

AM-86-318

Crystal-chemical aspects of nonstoichiometric pyroxenes

McCormick

To be deposited: Table 4

American Mineralogist, 71 ,11-12, 1434-1440

Table 4. Observed and calculated structure factors for final refinement cycle.

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
0	0	2	136.466	141.827	1	1	-1	24.031	22.477
0	0	4	103.168	105.159	1	1	0	13.089	10.138
0	0	6	37.801	38.159	1	1	1	6.754	6.179
0	0	8	40.864	41.253	1	1	2	75.550	74.404
0	2	0	50.131	48.682	1	1	3	13.534	13.375
0	2	1	40.707	38.098	1	1	4	3.770	3.240
0	2	2	61.675	60.086	1	1	5	1.518	1.021
0	2	3	10.681	10.572	1	1	6	26.597	26.474
0	2	4	13.979	13.279	1	1	7	11.230	10.991
0	2	5	8.508	8.118	1	3	-8	7.853	7.927
0	2	6	6.335	5.484	1	3	-7	45.314	45.643
0	2	7	2.461	1.398	1	3	-6	21.990	22.284
0	4	0	1.832	1.174	1	3	-5	81.702	82.969
0	4	1	91.361	91.446	1	3	-4	11.387	9.263
0	4	2	63.063	63.047	1	3	-3	108.220	110.012
0	4	3	33.168	33.073	1	3	-2	45.864	44.163
0	4	4	13.168	11.859	1	3	-1	71.387	70.834
0	4	5	17.094	15.832	1	3	0	3.246	3.856
0	4	6	37.277	37.340	1	3	1	22.173	21.338
0	4	7	16.545	16.725	1	3	2	37.461	35.873
0	6	0	97.644	98.723	1	3	3	13.560	14.227
0	6	1	38.508	38.231	1	3	4	7.277	7.241
0	6	2	99.476	101.777	1	3	5	12.120	11.888
0	6	3	31.832	31.256	1	3	6	10.105	10.112
0	6	4	24.974	23.753	1	3	7	3.455	1.653
0	6	5	19.319	19.107	1	5	-7	7.120	7.556
0	6	6	32.356	32.298	1	5	-6	1.440	.062
0	6	7	7.173	7.380	1	5	-5	6.754	6.782
0	8	0	.838	.499	1	5	-4	8.272	8.109
0	8	1	14.319	14.238	1	5	-3	14.110	14.260
0	8	2	19.398	18.698	1	5	-2	3.403	1.598
0	8	3	1.597	.212	1	5	-1	27.592	27.423
0	8	4	8.168	8.293	1	5	0	76.518	77.431
0	8	5	1.963	1.558	1	5	1	5.576	5.677
0	8	6	17.775	17.826	1	5	2	47.382	46.407
0	10	0	66.702	66.858	1	5	3	25.864	26.354
0	10	1	25.707	25.219	1	5	4	49.869	49.380
0	10	2	43.508	43.422	1	5	5	12.408	12.815
0	10	3	4.921	5.175	1	5	6	27.330	27.639
0	10	4	49.607	49.637	1	5	7	4.843	4.026
0	10	5	1.859	1.441	1	7	-7	26.361	27.307
0	12	0	44.162	43.738	1	7	-6	20.550	20.635
0	12	1	6.047	6.272	1	7	-5	32.435	32.643
0	12	2	20.445	19.842	1	7	-4	26.597	26.543
0	12	3	5.812	6.274	1	7	-3	58.639	58.506
0	12	4	15.209	14.712	1	7	-2	36.728	35.949
1	1	-8	12.487	13.009	1	7	-1	50.628	51.089
1	1	-7	1.911	1.418	1	7	0	19.450	19.220
1	1	-6	7.801	7.883	1	7	1	56.257	56.846
1	1	-5	6.230	6.232	1	7	2	5.654	5.526
1	1	-4	47.853	47.051	1	7	3	30.366	30.672
1	1	-3	16.885	16.041	1	7	4	9.215	8.866
1	1	-2	9.948	8.238	1	7	5	23.063	22.935

