

AM-96-613

7074

Structure refinement of a natural K-rich diopside: The effect of K on the average structure

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For deposit: Table 6

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Table 6: Structure factors for K18a diopside

Frel and Sigf Scales:

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3.0203

h	k	l	Frel	Fcalc	Sigf	h	k	l	Frel	Fcalc	Sigf
2	0	0	8.36	7.17	.05	2	8	0	26.04	26.08	.11
4	0	0	14.94	19.04	.07	4	8	0	38.18	38.03	.11
6	0	0	87.46	85.05	.08	6	8	0	4.76	3.96	.12
8	0	0	73.47	76.65	.10	8	8	0	8.26	7.98	.13
10	0	0	52.77	53.65	.12	10	8	0	29.09	28.35	.14
12	0	0	3.53	7.39	.13	1	9	0	2.74	4.07	.11
1	1	0	3.09	3.30	.04	3	9	0	20.83	21.34	.12
3	1	0	85.41	82.26	.06	5	9	0	15.03	14.74	.12
5	1	0	61.13	60.86	.08	7	9	0	14.65	14.72	.13
7	1	0	43.27	42.00	.09	9	9	0	7.91	7.50	.14
9	1	0	.00	.12	.00	0	10	0	72.19	71.25	.12
11	1	0	28.80	28.78	.12	2	10	0	7.56	7.36	.12
13	1	0	15.49	15.54	.14	4	10	0	53.03	52.95	.13
0	2	0	26.83	26.41	.05	6	10	0	21.42	21.53	.13
2	2	0	69.35	65.58	.06	8	10	0	18.97	19.06	.14
4	2	0	22.29	22.07	.07	1	11	0	9.16	5.13	.13
6	2	0	18.15	18.60	.09	3	11	0	26.06	24.52	.13
8	2	0	20.61	19.94	.10	5	11	0	31.12	30.86	.14
10	2	0	.00	2.96	.00	0	12	0	40.67	40.88	.14
12	2	0	16.80	17.33	.13	2	12	0	25.41	24.53	.14
1	3	0	13.24	12.42	.06	4	12	0	9.72	9.37	.14
3	3	0	62.48	60.30	.07	-13	1	1	.69	.75	.18
5	3	0	36.20	36.24	.08	-11	1	1	23.89	24.98	.12
7	3	0	8.04	8.34	.10	-9	1	1	4.42	2.98	.11
9	3	0	29.20	30.37	.11	-7	1	1	35.89	36.23	.09
11	3	0	16.16	16.73	.13	-5	1	1	15.46	15.81	.08
13	3	0	1.85	2.30	.14	-3	1	1	85.13	85.22	.06
0	4	0	.00	4.92	.00	-1	1	1	4.47	3.41	.05
2	4	0	18.35	15.56	.07	1	1	1	14.25	14.67	.05
4	4	0	65.91	65.53	.08	3	1	1	76.04	75.76	.07
6	4	0	27.68	29.04	.10	5	1	1	5.90	5.05	.08
8	4	0	11.24	11.92	.11	7	1	1	27.80	28.16	.10
10	4	0	43.86	44.15	.12	9	1	1	4.45	4.43	.11
12	4	0	18.25	18.01	.14	11	1	1	32.68	32.73	.13
1	5	0	99.73	97.20	.08	-12	2	1	65.16	64.25	.13
3	5	0	70.09	69.62	.08	-10	2	1	.00	1.04	.00
5	5	0	11.43	9.94	.09	-8	2	1	35.04	35.13	.10
7	5	0	109.97	111.46	.11	-6	2	1	45.45	47.36	.09
9	5	0	11.20	12.63	.12	-4	2	1	65.16	64.33	.07
11	5	0	40.49	39.31	.13	-2	2	1	143.57	143.84	.06
0	6	0	113.91	106.63	.09	0	2	1	38.93	39.12	.06
2	6	0	28.09	27.12	.09	2	2	1	111.76	112.49	.07
4	6	0	18.81	17.27	.10	4	2	1	28.00	27.50	.08
6	6	0	6.29	3.21	.11	6	2	1	71.63	74.14	.09
8	6	0	17.32	17.28	.12	8	2	1	38.78	39.52	.11
10	6	0	34.54	36.61	.13	10	2	1	4.48	3.90	.12
1	7	0	4.16	2.49	.09	12	2	1	45.38	43.49	.14
3	7	0	12.24	11.26	.10	-13	3	1	21.63	21.30	.14
5	7	0	45.02	45.05	.11	-11	3	1	23.92	26.17	.13
7	7	0	29.12	28.65	.12	-9	3	1	68.30	68.57	.11
9	7	0	20.89	20.67	.13	-7	3	1	42.22	43.95	.10
11	7	0	2.53	2.30	.14	-5	3	1	112.45	113.14	.08
0	8	0	5.23	3.54	.10	-3	3	1	95.97	93.67	.07

