	11.79	3	22	6	9.00	6.84	6	16	8	14.65	13.54
20	20	3	34.54	34.17	5	22	6	27.11	26.89	8	16	8	22.54	23.97
2	2	4	13.93	15.35	2	23	6	14.63	16.78	3	17	8	13.00	10.38
4	4	4	14.66	15.35	4	23	6	23.21	24.39	5	17	8	17.66	15.35
6	6	4	31.71	32.30	1	24	6	10.86	9.54	7	17	8	22.87	21.81
8	8	4	21.09	21.63	3	24	6	15.10	14.23	0	18	8	14.67	13.83
10	10	4	358.17	369.69	5	24	6	15.87	14.23	4	18	8	114.82	113.68
12	12	4	318.19	332.60	6	24	6	11.90	5.83	6	18	8	17.79	12.05
14	14	4	387.59	385.34	6	25	6	34.18	31.35	6	19	8	15.30	10.87
16	16	4	19.90	19.62	1	26	6	21.59	21.07	1	19	8	82.73	84.30
18	18	4	345.27	360.63	3	26	6	28.99	25.56	3	19	8	9.71	8.08
20	20	4	232.28	239.70	5	26	6	18.22	9.82	5	19	8	16.28	12.27
2	2	6	65.68	63.62	6	27	6	28.45	27.20	7	19	8	5.47	4.87
4	4	6	36.63	38.31	1	28	6	11.56	7.63	2	20	8	13.96	11.43
6	6	6	248.35	253.48	3	28	6	27.28	26.12	4	20	8	21.46	21.19
8	8	6	240.96	240.89	5	28	6	21.94	22.25	8	20	8	0.00	6.22
10	10	6	182.27	178.33	7	29	6	424.76	466.60	1	21	8	23.89	19.99
12	12	6	46.44	46.58	9	29	6	48.02	51.49	3	21	8	11.38	13.85
14	14	6	237.94	244.39	0	30	6	16.90	16.15	5	21	8	19.30	18.96
16	16	6	173.12	170.83	2	30	6	21.52	21.92	7	21	8	8.81	3.84
18	18	6	17.85	16.10	4	30	6	32.23	31.98	2	22	8	10.79	13.27
20	20	6	184.80	184.63	6	30	6	48.31	338.72	4	22	8	12.00	18.44
2	2	8	10.62	1.07	8	30	6	17.08	18.95	8	22	8	8.29	8.16
4	4	8	10.62	1.07	9	30	6	17.08	18.95	9	22	8	0.00	10.54

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
5	14	9	24.24	23.69	2	5	11	13.17	12.99	6	7	13	9.40	4.92
7	14	9	32.68	32.00	3	6	11	70.51	70.99	1	14	13	11.78	12.62
4	15	9	11.41	15.61	2	7	11	27.40	27.62	1	3	14	24.24	24.09
4	15	9	21.96	21.64	1	12	11	38.12	40.69	5	14	13	13.96	10.60
6	15	9	0.00	11.51	3	12	11	14.28	8.46	7	14	13	9.69	9.19
8	15	9	23.25	23.39	5	12	11	11.14	1.03	2	15	13	0.00	2.09
8	16	9	23.08	24.27	7	12	11	12.00	8.09	4	15	13	7.20	11.26
13	16	9	26.14	27.60	9	12	11	13.19	14.22	1	16	13	8.69	2.32
5	16	9	15.75	12.65	2	13	11	25.89	24.79	1	1	14	1.49	3.45
7	16	9	0.00	2.40	4	13	11	35.16	36.45	1	3	14	34.40	34.59
2	17	9	0.00	1.77	6	13	11	19.61	22.33	1	3	14	13.31	4.81
4	17	9	31.36	29.02	10	13	11	13.03	2.62	2	3	14	184.68	188.27
6	17	9	12.67	12.67	8	13	11	0.00	11.82	3	5	14	15.77	16.85
4	17	9	5.60	5.60	1	14	11	10.95	14.32	5	5	14	18.75	18.90
1	18	9	11.25	2.28	3	14	11	24.48	25.18	5	6	14	15.01	17.04
3	18	9	47.86	47.31	5	14	11	29.83	27.34	2	7	14	52.02	51.43
1	1	10	7.89	8.04	7	14	11	0.00	1.94	9	9	14	32.83	30.91
1	3	10	30.91	31.54	9	14	11	11.14	2.04	1	15	14	0.00	9.38
3	4	10	220.36	221.70	2	15	11	25.99	28.04	1	1	15	30.58	30.13
5	5	10	77.76	2.67	4	15	11	15.75	3.78	2	3	15	44.90	46.39
7	7	10	11.55	5.92	6	15	11	17.19	15.24	1	2	15	6.01	4.31
9	9	10	34.16	32.16	8	15	11	18.26	20.79	1	3	15	11.70	14.48
1	11	10	6.23	3.18	1	16	11	0.00	3.65	0	0	16	190.64	200.59
3	11	10	18.13	16.23	3	16	11	0.00	7.95	1	3	16	44.90	42.79
5	11	10	14.15	14.77	5	16	11	0.00	8.42	4	6	16	9.69	13.78
7	11	10	7.10	5.78	7	16	11	28.26	27.88	6	8	16	17.04	15.55
11	11	10	37.51	36.12	2	17	11	16.26	11.63	8	1	18	214.51	212.76
1	12	10	39.01	38.23	4	0	12	0.00	2.89	1	3	18	14.56	15.94
0	12	10	132.85	134.47	0	0	12	109.78	110.05	5	5	18	45.59	44.79
2	12	10	143.76	145.52	2	2	12	236.68	240.24	7	0	20	0.00	12.54
4	12	10	0.00	3.64	1	0	12	39.02	40.57	0	0	20	0.00	4.04
6	12	10	152.11	148.32	0	4	12	15.22	12.06	7	0	20	149.85	146.69
8	12	10	114.58	111.53	4	4	12	156.29	158.10	2	2	20	120.15	121.34
1	13	10	16.40	19.53	3	5	12	34.52	35.69	1	1	20	9.40	4.92
3	13	10	2.70	19.53	5	6	12	10.71	16.74	1	1	20	11.78	12.62
5	13	10	7.72	2.38	6	6	12	197.10	198.50	1	1	20	24.24	24.09
7	13	10	11.51	5.92	8	10	12	137.80	148.50	5	14	13	13.96	10.60
9	13	10	0.00	10.93	10	8	12	69.70	67.55	7	14	13	9.69	9.19
0	14	10	19.45	20.87	1	13	12	0.00	4.18	4	15	13	0.00	2.09
2	14	10	15.95	12.15	3	13	12	29.05	31.85	2	15	13	7.20	11.26
4	14	10	96.63	95.08	5	13	12	15.61	13.69	1	16	13	8.69	2.32
6	14	10	29.26	32.18	7	13	12	35.44	35.30	4	16	13	34.40	34.59
8	14	10	13.61	16.45	9	13	12	28.71	29.40	1	1	20	13.31	4.81
1	15	10	16.23	19.79	0	14	12	131.95	139.24	2	3	14	15.77	16.85
3	15	10	16.95	7.87	2	14	12	68.68	70.46	1	1	20	8.69	2.32
5	15	10	0.00	5.77	4	14	12	0.00	2.65	1	1	20	1.49	3.45
7	15	10	12.44	9.65	6	14	12	122.69	122.42	1	1	20	34.40	34.59
9	15	10	0.00	11.11	8	14	12	112.10	108.32	1	1	20	13.31	4.81
0	16	10	13.31	9.52	1	15	12	18.51	11.40	1	1	20	184.68	188.27
2	16	10	77.40	74.50	3	15	12	9.96	5.98	2	3	14	15.77	16.85
4	16	10	11.72	4.65	5	15	12	18.66	23.57	8	8	16	17.04	15.55
6	16	10	13.69	8.90	7	15	12	0.00	3.02	1	3	14	52.02	51.43
8	16	10	12.38	13.76	0	16	12	124.52	130.52	1	3	14	32.83	30.91
1	17	10	14.95	19.22	2	16	12	102.35	106.98	2	7	14	0.00	9.38
3	17	10	16.95	13.76	4	16	12	26.87	2.48	5	7	14	30.58	30.13
5	17	10	0.00	2.06	1	2	13	23.41	23.80	1	1	20	44.90	42.79
0	18	10	36.02	34.97	2	4	13	24.39	23.52	1	1	20	9.69	9.19
2	18	10	21.42	22.29	3	5	13	15.20	17.60	1	1	20	11.78	12.62
1	1	11	4.50	5.84	5	6	13	23.86	23.52	1	1	20	24.24	24.09

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
4	8	0	278.81	R	0	12	6	195.18	195.36	8	14	12	136.23	135.76
8	8	0	469.76	R	2	12	6	150.28	148.16	10	14	12	107.73	108.90
6	10	0	86.57	R	0	14	6	54.40	54.86	14	14	12	117.23	116.27
8	12	0	166.57	R	4	16	6	159.20	160.96	0	16	12	142.93	143.39
10	12	0	169.30	R	2	20	6	109.63	110.36	6	16	12	123.59	124.42
16	16	0	226.44	R	6	20	6	104.06	111.13	10	16	12	156.29	153.75
5	0	0	65.64	R	1	24	6	66.23	65.41	2	18	12	164.77	160.12
0	0	0	0.00	LR	4	4	7	71.52	72.51	0	18	12	99.81	96.29
1	1	1	46.49	LR	4	5	7	75.04	76.49	6	18	12	94.54	96.12
7	7	2	67.52	R	5	10	7	62.81	61.47	8	18	12	109.33	108.53
2	2	2	144.73	R	1	10	7	59.44	59.71	4	20	12	137.64	135.82
0	10	0	238.23	R	4	11	7	44.32	45.24	0	22	12	116.15	116.61
8	14	2	53.38	R	3	12	7	44.18	45.61	6	22	12	101.40	101.42
8	14	2	49.15	R	2	13	7	535.78	531.90	2	22	12	71.11	70.39
2	16	2	59.48	R	0	0	8	20.38	21.20	2	4	14	200.70	204.58
12	16	2	136.30	R	2	2	8	293.51	291.20	4	4	14	0.00	0.00
0	20	2	170.37	R	2	4	8	94.79	93.58	7	7	14	67.87	66.19
2	20	2	132.27	R	3	5	8	254.29	247.48	9	9	14	52.34	50.10
1	2	3	99.02	R	4	6	8	55.37	52.67	4	16	14	122.25	121.56
1	14	3	54.46	R	6	6	8	199.50	197.31	12	16	14	93.64	90.80
0	0	4	411.09	R	4	8	8	393.17	391.06	4	18	14	96.96	96.03
2	2	4	212.73	R	1	8	8	49.98	48.57	0	20	14	81.62	83.04
4	4	4	118.55	R	4	10	8	242.46	241.18	2	22	14	77.46	77.55
4	4	4	153.53	R	4	12	8	63.39	58.36	2	0	16	91.84	89.56
4	4	4	479.45	R	6	12	8	201.14	199.11	2	0	16	62.02	64.27
4	4	4	419.50	R	0	16	8	316.01	317.19	8	0	16	246.25	247.25
4	4	4	85.28	R	16	16	8	168.19	165.96	0	8	16	75.38	74.39
4	4	4	288.24	R	4	18	8	140.78	140.61	10	10	16	29.53	32.74
10	10	4	186.70	R	2	20	8	136.50	136.84	12	12	16	120.30	122.01
4	4	4	41.94	R	4	22	8	107.16	111.57	12	18	16	58.49	61.59
12	12	4	232.13	R	0	24	8	180.16	182.55	2	20	16	106.67	107.86
8	14	4	184.73	R	4	24	8	88.41	89.73	6	0	20	160.15	159.98
6	14	4	133.31	R	2	3	9	76.33	77.47	0	8	20	132.55	132.27
10	14	4	175.12	R	6	7	9	61.42	61.75	6	0	20	99.37	94.75
4	4	4	109.35	R	2	9	9	51.30	49.11	0	10	20	102.74	101.37
4	4	4	132.14	R	6	3	9	44.53	55.10	10	10	20	194.28	196.45
4	4	4	193.67	R	3	3	10	241.53	242.78	0	0	24	0.00	0.00
4	4	4	126.40	R	2	4	10	40.14	79.71	8	8	16	246.25	253.00
16	16	4	105.52	R	0	10	10	80.44	50.93	10	12	16	75.38	74.39
4	4	4	115.85	R	8	10	10	60.63	159.89	12	12	16	120.30	122.01
2	18	4	117.43	R	2	12	10	160.61	163.40	12	18	16	58.49	61.59
4	4	4	110.35	R	6	12	10	105.98	105.17	0	20	16	106.67	107.86
4	4	4	87.10	R	4	16	10	118.78	118.95	6	8	20	160.15	159.98
18	18	4	162.98	R	0	20	10	86.50	84.90	0	8	20	132.55	132.27
4	4	4	76.52	R	4	22	10	88.23	93.27	8	0	20	102.74	101.37
0	24	4	108.79	R	4	24	10	89.48	89.29	10	10	20	194.28	196.45
0	0	2	111.90	R	3	6	11	129.23	128.97	8	8	16	246.25	247.25
1	2	5	150.99	R	0	0	12	262.66	259.94	0	20	16	75.38	74.39
2	2	5	139.05	R	2	4	12	216.58	213.72	10	10	20	246.25	247.25
5	5	5	100.07	R	4	4	12	15.60	16.13	0	0	24	0.00	0.00
5	5	5	54.39	R	4	6	12	165.99	164.22	8	8	16	246.25	247.25
6	6	6	202.33	R	6	6	12	205.62	205.06	10	10	20	194.28	196.45
6	6	6	60.59	R	2	8	12	150.85	149.34	12	12	16	58.49	61.59
3	3	3	339.96	R	8	8	12	81.27	81.30	14	14	16	106.67	107.86
6	6	6	70.75	R	10	10	12	115.71	116.44	16	16	16	106.67	107.86
6	6	6	62.46	R	12	14	12	164.44	167.16	18	18	16	106.67	107.86
6	6	6	253.30	R	0	14	12	81.44	83.12	0	10	20	102.74	101.37
4	4	4	71.57	R	2	14	12	133.89	135.33	10	10	20	194.28	196.45
2	2	1	49.57	R	6	14	12	133.89	135.33	10	10	20	194.28	196.45