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
1	7	6	4.319	4.103	2	4	-7	2.199	2.119
1	9	-6	8.377	9.242	2	4	-6	10.157	10.025
1	9	-5	23.770	23.366	2	4	-5	5.157	4.465
1	9	-4	11.492	11.467	2	4	-4	15.733	15.964
1	9	-3	38.272	37.902	2	4	-3	52.147	52.096
1	9	-2	5.000	4.812	2	4	-2	17.173	15.856
1	9	-1	1.414	.467	2	4	-1	45.681	44.255
1	9	0	3.455	2.967	2	4	0	7.513	7.378
1	9	1	13.927	13.693	2	4	1	20.471	20.296
1	9	2	19.031	18.671	2	4	2	34.738	33.882
1	9	3	21.047	20.955	2	4	3	12.984	13.745
1	9	4	11.466	11.662	2	4	4	32.670	32.338
1	9	5	3.063	3.731	2	4	5	32.723	32.948
1	11	-5	4.686	4.465	2	4	6	28.194	28.479
1	11	-4	15.707	15.390	2	4	7	16.073	15.868
1	11	-3	13.796	14.099	2	6	-7	3.534	3.528
1	11	-2	7.042	6.982	2	6	-6	2.853	2.620
1	11	-1	2.984	2.986	2	6	-5	8.639	8.610
1	11	0	3.194	2.990	2	6	-4	21.466	21.336
1	11	1	12.958	13.060	2	6	-3	3.482	2.670
1	11	2	11.440	11.539	2	6	-2	60.340	61.009
1	11	3	10.314	10.602	2	6	-1	14.869	15.391
1	11	4	1.702	1.039	2	6	0	24.058	23.854
1	13	-3	22.199	22.581	2	6	1	1.152	1.493
1	13	-2	5.890	5.320	2	6	2	9.372	9.428
1	13	-1	32.147	32.541	2	6	3	12.487	12.266
1	13	0	16.126	15.713	2	6	4	13.743	13.764
1	13	1	19.241	18.690	2	6	5	3.874	4.007
1	13	2	24.581	23.849	2	6	6	19.267	19.099
2	0	-8	17.016	17.468	2	8	-6	15.183	15.709
2	0	-6	28.743	28.668	2	8	-5	30.105	30.436
2	0	-4	14.895	14.229	2	8	-4	21.623	21.850
2	0	-2	44.503	42.101	2	8	-3	48.534	48.397
2	0	0	6.859	8.022	2	8	-2	7.984	8.180
2	0	2	65.733	64.427	2	8	-1	79.869	80.544
2	0	4	7.513	6.487	2	8	0	21.623	22.227
2	0	6	2.461	2.380	2	8	1	58.246	58.849
2	2	-8	2.382	2.300	2	8	2	13.194	13.387
2	2	-7	15.759	16.366	2	8	3	68.377	69.079
2	2	-6	12.618	12.613	2	8	4	1.675	1.850
2	2	-5	38.403	38.112	2	8	5	51.073	51.554
2	2	-4	10.733	10.719	2	8	6	6.466	6.091
2	2	-3	103.927	105.236	2	10	-5	17.147	16.571
2	2	-2	15.471	14.284	2	10	-4	14.843	14.913
2	2	-1	124.005	131.632	2	10	-3	23.194	23.050
2	2	0	45.838	44.910	2	10	-2	14.005	13.913
2	2	1	93.115	97.121	2	10	-1	36.702	36.238
2	2	2	26.937	26.519	2	10	0	1.283	.185
2	2	3	79.764	81.223	2	10	1	5.000	4.140
2	2	4	45.681	45.910	2	10	2	3.796	3.229
2	2	5	74.450	76.078	2	10	3	14.398	14.256
2	2	6	31.440	31.879	2	10	4	10.785	10.608
2	2	7	44.319	44.978	2	10	5	9.869	9.748

