

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	9	0	77.004	73.624	-73.824	0.0	3.179	2.689
-1	9	0	75.276	73.824	-73.824	0.0	2.452	2.088
-3	9	0	3.415	0.819	-0.819	0.0	2.596	1.068
-5	9	0	22.440	22.490	22.490	0.0	-0.049	-0.063
-7	9	0	90.969	92.366	-92.366	0.0	-1.397	-0.988
-9	9	0	30.758	31.669	31.669	0.0	-0.911	-1.049
-11	9	0	6.970	6.849	-6.849	0.0	0.122	0.047
-12	10	0	17.661	17.654	17.654	0.0	0.097	0.005
-10	10	0	22.151	21.719	21.719	0.0	0.432	0.408
-8	10	0	24.326	23.718	23.718	0.0	0.608	0.674
-6	10	0	15.726	14.755	14.755	0.0	0.971	0.877
-4	10	0	49.991	50.299	50.299	0.0	-0.308	-0.362
-2	10	0	37.679	37.865	37.865	0.0	-0.186	-0.268
0	10	0	86.347	86.240	86.240	0.0	0.107	0.081
0	12	0	207.446	211.538	211.538	0.0	-4.092	-1.320
2	10	0	37.274	37.865	37.865	0.0	-0.591	-0.851
4	10	0	50.388	50.299	50.299	0.0	0.089	0.103
6	10	0	13.165	14.755	14.755	0.0	-1.650	-1.232
8	10	0	23.730	23.718	23.718	0.0	0.012	0.014
10	10	0	23.863	21.719	21.719	0.0	2.144	2.294
12	10	0	12.502	17.654	17.654	0.0	-5.152	-2.343
11	11	0	56.572	53.800	53.800	0.0	2.772	2.640
9	11	0	9.674	7.307	7.307	0.0	2.367	1.396
7	11	0	131.740	131.634	131.634	0.0	0.106	0.053
5	11	0	37.836	38.011	-38.011	0.0	-0.175	-0.225
3	11	0	90.638	91.507	91.507	0.0	-1.269	-0.908
1	11	0	127.391	125.502	125.502	0.0	1.489	0.776
-1	11	0	126.457	125.502	125.502	0.0	0.554	0.290
-3	11	0	90.944	91.507	91.507	0.0	-0.963	-0.689
-5	11	0	36.646	38.011	-38.011	0.0	-1.366	-1.739
-7	11	0	130.078	131.634	131.634	0.0	-1.556	-0.787
-9	11	0	7.169	7.307	7.307	0.0	-0.139	-0.061
-11	11	0	56.060	53.800	53.800	0.0	2.259	2.152
-10	12	0	60.012	60.381	60.381	0.0	-0.369	-0.344
-8	12	0	41.912	41.447	41.447	0.0	0.466	0.536
0	12	0	208.223	211.538	211.538	0.0	-3.315	-1.063
-6	12	0	23.044	23.785	-23.785	0.0	-0.741	-0.854
-4	12	0	50.396	48.606	48.606	0.0	1.790	2.042
-2	12	0	46.030	44.832	-44.832	0.0	1.198	1.464
0	12	0	207.404	211.538	211.538	0.0	-4.133	-1.333
2	12	0	46.725	44.832	-44.832	0.0	1.893	2.312
4	12	0	50.875	48.606	48.606	0.0	2.270	2.590
6	12	0	23.459	23.785	-23.785	0.0	-0.287	-0.336
8	12	0	40.672	41.447	41.447	0.0	-0.774	-0.909
10	12	0	61.261	60.381	60.381	0.0	0.879	0.806
11	13	0	19.563	18.172	18.172	0.0	1.391	1.129
9	13	0	19.282	21.599	-21.599	0.0	-2.317	-1.796
7	13	0	47.948	47.920	47.920	0.0	0.029	0.031
5	13	0	68.016	67.833	-67.833	0.0	0.183	0.165
3	13	0	10.278	10.176	-10.176	0.0	0.101	0.068
1	13	0	13.519	14.262	14.262	0.0	-0.743	-0.656
-1	13	0	13.395	14.262	14.262	0.0	-0.867	-0.723
-3	13	0	10.567	10.176	-10.176	0.0	0.391	0.264

H	K	L	F(OBS)	F(CALC)	AL(CALC)	B(CALC)	DELTA F	CELTA/SIGMA
-5	13	0	67.917	67.833	-67.833	0.0	0.084	0.076 *