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STRUCTURE FACTORS				STRUCTURE FACTORS				STRUCTURE FACTORS						
H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	4	0	71.15	71.85	2	4	1	10.60	10.32	1	1	1	10.60	10.32
6	6	0	165.20	164.62	1	1	1	17.48	10.63	2	4	6	35.16	37.14
8	4	0	475.46	475.83	1	1	1	13.02	20.79	6	1	7	47.89	47.89
10	10	0	295.89	303.31	2	2	2	407.32	71.34	8	8	8	8.98	10.29
12	12	0	73.76	74.78	3	3	3	112.32	396.96	1	1	1	93.61	94.82
14	14	0	20.55	18.92	4	4	4	112.65	113.98	2	2	2	69.53	71.71
16	16	0	213.98	214.35	5	5	5	33.88	25.44	3	3	3	43.95	45.00
18	18	0	175.85	176.17	6	6	6	341.53	338.42	9	9	9	58.49	58.07
20	20	0	186.74	185.55	7	7	7	76.45	77.01	13	13	13	19.33	20.30
22	22	0	46.01	47.64	8	8	8	47.77	69.64	10	10	10	62.69	61.63
24	24	0	201.22	205.45	9	9	9	70.04	156.38	18	18	18	45.07	44.71
26	26	0	31.88	30.00	10	10	10	150.42	33.80	3	3	3	32.81	34.11
28	28	0	9.78	5.59	11	11	11	35.21	38.02	4	4	4	13.03	13.02
30	30	0	53.58	53.94	12	12	12	39.05	28.57	6	6	6	98.96	99.75
32	32	0	32.74	31.90	13	13	13	29.88	38.02	7	7	7	26.11	25.93
34	34	0	244.49	245.78	14	14	14	256.78	256.55	11	11	11	9.51	9.86
36	36	0	32.09	33.13	15	15	15	158.34	157.85	12	12	12	39.39	39.49
38	38	0	21.15	19.15	16	16	16	224.24	222.20	14	14	14	34.31	34.61
40	40	0	25.23	23.86	17	17	17	8.32	6.92	15	15	15	44.49	44.66
42	42	0	42.88	44.20	18	18	18	52.28	51.78	16	16	16	22.36	22.45
44	44	0	65.74	67.33	19	19	19	27.12	26.07	17	17	17	33.18	31.91
46	46	0	167.31	165.26	20	20	20	49.05	48.67	18	18	18	61.39	61.35
48	48	0	16.82	17.84	21	21	21	45.32	45.06	19	19	19	43.28	43.61
50	50	0	216.04	214.16	22	22	22	27.51	28.55	20	20	20	36.59	35.63
52	52	0	34.05	33.08	23	23	23	17.64	17.85	21	21	21	32.97	32.37
54	54	0	71.49	70.89	24	24	24	63.86	63.37	22	22	22	35.86	36.30
56	56	0	54.96	54.67	25	25	25	17.00	10.69	23	23	23	29.47	30.38
58	58	0	64.67	64.67	26	26	26	68.48	71.80	24	24	24	10.62	5.20
60	60	0	22.12	22.12	27	27	27	9.97	8.32	25	25	25	17.14	17.14
62	62	0	65.04	66.73	28	28	28	8.94	6.55	26	26	26	24.40	25.57
64	64	0	16.40	16.18	29	29	29	13.72	17.26	27	27	27	18.86	19.21
66	66	0	53.34	52.11	30	30	30	10.69	14.11	28	28	28	34.51	34.37
68	68	0	84.67	85.81	31	31	31	67.35	67.06	29	29	29	39.02	38.72
70	70	0	57.65	58.94	32	32	32	2.59	7.27	30	30	30	69.30	69.33
72	72	0	45.05	43.41	33	33	33	148.43	151.74	31	31	31	48.34	48.88
74	74	0	67.84	63.84	34	34	34	4.19	10.96	32	32	32	21.20	21.20
76	76	0	49.34	48.20	35	35	35	32.93	32.98	33	33	33	10.70	11.72
78	78	0	42.85	43.43	36	36	36	12.37	13.74	34	34	34	5.69	5.69
80	80	0	24.34	24.23	37	37	37	39.87	40.48	35	35	35	14.79	14.79
82	82	0	30.49	30.76	38	38	38	3.48	0.00	36	36	36	12.11	14.53
84	84	0	4.58	2.65	39	39	39	36.48	35.51	37	37	37	23.63	24.18
86	86	0	7.65	7.84	40	40	40	34.66	32.45	38	38	38	40.71	40.09
88	88	0	7.87	0.43	41	41	41	41.80	41.55	39	39	39	392.19	382.61
90	90	0	7.87	13.28	42	42	42	6.73	18.53	40	40	40	218.19	223.07
92	92	0	11.54	52.11	43	43	43	13.67	18.52	41	41	41	490.52	473.50
94	94	0	53.72	56.11	44	44	44	39.79	41.60	42	42	42	409.95	413.44
96	96	0	4.52	6.03	45	45	45	4.16	6.06	43	43	43	260.62	261.45
98	98	0	43.55	44.12	46	46	46	10.32	6.54	44	44	44	307.07	308.80
100	100	0	12.31	13.56	47	47	47	45.37	46.53	45	45	45	16.78	15.97
102	102	0	4.74	5.74	48	48	48	15.41	7.88	46	46	46	206.51	205.76
104	104	0	9.64	1.62	49	49	49	119.07	111.45	47	47	47	251.57	251.57
106	106	0	27.18	27.07	50	50	50	158.20	154.24	48	48	48	195.73	194.73
108	108	0	8.81	5.69	51	51	51	77.59	75.62	49	49	49	9.52	5.81
110	110	0	9.75	5.67	52	52	52	77.59	75.62	50	50	50	9.52	5.81

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
4	15	5	25.78	26.42	1	11	8	29.65	28.85	8	15	9	24.51	23.73
6	15	5	17.34	17.69	7	11	8	26.56	25.58	8	16	9	27.33	27.56
8	15	5	32.22	32.10	4	12	8	70.08	68.17	3	16	9	28.10	27.29
12	16	5	19.85	21.77	6	12	8	215.78	217.15	5	16	9	11.83	11.98
1	16	5	11.18	12.34	12	13	8	15.24	17.15	7	16	9	10.41	3.27
3	16	5	15.36	12.68	1	13	8	22.44	22.43	4	17	9	31.62	31.06
5	16	5	17.79	0.00	3	13	8	34.76	33.02	6	17	9	33.52	33.59
11	16	5	11.22	7.79	7	14	8	32.61	33.17	8	17	9	7.90	4.62
4	17	5	14.22	14.49	14	14	8	13.06	9.56	5	18	9	38.31	37.69
6	17	5	30.61	30.76	13	14	8	16.67	16.55	7	18	9	39.29	39.81
8	17	5	15.23	15.95	7	15	8	13.06	24.76	2	19	9	16.74	14.94
10	17	5	10.39	10.99	0	16	8	25.39	24.76	4	19	9	39.81	39.58
3	18	5	39.92	39.99	2	16	8	337.06	336.33	6	19	9	25.75	26.12
5	18	5	7.11	5.64	6	16	8	21.84	18.79	8	19	9	35.94	38.03
5	18	5	10.91	12.76	16	16	8	15.32	5.36	6	20	9	29.59	28.71
5	18	5	50.76	51.68	1	17	8	194.01	189.71	1	20	9	0.00	1.30
5	18	5	2.97	3.54	3	17	8	8.60	10.71	3	20	9	0.00	12.38
5	18	5	25.26	26.59	7	17	8	8.97	23.67	5	20	9	13.39	12.18
5	18	5	12.15	11.79	4	18	8	159.11	156.26	7	21	9	14.75	11.74
3	18	5	34.83	35.07	6	18	8	25.62	23.79	2	21	9	11.30	13.95
2	18	5	25.97	25.74	1	19	8	12.41	10.41	6	21	9	31.42	31.89
5	18	5	30.83	32.27	3	19	8	10.92	11.29	8	21	9	21.58	22.67
5	18	5	17.32	18.17	5	19	8	6.56	6.37	3	22	9	6.62	6.36
5	18	5	33.46	33.46	7	19	8	86.26	88.72	5	22	9	11.92	10.76
5	18	5	12.70	15.23	0	20	8	150.08	152.02	5	23	9	0.00	0.69
5	18	5	32.08	34.13	4	20	8	44.01	45.50	4	23	9	0.00	38.93
7	18	5	4.20	6.53	6	20	8	142.76	147.29	6	23	9	0.00	0.69
5	18	5	9.57	9.52	2	21	8	9.26	9.34	6	24	9	2.64	5.35
6	18	5	81.90	83.00	1	21	8	27.27	27.62	3	24	9	18.43	20.07
6	18	5	270.96	266.90	3	21	8	11.73	11.73	5	24	9	31.16	29.58
6	18	5	44.12	43.66	5	21	8	10.31	5.79	7	24	9	24.62	26.41
6	18	5	96.63	97.78	0	22	8	13.78	5.40	9	24	10	58.70	57.82
6	18	5	38.07	36.00	2	22	8	16.45	16.87	10	24	10	29.93	29.72
6	18	5	196.28	193.26	2	22	8	118.00	124.94	7	24	10	59.29	58.91
6	18	5	25.77	24.76	6	22	8	27.41	26.56	11	24	10	59.56	58.66
6	18	5	9.91	6.55	6	22	8	14.57	13.82	11	24	10	171.31	171.04
6	18	5	21.61	16.44	3	23	8	4.57	6.00	4	24	10	8.90	3.03
6	18	5	12.99	11.74	5	23	8	28.98	28.32	6	24	10	174.92	173.93
6	18	5	59.33	56.75	0	24	8	204.94	204.58	8	24	10	158.23	159.85
6	18	5	64.46	65.09	2	24	8	16.46	9.98	8	24	10	44.05	44.13
6	18	5	22.32	22.29	4	24	8	102.35	100.06	13	24	10	30.67	27.99
6	18	5	12.34	13.41	6	24	8	11.16	11.56	7	24	10	20.86	18.99
6	18	5	33.31	33.41	1	25	8	15.33	16.31	9	24	10	33.52	33.53
6	18	5	6.69	9.01	3	25	8	34.79	35.01	13	24	10	33.21	30.34
6	18	5	22.03	21.53	1	25	8	28.95	28.90	6	24	10	37.71	38.27
6	18	5	53.06	54.03	4	25	8	22.71	21.00	5	24	10	28.21	27.18
6	18	5	178.81	177.63	6	25	8	12.77	12.00	8	24	10	8.26	14.03
6	18	5	35.66	35.76	8	25	8	8.77	6.78	7	24	10	14.73	13.85
6	18	5	38.70	38.00	3	25	8	21.99	21.12	15	24	10	14.73	13.85
6	18	5	27.77	24.80	7	25	8	18.22	12.00	15	24	10	28.08	27.66
6	18	5	26.73	63.82	7	25	8	18.69	18.36	0	24	10	9.36	6.91
6	18	5	63.86	19.01	2	26	8	20.99	21.29	4	16	10	124.62	122.70
6	18	5	19.40	116.04	8	26	8	8.18	9.28	6	16	10	26.57	26.38
6	18	5	119.37	120.58	6	26	8	36.33	34.49	8	16	10	17.73	17.15
6	18	5	12.91	14.84	8	26	8	18.13	19.10	1	17	10	32.02	32.09
1	19	6	43.95	47.09	8	26	8	47.70	46.35	1	17	10	14.60	11.40
3	19	6	7.58	9.78	9	26	8	31.88	30.81	9	17	10	99.96	100.09
5	19	6	7.58	9.78	6	26	8	31.88	30.81	4	18	10	23.62	19.63