h	k	l	Frel	Fcalc	Sigf	h	k	l	Frel	Fcalc	Sigf
-1	3	1	87.10	89.61	.06	7	7	1	10.18	10.54	.12
1	3	1	20.34	15.24	.07	9	7	1	48.77	48.57	.13
3	3	1	39.11	38.40	.08	-10	8	1	.00	.01	.00
5	3	1	149.79	149.60	.09	-8	8	1	35.70	36.17	.13
7	3	1	16.90	16.49	.10	-6	8	1	20.46	21.55	.12
9	3	1	44.13	45.07	.12	-4	8	1	19.08	19.78	.11
11	3	1	9.53	10.57	.13	-2	8	1	92.73	96.46	.11
-12	4	1	28.29	27.03	.14	0	8	1	21.52	22.81	.11
-10	4	1	28.59	28.82	.12	2	8	1	56.53	56.32	.11
-8	4	1	14.48	15.51	.11	4	8	1	17.26	18.71	.11
-6	4	1	9.82	9.85	.09	6	8	1	56.06	55.76	.12
-4	4	1	8.94	8.43	.08	8	8	1	17.45	17.41	.13
-2	4	1	22.36	23.51	.07	-9	9	1	4.94	5.32	.14
0	4	1	88.98	91.83	.07	-7	9	1	55.89	56.19	.13
2	4	1	24.10	22.09	.08	-5	9	1	39.93	40.39	.12
4	4	1	37.67	37.49	.09	-3	9	1	10.21	9.12	.12
6	4	1	7.38	7.14	.10	-1	9	1	9.54	8.42	.11
8	4	1	4.06	2.37	.11	1	9	1	18.91	19.93	.11
10	4	1	32.33	32.05	.13	3	9	1	15.99	15.91	.12
12	4	1	6.41	6.36	.14	5	9	1	31.33	31.10	.12
-11	5	1	8.72	9.83	.13	7	9	1	35.46	34.42	.13
-9	5	1	7.40	8.34	.12	-8	10	1	13.01	12.88	.14
-7	5	1	5.46	5.05	.10	-6	10	1	.00	1.07	.00
-5	5	1	9.95	9.57	.09	-4	10	1	.00	1.93	.00
-3	5	1	16.41	16.35	.08	-2	10	1	35.09	37.13	.12
-1	5	1	28.86	28.89	.08	0	10	1	16.59	16.46	.12
1	5	1	8.47	8.26	.08	2	10	1	8.21	8.54	.12
3	5	1	21.84	21.03	.09	4	10	1	7.91	7.77	.13
5	5	1	19.84	19.63	.10	6	10	1	19.93	20.02	.14
7	5	1	3.24	3.54	.11	-7	11	1	20.86	19.84	.14
9	5	1	4.92	5.02	.12	-5	11	1	20.64	20.76	.14
11	5	1	7.72	6.70	.14	-3	11	1	5.45	6.54	.13
-12	6	1	7.24	7.29	.14	-1	11	1	9.21	8.99	.13
-10	6	1	20.34	20.01	.13	1	11	1	30.71	29.47	.13
-8	6	1	.00	1.29	.00	3	11	1	13.31	12.61	.13
-6	6	1	23.84	25.01	.10	5	11	1	.00	.76	.00
-4	6	1	35.27	34.97	.10	-4	12	1	16.22	16.04	.14
-2	6	1	8.45	9.43	.09	-2	12	1	28.83	29.39	.14
0	6	1	44.91	45.97	.09	0	12	1	1.15	.84	.13
2	6	1	18.94	18.52	.09	2	12	1	46.22	44.44	.14
4	6	1	22.97	23.05	.10	-12	0	2	8.79	10.48	.13
6	6	1	7.59	6.83	.11	-10	0	2	67.36	68.20	.11
8	6	1	20.56	20.79	.12	-8	0	2	30.55	31.66	.10
10	6	1	18.43	18.10	.14	-6	0	2	100.24	99.57	.09
-11	7	1	11.63	11.60	.14	-4	0	2	108.12	109.14	.07
-9	7	1	29.95	29.46	.13	-2	0	2	37.57	33.42	.06
-7	7	1	.00	1.48	.00	0	0	2	156.64	158.51	.06
-5	7	1	82.10	84.26	.11	2	0	2	90.19	89.67	.07
-3	7	1	6.12	7.37	.10	4	0	2	115.48	116.80	.09
-1	7	1	43.86	45.39	.10	6	0	2	6.64	6.94	.10
1	7	1	56.71	59.83	.10	8	0	2	45.31	46.35	.11
3	7	1	7.53	5.94	.10	10	0	2	74.23	74.97	.13
5	7	1	47.85	48.43	.11						