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
2	12	-4	19.764	19.851	3	5	6	22.775	22.595
2	12	-3	34.058	34.080	3	7	-7	1.832	3.309
2	12	-2	25.445	25.557	3	7	-6	32.120	32.066
2	12	-1	28.168	27.585	3	7	-5	17.356	17.059
2	12	0	20.393	20.518	3	7	-4	9.031	8.719
2	12	1	42.670	42.214	3	7	-3	13.770	13.711
2	12	2	7.592	7.795	3	7	-2	13.534	13.278
2	12	3	23.770	23.363	3	7	-1	12.853	13.191
3	1	-8	35.366	35.667	3	7	0	15.105	14.657
3	1	-7	21.990	22.340	3	7	1	1.257	.866
3	1	-6	40.916	40.571	3	7	2	30.550	30.617
3	1	-5	45.524	45.187	3	7	3	8.508	8.545
3	1	-4	87.120	88.069	3	7	4	4.372	.190
3	1	-3	66.361	64.912	3	7	5	23.953	24.051
3	1	-2	6.335	6.157	3	7	6	1.152	.545
3	1	-1	73.927	73.599	3	9	-6	6.885	6.863
3	1	0	85.052	86.639	3	9	-5	31.178	31.182
3	1	1	69.634	69.876	3	9	-4	26.126	25.889
3	1	2	34.869	35.070	3	9	-3	12.801	12.823
3	1	3	30.838	30.039	3	9	-2	10.576	10.704
3	1	4	45.497	45.022	3	9	-1	6.518	6.513
3	1	5	1.859	.423	3	9	0	26.361	26.671
3	1	6	10.157	10.134	3	9	1	12.618	12.663
3	1	7	11.126	10.720	3	9	2	1.675	.295
3	3	-8	8.743	9.156	3	9	3	21.597	21.684
3	3	-7	17.565	17.804	3	9	4	13.141	12.817
3	3	-6	10.236	9.810	3	9	5	5.052	4.053
3	3	-5	18.770	18.933	3	11	-5	3.403	.776
3	3	-4	24.764	25.226	3	11	-4	45.864	45.569
3	3	-3	21.937	20.631	3	11	-3	9.293	9.237
3	3	-2	21.963	20.136	3	11	-2	29.738	29.762
3	3	-1	79.817	80.197	3	11	-1	7.592	7.809
3	3	0	52.644	53.325	3	11	0	40.864	40.901
3	3	1	26.911	25.903	3	11	1	5.209	5.350
3	3	2	8.770	7.705	3	11	2	22.984	23.046
3	3	3	5.262	4.705	3	11	3	1.099	1.127
3	3	4	23.691	24.089	3	11	4	17.984	18.157
3	3	5	17.513	17.208	3	13	-3	13.534	13.074
3	3	6	2.880	3.083	3	13	-2	3.063	3.272
3	3	7	23.010	23.066	3	13	-1	6.309	5.820
3	5	-7	7.958	7.129	3	13	0	8.874	9.050
3	5	-6	79.031	80.419	3	13	1	3.508	3.848
3	5	-5	16.204	16.496	3	13	2	10.288	10.915
3	5	-4	77.225	78.141	4	0	-8	2.277	1.611
3	5	-3	20.550	20.620	4	0	-6	48.246	48.169
3	5	-2	109.817	114.555	4	0	-4	54.869	53.263
3	5	-1	10.812	9.847	4	0	-2	85.209	84.150
3	5	0	67.801	71.541	4	0	0	5.654	4.856
3	5	1	24.188	23.789	4	0	2	104.895	109.870
3	5	2	100.576	105.685	4	0	4	70.812	71.709
3	5	3	9.555	9.240	4	0	6	62.120	63.765
3	5	4	37.068	36.587	4	2	-8	25.628	25.811
3	5	5	6.702	6.611	4	2	-7	31.937	32.225