-7	13	0	47.494	47.920	47.920	0.0	-0.426	-0.477 *
-9	13	0	20.580	21.599	-21.599	0.0	-1.019	-0.880 *
0	12	0	206.561	211.538	211.538	0.0	-4.976	-1.609 *
-11	13	0	18.025	18.172	18.172	0.0	-0.147	-0.114 *
-6	14	0	4.639	6.873	-6.873	0.0	-2.234	-0.757 *
-4	14	0	2.464	4.163	4.163	0.0	-1.699	-0.448 *
-2	14	0	23.887	24.340	24.340	0.0	-0.453	-0.542 *
0	14	0	1.160	10.026	-10.026	0.0	0.434	0.282
2	14	0	23.623	24.340	24.340	0.0	-0.717	-0.842
6	14	0	1.836	6.873	-6.873	0.0	-5.037	-1.120
8	14	0	3.539	1.403	1.403	0.0	2.135	0.590
9	15	0	32.313	31.874	31.874	0.0	0.438	0.465
7	15	0	47.618	46.589	-46.589	0.0	0.629	0.679
5	15	0	37.902	38.052	38.052	0.0	-0.150	-0.179
3	15	0	7.392	3.124	3.124	0.0	4.268	2.435
1	15	0	5.540	0.304	-0.304	0.0	5.236	2.125
-1	15	0	9.219	0.304	-0.304	0.0	8.916	5.925 *
-5	15	0	38.026	38.052	38.052	0.0	-0.032	-0.032 *
0	12	0	207.404	211.538	211.538	0.0	-4.133	-1.333 *
-7	15	0	47.841	46.589	-46.589	0.0	0.852	0.945 *
-9	15	0	31.015	31.874	31.874	0.0	-0.860	-0.889 *
-10	16	0	27.616	27.629	-27.629	0.0	-0.013	-0.012 *
-8	16	0	6.391	2.513	-2.513	0.0	3.478	1.446 *
-6	16	0	24.144	26.544	26.544	0.0	-2.400	-2.481 *
-4	16	0	51.711	52.370	-52.370	0.0	-0.660	-0.712 *
-2	16	0	6.896	4.529	4.529	0.0	1.967	1.017 *
2	16	0	8.607	4.929	4.929	0.0	3.679	2.379
4	16	0	53.050	52.370	-52.370	0.0	0.680	0.734
6	16	0	24.268	26.544	26.544	0.0	-2.276	-2.480
10	16	0	29.518	27.629	-27.629	0.0	1.889	1.872
9	17	0	14.412	14.715	14.715	0.0	-0.304	-0.192
7	17	0	16.611	16.702	-16.702	0.0	-0.090	-0.070
3	17	0	25.574	26.248	26.248	0.0	-0.674	-0.815
1	17	0	13.238	14.137	-14.137	0.0	-0.900	-0.711
-1	17	0	14.379	14.137	-14.137	0.0	0.242	0.221 *
-3	17	0	25.243	26.248	26.248	0.0	-1.005	-1.253 *
0	12	0	207.380	211.538	211.538	0.0	-4.158	-1.341 *
-7	17	0	17.107	16.702	-16.702	0.0	0.406	0.356 *
-9	17	0	13.990	14.715	14.715	0.0	-0.725	-0.462 *
-8	18	0	9.715	7.837	-7.837	0.0	1.879	1.005 *
-6	18	0	18.604	18.783	18.783	0.0	-0.179	-0.155 *
-4	18	0	8.409	1.651	1.651	0.0	6.758	4.006 *
-2	18	0	16.892	16.936	16.936	0.0	-0.044	-0.039 *
0	18	0	14.734	14.204	14.204	0.0	0.531	0.465
2	18	0	16.413	16.536	16.536	0.0	-0.524	-0.456
6	18	0	18.066	18.783	18.783	0.0	-0.717	-0.615
8	18	0	12.138	7.837	-7.837	0.0	4.301	2.738
7	19	0	22.267	22.220	-22.220	0.0	0.046	0.040
5	19	0	6.317	7.236	7.236	0.0	-0.919	-0.348
3	19	0	25.095	23.801	-23.801	0.0	1.293	1.519
1	19	0	1.910	0.477	0.477	0.0	1.433	0.328
-1	19	0	3.481	0.477	0.477	0.0	3.004	0.886 *

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-3	19	0	26.186	23.801	-23.801	0.0	2.385	2.036 *
-5	19	0	8.235	7.236	7.236	0.0	0.999	0.483 *
-7	19	0	24.135	22.220	-22.220	0.0	1.915	1.914 *