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
8	1	18	38.95	39.65	9	20	11	9.18	0.18	1	21	12	10.36	10.60	2	16	14	21.94	21.66
1	19	10	10.57	6.34	2	21	11	15.19	16.87	3	21	12	13.53	1.40	4	16	14	136.52	136.38
3	19	10	17.76	19.84	6	21	11	13.69	14.84	5	21	12	14.27	16.29	6	16	14	136.52	136.38
7	19	10	32.05	38.84	1	22	11	20.55	23.13	0	22	12	132.43	130.73	8	16	14	19.57	17.60
9	19	10	12.97	32.95	3	22	11	14.33	21.00	2	22	12	112.45	109.32	10	16	14	44.03	43.22
2	20	10	132.31	23.46	5	22	11	15.47	12.62	4	22	12	13.87	5.37	12	16	14	107.29	105.20
4	20	10	73.55	72.26	6	22	11	15.46	16.05	6	22	12	75.23	77.23	12	17	14	48.00	47.86
6	20	10	24.03	24.03	4	23	11	24.66	23.64	1	23	12	19.33	19.60	1	17	14	2.32	7.37
8	20	10	92.84	90.95	6	23	11	18.90	20.03	3	23	12	5.19	9.51	5	17	14	52.18	54.63
3	21	10	110.18	110.18	1	24	11	38.40	37.54	5	14	13	11.92	10.39	7	17	14	15.41	11.43
5	21	10	5.35	16.83	0	24	12	22.00	20.03	3	14	13	36.30	35.79	9	17	14	35.86	35.56
7	21	10	15.56	38.18	2	24	12	130.69	134.79	7	14	13	43.71	43.93	1	18	14	36.56	35.94
0	22	10	36.06	34.73	6	24	12	270.64	267.38	1	18	14	32.89	30.91	2	18	14	13.45	8.59
2	22	10	34.42	31.65	8	24	12	176.76	174.33	4	18	14	13.46	13.86	4	18	14	102.93	103.67
4	22	10	20.87	20.87	6	24	12	156.35	159.75	6	18	14	32.95	32.84	6	18	14	17.90	15.59
6	22	10	93.42	93.42	10	24	12	87.48	87.80	8	18	14	45.25	45.01	8	18	14	26.57	25.40
1	23	10	2.90	15.67	12	24	12	138.77	140.12	10	18	14	17.88	15.12	10	19	14	26.57	25.40
3	23	10	15.67	24.45	1	25	13	34.27	33.18	12	19	14	8.65	7.49	12	19	14	33.07	34.18
5	23	10	24.45	31.17	9	25	13	28.66	28.14	13	19	14	13.31	13.91	13	19	14	12.50	16.82
0	24	10	30.77	31.36	1	26	14	13.53	15.56	5	20	14	17.78	18.63	7	20	14	14.35	15.84
2	24	10	5.81	1.36	11	26	14	183.29	183.25	9	20	14	3.67	12.37	9	20	14	96.38	96.62
4	24	10	28.16	28.16	2	26	14	91.48	90.89	1	20	14	18.10	17.58	2	20	14	81.54	85.35
2	24	10	107.52	107.52	6	26	14	146.77	145.28	2	20	14	53.93	54.66	2	20	14	15.90	12.63
4	24	10	37.01	37.01	8	26	14	154.05	151.84	4	20	14	9.69	9.66	4	20	14	84.29	85.00
1	25	11	8.98	8.98	10	26	14	118.21	117.44	6	21	14	27.85	28.61	6	21	14	33.73	33.90
3	25	11	11.45	10.36	14	26	14	130.57	128.07	1	21	14	0.00	4.56	1	21	14	12.24	8.43
7	25	11	12.18	9.36	14	26	14	12.76	13.07	5	21	14	14.93	14.72	5	21	14	18.61	19.41
9	25	11	4.97	5.38	3	27	15	10.42	5.03	12	21	14	6.98	9.22	12	21	14	34.04	34.07
8	13	11	8.43	35.38	7	27	15	8.56	8.86	1	22	14	41.46	43.45	1	22	14	12.35	14.13
1	14	11	39.09	38.38	11	27	15	5.44	6.86	3	22	14	68.80	68.24	3	22	14	15.47	6.87
7	14	11	5.90	5.52	1	28	15	3.09	5.11	5	22	14	6.51	9.27	5	22	14	5.50	98.60
9	14	11	23.30	22.95	4	28	15	155.78	153.78	7	22	14	30.88	30.04	7	22	14	8.64	5.60
1	15	11	24.83	24.83	0	28	15	27.81	25.27	9	22	14	13.49	16.35	9	22	14	16.32	13.51
4	15	11	0.00	4.10	6	28	15	141.41	140.30	2	23	14	10.67	9.99	2	23	14	3.68	5.61
6	15	11	36.08	35.56	8	28	15	102.56	102.59	4	23	14	35.72	33.90	4	23	14	7.39	6.62
8	15	11	25.26	24.21	10	28	15	169.20	168.92	6	23	14	10.36	11.82	6	23	14	4.55	2.16
10	15	11	13.63	13.72	1	29	16	18.33	19.32	8	23	14	17.54	17.54	8	23	14	27.65	26.06
3	16	11	6.01	6.99	3	29	16	24.40	25.22	1	24	15	10.83	11.43	1	24	15	27.65	29.04
7	16	11	30.36	30.06	5	29	16	0.00	5.73	3	24	15	6.70	6.70	3	24	15	13.65	14.57
9	16	11	16.60	16.80	7	29	16	0.00	5.36	5	24	15	34.71	33.75	5	24	15	17.01	18.62
4	17	11	5.08	4.77	9	29	16	16.81	16.61	2	24	15	24.15	25.50	2	24	15	8.03	9.15
6	17	11	62.96	60.77	1	30	17	0.00	0.82	4	24	15	11.79	12.74	4	24	15	8.03	6.29
8	17	11	18.93	16.92	1	30	17	172.44	174.86	6	24	15	34.71	33.75	6	24	15	30.66	31.22
1	18	11	22.90	22.90	4	30	17	106.13	106.13	8	24	15	24.07	25.38	8	24	15	20.65	20.60
3	18	11	33.55	33.55	6	30	17	8.83	8.91	1	25	15	14.45	15.36	1	25	15	14.53	14.55
5	18	11	44.60	44.60	8	30	17	105.15	104.69	3	25	15	37.51	37.51	3	25	15	6.87	7.51
7	18	11	12.69	12.69	10	30	17	125.18	123.70	5	25	15	24.07	23.38	5	25	15	12.79	12.79
9	18	11	17.97	17.97	1	31	18	96.59	95.37	7	25	15	54.85	54.91	7	25	15	11.94	8.34
2	19	11	18.31	18.31	3	31	18	5.85	3.92	9	25	15	18.96	17.71	9	25	15	8.71	7.20
4	19	11	25.25	25.25	5	31	18	26.09	26.09	1	26	16	15.07	14.42	1	26	16	15.67	17.38
6	19	11	16.31	16.31	7	31	18	19.62	19.62	3	26	16	39.55	39.42	3	26	16	14.51	12.71
8	19	11	8.87	8.87	9	31	18	20.07	20.07	5	26	16	12.31	12.31	5	26	16	32.95	27.01
1	20	11	19.27	19.27	1	32	19	9.27	9.40	7	26	16	40.92	40.92	7	26	16	268.71	270.13
3	20	11	20.01	20.01	3	32	19	67.23	67.18	9	26	16	36.24	36.24	9	26	16	15.94	15.94
5	20	11	27.59	27.59	5	32	19	154.68	157.28	1	27	17	29.04	29.04	1	27	17	32.95	35.64
7	20	11	4.42	4.42	7	32	19	30.81	30.19	3	27	17	41.41	41.41	3	27	17	269.80	274.66
1	20	11	12.32	12.32	9	32	19	23.00	19.99	5	27	17	41.41	41.41	5	27	17	80.67	82.93