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
4	2	-6	4.895	1.511	4	8	4	30.052	29.845
4	2	-5	23.953	24.092	4	8	5	10.157	10.148
4	2	-4	15.654	14.935	4	10	-5	7.225	6.891
4	2	-3	24.686	25.151	4	10	-4	19.136	19.290
4	2	-2	36.047	33.865	4	10	-3	4.948	5.051
4	2	-1	55.812	55.343	4	10	-2	47.853	48.111
4	2	0	16.806	16.366	4	10	-1	12.382	11.793
4	2	1	16.178	15.537	4	10	0	45.524	45.665
4	2	2	55.393	55.827	4	10	1	11.754	11.554
4	2	3	17.723	17.939	4	10	2	61.335	62.424
4	2	4	12.120	11.926	4	10	3	10.157	10.505
4	2	5	15.209	15.196	4	10	4	40.340	40.166
4	2	6	15.969	15.718	4	12	-4	3.063	3.160
4	2	7	1.152	.695	4	12	-3	11.152	10.823
4	4	-8	6.257	6.390	4	12	-2	4.529	3.613
4	4	-7	5.288	4.813	4	12	-1	13.351	12.919
4	4	-6	12.304	12.187	4	12	0	8.534	7.966
4	4	-5	10.602	10.181	4	12	1	6.440	5.476
4	4	-4	31.832	31.351	4	12	2	13.927	14.245
4	4	-3	18.272	17.527	5	1	-8	16.387	16.960
4	4	-2	15.550	15.740	5	1	-7	25.471	25.471
4	4	-1	9.869	9.998	5	1	-6	18.927	18.703
4	4	0	74.869	77.232	5	1	-5	29.738	29.146
4	4	1	20.052	19.498	5	1	-4	10.366	10.654
4	4	2	43.848	44.329	5	1	-3	32.251	31.705
4	4	3	38.560	38.574	5	1	-2	31.047	29.854
4	4	4	58.482	58.849	5	1	-1	31.361	30.610
4	4	5	32.094	31.794	5	1	0	60.209	59.773
4	4	6	15.759	15.633	5	1	1	19.188	18.875
4	6	-7	1.152	.917	5	1	2	35.497	35.044
4	6	-6	7.120	5.464	5	1	3	6.283	6.083
4	6	-5	5.995	5.672	5	1	4	2.251	.995
4	6	-4	38.770	37.645	5	1	5	8.377	8.278
4	6	-3	5.969	5.455	5	1	6	1.126	1.426
4	6	-2	2.435	2.181	5	3	-8	5.314	5.167
4	6	-1	20.838	20.791	5	3	-7	44.634	44.674
4	6	0	22.958	22.412	5	3	-6	11.440	11.574
4	6	1	12.984	12.699	5	3	-5	45.812	44.865
4	6	2	23.770	23.372	5	3	-4	19.791	18.904
4	6	3	16.571	16.324	5	3	-3	67.670	69.105
4	6	4	54.791	54.533	5	3	-2	24.791	23.658
4	6	5	10.733	10.974	5	3	-1	109.974	116.075
4	6	6	21.021	20.957	5	3	0	27.775	27.608
4	8	-6	2.068	.607	5	3	1	126.990	135.408
4	8	-5	16.545	16.116	5	3	2	20.105	19.713
4	8	-4	24.398	24.902	5	3	3	69.660	71.465
4	8	-3	18.351	18.405	5	3	4	19.398	19.205
4	8	-2	6.335	6.051	5	3	5	40.026	40.358
4	8	-1	11.832	11.004	5	3	6	8.665	8.031
4	8	0	27.696	27.833	5	5	-7	22.696	22.597
4	8	1	2.068	1.887	5	5	-6	8.089	8.111
4	8	2	16.492	16.672	5	5	-5	13.770	13.433
4	8	3	20.995	20.863	5	5	-4	1.832	1.688