0	12	0	207.644	211.538	211.538	0.0	-3.893	-1.252 *
-6	20	0	4.010	0.607	-0.807	0.0	3.203	0.883 *
-4	20	0	35.314	34.203	-34.203	0.0	1.111	1.317 *
-2	20	0	24.541	24.825	24.825	0.0	-0.284	-0.310 *
0	20	0	55.423	55.366	-55.366	0.0	0.057	0.057 *
2	20	0	23.788	24.825	24.825	0.0	-1.037	-1.045 *
4	20	0	34.603	34.203	-34.203	0.0	0.400	0.452 *
6	20	0	7.714	0.607	-0.807	0.0	6.908	3.060 *
7	21	0	5.813	7.573	-7.573	0.0	-1.760	-0.543 *
5	21	0	36.703	37.764	37.764	0.0	-1.061	-1.060 *
3	21	0	6.168	3.734	3.734	0.0	2.434	0.926 *
1	21	0	23.044	24.173	24.173	0.0	-1.129	-1.075 *
-1	21	0	26.145	24.173	24.173	0.0	1.972	2.272 *
-3	21	0	6.582	3.734	3.734	0.0	2.848	1.144 *
-5	21	0	38.142	37.764	37.764	0.0	0.378	0.354 *
-7	21	0	10.220	7.573	-7.573	0.0	2.647	1.339 *
-6	22	0	13.072	9.894	9.894	0.0	3.178	2.055 *
-4	22	0	40.110	39.865	39.865	0.0	0.245	0.265 *
-2	22	0	21.531	19.223	19.223	0.0	2.308	2.470 *
0	22	0	52.802	52.934	52.934	0.0	-0.132	-0.131 *
2	22	0	18.951	19.223	19.223	0.0	-0.272	-0.229 *
0	12	0	206.693	211.538	211.538	0.0	-4.844	-1.566 *
4	22	0	39.458	39.865	39.865	0.0	-0.367	-0.382 *
6	22	0	8.244	9.894	9.894	0.0	-1.651	-0.612 *
5	23	0	39.101	40.190	40.190	0.0	-1.089	-0.997 *
3	23	0	35.562	36.361	36.361	0.0	-0.799	-0.819 *
1	23	0	14.734	13.294	13.294	0.0	1.440	1.019 *
-1	23	0	14.478	13.294	13.294	0.0	1.184	0.813 *
-3	23	0	36.315	36.361	36.361	0.0	-0.046	-0.047 *
-5	24	0	42.417	40.190	40.190	0.0	2.227	2.447 *
-2	24	0	41.160	42.173	42.173	0.0	-1.013	-0.996 *
0	24	0	80.179	82.097	82.097	0.0	-1.919	-1.432 *
2	24	0	42.070	42.173	42.173	0.0	-0.103	-0.103 *
-1	24	0	4.655	3.452	3.452	0.0	1.203	0.354 *
2	24	1	13.428	11.392	11.392	0.0	2.036	1.383 *
0	23	1	18.215	17.743	17.743	0.0	0.472	0.391 *
-2	23	1	1.860	5.541	5.541	0.0	-4.081	-0.806 *
-4	23	1	9.219	10.886	10.886	0.0	-1.666	-0.720 *
-5	22	1	26.293	26.608	26.608	0.0	-0.314	-0.292 *
0	12	0	206.338	211.538	211.538	0.0	-5.200	-1.686 *
-3	22	1	18.754	16.567	16.567	0.0	1.827	1.567 *
-1	22	1	2.431	5.521	5.521	0.0	-3.090	-0.680 *
1	22	1	21.655	20.505	20.505	0.0	1.150	1.149 *
3	22	1	9.914	10.941	10.941	0.0	-1.027	-0.503 *
5	22	1	4.490	7.502	7.502	0.0	-3.012	-0.762 *
4	21	1	3.613	4.703	4.703	0.0	-1.090	-0.285 *
2	21	1	26.219	25.281	25.281	0.0	0.938	1.051 *
0	21	1	31.263	31.386	31.386	0.0	-0.123	-0.145 *
-2	21	1	38.390	37.537	37.537	0.0	0.453	0.512 *
-4	21	1	13.502	12.294	12.294	0.0	1.208	0.854 *

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-6	21	1	4.043	3.403	3.403	0.0	0.641	0.171
-7	20	1	15.404	15.318	15.318	0.0	0.086	0.057
-5	20	1	2.398	3.739	-3.739	0.0	-1.341	-0.305
-3	20	1	11.386	14.045	14.045	0.0	-2.659	-1.531
3	20	1	10.964	12.523	12.523	0.0	-1.559	-0.938