h	k	l	Frel	Fcalc	Sigf	h	k	l	Frel	Fcalc	Sigf
-13	1	2	16.19	16.87	.14	-7	5	2	88.68	90.95	.11
-11	1	2	3.21	3.21	.12	-5	5	2	6.15	9.76	.10
-9	1	2	26.09	27.06	.11	-3	5	2	104.53	105.31	.09
-7	1	2	95.72	97.57	.09	-1	5	2	12.08	12.91	.09
-5	1	2	31.55	33.20	.08	1	5	2	71.43	70.92	.09
-3	1	2	7.55	4.24	.07	3	5	2	107.44	109.86	.10
-1	1	2	3.20	4.21	.06	5	5	2	11.61	2.59	.11
1	1	2	64.95	64.84	.07	7	5	2	55.39	56.05	.12
3	1	2	25.06	24.71	.08	9	5	2	13.64	14.66	.13
5	1	2	36.52	35.87	.09	-12	6	2	23.07	22.73	.14
7	1	2	49.19	50.39	.11	-10	6	2	7.94	8.00	.13
9	1	2	26.19	25.85	.12	-8	6	2	4.32	3.55	.12
11	1	2	25.96	24.33	.14	-6	6	2	53.15	56.03	.11
-12	2	2	31.33	31.08	.13	-4	6	2	4.78	4.33	.10
-10	2	2	23.49	24.62	.12	-2	6	2	64.44	66.56	.09
-8	2	2	26.28	26.83	.10	0	6	2	96.71	98.93	.10
-6	2	2	48.28	49.78	.09	2	6	2	7.41	5.37	.10
-4	2	2	19.08	19.79	.08	4	6	2	23.11	22.82	.11
-2	2	2	20.41	22.32	.07	6	6	2	14.61	14.65	.12
0	2	2	60.13	59.19	.07	8	6	2	14.27	14.86	.13
2	2	2	41.30	43.35	.08	10	6	2	20.60	20.15	.14
4	2	2	37.70	37.32	.09	-11	7	2	3.20	2.91	.14
6	2	2	41.74	42.20	.10	-9	7	2	17.00	17.23	.13
8	2	2	30.30	31.72	.12	-7	7	2	14.15	16.66	.12
10	2	2	11.29	10.60	.13	-5	7	2	29.28	30.77	.11
-13	3	2	18.05	17.95	.14	-3	7	2	12.57	12.81	.10
-11	3	2	2.04	2.76	.12	-1	7	2	36.10	37.46	.10
-9	3	2	13.06	13.24	.11	1	7	2	5.34	5.39	.10
-7	3	2	28.69	29.01	.10	3	7	2	20.21	20.42	.11
-5	3	2	31.70	31.29	.09	5	7	2	34.46	33.95	.12
-3	3	2	9.93	8.69	.08	7	7	2	.00	2.02	.00
-1	3	2	56.12	58.00	.07	9	7	2	16.68	16.71	.14
1	3	2	45.19	44.39	.08	-10	8	2	15.84	14.99	.14
3	3	2	3.94	3.33	.09	-8	8	2	19.07	18.49	.13
5	3	2	29.22	29.16	.10	-6	8	2	15.16	14.71	.12
7	3	2	23.11	24.25	.11	-4	8	2	15.90	16.44	.11
9	3	2	13.74	13.44	.12	-2	8	2	23.19	23.66	.11
11	3	2	.58	3.01	.18	0	8	2	22.48	23.48	.11
-12	4	2	22.97	22.09	.13	2	8	2	11.17	11.22	.11
-10	4	2	21.83	20.66	.12	4	8	2	24.56	24.62	.12
-8	4	2	.00	.05	.00	6	8	2	20.61	21.29	.13
-6	4	2	14.79	14.62	.10	8	8	2	6.08	7.05	.14
-4	4	2	5.95	5.83	.09	-9	9	2	11.55	11.60	.14
-2	4	2	21.33	21.41	.08	-7	9	2	24.44	24.09	.13
0	4	2	60.86	60.46	.08	-5	9	2	13.79	14.00	.12
2	4	2	41.06	42.15	.09	-3	9	2	10.61	11.76	.12
4	4	2	36.08	36.69	.10	-1	9	2	3.27	3.69	.12
6	4	2	2.00	.86	.11	1	9	2	9.11	9.29	.12
8	4	2	6.42	6.03	.12	3	9	2	5.32	5.13	.12
10	4	2	8.92	8.09	.13	5	9	2	11.94	11.44	.13
-11	5	2	35.87	35.09	.13	7	9	2	20.83	19.94	.14
-9	5	2	16.06	16.53	.12						