PYROPE 293 K

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	0	4	213.13	204.49	7	18	3	8.69	8.52	2	4	6	56.04	55.61
10	10	14	297.03	283.56	9	18	3	14.70	14.66	4	6	6	68.37	70.60
14	14	14	108.64	105.78	15	18	3	35.47	35.88	7	7	5	29.74	29.50
16	16	15	14.78	14.39	1	20	3	18.79	18.87	3	2	2	87.47	89.12
6	20	16	120.57	120.10	5	20	3	3.45	1.01	3	8	5	20.50	20.66
12	20	0	35.10	34.71	7	20	3	9.45	9.23	9	9	5	9.75	11.22
14	20	0	24.79	24.35	13	21	3	12.81	12.85	6	8	5	5.10	4.36
14	20	0	29.64	28.59	2	21	3	12.88	12.85	1	10	5	26.57	26.03
6	22	0	17.98	15.57	4	22	3	11.49	11.38	3	11	5	9.32	8.68
10	22	0	9.85	9.52	2	23	3	16.76	16.34	4	11	5	3.93	2.23
2	24	0	5.20	3.68	0	23	4	251.62	227.25	6	11	5	9.96	8.48
1	2	3	36.77	35.39	10	11	4	124.25	130.13	10	11	5	31.59	31.46
1	2	3	39.71	38.25	11	17	4	83.28	78.97	11	12	5	7.17	5.96
3	4	5	112.19	105.05	2	4	4	251.98	241.01	3	12	5	34.56	34.27
2	4	5	19.57	18.75	0	4	4	255.12	246.03	7	12	5	7.38	6.95
4	5	6	131.01	126.44	0	6	4	240.81	234.45	2	13	5	66.83	67.01
3	4	7	43.85	42.77	6	6	4	186.11	184.60	4	13	5	22.06	21.52
4	5	6	62.64	65.46	0	6	4	203.26	201.50	7	13	5	33.62	33.13
4	5	7	64.06	65.46	1	8	4	79.10	79.10	6	13	5	33.41	33.13
7	8	8	18.33	18.57	0	9	4	44.68	44.66	8	14	5	50.69	51.08
4	10	13	2.47	1.31	0	9	4	181.10	180.80	1	14	5	33.93	33.35
15	16	17	2.99	1.38	2	10	4	181.51	180.80	3	14	5	38.13	37.98
14	17	17	6.59	6.43	0	10	4	152.16	152.33	5	14	5	7.19	6.08
14	19	17	15.42	15.38	8	10	4	139.23	139.90	13	14	5	27.37	27.55
5	20	20	7.70	7.18	1	11	4	40.18	40.96	4	15	5	24.29	24.16
1	20	20	22.77	22.73	3	11	4	16.14	16.35	6	15	5	19.62	19.66
1	20	21	3.55	2.43	0	12	4	31.24	32.79	1	16	5	12.65	12.60
1	21	21	2.92	2.43	8	12	4	21.82	20.24	15	16	5	12.11	12.16
1	21	21	11.57	11.51	0	14	4	105.60	105.91	2	17	5	24.75	24.73
3	22	22	9.95	9.60	14	14	4	52.75	52.75	4	17	5	30.08	30.18
5	22	22	26.24	26.40	1	15	4	4.61	4.17	1	18	5	38.20	38.51
6	23	23	4.18	0.77	1	15	4	14.19	13.99	5	18	5	4.19	4.99
3	24	24	6.85	6.43	0	16	4	91.28	92.00	11	18	5	5.41	4.99
0	3	5	28.26	28.95	16	16	4	5.99	3.25	15	18	5	5.41	4.99
3	5	5	32.02	29.30	7	16	4	67.71	67.71	2	19	5	23.53	23.88
5	6	7	158.78	148.19	3	17	4	24.26	24.30	6	19	5	16.94	16.93
0	3	5	40.47	40.32	1	17	4	24.14	23.87	10	19	5	5.06	4.66
7	7	8	105.93	101.31	1	17	4	25.46	25.39	14	20	5	14.42	14.55
0	7	8	16.87	15.41	11	17	4	3.04	2.39	9	20	5	12.67	12.34
1	8	8	50.56	51.73	13	17	4	3.75	3.61	2	21	5	9.47	9.15
0	8	8	39.33	39.76	15	18	4	22.07	23.07	6	21	5	11.77	11.66
2	8	8	175.34	174.12	14	18	4	61.20	61.14	8	21	5	23.63	23.68
6	9	9	22.79	22.42	16	18	4	7.73	62.01	5	22	5	3.26	3.47
8	9	9	12.45	13.51	3	19	4	3.52	0.24	7	22	5	18.27	18.24
8	9	9	9.54	8.23	1	19	4	9.58	9.08	9	22	5	5.09	5.07
0	11	11	89.07	91.61	5	19	4	33.20	33.74	2	23	6	5.48	4.66
1	15	11	32.82	32.74	15	19	4	13.20	13.25	6	23	6	5.80	5.84
2	2	2	6.51	5.85	1	20	4	19.43	19.04	7	23	6	80.46	81.84
2	2	2	8.98	8.35	12	20	4	49.31	49.60	8	23	6	58.81	58.12
2	2	2	16.97	16.80	12	20	4	29.26	28.26	0	24	6	8.19	8.15
1	9	11	144.71	145.42	0	22	4	57.04	56.96	4	24	6	146.35	145.29
2	11	11	197.85	199.15	6	22	4	3.51	1.57	1	24	6	1.82	1.23
2	12	12	8.11	6.67	1	23	4	25.75	26.25	3	24	6	3.89	2.19
6	12	12	105.71	105.71	3	24	4	44.45	44.53	7	24	6	33.98	34.18
8	12	13	124.48	124.51	0	24	4	4.14	4.16	9	24	6	82.12	82.58
1	13	13	45.37	45.92	5	24	4	18.44	18.83	0	24	6	41.59	41.85



H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
4	10	6	135.10	135.07	2	16	8	20.25	19.65	1	20	9	22.53	22.73
1	11	6	25.16	25.03	4	16	8	87.21	87.42	3	20	9	4.34	3.18
1	11	6	47.46	47.64	6	16	8	5.90	5.32	1	20	9	3.13	2.36
1	11	6	108.57	109.12	8	16	8	144.45	145.00	1	21	9	19.38	19.50
4	12	6	108.57	109.12	12	16	8	59.49	59.79	4	21	9	11.10	10.85
4	12	6	16.55	16.15	5	17	8	13.96	13.79	6	21	9	5.29	5.11
6	12	6	119.21	119.29	3	17	8	20.40	20.58	1	21	9	4.53	2.97
10	12	6	117.36	117.93	5	17	8	10.28	9.71	1	21	9	68.81	70.00
1	13	6	28.17	27.82	7	17	8	14.33	14.09	3	21	10	10.47	8.24
3	13	6	35.82	35.95	9	17	8	5.17	4.69	5	21	10	19.05	18.36
0	14	6	16.86	16.47	13	17	8	9.11	8.88	1	21	10	16.15	15.35
4	14	6	92.98	92.98	10	18	8	18.84	18.76	0	21	10	90.94	90.40
4	14	6	29.27	29.35	4	18	8	73.25	73.18	2	21	10	115.55	116.32
3	15	6	4.71	3.58	6	18	8	13.84	13.34	4	21	10	4.94	4.04
9	15	6	5.73	5.24	10	18	8	7.11	5.56	2	21	10	2.26	0.34
15	15	6	24.59	25.10	12	18	8	47.79	47.62	1	21	10	14.59	14.27
0	16	6	20.88	20.14	1	19	8	9.43	9.06	3	21	10	15.84	15.24
2	16	6	11.41	11.10	0	20	8	51.18	50.36	5	21	10	22.23	22.26
4	16	6	87.73	88.32	1	20	8	10.57	10.40	9	21	10	6.08	5.09
6	16	6	19.59	19.18	1	21	8	8.53	7.99	13	21	10	14.49	14.33
14	16	6	4.40	4.48	1	21	8	23.18	23.18	0	21	10	33.57	33.66
1	17	6	31.35	31.35	7	21	8	4.37	4.65	2	21	10	12.44	11.27
3	17	6	7.56	7.06	0	22	8	7.84	6.09	4	21	10	72.51	72.64
5	17	6	48.99	49.01	2	22	8	52.56	52.87	6	21	10	28.95	29.15
7	17	6	4.57	4.57	6	22	8	9.78	8.62	8	21	10	3.10	0.77
9	17	6	2.78	2.78	1	23	8	14.33	14.39	12	21	10	72.32	72.53
0	18	6	15.90	14.51	3	23	8	2.43	2.24	1	15	10	4.74	3.04
2	18	6	72.91	72.77	1	23	8	21.49	21.39	3	15	10	10.85	10.56
4	18	6	19.37	19.37	1	23	8	13.71	13.23	5	15	10	12.31	11.80
1	19	6	22.94	22.91	3	23	8	28.61	28.50	1	16	10	21.71	21.78
3	19	6	4.68	4.68	1	23	8	34.59	34.60	0	16	10	9.97	9.32
7	19	6	15.29	14.86	9	23	8	10.50	10.27	4	16	10	39.30	38.85
13	19	6	74.23	74.54	4	23	8	19.16	19.16	6	16	10	11.63	10.36
6	20	6	49.98	49.73	6	23	8	48.88	49.02	8	16	10	15.41	14.56
10	20	6	10.89	10.68	8	23	8	6.36	5.70	10	16	10	38.47	38.52
1	21	6	36.46	36.77	10	23	8	18.45	18.36	12	16	10	87.27	88.07
3	21	6	9.82	9.67	1	23	8	17.70	17.68	14	16	10	5.94	4.95
1	21	6	18.92	19.02	3	23	8	22.49	22.33	5	17	10	3.08	0.83
1	21	6	27.12	27.42	5	23	8	11.91	11.90	4	17	10	4.27	3.45
5	23	7	13.86	13.86	2	23	8	20.48	20.30	2	17	10	25.43	25.66
2	1	8	18.31	18.31	6	23	8	6.74	6.74	11	17	10	18.66	18.70
1	8	7	32.62	33.10	8	23	8	19.70	19.28	13	17	10	12.63	12.30
3	8	7	18.09	18.51	8	23	8	22.87	22.80	0	18	10	29.94	29.78
5	8	7	37.62	38.51	3	23	8	8.75	8.53	6	18	10	19.22	18.81
2	9	7	20.74	20.31	5	23	8	5.22	4.79	7	19	10	4.02	1.77
4	9	7	28.21	27.80	2	23	8	43.62	43.62	9	19	10	8.98	8.95
5	10	7	22.88	22.47	4	23	8	29.02	29.18	1	19	10	14.15	14.23
9	10	7	14.48	14.48	8	23	8	21.86	22.01	1	20	10	55.87	56.12
4	11	7	54.45	54.78	4	23	8	23.07	22.85	0	20	10	33.73	33.38
6	11	7	19.37	19.68	10	23	8	23.80	24.11	8	20	10	36.38	36.20
8	11	7	24.77	24.71	1	23	8	24.96	25.02	1	21	10	61.58	61.57
10	11	7	11.81	11.80	5	23	8	10.76	10.35	3	21	10	16.13	16.00
1	12	7	44.64	44.69	15	23	8	3.93	4.82	5	21	10	14.69	14.90
3	12	7	18.68	18.73	1	23	8	5.60	5.33	2	21	10	19.74	19.69
9	12	7	18.68	18.73	1	23	8	11.38	10.78	1	21	10	18.04	17.90
1	12	7	16.47	16.47	7	23	8	33.09	33.37	0	21	10	39.10	39.29
1	12	7	5.83	5.83	12	23	8	5.5	5.5	5	21	10	8.23	7.88
1	12	7	196.27	196.27	12	23	8	33.09	33.37	5	21	10	3.19	2.59