5	20	1	5.465	9.523	-9.523	0.0	-4.058	-1.268
7	20	1	18.976	17.049	17.049	0.0	1.927	1.653
0	12	0	207.173	211.538	211.538	0.0	-4.365	-1.408
6	19	1	28.691	28.488	28.488	0.0	0.203	0.217
4	19	1	14.858	13.416	-13.416	0.0	1.442	1.187
2	19	1	10.228	8.950	8.050	0.0	2.178	1.337
0	19	1	39.200	38.393	-38.393	0.0	0.803	0.940
-2	19	1	41.607	41.522	41.522	0.0	0.084	0.099
-4	19	1	10.873	11.662	-11.662	0.0	-0.789	-0.457
-6	19	1	0.661	6.669	-6.669	0.0	-6.008	-1.041
-8	19	1	5.358	1.555	-1.555	0.0	3.803	1.217
-9	18	1	33.942	35.824	35.824	0.0	-1.883	-1.822
-7	18	1	80.658	81.002	-81.002	0.0	-0.344	-0.262
-5	18	1	75.029	79.990	79.990	0.0	-0.960	-0.749
-3	18	1	5.556	3.044	3.044	0.0	2.513	1.003
-1	18	1	6.251	5.510	-5.510	0.0	0.741	0.309
1	18	1	23.069	23.751	-23.751	0.0	-0.682	-0.724
3	18	1	19.770	19.280	-19.280	0.0	0.490	0.485
5	18	1	72.613	72.912	72.912	0.0	-0.299	-0.249
7	18	1	42.731	42.507	-42.507	0.0	-0.176	-0.179
8	17	1	10.046	12.325	12.325	0.0	-2.279	-1.025
6	17	1	76.855	75.378	75.378	0.0	1.477	1.175
4	17	1	8.045	5.811	5.811	0.0	2.234	1.130
0	12	0	206.363	211.538	211.538	0.0	-5.175	-1.678
2	17	1	74.407	73.547	73.547	0.0	0.860	0.717
0	17	1	44.651	45.316	-45.316	0.0	-0.625	-0.727
-2	17	1	118.660	117.896	117.896	0.0	0.764	0.420
-4	17	1	19.207	19.847	19.847	0.0	-0.640	-0.629
-6	17	1	47.022	46.332	46.332	0.0	0.691	0.759
-8	17	1	12.593	14.530	14.530	0.0	-1.937	-1.171
-10	17	1	8.384	6.869	-6.869	0.0	1.515	0.623
-9	16	1	33.107	32.901	32.901	0.0	0.205	0.228
-7	16	1	21.581	20.244	20.244	0.0	1.337	1.382
-5	16	1	56.300	56.526	56.526	0.0	-0.227	-0.228
-3	16	1	45.509	45.320	45.320	0.0	0.189	0.222
-1	16	1	58.011	57.07	57.07	0.0	0.204	0.207
1	16	1	45.526	45.053	45.853	0.0	-0.328	-0.385
3	16	1	36.522	35.756	35.756	0.0	0.765	0.974
5	16	1	50.214	51.148	51.148	0.0	-0.934	-1.000
7	16	1	25.905	26.763	26.763	0.0	-0.858	-0.872
9	16	1	33.909	33.226	33.226	0.0	0.682	0.671
8	15	1	12.146	9.795	9.795	0.0	2.351	1.615
6	15	1	3.266	5.822	-5.822	0.0	-2.556	-0.684
4	15	1	3.919	1.107	1.107	0.0	2.813	0.927
0	12	0	205.412	211.538	211.538	0.0	-6.126	-1.992
2	15	1	22.647	22.587	-22.987	0.0	-0.340	-0.395
0	15	1	55.365	55.361	55.361	0.0	0.004	0.005
-2	15	1	55.506	54.679	-54.679	0.0	0.827	0.877

*

*

*

H	K	L	F(0BS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-4	15	1	17.851	17.677	17.677	0.0	0.174	0.177
-6	15	1	22.755	20.590	20.990	0.0	1.765	2.114
-8	15	1	8.516	11.493	-11.493	0.0	-2.976	-1.369
-10	15	1	10.832	12.950	12.850	0.0	-2.019	-1.001
-11	14	1	4.043	3.656	3.656	0.0	0.387	0.099
-9	14	1	28.997	25.751	-23.751	0.0	0.247	0.274
-7	14	1	27.046	27.601	27.601	0.0	-0.555	-0.605
-5	14	1	78.269	80.676	-80.676	0.0	-2.408	-1.929