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
5	5	-3	21.937	22.013	6	0	6	4.084	4.012
5	5	-2	1.099	2.378	6	2	-8	10.471	9.981
5	5	-1	16.597	16.286	6	2	-7	3.639	3.648
5	5	0	16.492	17.085	6	2	-6	16.387	16.426
5	5	1	21.728	21.657	6	2	-5	8.743	8.531
5	5	2	4.267	4.072	6	2	-4	8.639	7.595
5	5	3	9.372	9.341	6	2	-3	4.084	3.963
5	5	4	16.832	16.969	6	2	-2	36.545	34.872
5	5	5	4.188	4.273	6	2	-1	40.131	41.462
5	5	6	18.665	18.230	6	2	0	12.304	12.408
5	7	-7	35.000	35.435	6	2	1	65.916	67.583
5	7	-6	14.188	14.329	6	2	2	35.079	34.741
5	7	-5	59.005	59.884	6	2	3	53.770	53.835
5	7	-4	7.853	7.586	6	2	4	4.895	5.174
5	7	-3	58.325	58.815	6	2	5	30.497	30.475
5	7	-2	22.906	22.841	6	2	6	6.047	5.767
5	7	-1	74.974	76.297	6	4	-8	9.712	9.920
5	7	0	45.105	46.032	6	4	-7	11.754	11.485
5	7	1	47.801	48.552	6	4	-6	23.796	24.123
5	7	2	29.817	29.899	6	4	-5	16.675	16.872
5	7	3	38.063	37.849	6	4	-4	2.094	1.714
5	7	4	12.199	11.930	6	4	-3	38.822	39.165
5	7	5	14.188	14.127	6	4	-2	24.660	24.373
5	9	-6	3.037	2.233	6	4	-1	9.372	9.310
5	9	-5	15.995	16.507	6	4	0	20.654	19.819
5	9	-4	9.607	9.873	6	4	1	17.356	17.242
5	9	-3	9.843	9.338	6	4	2	6.518	6.434
5	9	-2	11.309	11.344	6	4	3	19.607	19.107
5	9	-1	45.052	45.063	6	4	4	5.864	5.816
5	9	0	9.267	9.416	6	4	5	3.796	4.094
5	9	1	37.277	37.226	6	4	6	7.644	6.797
5	9	2	13.168	13.004	6	6	-7	10.838	11.035
5	9	3	29.058	28.838	6	6	-6	35.445	35.502
5	9	4	9.319	9.364	6	6	-5	19.267	19.159
5	11	-5	9.712	9.589	6	6	-4	39.058	38.899
5	11	-4	17.984	18.021	6	6	-3	10.236	9.936
5	11	-3	4.398	5.152	6	6	-2	61.283	61.718
5	11	-2	21.204	20.981	6	6	-1	17.984	18.061
5	11	-1	12.435	12.400	6	6	0	2.016	1.799
5	11	0	22.539	22.525	6	6	1	4.424	4.463
5	11	1	2.592	1.104	6	6	2	5.916	5.936
5	11	2	12.513	12.735	6	6	3	3.220	2.777
5	11	3	1.204	1.122	6	6	4	17.330	17.166
5	13	-2	6.911	6.680	6	6	5	8.194	8.005
5	13	-1	30.602	30.651	6	8	-6	5.916	5.638
5	13	0	5.419	5.054	6	8	-5	3.482	2.512
6	0	-8	44.607	44.881	6	8	-4	3.037	2.325
6	0	-6	44.476	43.950	6	8	-3	14.424	14.057
6	0	-4	109.241	112.890	6	8	-2	16.649	17.191
6	0	-2	92.775	93.957	6	8	-1	23.037	22.589
6	0	0	72.853	72.098	6	8	0	6.597	7.039
6	0	2	4.686	5.072	6	8	1	46.257	47.155
6	0	4	16.466	16.058	6	8	2	11.178	11.274