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
9	12	11	13.63	13.12	6	12	16	59.53	59.74	4	5	23	15.35	15.36
2	13	11	6.80	6.17	3	13	16	8.31	8.09	0	0	24	98.45	98.29
4	13	11	33.71	33.79	5	13	16	10.63	10.52	4	4	24	4.53	2.03
6	13	11	36.80	36.92	2	14	16	15.78	14.80					
10	13	11	4.33	4.29	4	14	16	57.90	57.82					
1	14	11	4.99	4.29	8	16	16	75.46	75.53					
3	14	11	36.03	36.13	1	17	16	3.49	3.55	LR				
5	14	11	10.82	10.00	1	17	16	11.80	11.91					
7	14	11	14.42	14.26	0	18	16	18.81	18.55					
9	14	11	18.43	18.50	7	10	17	16.08	15.95					
13	14	11	3.66	2.41	6	11	17	20.62	20.47					
2	15	11	39.74	40.12	8	11	17	14.79	14.92					
4	15	11	2.01	2.01	1	12	17	18.81	18.87					
6	15	11	2.44	0.34	1	12	17	20.86	21.03					
8	15	11	16.18	16.12	5	12	17	8.35	7.60					
12	15	11	6.01	5.89	5	12	17	5.13	5.14					
14	15	11	3.34	1.89	2	13	17	15.36	15.51					
1	16	11	3.50	0.68	7	13	17	14.14	14.27					
3	16	11	7.94	7.74	7	16	17	14.14	14.24	LR				
5	16	11	8.50	8.10	1	7	18	2.88	3.24					
9	16	11	14.23	14.13	5	9	18	4.29	1.93	LR				
15	16	11	2.77	2.26	4	10	18	54.39	54.27					
2	19	11	8.15	7.97	1	11	18	13.38	13.15					
4	19	11	9.99	9.49	3	11	18	8.60	8.60					
6	19	11	22.00	21.52	7	11	18	21.44	21.71					
3	20	11	3.68	3.66	1	10	18	17.63	17.66					
5	20	11	6.90	6.16	5	13	18	26.07	26.00					
2	21	11	15.55	15.39	8	14	18	8.61	7.58					
1	22	11	14.65	14.70	2	16	18	7.76	6.82					
0	0	12	87.63	87.47	3	3	19	13.29	13.30					
8	8	12	105.87	106.26	5	5	19	17.72	17.63					
10	10	12	48.77	48.60	7	8	19	24.69	24.91					
0	12	12	10.07	9.73	2	9	19	19.46	19.37					
4	12	12	120.80	120.82	6	9	19	6.63	6.19					
8	12	12	20.02	19.15	8	10	19	32.50	32.62					
12	12	12	29.01	28.75	1	10	19	26.25	26.62					
1	13	12	5.31	4.09	1	10	19	17.28	17.25					
3	13	12	26.95	26.77	3	11	19	17.52	17.55					
5	13	12	12.37	12.29	8	11	19	2.72	1.96	LR				
7	13	12	32.07	32.30	1	12	19	3.89	1.15	LR				
9	13	12	23.52	23.80	5	12	19	23.20	23.67					
11	13	12	14.42	14.22	7	12	19	16.86	17.16					
0	14	12	96.37	96.13	2	15	19	14.57	14.57					
2	14	12	49.81	49.82	0	0	20	112.80	113.10					
4	14	12	4.16	2.49	4	4	20	65.30	65.79					
6	14	12	93.83	94.03	6	4	20	67.74	68.01					
8	14	12	67.88	68.16	8	8	20	53.89	54.18					
1	15	12	11.14	10.67	8	8	20	19.78	19.36					
7	15	12	3.33	1.39	4	10	20	25.64	25.45					
0	16	12	100.86	101.18	6	12	20	19.39	19.85					
2	16	12	66.90	67.18	8	7	21	3.00	0.52	LR				
4	16	12	12.81	12.08	4	10	21	12.90	12.73					
12	16	12	5.76	4.40	7	4	21	2.55	0.23	LR				
19	17	12	2.89	0.67	3	12	21	36.32	36.80					
11	17	12	14.31	14.54	1	3	22	23.79	24.28					
0	18	12	93.84	93.78	1	3	22	37.95	38.02					
4	18	12	7.74	6.89	2	3	22	26.32	26.74					
6	18	12	62.16	62.06	3	4	22	51.91	52.10					
2	18	12	8.68	8.10	4	10	22	26.74	26.74					

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	4	0	16.32	9.19	1	10	7	24.02	26.90	4	15	9	24.47	21.51	1	4	15	24.47	21.51
4	6	0	99.34	97.25	5	10	7	15.23	18.73	7	16	9	19.66	22.16	1	5	16	19.66	22.16
8	8	0	359.89	358.67	2	11	7	2.38	13.20	7	16	9	17.78	10.88	1	5	16	17.78	10.88
10	10	0	102.47	101.65	6	11	7	55.11	50.14	7	17	9	0.00	0.86	1	6	17	0.00	0.86
12	12	0	13.51	15.93	4	11	7	12.38	10.75	7	17	9	17.15	11.41	1	6	17	17.15	11.41
16	16	0	130.45	136.54	1	12	7	0.00	5.47	7	18	9	0.00	4.19	1	7	18	0.00	4.19
1	1	3	17.84	15.18	1	13	7	43.36	44.04	1	18	9	13.65	9.17	1	8	18	13.65	9.17
1	3	3	14.08	19.29	2	13	7	18.18	13.27	1	10	10	58.24	58.24	1	9	19	58.24	58.24
1	3	4	157.52	146.50	5	14	7	12.69	9.66	2	10	10	102.56	103.44	1	10	20	102.56	103.44
0	1	5	300.80	296.43	2	15	7	0.00	1.39	3	4	10	18.37	18.85	1	10	30	18.37	18.85
1	1	5	104.77	97.34	6	15	7	0.00	5.57	0	4	10	215.71	212.03	1	10	40	215.71	212.03
1	7	7	54.09	53.60	6	17	7	0.00	9.00	2	2	10	206.09	201.58	1	10	50	206.09	201.58
1	7	9	10.07	2.59	1	18	7	16.67	0.95	1	5	10	5.63	8.66	1	10	60	5.63	8.66
1	9	9	17.83	24.07	2	19	7	18.91	10.56	3	7	10	17.03	4.43	1	10	70	17.03	4.43
1	11	11	7.29	1.72	0	20	8	401.82	399.35	8	8	10	16.99	14.74	1	10	80	16.99	14.74
1	11	11	7.64	7.49	0	22	4	51.66	27.92	8	8	10	17.40	17.82	1	10	90	17.40	17.82
1	11	12	168.30	168.50	6	24	4	28.80	34.27	9	9	10	14.77	17.24	1	10	100	14.77	17.24
1	13	13	38.30	37.65	4	26	8	14.88	18.31	4	10	10	151.63	151.12	1	10	110	151.63	151.12
1	13	14	19.35	9.08	6	28	8	13.99	0.00	8	11	10	8.23	8.21	1	10	120	8.23	8.21
1	15	15	17.32	16.68	8	30	8	44.84	44.92	8	11	10	13.68	28.01	1	10	130	13.68	28.01
1	17	17	18.64	23.14	8	32	8	20.10	26.88	9	11	10	15.63	23.86	1	10	140	15.63	23.86
1	17	18	0.60	3.91	7	34	9	173.93	173.46	9	11	10	16.71	7.61	1	10	150	16.71	7.61
1	19	19	5.37	22.92	1	36	9	10.91	13.36	0	14	10	24.84	0.81	1	10	160	24.84	0.81
1	2	3	191.15	187.30	6	38	8	24.49	20.43	8	15	10	0.00	5.20	1	10	170	0.00	5.20
1	2	3	28.99	27.97	10	40	8	20.93	26.60	8	15	10	9.77	4.95	1	10	180	9.77	4.95
1	2	3	47.43	46.82	3	42	8	20.84	23.07	8	16	10	3.77	7.68	1	10	190	3.77	7.68
1	2	3	10.28	12.98	5	44	8	40.95	41.59	8	16	10	20.46	24.35	1	10	200	20.46	24.35
1	2	3	13.80	19.07	7	46	8	27.25	24.95	8	17	10	51.52	51.19	1	10	210	51.52	51.19
1	2	3	9.10	19.07	3	48	8	132.85	130.07	8	17	10	10.95	3.64	1	10	220	10.95	3.64
1	2	3	0.00	3.73	7	50	8	142.98	142.50	8	18	10	0.00	8.00	1	10	230	0.00	8.00
1	2	3	12.00	13.16	2	52	8	23.12	27.50	2	20	10	66.37	66.07	1	10	240	66.37	66.07
1	2	3	19.50	12.34	6	54	8	137.62	138.23	0	20	10	45.54	45.63	1	10	250	45.54	45.63
1	2	3	19.06	16.08	12	56	8	0.00	14.00	8	22	10	56.56	56.45	1	10	260	56.56	56.45
1	2	3	358.92	353.05	2	58	8	5.24	21.74	2	23	11	9.45	10.82	1	10	270	9.45	10.82
1	2	4	151.89	158.08	7	60	8	12.98	20.38	6	6	11	18.23	16.44	1	10	280	18.23	16.44
1	2	4	333.64	337.12	9	62	8	92.30	90.75	6	6	11	55.93	55.57	1	10	290	55.93	55.57
1	2	4	20.14	18.88	16	64	8	15.07	12.82	9	9	11	14.08	15.57	1	10	300	14.08	15.57
1	2	4	23.11	18.88	2	66	8	22.15	13.56	5	10	11	25.61	24.23	1	10	310	25.61	24.23
1	2	4	329.97	326.17	4	68	8	85.08	83.55	4	10	11	39.13	37.99	1	10	320	39.13	37.99
1	2	6	294.96	290.98	5	70	8	20.99	9.22	1	15	11	0.00	1.46	1	10	330	0.00	1.46
1	2	6	64.86	62.20	6	72	8	77.18	77.91	5	15	11	32.66	33.52	1	10	340	32.66	33.52
1	2	6	35.66	36.28	6	74	8	0.00	18.04	6	16	11	3.18	2.11	1	10	350	3.18	2.11
1	2	6	238.66	234.56	1	76	8	15.45	10.83	1	16	11	12.61	12.52	1	10	360	12.61	12.52
1	2	6	212.32	210.13	1	78	8	16.58	18.20	1	16	11	15.44	5.01	1	10	370	15.44	5.01
1	2	6	164.10	162.15	4	80	8	14.92	14.30	1	16	11	0.00	1.02	1	10	380	0.00	1.02
1	2	6	81.59	80.58	5	82	8	23.85	26.43	5	17	11	25.28	24.87	1	10	390	25.28	24.87
1	2	6	44.75	44.63	1	84	8	16.52	17.57	7	17	11	5.56	5.68	1	10	400	5.56	5.68
1	2	6	41.19	41.57	1	86	8	41.75	42.79	7	17	11	16.35	16.35	1	10	410	41.75	42.79
1	2	6	142.56	141.57	5	88	8	14.51	16.24	8	18	11	19.70	19.68	1	10	420	14.51	16.24
1	2	6	124.14	122.91	12	90	8	19.02	17.73	8	18	11	22.70	22.70	1	10	430	19.02	17.73
1	2	6	56.28	57.31	4	92	8	23.35	23.03	1	19	11	38.63	38.63	1	10	440	23.35	23.03
1	2	6	21.00	21.44	6	94	8	41.68	42.54	3	19	11	23.03	23.03	1	10	450	41.68	42.54