-3	14	1	35.471	37.890	37.890	0.0	-2.419	-2.955
-1	14	1	34.479	35.884	-35.884	0.0	-1.404	-1.751
1	14	1	54.943	58.387	-58.387	0.0	-3.443	-3.521
3	14	1	19.315	21.213	21.213	0.0	-1.898	-1.929
5	14	1	44.831	44.168	-44.168	0.0	0.653	0.764
7	14	1	8.053	9.520	9.520	0.0	-1.467	-0.664
9	14	1	36.505	35.654	-35.654	0.0	0.851	0.927
10	13	1	3.754	4.710	-4.710	0.0	-0.957	-0.231
8	13	1	11.791	13.619	13.619	0.0	-1.829	-1.074
0	12	0	204.916	211.538	211.538	0.0	-6.522	-2.159
6	13	1	4.176	3.637	-3.637	0.0	0.539	0.176
4	13	1	17.223	13.355	18.355	0.0	-1.132	-1.037
2	13	1	23.606	24.300	-24.300	0.0	-0.694	-0.791
0	13	1	43.161	43.281	43.281	0.0	-0.120	-0.147
-2	13	1	35.926	35.451	-35.451	0.0	0.475	0.624
-4	13	1	36.546	36.160	36.160	0.0	0.386	0.481
-8	13	1	4.878	4.384	-4.384	0.0	0.495	0.169
-10	13	1	3.307	4.084	4.084	0.0	-0.776	-0.192
-11	12	1	10.063	9.678	9.678	0.0	0.384	0.155
-7	12	1	10.319	13.243	13.243	0.0	-2.924	-1.700
-5	12	1	15.032	13.836	13.836	0.0	1.196	0.991
-3	12	1	6.921	10.520	10.520	0.0	-3.600	-1.637
-1	12	1	18.075	18.571	18.571	0.0	-0.496	-0.561
1	12	1	19.795	20.160	20.160	0.0	-0.365	-0.438
3	12	1	6.284	8.400	8.400	0.0	-2.116	-0.914
5	12	1	12.171	10.554	10.554	0.0	1.617	1.286
7	12	1	10.129	10.877	10.877	0.0	-0.748	-0.437
9	12	1	6.730	5.860	5.860	0.0	0.870	0.343
0	12	0	205.031	211.538	211.538	0.0	-6.506	-2.121
10	11	1	8.979	10.140	-10.140	0.0	-1.161	-0.509
6	11	1	8.889	9.013	-9.013	0.0	-0.125	-0.074
4	11	1	2.274	6.506	-6.506	0.0	-4.633	-1.105
2	11	1	45.600	46.175	-46.175	0.0	-0.575	-0.703
0	11	1	6.292	2.783	2.783	0.0	3.509	1.947
-2	11	1	24.598	23.872	-23.872	0.0	0.726	0.965
-4	11	1	6.888	11.158	-11.158	0.0	-4.270	-1.971
-6	11	1	11.344	12.283	-12.283	0.0	-0.938	-0.630
-8	11	1	11.964	11.742	11.742	0.0	0.222	0.163
-10	11	1	5.459	10.764	-10.764	0.0	-1.305	-0.692
-11	10	1	18.910	17.610	-17.610	0.0	1.300	1.123
-9	10	1	19.952	21.170	-21.170	0.0	-1.218	-1.116
-7	10	1	21.440	20.874	20.874	0.0	0.566	0.658
-5	10	1	32.123	32.528	-32.528	0.0	-0.405	-0.522
-3	10	1	55.555	54.651	54.651	0.0	0.704	0.774
-1	10	1	37.613	37.648	-37.648	0.0	-0.035	-0.050

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	10	1	8.789	11.667	-11.667	0.0	-2.878	-2.047
3	10	1	50.371	49.665	49.665	0.0	0.706	0.829
0	12	0	204.618	211.538	211.538	0.0	-6.920	-2.262 *
5	10	1	39.630	39.297	-39.297	0.0	0.334	0.408
7	10	1	21.523	21.219	21.219	0.0	0.304	0.328
9	10	1	15.387	14.560	-14.560	0.0	0.828	0.667
11	10	1	14.370	17.283	17.283	0.0	-2.912	-1.512
10	9	1	23.259	22.583	22.583	0.0	0.676	0.659
8	9	1	4.308	0.728	0.728	0.0	3.580	1.203
4	9	1	33.694	33.553	33.553	0.0	0.141	0.190
2	9	1	53.546	53.505	-53.505	0.0	0.041	0.047