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
6	8	3	31.492	31.847	7	5	1	11.152	11.485
6	8	4	10.393	10.755	7	5	2	46.152	46.128
6	10	-5	10.262	9.521	7	5	3	7.304	7.258
6	10	-4	31.963	32.048	7	5	4	57.801	59.061
6	10	-3	9.948	10.002	7	5	5	7.304	7.246
6	10	-2	17.644	17.615	7	7	-7	3.272	3.693
6	10	-1	7.461	6.995	7	7	-6	8.560	8.575
6	10	0	23.639	23.508	7	7	-5	4.686	4.221
6	10	1	18.743	18.985	7	7	-4	27.749	27.268
6	10	2	8.377	8.159	7	7	-3	3.639	3.308
6	10	3	9.869	9.486	7	7	-2	26.335	26.327
6	12	-3	2.539	1.550	7	7	-1	1.963	1.181
6	12	-2	11.152	11.019	7	7	0	39.712	40.545
6	12	-1	13.010	13.164	7	7	1	5.340	5.148
6	12	0	2.984	1.967	7	7	2	2.356	1.048
6	12	1	8.717	8.954	7	7	3	1.257	.061
7	1	-8	2.277	2.955	7	7	4	19.267	19.309
7	1	-7	9.948	10.141	7	9	-6	18.743	18.577
7	1	-6	29.188	28.815	7	9	-5	10.105	10.921
7	1	-5	12.461	11.957	7	9	-4	10.995	10.985
7	1	-4	28.796	27.954	7	9	-3	34.634	34.495
7	1	-3	23.482	22.859	7	9	-2	32.461	32.169
7	1	-2	99.948	103.381	7	9	-1	45.838	45.784
7	1	-1	23.508	23.088	7	9	0	20.000	19.870
7	1	0	42.592	43.706	7	9	1	27.644	27.815
7	1	1	13.115	12.869	7	9	2	34.319	34.185
7	1	2	54.005	54.431	7	9	3	18.508	18.604
7	1	3	14.817	14.783	7	11	-4	17.120	17.042
7	1	4	21.178	21.102	7	11	-3	9.503	9.724
7	1	5	21.440	21.194	7	11	-2	38.298	38.189
7	1	6	37.199	36.723	7	11	-1	11.283	10.754
7	3	-8	4.686	4.826	7	11	0	22.225	22.486
7	3	-7	17.094	15.954	7	11	1	19.607	19.917
7	3	-6	13.272	13.130	7	11	2	26.335	26.402
7	3	-5	6.649	6.461	8	0	-8	7.408	7.752
7	3	-4	14.634	14.146	8	0	-6	29.895	29.748
7	3	-3	33.115	33.305	8	0	-4	11.649	11.465
7	3	-2	21.623	21.183	8	0	-2	21.885	21.777
7	3	-1	48.717	48.723	8	0	0	57.827	60.069
7	3	0	20.681	20.696	8	0	2	26.754	26.699
7	3	1	19.450	19.576	8	0	4	35.105	35.153
7	3	2	13.351	13.017	8	2	-8	1.335	.171
7	3	3	4.607	4.631	8	2	-7	45.262	45.675
7	3	4	10.314	10.220	8	2	-6	16.545	16.185
7	3	5	9.267	8.478	8	2	-5	65.916	65.770
7	5	-7	1.152	.096	8	2	-4	12.277	12.914
7	5	-6	24.084	24.553	8	2	-3	66.099	65.845
7	5	-5	4.346	4.632	8	2	-2	23.534	22.350
7	5	-4	73.796	74.962	8	2	-1	42.199	41.445
7	5	-3	1.309	1.995	8	2	0	11.623	11.078
7	5	-2	73.560	75.321	8	2	1	45.105	44.720
7	5	-1	2.147	2.296	8	2	2	32.723	32.720
7	5	0	93.534	97.835	8	2	3	34.058	33.752

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
8	2	4	10.131	10.113	9	1	0	4.319	4.513
8	2	5	14.293	14.028	9	1	1	15.105	14.863
8	4	-7	26.073	25.858	9	1	2	24.005	24.188
8	4	-6	5.183	5.789	9	1	3	26.832	26.899
8	4	-5	34.660	34.190	9	1	4	21.126	21.055
8	4	-4	18.298	17.736	9	1	5	20.079	19.956
8	4	-3	26.728	26.966	9	3	-7	15.079	14.883
8	4	-2	2.147	2.154	9	3	-6	1.073	.268
8	4	-1	4.293	4.700	9	3	-5	53.325	53.603
8	4	0	15.393	15.266	9	3	-4	17.120	17.641
8	4	1	6.963	6.661	9	3	-3	65.812	65.789
8	4	2	3.455	3.451	9	3	-2	7.958	7.838
8	4	3	4.084	3.919	9	3	-1	55.942	56.011
8	4	4	6.204	6.323	9	3	0	23.272	23.515
8	4	5	2.749	3.704	9	3	1	44.738	44.597
8	6	-7	5.681	4.824	9	3	2	7.723	7.646
8	6	-6	28.901	29.213	9	3	3	52.723	52.665
8	6	-5	10.969	11.095	9	3	4	12.487	12.004
8	6	-4	32.356	33.240	9	5	-7	8.901	8.746
8	6	-3	2.906	1.966	9	5	-6	25.209	25.134
8	6	-2	5.524	5.417	9	5	-5	4.895	4.665
8	6	-1	7.304	7.350	9	5	-4	2.984	2.489
8	6	0	10.497	10.375	9	5	-3	1.990	1.380
8	6	1	10.759	10.684	9	5	-2	18.639	18.388
8	6	2	13.482	13.032	9	5	-1	2.775	2.907
8	6	3	6.806	7.484	9	5	0	6.728	6.372
8	6	4	5.052	4.578	9	5	1	4.162	3.861
8	8	-6	8.325	8.266	9	5	2	1.335	.200
8	8	-5	49.267	50.162	9	5	3	23.246	22.688
8	8	-4	3.796	3.199	9	5	4	15.838	15.702
8	8	-3	39.738	39.589	9	7	-6	3.351	2.245
8	8	-2	15.550	15.673	9	7	-5	10.838	11.260
8	8	-1	39.529	39.987	9	7	-4	25.916	26.503
8	8	0	2.958	2.893	9	7	-3	32.068	32.371
8	8	1	27.984	28.053	9	7	-2	9.581	9.506
8	8	2	1.073	.623	9	7	-1	30.550	30.702
8	8	3	31.859	31.164	9	7	0	10.995	10.820
8	10	-5	27.618	27.627	9	7	1	46.257	46.705
8	10	-4	3.639	2.824	9	7	2	11.649	11.415
8	10	-3	8.482	8.423	9	7	3	39.843	39.833
8	10	-2	2.435	1.507	9	9	-5	14.005	14.152
8	10	-1	4.110	4.871	9	9	-4	2.670	2.036
8	10	0	9.869	9.904	9	9	-3	29.162	29.199
8	10	1	2.094	2.072	9	9	-2	12.408	12.460
8	10	2	5.314	5.681	9	9	-1	8.796	8.244
9	-11	-3	6.361	6.269	9	9	0	6.387	7.054
9	1	-7	11.335	11.068	9	9	1	15.602	15.708
9	1	-6	3.377	3.310	9	9	2	8.534	8.659
9	1	-5	2.853	2.323	9	11	-2	6.414	6.499
9	1	-4	7.173	6.749	9	11	-1	9.241	9.006
9	1	-3	1.545	1.250	9	11	0	4.398	3.072
9	1	-2	17.827	17.754	10	0	-6	66.073	67.058
9	1	-1	5.236	4.718	10	0	-4	34.843	34.081