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	4	4	15.10	7.59	1	12	15	21.23	10.90	2	2	20	102.59	101.96
4	4	12	120.16	118.34	7	12	13	21.94	31.73	0	4	20	21.21	12.71
1	0	5	18.23	5.06	9	12	13	25.85	24.11	2	4	20	18.11	1.33
6	12	12	128.87	128.16	6	13	13	12.71	21.72	4	4	20	82.16	81.61
2	4	6	116.26	116.24	1	14	13	16.23	2.98	4	4	20	80.33	81.10
6	6	12	16.68	16.86	3	7	14	10.37	11.71	6	6	20	70.60	68.82
4	6	12	128.26	130.31	7	14	13	0.00	0.65	10	10	20	60.39	60.26
5	7	12	9.65	6.04	0	0	16	0.00	12.05	4	8	22	111.92	114.30
8	8	12	113.47	114.89	2	4	14	21.26	23.06	0	0	24		
3	8	12	21.69	21.86	4	4	16	14.36	3.14					
5	9	12	17.38	11.70	4	6	16	165.66	166.67					
0	10	12	105.89	105.47	0	4	16	40.60	42.70					
2	10	12	129.30	126.51	6	6	16	31.27	29.95					
4	10	12	10.32	3.55	1	3	16	22.26	22.94					
6	10	12	125.57	127.98	1	7	16	19.48	12.86					
8	10	12	82.69	84.46	5	7	16	4.72	0.88					
10	10	12	53.38	55.18	0	4	16	35.24	36.44					
3	11	12	19.86	7.78	0	8	16	27.90	28.26					
7	11	12	11.06	7.31	6	8	16	21.70	23.55					
9	11	12	4.32	12.09	8	8	16	115.78	114.91					
12	12	12	9.50	0.00	3	9	16	24.53	11.51					
1	13	12	43.36	44.20	6	10	16	20.74	15.88					
3	13	12	23.10	27.65	1	9	14	11.29	11.36					
5	13	12	12.97	11.92	5	9	14	36.80	37.36					
8	14	12	77.66	78.91	2	10	14	23.33	19.25					
10	14	12	82.85	81.96	4	10	14	15.63	10.68					
14	14	12	20.70	18.51	6	10	14	25.82	28.84					
3	15	12	19.03	5.37	3	11	14	24.67	30.07					
5	16	12	18.17	18.85	5	11	14	21.97	15.98					
6	16	12	71.24	70.80	7	11	14	19.44	8.02					
10	18	12	98.66	98.14	9	11	14	18.32	11.72					
2	18	12	67.34	66.84	2	12	14	55.72	56.75					
6	18	12	56.81	67.31	4	12	14	17.43	1.74					
4	20	12	60.74	61.75	4	12	14	99.51	101.31					
4	4	13	6.81	1.42	6	13	14	13.05	0.78					
1	3	13	19.77	21.91	0	14	14	14.34	19.04					
2	4	13	60.62	60.06	2	2	14	48.46	36.22					
5	5	13	16.10	22.13	2	3	15	26.21	30.07					
3	6	13	21.78	28.31	3	4	15	16.61	14.02					
5	6	13	14.54	10.45	3	5	15	26.11	27.21					
4	6	13	14.53	15.21	1	6	15	26.60	22.38					
4	7	13	13.13	7.09	6	7	15	14.50	2.17					
3	8	13	31.83	31.56	6	8	15	44.68	17.19					
5	8	13	24.43	34.32	1	8	15	19.12	45.60					
7	8	13	22.91	29.29	3	8	15	21.09	14.11					
2	9	13	15.24	13.86	5	9	15	25.71	23.92					
4	9	13	17.85	13.87	6	9	15	20.93	0.86					
6	9	13	15.91	18.73	8	9	15	25.92	22.72					
8	9	13	0.00	9.06	1	10	15	19.02	8.42					
1	10	13	0.00	7.06	5	10	15	5.32	6.44					
5	10	13	14.23	15.61	7	10	15	22.03	16.92					
7	10	13	11.52	11.58	9	10	15	16.67	19.11					
2	11	13	23.71	30.91	4	11	15	36.84	35.15					
8	11	13	8.71	3.11	8	11	15	0.00	2.20					



PYROPE 60 - ALMANDINE 40 293 K				STRUCTURE FACTORS				PAGE . 2						
H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
6	8	12	150.30	150.75	1	3	14	30.19	30.14	1	3	7	16	17.93
8	8	12	120.53	120.74	3	3	14	8.90	5.07	3	7	16	24.10	23.08
1	3	9	13.47	18.30	0	4	14	136.19	136.70	5	4	16	16.01	20.71
3	9	12	19.92	20.98	2	5	14	171.46	174.05	4	8	16	100.55	101.11
5	9	12	8.92	10.01	5	5	14	22.61	21.67	8	8	16	179.56	180.28
7	9	12	16.68	17.82	0	6	14	30.83	31.01	1	5	16	24.15	22.59
2	10	12	132.83	132.28	2	6	14	14.74	14.88	5	9	16	10.76	9.92
4	10	12	11.18	12.35	4	6	14	106.92	107.24	0	10	16	21.10	18.71
8	10	12	132.61	134.24	3	7	14	11.70	7.75	6	10	16	5.60	1.88
6	10	12	95.42	96.44	7	7	14	7.78	3.24	2	10	16	2.84	7.72
10	10	12	59.91	59.35	5	7	14	41.32	41.28	5	10	16	25.14	25.25
5	11	12	11.22	1.45	2	8	14	31.71	30.72	7	11	16	10.72	0.91
7	11	12	12.27	7.21	6	8	14	12.88	4.54	1	13	16	11.43	6.30
9	11	12	9.38	11.12	3	9	14	0.00	17.52	2	12	16	23.26	24.02
4	12	12	160.41	159.91	5	9	14	16.90	30.38	1	13	16	28.21	22.96
8	12	12	6.40	7.99	7	9	14	30.46	25.13	4	5	17	37.43	37.63
10	12	12	5.59	0.00	9	9	14	26.01	10.60	4	5	17	28.97	28.97
0	14	12	118.08	118.84	2	10	14	9.80	10.60	5	2	17	11.24	4.06
4	14	12	8.82	1.44	4	10	14	84.17	84.64	5	2	17	9.61	12.08
1	15	12	13.78	11.05	8	10	14	13.93	10.75	1	8	17	18.68	20.32
3	15	12	15.95	6.26	1	11	14	13.61	9.16	3	8	17	0.00	6.62
7	15	12	0.00	3.34	5	11	14	22.99	22.15	6	10	17	4.84	4.76
0	16	12	114.61	113.41	7	11	14	4.72	3.17	2	12	17	0.00	13.47
2	16	12	89.96	89.62	9	11	14	1.99	5.09	4	11	17	0.00	2.84
4	16	12	2.85	2.97	2	12	14	61.44	60.80	1	11	17	0.00	12.80
2	16	12	18.21	19.30	6	12	14	106.23	106.39	1	11	18	12.81	12.30
3	4	13	21.12	21.23	8	12	14	89.92	89.19	4	1	18	10.50	12.49
5	5	13	22.39	21.85	1	13	14	11.12	8.78	1	3	18	37.79	38.12
6	6	13	13.21	14.35	5	13	14	8.41	5.27	0	3	18	63.18	62.58
3	6	13	12.80	20.12	7	13	14	7.82	5.52	1	5	18	17.62	25.18
5	6	13	18.26	18.12	0	14	14	25.24	24.17	5	5	18	6.52	12.48
4	7	13	13.96	14.99	4	14	14	59.99	60.31	2	6	18	23.91	22.77
6	7	13	6.36	1.79	3	15	14	20.84	24.20	4	6	18	82.97	83.54
3	8	13	30.77	31.30	1	4	15	0.00	4.49	1	7	18	10.14	5.21
5	8	13	35.28	35.43	3	4	15	12.85	14.96	7	7	18	4.54	17.37
7	8	13	29.79	29.91	2	5	15	26.10	25.90	0	8	18	17.55	17.37
2	9	13	12.88	7.65	4	3	15	2.57	9.44	6	6	18	5.23	8.74
4	9	13	13.66	12.64	3	6	15	7.57	8.44	2	6	18	7.01	3.47
6	9	13	17.55	15.93	5	6	15	15.23	10.98	5	9	18	0.00	10.20
8	9	13	1.52	18.70	2	7	15	9.52	8.29	0	10	18	9.26	3.75
3	10	13	12.77	4.36	6	7	15	24.58	23.87	1	12	19	13.19	16.69
5	10	13	11.47	6.63	5	8	15	27.63	28.29	3	4	19	12.35	0.29
7	10	13	11.55	9.23	7	8	15	20.50	21.48	4	5	19	30.46	8.93
8	11	13	33.54	24.63	4	9	15	22.61	21.01	1	6	19	9.14	30.49
6	11	13	7.69	4.47	8	9	15	17.37	22.26	3	6	19	9.14	12.78
10	11	13	6.58	7.81	5	10	15	14.10	1.37	0	20	20	107.04	122.79
1	12	13	8.65	3.44	9	10	15	11.86	12.65	2	3	20	16.02	18.60
3	12	13	27.45	12.29	6	11	15	18.45	9.89	1	0	20	12.66	6.78
5	12	13	16.21	30.80	5	12	15	13.92	12.45	0	2	20	0.00	0.52
7	12	13	30.85	23.63	1	14	15	174.53	175.53	2	4	20	107.04	107.52
9	12	13	2.00	0.00	2	2	16	38.81	38.37	0	2	20	16.02	16.60
4	13	13	26.90	26.87	2	3	16	16.51	14.06	1	4	20	0.00	0.00
6	13	13	0.00	0.00	1	4	16	4.35	5.56	4	4	20	0.00	0.00
8	13	13	18.17	16.14	4	4	16	19.08	21.70	3	4	20	0.00	0.00
3	14	13	5.12	6.51	0	6	16	23.50	25.05	2	3	20	0.00	0.00
2	15	13	11.92	8.42	4	6	16	114.20	113.85	1	0	2	0.00	0.00
4	15	13	7.88	4.62	6	6	16	0.00	4.73	2	2	20	0.00	0.00