0	9	1	58.195	58.771	98.771	0.0	-0.576	-0.387
-2	9	1	52.694	51.482	-51.482	0.0	1.213	1.410
-4	9	1	25.588	24.808	24.808	0.0	1.180	1.719
-6	9	1	18.918	20.397	20.397	0.0	-1.479	-1.454
-8	9	1	5.881	3.701	-3.701	0.0	6.180	4.397
-10	9	1	13.014	14.542	14.542	0.0	-1.528	-0.983
-12	9	1	26.566	25.543	-25.543	0.0	0.623	0.589
-11	8	1	12.932	13.796	-13.796	0.0	-0.864	-0.559
-9	8	1	12.866	11.554	-11.554	0.0	1.312	0.928
-7	8	1	9.170	6.663	6.663	0.0	2.506	1.443
-5	8	1	14.951	17.255	-17.255	0.0	-2.264	-2.059
0	12	0	204.750	211.538	211.538	0.0	-6.787	-2.213 *
-3	8	1	6.780	3.039	3.039	0.0	3.741	2.528
-1	8	1	11.179	10.561	-10.561	0.0	0.518	0.712
1	8	1	10.046	10.514	-10.514	0.0	-0.468	-0.472
3	8	1	8.541	8.270	-8.270	0.0	0.271	0.193
5	8	1	20.572	20.491	-20.491	0.0	0.081	0.091
7	8	1	15.611	15.871	15.871	0.0	-0.260	-0.246
11	8	1	12.328	12.265	-12.265	0.0	0.063	0.035
12	7	1	20.514	20.453	20.453	0.0	0.061	0.047
10	7	1	29.229	29.460	-29.460	0.0	-0.231	-0.243
6	7	1	59.524	60.960	60.960	0.0	-1.436	-1.435
4	7	1	47.047	47.279	-47.279	0.0	-0.232	-0.286
2	7	1	28.245	28.142	28.142	0.0	0.103	0.174
0	7	1	129.351	130.546	-130.546	0.0	-1.195	-0.615
-2	7	1	76.813	76.675	76.675	0.0	0.139	0.118
-4	7	1	10.542	6.266	6.266	0.0	4.276	4.274
-6	7	1	32.809	32.843	32.843	0.0	-0.034	-0.046
-8	7	1	17.066	19.549	-19.549	0.0	-2.483	-2.241
-10	7	1	22.639	21.145	-21.145	0.0	1.494	1.531
0	12	0	204.552	211.538	211.538	0.0	-6.985	-2.283 *
-12	7	1	49.404	50.440	50.440	0.0	-1.037	-1.036
-13	6	1	42.425	42.074	42.074	0.0	0.352	0.357
-11	6	1	10.079	4.538	4.538	0.0	5.541	3.419
-9	6	1	101.131	102.820	102.820	0.0	-1.690	-1.081
-7	6	1	98.253	101.527	-101.527	0.0	-3.273	-2.163
-5	6	1	189.412	200.536	200.536	0.0	-11.124	-3.922 *
-3	6	1	160.175	159.134	159.134	0.0	1.042	0.434
-1	6	1	126.779	130.333	130.333	0.0	-3.554	-1.869
1	6	1	52.909	43.516	-43.516	0.0	9.394	11.248
3	6	1	52.893	52.167	52.167	0.0	0.726	0.853
5	6	1	233.210	246.147	246.147	0.0	-12.937	-3.708 *

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
7	6	1	41.168	41.415	-41.415	0.0	-0.247	-0.299
9	6	1	74.606	75.091	75.091	0.0	-0.485	-0.399
11	6	1	22.531	19.814	-19.814	0.0	2.717	2.693
12	5	1	48.254	46.654	46.654	0.0	1.600	1.613
10	5	1	13.618	13.413	-13.413	0.0	0.205	0.146
8	5	1	39.333	39.038	39.038	0.0	0.295	0.368
6	5	1	135.759	139.713	139.713	0.0	-3.954	-1.928
4	5	1	25.045	24.755	24.755	0.0	0.290	0.434
2	5	1	127.135	133.340	133.340	0.0	-6.205	-3.249
0	12	0	204.188	211.538	211.538	0.0	-7.350	-2.402
0	5	1	73.862	71.513	-71.513	0.0	1.949	1.733
-2	5	1	211.332	220.143	220.143	0.0	-8.811	-2.757
-4	5	1	96.434	96.599	96.599	0.0	-0.164	-0.112
-6	5	1	91.341	95.252	95.252	0.0	-3.911	-2.783