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
10	0	-2	68.508	68.198	11	1	-4	10.681	10.239
10	0	0	54.555	54.025	11	1	-3	1.859	.266
10	0	2	65.026	65.418	11	1	-2	6.728	6.635
10	0	4	17.539	17.550	11	1	-1	15.105	14.973
10	2	-7	14.869	15.250	11	1	0	34.005	33.686
10	2	-6	26.230	26.129	11	1	1	26.257	26.286
10	2	-5	10.864	10.561	11	1	2	25.471	25.020
10	2	-4	2.199	1.867	11	1	3	22.801	22.220
10	2	-3	2.696	1.284	11	3	-7	14.948	14.879
10	2	-2	35.000	34.867	11	3	-6	2.670	.520
10	2	-1	11.990	11.687	11	3	-5	20.079	19.668
10	2	0	11.230	10.949	11	3	-4	13.298	12.978
10	2	1	12.487	12.431	11	3	-3	39.293	39.354
10	2	2	22.147	22.304	11	3	-2	4.188	4.107
10	2	3	5.681	5.247	11	3	-1	27.670	27.290
10	2	4	14.921	14.713	11	3	0	14.267	14.274
10	4	-7	22.565	23.340	11	3	1	4.843	4.791
10	4	-6	21.440	21.434	11	3	2	3.796	3.030
10	4	-5	19.581	19.470	11	3	3	4.398	3.879
10	4	-4	49.581	50.088	11	5	-6	18.848	18.215
10	4	-3	11.021	11.068	11	5	-5	1.911	1.609
10	4	-2	30.602	30.320	11	5	-4	8.743	8.919
10	4	-1	25.340	24.925	11	5	-3	7.853	8.115
10	4	0	53.403	53.867	11	5	-2	30.471	30.366
10	4	1	27.277	27.370	11	5	-1	6.126	5.997
10	4	2	15.209	14.641	11	5	0	34.293	34.075
10	4	3	10.812	10.943	11	5	1	12.618	12.391
10	4	4	14.267	13.751	11	5	2	55.105	54.248
10	6	-6	24.634	24.501	11	5	3	12.173	11.665
10	6	-5	10.995	11.616	11	7	-5	21.126	21.900
10	6	-4	32.539	32.754	11	7	-4	11.073	11.294
10	6	-3	15.236	15.262	11	7	-3	12.199	11.993
10	6	-2	14.110	13.587	11	7	-2	3.272	3.775
10	6	-1	8.848	9.246	11	7	-1	7.042	7.448
10	6	0	46.230	46.438	11	7	0	1.152	2.000
10	6	1	8.560	8.106	11	7	1	8.010	7.991
10	6	2	20.340	19.728	11	7	2	18.665	18.215
10	6	3	7.173	6.874	11	9	-3	8.927	8.396
10	8	-5	9.241	10.105	11	9	-2	2.513	1.716
10	8	-4	15.733	15.883	11	9	-1	8.927	8.641
10	8	-3	9.162	9.343	11	9	0	9.869	9.566
10	8	-2	3.979	4.443	12	0	-6	12.147	11.201
10	8	-1	11.728	11.631	12	0	-4	4.346	4.783
10	8	0	28.089	28.274	12	0	-2	21.649	21.550
10	8	1	12.723	12.176	12	0	0	17.173	16.732
10	8	2	6.806	6.243	12	0	2	2.435	2.453
10	10	-3	4.843	4.790	12	2	-6	13.953	14.438
10	10	-2	49.921	50.181	12	2	-5	35.785	35.778
10	10	-1	1.754	.863	12	2	-4	16.178	16.203
10	10	0	33.796	34.003	12	2	-3	52.984	53.357
11	1	-7	8.901	8.973	12	2	-2	25.393	25.439
11	1	-6	2.016	.630	12	2	-1	62.749	62.726
11	1	-5	3.927	3.615	12	2	0	12.801	12.728