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
4	14	0	163.22	167.27	0	12	8	149.59	151.91	2	20	14	60.81	62.49
12	14	0	141.07	142.10	0	16	8	277.72	277.62	1	2	15	40.27	39.69
14	20	0	125.10	125.14	2	20	8	111.67	111.66	0	3	10	51.67	54.14
14	24	0	63.38	63.50	6	20	8	108.45	107.08	0	0	16	213.90	217.66
0	24	0	64.20	64.69	2	3	9	58.73	55.72	2	2	16	43.63	52.12
0	1	2	6.29	6.00	1	4	9	81.98	82.61	4	4	16	172.70	172.68
1	1	2	43.37	46.15	1	6	9	37.63	45.15	4	6	16	143.20	141.18
8	14	2	45.24	45.21	6	7	9	68.42	70.23	8	8	16	218.56	215.64
0	20	2	140.73	143.72	1	8	9	44.52	44.52	4	10	16	91.85	89.60
2	20	2	119.61	120.00	2	9	9	54.17	53.20	10	10	16	62.95	61.12
1	2	3	36.07	39.88	6	9	9	49.87	50.30	2	12	16	113.73	114.08
1	3	3	98.01	88.84	0	2	10	133.20	135.86	12	12	16	33.31	20.31
1	14	4	48.74	47.43	3	3	10	47.23	48.49	0	16	16	184.19	184.31
0	0	4	414.15	404.77	2	4	10	236.15	231.33	4	16	16	89.80	90.42
0	2	4	404.70	400.36	1	5	10	46.85	48.71	8	16	16	129.69	130.59
0	2	4	202.22	208.95	1	7	10	57.21	55.26	4	18	16	91.15	92.17
1	0	4	117.84	111.21	4	8	10	220.86	220.20	2	4	18	104.63	104.63
4	4	4	149.03	147.62	0	10	10	80.90	170.87	4	8	18	112.82	114.53
4	4	4	466.45	463.27	4	10	10	172.05	170.87	6	12	18	81.33	80.53
0	6	4	402.54	400.61	8	10	10	16.90	42.25	8	12	18	85.41	83.13
0	0	4	271.02	271.80	0	12	10	150.43	150.49	0	0	20	130.41	128.70
0	0	4	267.01	269.35	0	20	10	96.38	95.74	6	6	22	95.97	96.07
12	12	4	200.37	201.23	8	20	10	72.45	74.29	4	8	22	81.55	83.08
2	14	4	190.48	190.74	10	20	10	86.09	84.57	4	10	22	69.09	67.26
0	16	4	99.57	97.09	1	4	11	34.65	39.83	0	2	24	156.09	158.70
0	16	4	120.31	123.13	3	6	11	81.36	81.71	2	0	4	84.98	84.64
8	16	4	114.09	114.79	4	7	11	53.90	55.09	0	2	4		
8	18	4	84.86	88.76	0	0	12	114.38	114.32					
6	18	4	95.28	94.57	0	0	12	221.58	225.10					
4	20	4	128.08	128.96	2	2	12	246.95	249.20					
1	2	5	154.58	146.95	4	4	12	192.43	192.57					
2	3	5	140.99	136.09	2	6	12	142.07	141.19					
2	5	5	96.69	96.48	4	6	12	19.22	17.49					
5	5	6	205.89	199.13	6	6	12	155.90	153.68					
6	6	6	61.92	59.15	3	7	12	43.49	40.97					
2	5	6	335.05	330.15	2	8	12	188.32	188.46					
5	6	6	64.03	62.16	4	8	12	51.69	51.08					
6	6	6	56.30	50.79	6	8	12	180.98	179.90					
6	6	6	248.32	245.28	8	8	12	136.51	134.48					
6	6	6	79.22	78.96	2	10	12	149.08	149.29					
0	10	6	182.42	180.50	10	10	12	70.73	70.28					
10	12	6	146.08	149.36	12	12	12	92.64	91.73					
0	14	6	49.77	47.25	2	14	12	121.65	119.46					
2	2	6	98.25	97.09	6	14	12	110.97	111.87					
1	4	7	64.99	64.15	8	14	12	91.24	92.59					
5	7	7	68.11	69.32	10	14	12	102.72	103.49					
7	7	7	58.70	60.81	10	16	12	124.77	124.31					
7	14	7	52.27	54.48	0	18	12	82.56	80.25					
0	0	8	517.28	511.14	2	18	12	104.37	103.02					
2	2	8	17.52	11.69	4	20	12	104.37	103.02					
2	4	8	284.27	281.88	2	4	13	32.35	39.11					
3	5	8	65.18	64.65	4	4	14	25.65	0.00					
3	6	8	91.58	91.04	4	6	14	121.72	121.04					
6	6	8	66.14	66.43	4	8	14	154.29	153.66					
6	6	8	238.82	235.35	9	9	14	27.10	40.37					
8	8	8	47.30	45.99	12	14	14	98.80	98.15					
8	8	8	441.82	442.90	12	16	14	97.39	97.33					
0	4	8	187.17	188.77	12	16	14	68.80	68.52					
8	8	8	363.71	363.10	4	18	14	73.03	75.51					

ALMANDINE 293K A = 11.525(1) A

STRUCTURE FACTORS

PAGE 1

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	0	0	68.31	71.20	0	18	0	25.45	25.05	6	15	3	28.71	28.79
0	0	0	397.39	380.07	8	18	6	22.73	22.02	10	16	3	21.55	21.76
2	4	0	405.05	394.10	8	18	2	26.04	26.47	1	16	3	15.75	16.46
4	4	0	165.10	163.38	12	18	2	92.36	91.30	7	16	3	24.07	23.85
6	0	0	65.40	63.20	4	19	2	8.25	7.44	15	16	3	11.07	11.82
2	8	0	48.01	48.83	5	19	2	8.86	7.17	15	16	3	11.13	11.82
8	0	0	460.02	459.00	15	19	2	6.93	5.18	14	17	3	7.80	7.80
6	10	0	89.49	90.35	10	20	2	163.31	165.41	3	18	3	63.23	63.24
10	10	0	76.63	76.93	12	20	2	131.77	132.74	7	18	3	42.92	43.64
6	12	0	200.45	202.12	8	20	2	10.22	11.94	11	18	3	26.44	26.65
10	12	0	161.08	162.38	12	20	2	9.77	8.80	11	18	3	8.04	9.47
8	12	0	168.10	170.15	7	21	2	32.79	33.23	15	18	3	13.32	12.51
12	12	0	49.89	46.22	0	22	2	32.30	31.91	2	19	3	42.59	43.03
14	14	0	28.96	26.96	8	22	2	63.81	62.14	12	19	3	0.00	4.40
14	14	0	43.56	43.25	8	22	2	9.32	8.63	14	19	3	24.45	24.62
2	16	0	22.84	22.59	3	22	2	20.70	18.48	2	21	3	8.28	8.92
4	16	0	134.29	134.60	10	22	2	7.35	4.11	6	21	3	33.37	33.57
6	16	0	26.21	25.95	15	23	2	8.18	6.64	8	21	3	28.37	26.52
6	16	0	26.21	25.95	15	23	2	26.94	26.51	5	22	3	22.26	22.52
10	16	0	11.53	1.33	4	23	2	13.82	13.97	7	22	3	37.12	37.18
12	16	0	140.01	138.71	0	24	2	101.85	103.91	9	22	3	9.57	4.32
16	16	0	216.29	214.45	4	24	2	155.85	151.14	11	22	3	8.66	7.96
0	18	0	14.72	18.23	5	25	2	76.44	74.37	8	23	3	4.23	5.96
0	18	0	146.00	148.70	3	25	2	9.91	9.71	2	23	3	11.28	7.44
0	20	0	143.40	142.62	5	25	2	10.47	10.10	2	23	3	214.28	220.74
0	20	0	69.86	68.44	3	26	2	34.99	35.75	4	24	4	684.80	667.00
8	20	0	59.13	61.15	2	26	2	44.69	44.08	0	26	4	407.26	404.98
14	20	0	79.44	80.52	6	26	2	91.95	92.85	6	26	4	335.38	333.31
4	22	0	11.05	7.19	8	26	2	66.64	67.28	0	28	4	285.40	255.72
0	24	0	67.00	66.62	5	27	2	44.57	43.06	0	28	4	303.52	282.11
1	2	3	58.67	59.32	0	27	2	53.64	52.66	8	28	4	201.19	199.95
3	4	5	118.31	110.63	7	27	2	59.47	57.97	0	28	4	288.17	289.34
5	5	5	166.16	162.22	9	27	2	59.47	57.97	0	28	4	242.65	242.00
4	4	4	17.85	16.75	5	27	2	56.67	56.51	10	10	4	183.81	182.51
1	6	6	217.90	212.36	10	27	2	40.42	40.98	1	11	4	41.49	42.17
3	6	6	32.67	31.99	9	27	2	16.64	15.51	2	12	4	19.93	18.34
5	6	6	68.82	68.74	10	27	2	16.64	15.51	2	12	4	9.02	9.84
7	7	7	49.96	51.24	4	27	2	10.43	11.99	12	12	4	229.82	231.04
7	7	7	66.19	63.93	6	27	2	92.15	93.32	0	14	4	185.62	188.07
6	8	8	23.98	24.13	11	27	2	26.08	26.27	14	14	4	79.44	76.73
1	8	8	6.53	0.00	11	27	2	5.15	5.37	11	15	4	4.90	2.79
3	8	8	9.72	10.17	10	27	2	39.47	38.40	13	15	4	8.49	6.44
5	8	8	65.06	66.86	15	27	2	33.90	33.39	2	16	4	191.98	194.04
7	8	8	16.13	15.97	5	27	2	33.90	33.39	10	16	4	107.98	107.26
9	9	9	48.38	47.58	6	27	2	42.68	43.12	12	16	4	14.80	14.94
9	9	9	82.51	83.94	9	27	2	20.21	19.51	14	16	4	115.06	115.12
4	9	9	53.53	55.39	11	27	2	6.58	8.27	16	16	4	103.41	103.98
6	9	9	8.29	12.84	11	27	2	44.86	45.55	1	17	4	25.93	25.31
10	10	10	44.20	41.91	2	28	2	22.18	20.34	3	17	4	22.70	23.12
3	10	10	59.84	59.75	6	28	2	6.57	6.57	13	17	4	13.08	28.82
5	10	10	28.07	29.07	15	28	2	31.59	31.38	15	17	4	29.01	4.06
9	10	10	43.72	44.85	10	28	2	22.36	23.07	15	17	4	25.07	25.34
2	11	11	18.87	18.97	6	28	2	57.67	57.54	2	18	4	105.02	105.33
8	11	11	29.57	29.17	5	28	2	39.23	38.62	0	18	4	114.76	114.95
5	12	12	3.92	3.16	11	28	2	33.25	32.73	6	18	4	106.06	105.56
12	12	12	7.77	8.19	9	28	2	25.68	25.44	8	18	4	132.95	132.87
1	12	12	35.36	35.55	13	28	2	34.45	35.15	10	18	4	12.10	87.05
1	12	12			13	28	2			12	18	4		5.89