-8	5	1	21.663	20.368	20.368	0.0	1.295	1.437
-10	5	1	6.888	3.876	3.876	0.0	3.011	1.401
-12	5	1	77.450	76.592	76.592	0.0	0.859	0.670
-13	4	1	18.405	19.771	19.771	0.0	-1.365	-0.933
-11	4	1	12.163	12.808	-12.808	0.0	-0.645	-0.411
-7	4	1	11.056	10.687	10.687	0.0	0.410	0.290
-5	4	1	20.322	19.809	19.809	0.0	0.515	0.788
-3	4	1	6.524	5.322	5.322	0.0	1.202	1.038
-1	4	1	10.592	10.247	10.247	0.0	0.345	0.409
1	4	1	9.693	4.642	4.642	0.0	5.056	6.115
3	4	1	6.003	0.549	0.549	0.0	5.453	4.487
5	4	1	8.715	4.158	4.158	0.0	4.557	3.281
7	4	1	15.197	14.554	14.554	0.0	0.644	0.560
9	4	1	16.793	16.996	16.996	0.0	-0.203	-0.167
11	4	1	15.627	14.638	-14.638	0.0	0.989	0.708
0	12	0	204.430	211.538	211.538	0.0	-7.110	-2.324
12	3	1	31.676	29.635	-29.635	0.0	2.041	2.165
10	3	1	9.327	11.814	11.814	0.0	-2.488	-1.223
8	3	1	10.559	12.578	-12.578	0.0	-2.020	-1.234
6	3	1	27.873	28.812	-28.812	0.0	-0.939	-1.248
4	3	1	23.150	23.134	-23.134	0.0	0.025	0.040
2	3	1	113.079	118.256	-118.256	0.0	-5.178	-3.055
-2	3	1	141.662	143.390	-143.390	0.0	-1.727	-0.816
-4	3	1	20.332	19.150	-19.150	0.0	1.182	2.166
-6	3	1	1.406	2.117	-2.117	0.0	-0.712	-0.177
-8	3	1	24.921	23.087	-23.087	0.0	1.834	2.175
-10	3	1	12.080	8.710	8.710	0.0	3.370	2.516
-12	3	1	39.738	38.477	-38.477	0.0	1.261	1.425
-13	2	1	16.413	17.188	-17.188	0.0	-0.775	-0.515
-11	2	1	21.093	20.546	20.546	0.0	0.546	0.565
-9	2	1	26.310	27.055	-27.055	0.0	-0.745	-0.901
-7	2	1	46.038	47.368	47.368	0.0	-1.330	-1.608
-5	2	1	50.247	50.584	-50.584	0.0	-0.337	-0.412
-3	2	1	124.729	128.578	-128.578	0.0	-3.849	-2.060
1	2	1	11.336	6.975	-6.975	0.0	4.361	5.926
3	2	1	105.331	107.192	107.192	0.0	-1.861	-1.172
0	12	0	204.155	211.538	211.538	0.0	-7.383	-2.413
5	2	1	31.081	30.305	-30.305	0.0	0.776	1.104
7	2	1	40.499	40.306	40.306	0.0	0.193	0.236

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
9	2	1	22.399	23.245	-23.245	0.0	-0.846	-0.874
11	2	1	32.098	30.156	30.156	0.0	1.942	2.135
12	1	1	7.896	1.202	1.202	0.0	6.694	2.735
8	1	1	13.287	14.816	14.816	0.0	-1.528	-1.257
6	1	1	5.317	4.202	-4.202	0.0	1.115	0.475
4	1	1	12.354	12.018	12.018	0.0	0.376	0.446
2	1	1	49.428	50.894	-50.894	0.0	-1.465	-1.885
-4	1	1	22.937	24.040	24.040	0.0	-1.104	-1.963
-6	1	1	4.085	6.633	6.633	0.0	-2.549	-1.056
-10	1	1	6.582	4.655	-4.655	0.0	1.727	0.754
-12	1	1	7.160	1.439	1.439	0.0	5.722	2.621
-13	0	1	16.611	15.362	-15.362	0.0	1.249	0.904
-9	0	1	6.896	8.895	-8.895	0.0	-1.999	-0.905
-7	0	1	6.921	7.069	-7.069	0.0	-0.149	-0.075
-5	0	1	7.797	9.492	-9.492	0.0	-1.695	-1.358
0	12	0	204.907	211.538	211.538	0.0	-6.630	-2.161
-3	0	1	19.464	18.612	-18.612	0.0	0.852	1.451
3	0	1	30.841	31.844	-31.844	0.0	-1.003	-1.733