h	k	l	Frel	Fcalc	Sigf	h	k	l	Frel	Fcalc	Sigf
-8	10	2	15.47	15.08	.14	-10	4	3	19.86	19.87	.12
-6	10	2	23.95	23.89	.13	-8	4	3	16.70	17.64	.11
-4	10	2	47.20	47.88	.13	-6	4	3	36.68	38.32	.10
-2	10	2	15.08	14.92	.12	-4	4	3	29.39	30.10	.09
0	10	2	52.90	54.77	.13	-2	4	3	40.77	42.88	.09
2	10	2	4.92	3.99	.13	0	4	3	42.03	44.26	.09
4	10	2	65.93	64.71	.13	2	4	3	3.98	3.26	.10
6	10	2	11.55	12.40	.14	4	4	3	42.24	42.55	.11
-5	11	2	19.59	20.85	.14	6	4	3	14.33	13.59	.12
-3	11	2	18.90	19.57	.13	8	4	3	8.84	8.96	.13
-1	11	2	12.64	12.52	.13	-11	5	3	6.71	7.25	.13
1	11	2	15.42	16.11	.13	-9	5	3	5.10	5.99	.12
3	11	2	22.56	22.87	.14	-7	5	3	3.67	4.60	.11
-2	12	2	33.80	34.95	.14	-5	5	3	30.94	32.82	.10
0	12	2	23.30	23.68	.14	-3	5	3	19.38	21.86	.10
-13	1	3	6.90	5.99	.14	-1	5	3	2.05	.51	.09
-11	1	3	8.58	8.81	.12	1	5	3	25.58	26.79	.10
-9	1	3	6.50	7.29	.11	3	5	3	2.81	1.71	.10
-7	1	3	37.73	38.71	.10	5	5	3	9.57	9.46	.12
-5	1	3	24.63	24.78	.09	7	5	3	2.18	3.21	.12
-3	1	3	65.15	67.47	.08	9	5	3	20.96	20.16	.14
-1	1	3	7.76	8.23	.08	-12	6	3	4.63	5.03	.14
1	1	3	4.79	3.97	.08	-10	6	3	22.17	21.76	.13
3	1	3	35.24	34.58	.09	-8	6	3	11.79	11.29	.12
5	1	3	14.96	15.48	.10	-6	6	3	13.22	13.04	.11
7	1	3	25.46	26.48	.12	-4	6	3	16.15	17.09	.11
9	1	3	15.50	14.39	.13	-2	6	3	15.88	17.42	.10
-12	2	3	51.48	49.73	.13	0	6	3	30.65	31.71	.10
-10	2	3	7.27	7.27	.12	2	6	3	5.30	5.26	.11
-8	2	3	62.23	63.49	.11	4	6	3	34.26	34.91	.12
-6	2	3	8.74	7.64	.09	6	6	3	10.75	11.87	.13
-4	2	3	24.91	25.88	.09	8	6	3	7.72	8.13	.14
-2	2	3	117.21	119.66	.08	-11	7	3	12.85	11.98	.14
0	2	3	10.39	10.10	.08	-9	7	3	39.07	38.52	.13
2	2	3	74.10	74.77	.09	-7	7	3	1.05	.83	.12
4	2	3	7.17	6.64	.10	-5	7	3	55.13	55.63	.11
6	2	3	63.80	64.46	.11	-3	7	3	3.17	2.87	.11
8	2	3	30.63	31.13	.13	-1	7	3	58.42	59.54	.11
10	2	3	8.75	8.57	.14	1	7	3	26.06	26.52	.11
-13	3	3	2.07	1.61	.14	3	7	3	11.86	12.22	.12
-11	3	3	32.49	32.26	.13	5	7	3	43.01	42.60	.13
-9	3	3	73.62	73.44	.11	7	7	3	3.97	2.66	.13
-7	3	3	24.38	25.81	.10	-10	8	3	2.07	2.45	.14
-5	3	3	67.93	70.16	.09	-8	8	3	35.47	35.37	.13
-3	3	3	26.10	26.35	.09	-6	8	3	14.50	14.39	.12
-1	3	3	116.53	118.62	.09	-4	8	3	20.55	21.19	.12
1	3	3	21.93	22.65	.09	-2	8	3	56.02	59.90	.12
3	3	3	4.93	4.04	.10	0	8	3	2.65	1.77	.11
5	3	3	76.56	77.58	.11	2	8	3	65.96	65.52	.12
7	3	3	10.11	10.99	.12	4	8	3	15.49	15.67	.13
9	3	3	51.03	51.80	.13	6	8	3	43.04	42.53	.14
-12	4	3	14.23	12.34	.14						