H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	R	F(CALC)
3	19	4	4.48 LR	1.31	6	17	5	19.04	20.69	2	22	6	9.52 LR	6.70		24.71
9	19	4	36.03 LR	35.52	8	17	5	12.56 LR	9.25	6	22	6	13.16 LR	0.00		11.88
13	19	4	7.99 LR	4.74	12	17	5	43.37 LR	5.06	8	22	6	18.19 LR	16.21		56.21
2	20	4	22.37 LR	18.11	14	17	5	7.22 LR	44.16	8	23	6	19.45 LR	20.88		388.26
2	20	4	9.60 LR	5.79	3	18	5	7.22 LR	5.20	1	23	6	6.93 LR	3.31		44.26
3	21	4	6.22 LR	5.26	5	18	5	13.02 LR	10.97	3	23	6	9.42 LR	8.45		15.34
3	21	4	29.02 LR	28.94	7	18	5	37.04 LR	37.28	10	24	6	31.58 LR	31.94		29.96
5	21	4	10.86 LR	9.86	4	19	5	9.84 LR	9.45	2	24	6	10.72 LR	6.78		241.32
9	21	4	84.26 LR	84.32	8	19	5	7.08 LR	8.53	4	24	6	14.02 LR	14.13		20.58
6	22	4	4.26 LR	8.91	2	20	5	7.85 LR	3.54	10	10	8	20.32 LR	20.40		53.03
1	23	4	1.34 LR	0.32	6	20	5	3.04 LR	8.00	2	12	8	80.87 LR	79.53		209.55
3	23	4	6.35 LR	1.30	11	20	5	10.84 LR	7.28	4	12	8	12.00 LR	14.65		61.72
7	23	4	75.99 LR	75.99	8	21	5	10.59 LR	15.69	6	12	8	24.65 LR	24.65		201.00
0	24	4	75.78 LR	72.37	7	21	5	5.95 LR	7.74	12	12	8	25.38 LR	21.63		14.53
5	2	7	6.30 LR	6.32	2	22	5	28.58 LR	29.68	4	14	8	48.54 LR	47.44		55.47
4	7	5	67.12 LR	69.90	1	22	5	15.11 LR	13.22	2	11	7	57.06 LR	56.75		173.37
6	7	5	80.63 LR	81.90	5	22	5	25.43 LR	25.99	6	11	7	25.99 LR	24.87		16.29
5	8	5	5.30 LR	0.00	8	23	5	21.46 LR	21.68	8	11	7	24.11 LR	23.12	LR	4.23
5	8	5	20.65 LR	20.99	4	23	5	13.85 LR	17.27	10	11	7	24.70 LR	24.00		15.90
7	8	5	31.11 LR	30.56	5	24	5	29.21 LR	29.63	10	11	7	18.94 LR	18.16		306.19
2	9	5	10.70 LR	12.39	1	24	5	16.52 LR	15.93	11	12	7	11.28 LR	8.82	LR	128.32
4	9	5	42.45 LR	42.83	3	24	5	10.02 LR	13.50	4	13	7	10.15 LR	17.20	LR	13.64
6	9	5	30.42 LR	27.28	7	0	8	6.53 LR	3.75	6	13	7	23.68 LR	23.83	LR	157.10
8	9	5	32.58 LR	27.88	0	8	6	78.53 LR	79.76	8	13	7	31.35 LR	31.33	LR	10.24
5	10	5	19.09 LR	18.65	2	8	6	259.56 LR	256.84	10	13	7	9.14 LR	11.48	LR	21.28
7	10	5	8.97 LR	9.23	4	8	6	47.76 LR	46.23	12	13	7	31.30 LR	30.70	LR	5.60
2	11	5	11.10 LR	9.33	6	6	6	35.88 LR	34.54	7	14	7	64.75 LR	63.99	LR	16.47
4	11	5	7.50 LR	2.43	2	10	6	184.56 LR	183.68	9	14	7	11.52 LR	10.15	LR	100.24
6	11	5	33.09 LR	33.23	4	11	6	9.01 LR	10.12	11	14	7	16.06 LR	17.59	LR	16.64
8	11	5	41.18 LR	41.11	11	11	6	152.77 LR	153.12	13	14	7	24.05 LR	24.88	LR	8.27
10	11	5	5.38 LR	7.51	4	12	6	20.99 LR	19.82	1	15	7	5.41 LR	5.45	LR	9.40
9	12	5	4.87 LR	5.99	13	13	6	45.06 LR	45.04	6	15	7	45.88 LR	45.96	LR	26.88
11	12	5	11.80 LR	6.41	0	14	6	57.92 LR	57.91	8	15	7	23.97 LR	22.69	LR	35.05
6	13	5	24.41 LR	23.77	1	15	6	6.04 LR	6.25	10	15	7	9.45 LR	8.18	LR	39.79
6	13	5	43.40 LR	43.54	15	15	6	8.81 LR	6.25	12	15	7	21.50 LR	21.33	LR	126.98
10	13	5	39.62 LR	39.91	12	16	6	159.70 LR	161.24	1	16	7	21.50 LR	21.34	LR	75.49
12	13	5	15.60 LR	15.62	1	16	6	121.83 LR	122.86	8	20	8	28.66 LR	28.69	LR	15.64
12	13	5	12.01 LR	12.98	3	17	6	5.99 LR	6.27	1	21	8	11.43 LR	11.43	LR	6.94
7	14	5	21.12 LR	20.53	11	17	6	27.18 LR	26.52	15	16	7	23.98 LR	23.78	LR	5.24
9	14	5	39.13 LR	39.16	6	17	6	49.20 LR	47.87	4	22	8	19.85 LR	19.85	LR	98.86
11	14	5	45.31 LR	44.69	13	17	6	15.63 LR	18.50	9	22	8	50.60 LR	50.60	LR	49.88
13	14	5	24.54 LR	24.50	15	17	6	9.02 LR	6.24	2	22	9	30.56 LR	30.70	LR	30.70
2	15	5	7.99 LR	11.42	17	17	6	28.39 LR	28.22	4	22	9	16.42 LR	16.42	LR	21.13
4	15	5	24.35 LR	24.15	8	18	6	16.38 LR	16.80	6	22	9	7.32 LR	7.32	LR	16.52
6	15	5	12.42 LR	11.51	10	18	6	15.71 LR	17.97	8	22	9	50.74 LR	50.94	LR	7.38
8	15	5	30.93 LR	31.09	12	18	6	92.30 LR	90.62	10	22	9	19.30 LR	19.30	LR	50.94
10	15	5	32.68 LR	33.11	1	19	6	8.15 LR	51.40	11	18	7	7.90 LR	7.90	LR	9.04
14	15	5	11.58 LR	12.26	2	19	6	13.81 LR	12.45	11	18	7	33.23 LR	32.68	LR	9.70
3	16	5	12.65 LR	12.21	4	19	6	6.21 LR	6.35	12	19	7	31.40 LR	31.70	LR	26.83
7	16	5	23.04 LR	22.70	14	19	6	8.57 LR	5.66	14	19	7	22.08 LR	22.50	LR	20.17
9	16	5	11.71 LR	9.95	1	20	6	100.81 LR	101.43	1	20	7	9.78 LR	6.91	LR	26.38
11	16	5	6.09 LR	8.12	2	20	6	111.13 LR	111.04	3	20	7	9.20 LR	5.74	LR	24.01
13	16	5	13.38 LR	11.85	4	20	6	35.53 LR	35.66	5	20	7	13.25 LR	14.74	LR	14.88
15	16	5	11.52 LR	13.01	1	21	6	11.08 LR	5.43	4	21	7	14.50 LR	15.23	LR	47.87
2	17	5	7.31 LR	7.40	6	21	6	19.29 LR	19.89	6	21	7	14.41 LR	17.86	LR	17.50
6	17	5	29.09 LR	28.93	0	22	6	11.11 LR	6.43	0	22	8	516.28 LR	507.38	LR	21.82

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
6	15	9	22.62	22.04	10	20	10	99.07	99.90	5	15	12	18.68	18.97
8	15	9	23.73	23.76	1	21	10	10.91	9.88	8	16	12	90.89	90.21
10	15	9	10.09	10.52	3	21	10	3.52	7.97	10	16	12	144.06	145.80
12	15	9	10.97	10.52	5	21	10	27.54	28.97	3	17	12	22.63	23.50
14	15	9	30.61	30.52	7	21	10	21.72	22.47	7	17	12	1.33	3.19
3	16	9	25.62	25.66	0	22	10	20.59	17.56	1	19	12	1.18	4.75
11	16	9	14.77	14.77	4	22	10	78.26	77.29	5	19	12	13.35	21.97
13	16	9	9.40	9.40	3	19	11	34.19	34.79	7	19	12	17.17	16.06
15	16	9	3.99	4.55	6	13	11	9.46	6.79	9	19	12	6.35	5.49
2	17	9	12.84	12.55	8	13	11	0.00	7.13	4	20	12	31.00	128.78
4	17	9	29.28	29.09	10	13	11	28.40	28.40	6	20	12	8.58	8.56
6	17	9	24.44	23.69	12	13	11	14.06	15.74	1	18	17	0.00	0.45
8	17	9	10.95	4.37	1	14	11	31.94	32.17	3	21	12	12.13	14.26
10	17	9	6.61	4.88	3	14	11	9.25	5.12	5	14	13	30.46	29.83
12	17	9	8.95	1.72	11	14	11	14.44	12.83	13	14	13	11.66	14.24
1	18	9	22.28	22.91	13	14	11	22.33	22.60	13	15	13	23.85	23.52
3	18	9	17.51	17.51	2	15	11	0.00	10.60	8	15	13	41.39	40.94
5	18	9	32.79	32.11	6	15	11	27.54	26.52	10	15	13	9.42	6.77
9	18	9	9.53	9.26	8	15	11	22.90	21.79	12	15	13	20.55	19.32
2	19	9	7.91	6.68	10	15	11	9.52	6.25	14	15	13	7.89	1.29
6	19	9	16.81	15.77	12	15	11	3.01	4.30	3	16	13	8.12	8.31
10	19	9	14.39	15.40	14	15	11	26.48	26.26	7	17	13	16.01	17.89
1	20	9	28.43	27.72	3	16	11	10.17	6.26	2	17	13	40.95	41.41
3	20	9	8.14	0.71	11	16	11	4.68	0.00	12	17	13	9.27	10.96
5	20	9	11.06	11.49	13	16	11	12.61	15.18	5	18	13	34.55	35.18
7	20	9	9.18	9.23	4	17	11	7.51	4.64	7	18	13	5.35	4.41
2	21	9	10.29	3.60	8	17	11	10.32	13.41	9	18	13	22.52	22.65
5	22	9	2.96	7.67	10	17	11	8.70	4.02	11	18	13	7.78	3.96
7	22	9	25.30	26.44	12	17	11	13.48	14.78	2	19	13	7.63	6.25
1	11	10	26.33	26.54	14	17	11	7.46	3.18	8	19	13	22.70	23.10
11	11	10	48.54	47.92	1	18	11	17.96	19.12	6	19	13	11.25	8.68
12	12	10	161.41	162.34	9	18	11	11.07	14.12	3	20	13	11.18	12.59
4	12	10	7.93	0.50	2	19	11	17.80	16.86	2	21	13	22.65	22.10
6	12	10	161.74	162.45	4	19	11	14.16	14.61	1	14	14	1.88	5.71
8	12	10	142.17	143.17	8	19	11	14.68	15.62	0	16	14	40.53	41.84
1	13	10	35.31	36.08	10	19	11	11.41	10.58	6	16	14	24.13	23.29
13	13	10	9.29	12.34	3	20	11	16.47	5.20	10	16	14	35.40	35.89
0	14	10	0.00	6.61	7	20	11	3.45	19.01	7	17	14	84.72	84.12
2	14	10	9.96	10.29	9	20	11	3.45	0.47	9	17	14	6.51	5.65
4	14	10	108.67	107.58	2	21	11	0.00	8.31	2	18	14	27.36	27.32
6	14	10	30.74	28.70	4	21	11	12.75	13.17	5	19	14	9.59	7.64
8	14	10	29.57	29.26	6	21	11	9.64	12.72	2	20	14	8.87	10.40
15	15	10	16.80	17.49	1	22	11	11.32	12.72	4	20	14	72.93	72.96
16	15	10	23.88	21.60	0	0	12	120.79	122.64	2	20	14	16.29	16.29
8	16	10	19.18	19.18	2	4	12	261.88	261.40	1	16	15	5.71	1.26
1	17	10	23.77	24.61	4	4	12	219.13	222.13	1	16	15	11.76	11.71
3	17	10	26.79	27.68	6	6	12	165.59	166.20	8	17	15	15.03	16.26
5	17	10	31.14	31.12	8	8	12	145.65	146.27	2	17	15	14.30	17.66
13	17	10	8.32	6.39	10	10	12	81.73	79.31	8	17	15	16.53	16.53
8	18	10	28.85	28.66	12	12	12	115.16	115.96	5	19	14	14.76	14.76
12	18	10	29.46	30.10	1	13	12	1.21	2.14	2	20	14	9.63	9.94
3	19	10	81.99	80.11	3	13	12	28.72	29.19	4	20	14	17.66	17.66
5	19	10	12.50	9.93	0	14	12	161.71	161.73	1	16	15	16.26	16.26
7	19	10	26.10	27.04	2	14	12	81.19	81.36	8	17	15	16.53	16.53
0	20	10	112.78	114.54	4	14	12	9.90	0.43	1	16	15	14.76	14.76
2	20	10	66.27	65.51	6	14	12	132.46	131.67	5	19	14	19.94	19.94
4	20	10	26.81	26.81	8	14	12	132.21	131.21	4	20	14	14.23	14.23
6	20	10	80.85	82.69	10	14	12	106.04	104.16	7	18	15	19.62	19.62
8	20	10	91.73	91.51	14	14	12	112.36	111.47	4	24	24	11.24	11.24
					3	15	12	7.09	6.08	9	19	15		