h	k	l	f(obs)	f(calc)	h	k	l	f(obs)	f(calc)
12	2	1	39.948	39.612	14	2	-4	15.026	15.252
12	2	2	1.178	1.084	14	2	-3	10.262	9.606
12	4	-6	9.686	9.928	14	2	-2	7.906	7.783
12	4	-5	11.702	11.789	14	2	-1	1.597	1.906
12	4	-4	18.272	18.889	14	2	0	4.921	3.922
12	4	-3	23.665	23.345	14	4	-4	8.613	8.654
12	4	-2	18.351	18.389	14	4	-3	20.707	20.510
12	4	-1	36.545	36.281	14	4	-2	23.665	23.324
12	4	0	12.565	12.667	14	4	-1	13.665	13.313
12	4	1	15.471	14.978	14	4	0	3.613	3.766
12	4	2	2.042	.160	15	1	-4	7.723	8.021
12	6	-5	2.723	1.045	15	1	-3	7.173	6.832
12	6	-4	9.293	9.533	15	1	-2	1.178	.076
12	6	-3	8.455	8.329					
12	6	-2	25.366	25.443					
12	6	-1	2.016	1.398					
12	6	0	27.147	26.355					
12	6	1	11.649	11.079					
12	8	-3	46.178	46.991					
12	8	-2	1.204	.453					
12	8	-1	40.288	40.679					
12	8	0	5.314	4.816					
13	1	-6	36.309	37.134					
13	1	-5	8.325	8.795					
13	1	-4	22.644	22.057					
13	1	-3	2.356	1.279					
13	1	-2	23.220	23.143					
13	1	-1	5.681	5.507					
13	1	0	7.775	7.543					
13	1	1	2.827	2.182					
13	1	2	12.277	12.621					
13	3	-6	7.147	7.295					
13	3	-5	21.099	20.744					
13	3	-4	9.398	9.063					
13	3	-3	6.806	6.386					
13	3	-2	9.110	9.287					
13	3	-1	15.733	14.941					
13	3	0	5.471	5.878					
13	3	1	22.277	21.594					
13	5	-5	3.429	3.107					
13	5	-4	44.764	45.265					
13	5	-3	6.859	6.911					
13	5	-2	15.183	15.129					
13	5	-1	9.817	9.607					
13	5	0	19.921	20.009					
13	5	1	5.916	6.005					
13	7	-3	6.754	6.544					
13	7	-2	2.644	2.814					
13	7	-1	17.932	17.563					
14	0	-4	58.822	58.956					
14	0	-2	43.639	43.418					
14	0	0	49.581	49.239					
14	2	-5	2.277	3.784					