h	k	l	Frel	Fcalc	Sigf	h	k	l	Frel	Fcalc	Sigf
-9	9	3	30.75	30.78	.14	-7	3	4	4.59	5.24	.11
-7	9	3	39.62	39.51	.13	-5	3	4	27.46	26.97	.10
-5	9	3	.00	2.55	.00	-3	3	4	26.20	27.76	.10
-3	9	3	15.54	14.97	.12	-1	3	4	14.80	14.53	.10
-1	9	3	35.70	36.45	.12	1	3	4	8.76	8.61	.10
1	9	3	31.84	31.85	.13	3	3	4	29.36	30.91	.11
3	9	3	31.01	30.68	.13	5	3	4	18.82	18.78	.12
5	9	3	28.82	27.94	.14	7	3	4	2.47	.17	.13
-6	10	3	1.81	2.56	.13	-12	4	4	22.27	22.03	.14
-4	10	3	5.83	4.96	.13	-10	4	4	37.02	35.95	.13
-2	10	3	14.90	15.78	.13	-8	4	4	15.77	15.50	.12
0	10	3	4.56	2.53	.13	-6	4	4	.00	.67	.00
2	10	3	21.50	22.40	.13	-4	4	4	23.21	22.91	.10
4	10	3	13.08	12.95	.14	-2	4	4	3.27	1.81	.10
-5	11	3	5.84	6.88	.14	0	4	4	12.06	11.96	.10
-3	11	3	14.33	14.60	.14	2	4	4	30.02	30.83	.11
-1	11	3	15.10	14.63	.14	4	4	4	45.70	45.87	.12
1	11	3	16.01	15.56	.14	6	4	4	11.92	11.81	.13
-12	0	4	13.04	12.11	.13	8	4	4	4.76	4.58	.14
-10	0	4	39.58	39.35	.12	-11	5	4	20.21	19.13	.14
-8	0	4	.00	1.80	.00	-9	5	4	.21	.61	.11
-6	0	4	103.30	106.23	.10	-7	5	4	81.39	81.23	.12
-4	0	4	69.65	70.98	.10	-5	5	4	12.15	13.17	.11
-2	0	4	6.89	5.62	.09	-3	5	4	75.54	77.35	.11
0	0	4	103.00	103.21	.10	-1	5	4	13.10	11.73	.11
2	0	4	22.14	20.22	.10	1	5	4	55.90	56.69	.11
4	0	4	86.96	87.88	.11	3	5	4	47.84	49.13	.12
6	0	4	21.50	19.77	.12	5	5	4	23.43	24.01	.13
8	0	4	34.96	35.36	.14	7	5	4	57.31	57.23	.14
-11	1	4	13.63	13.47	.13	-10	6	4	29.05	27.53	.14
-9	1	4	14.71	14.19	.12	-8	6	4	34.65	33.52	.13
-7	1	4	25.03	25.36	.11	-6	6	4	31.49	32.67	.12
-5	1	4	11.63	11.73	.10	-4	6	4	41.24	42.62	.11
-3	1	4	72.89	75.62	.09	-2	6	4	28.24	29.56	.11
-1	1	4	49.14	50.65	.09	0	6	4	19.88	18.75	.11
1	1	4	7.91	4.90	.10	2	6	4	10.57	7.66	.12
3	1	4	43.71	44.85	.11	4	6	4	52.56	53.47	.13
5	1	4	8.11	7.28	.12	6	6	4	26.11	24.79	.14
7	1	4	13.07	12.78	.13	-9	7	4	26.16	26.10	.14
9	1	4	19.41	17.54	.14	-7	7	4	18.38	18.47	.13
-12	2	4	24.52	23.38	.14	-5	7	4	20.37	19.99	.12
-10	2	4	7.49	7.21	.12	-3	7	4	6.25	7.10	.12
-8	2	4	11.18	11.11	.11	-1	7	4	26.48	27.46	.12
-6	2	4	.00	2.39	.00	1	7	4	.00	1.72	.00
-4	2	4	30.16	32.08	.10	3	7	4	4.59	4.40	.13
-2	2	4	18.88	19.18	.10	5	7	4	15.11	14.94	.14
0	2	4	13.62	14.75	.10	-8	8	4	14.67	14.90	.14
2	2	4	52.75	54.98	.10	-6	8	4	2.82	4.43	.13
4	2	4	.00	2.24	.00	-4	8	4	20.27	20.04	.13
6	2	4	2.79	2.61	.12	-2	8	4	25.61	25.84	.12
8	2	4	15.77	15.45	.14	0	8	4	10.37	10.55	.13
-11	3	4	17.75	17.37	.13	2	8	4	8.27	7.65	.13
-9	3	4	21.27	22.50	.12	4	8	4	26.92	26.44	.14

h	k	l	Frel	Fcalc	Sigf	h	k	l	Frel	Fcalc	Sigf
-7	9	4	7.31	8.86	.14	-1	5	5	5.54	4.78	.12
-5	9	4	11.03	11.89	.13	1	5	5	2.50	.96	.12
-3	9	4	22.87	22.63	.13	3	5	5	8.15	7.80	.13
-1	9	4	13.25	12.67	.13	5	5	5	2.18	3.09	.14
1	9	4	4.50	3.26	.13	-10	6	5	17.22	16.61	.14
3	9	4	8.40	8.38	.14	-8	6	5	5.17	3.99	.13
-6	10	4	33.02	33.07	.14	-6	6	5	24.25	23.19	.13
-4	10	4	28.24	27.88	.14	-4	6	5	17.37	16.54	.12
-2	10	4	18.21	17.77	.14	-2	6	5	1.16	1.80	.12
0	10	4	50.48	49.95	.14	0	6	5	25.22	25.14	.13
2	10	4	5.28	3.26	.14	2	6	5	9.81	9.25	.13
-11	1	5	4.32	4.02	.13	4	6	5	18.53	18.15	.14
-9	1	5	4.60	4.50	.12	-9	7	5	17.68	16.57	.14
-7	1	5	28.86	28.56	.12	-7	7	5	.00	1.10	.00
-5	1	5	15.88	16.00	.11	-5	7	5	61.65	58.31	.13
-3	1	5	41.30	41.88	.11	-3	7	5	11.82	11.77	.13
-1	1	5	5.34	5.18	.11	-1	7	5	32.64	31.78	.13
1	1	5	14.59	15.52	.11	1	7	5	26.87	26.90	.13
3	1	5	8.59	8.58	.12	3	7	5	25.53	25.11	.14
5	1	5	13.97	13.32	.13	-8	8	5	54.48	52.58	.14
7	1	5	29.23	29.21	.14	-6	8	5	.00	1.51	.00
-10	2	5	4.89	4.86	.13	-4	8	5	10.39	10.30	.13
-8	2	5	61.39	60.27	.12	-2	8	5	43.20	42.84	.13
-6	2	5	14.22	13.95	.11	0	8	5	7.19	6.79	.14
-4	2	5	19.85	19.33	.11	2	8	5	46.77	45.91	.14
-2	2	5	44.85	45.43	.11	-5	9	5	10.44	9.93	.14
0	2	5	15.24	15.28	.11	-3	9	5	39.62	39.93	.14
2	2	5	72.10	71.69	.12	-1	9	5	20.06	19.81	.14
4	2	5	14.77	13.40	.13	-8	0	6	21.51	21.21	.13
6	2	5	36.36	36.33	.14	-6	0	6	39.65	38.80	.13
-11	3	5	10.74	10.26	.14	-4	0	6	64.04	63.08	.12
-9	3	5	60.35	58.77	.13	-2	0	6	31.55	32.31	.12
-7	3	5	12.18	11.55	.12	0	0	6	35.98	35.70	.13
-5	3	5	42.90	42.88	.11	2	0	6	6.73	7.04	.13
-3	3	5	15.49	15.56	.11	4	0	6	73.80	73.45	.14
-1	3	5	85.79	88.27	.11	-9	1	6	8.86	9.04	.13
1	3	5	21.19	22.42	.12	-7	1	6	27.02	26.65	.13
3	3	5	14.19	14.15	.12	-5	1	6	22.24	21.98	.12
5	3	5	39.04	39.21	.13	-3	1	6	35.62	35.23	.12
-10	4	5	27.48	25.95	.14	-1	1	6	9.07	8.45	.12
-8	4	5	18.31	17.63	.13	1	1	6	14.51	14.60	.13
-6	4	5	16.32	16.18	.12	3	1	6	9.66	9.38	.13
-4	4	5	18.25	18.38	.12	-8	2	6	21.11	19.63	.13
-2	4	5	4.69	3.59	.11	-6	2	6	14.53	13.74	.13
0	4	5	21.32	21.28	.12	-4	2	6	8.10	8.09	.12
2	4	5	22.96	23.19	.12	-2	2	6	5.66	7.76	.12
4	4	5	43.67	42.39	.13	0	2	6	8.73	8.38	.13
6	4	5	3.04	2.01	.14	2	2	6	28.49	28.00	.13
-11	5	5	3.02	3.00	.14	4	2	6	3.36	2.35	.14
-9	5	5	6.94	6.57	.13	-9	3	6	7.52	7.10	.14
-7	5	5	4.74	5.10	.12	-7	3	6	18.94	18.45	.13
-5	5	5	11.79	12.03	.12	-5	3	6	16.15	16.09	.13
-3	5	5	4.17	4.69	.12	-3	3	6	2.71	2.21	.12

h	k	l	Frel	Fcalc	Sigf	h	k	l	Frel	Fcalc	Sigf
-1	3	6	28.20	26.54	.13	-2	6	6	2.44	.95	.13
1	3	6	15.92	15.76	.13	0	6	6	20.32	19.91	.14
3	3	6	5.59	5.33	.14	-5	7	6	20.59	19.67	.14
-8	4	6	6.07	6.32	.14	-3	7	6	22.97	21.75	.14
-6	4	6	19.30	18.22	.13	-1	7	6	24.34	23.07	.14
-4	4	6	13.10	13.33	.13	-5	1	7	11.56	10.70	.14
-2	4	6	.00	1.82	.00	-3	1	7	26.15	24.15	.14
0	4	6	32.20	31.23	.13	-1	1	7	7.50	6.87	.14
2	4	6	30.72	29.33	.14	1	1	7	19.74	19.62	.14
-9	5	6	19.32	17.38	.14	-6	2	7	9.77	8.88	.14
-7	5	6	31.06	29.61	.14	-4	2	7	26.79	24.84	.14
-5	5	6	4.61	4.51	.13	-2	2	7	21.36	20.59	.14
-3	5	6	79.76	78.62	.13	0	2	7	6.94	4.62	.14
-1	5	6	3.87	2.70	.13	-5	3	7	49.98	47.74	.14
1	5	6	32.33	31.75	.14	-3	3	7	20.38	19.85	.14
3	5	6	32.19	32.42	.14	-1	3	7	42.41	41.68	.14
-8	6	6	28.60	27.83	.14	-6	4	7	15.93	15.27	.14
-6	6	6	22.35	21.02	.14	-4	4	7	5.87	5.28	.14
-4	6	6	11.99	12.56	.14	-2	4	7	7.44	6.34	.14