9	0	1	8.211	6.334	-6.334	0.0	1.877	1.000
11	0	1	2.414	0.112	-0.112	0.0	2.303	0.507
-12	0	2	50.437	49.697	-49.697	0.0	0.740	0.772
-10	0	2	82.502	83.118	83.118	0.0	-0.616	-0.469
-8	0	2	64.502	66.757	66.757	0.0	-2.256	-2.131
-6	0	2	105.207	107.677	107.677	0.0	-2.470	-1.548
-4	0	2	155.628	163.557	163.557	0.0	-7.929	-3.401
-2	0	2	110.821	108.273	-108.273	0.0	2.548	1.525
0	0	2	247.705	271.635	271.635	0.0	-23.930	-6.475
2	0	2	127.523	127.751	127.751	0.0	-0.228	-0.119
4	0	2	193.017	202.349	202.349	0.0	-9.331	-3.224
6	0	2	44.410	45.468	-45.468	0.0	-1.058	-1.255
8	0	2	50.958	50.665	50.665	0.0	-0.567	-0.612
10	0	2	86.132	85.432	85.432	0.0	0.700	0.501
11	1	2	53.836	52.768	52.768	0.0	1.068	1.025
9	1	2	27.236	27.338	-27.338	0.0	-0.102	-0.109
0	12	0	204.544	211.538	211.538	0.0	-6.994	-2.286
7	1	2	61.856	62.435	62.435	0.0	-0.579	-0.560
5	1	2	43.748	44.334	-44.334	0.0	-0.586	-0.723
3	1	2	78.650	80.719	80.719	0.0	-2.029	-1.669
1	1	2	116.923	115.926	115.926	0.0	0.998	0.567
-1	1	2	7.086	4.621	-4.621	0.0	2.465	2.225
-5	1	2	23.838	23.748	-23.748	0.0	0.090	0.139
-7	1	2	164.086	171.377	171.377	0.0	-7.291	-2.959
-9	1	2	29.576	30.103	-30.103	0.0	-0.527	-0.685
-11	1	2	23.821	25.686	25.686	0.0	-1.865	-1.880
-13	1	2	9.930	6.255	6.255	0.0	3.676	1.771
-12	2	2	6.995	0.415	-0.415	0.0	6.580	2.842
-10	2	2	2.786	0.922	-0.922	0.0	1.864	0.477
-8	2	2	3.679	6.070	6.070	0.0	-2.390	-0.657
-6	2	2	26.872	27.295	-27.295	0.0	-0.423	-0.568
-4	2	2	18.687	18.541	-18.541	0.0	-0.254	-0.389
-2	2	2	20.605	20.533	-20.533	0.0	-0.328	-0.592
0	2	2	30.428	29.979	-29.979	0.0	0.449	0.775
2	2	2	10.112	9.127	-9.127	0.0	0.986	1.010

H	K	L	F(I OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
4	2	2	9.500	6.548	6.948	0.0	2.552	1.816
0	12	0	205.156	211.538	211.538	0.0	-6.382	-2.080 *
6	2	2	14.023	12.205	-12.205	0.0	1.818	1.516
8	2	2	15.975	14.823	-14.823	0.0	1.152	1.017
10	2	2	14.858	14.131	-14.131	0.0	0.727	0.523
11	3	2	16.314	16.517	-16.517	0.0	-0.204	-0.138
9	3	2	33.437	32.557	32.557	0.0	0.880	1.054
7	3	2	65.684	67.349	-67.349	0.0	-1.665	-1.525
5	3	2	47.866	49.879	49.879	0.0	-2.013	-2.257
1	3	2	71.513	69.379	-69.379	0.0	2.134	1.941
-1	3	2	6.524	5.985	5.985	0.0	0.539	0.432
-3	3	2	24.499	20.478	20.478	0.0	4.022	7.259
-5	3	2	21.738	23.033	23.033	0.0	-1.296	-1.844
-7	3	2	85.860	88.268	-88.268	0.0	-1.408	-1.045
-9	3	2	61.732	61.505	61.505	0.0	0.227	0.223
-11	3	2	6.243	8.957	-8.957	0.0	-2.714	-1.004
-13	3	2	15.075	18.748	-18.748	0.0	0.328	0.242
-12	4	2	44.864	44.302	44.302	0.0	0.562	0.591
-10	4	2	44.368	44.479	-44.479	0.0	-0.111	-0.127
-8	4	2	13.494	8.663	8.663	0.0	4.831	4.173
-6	4	2	80.212	81.193	81.193	0.0	-0.982	-0.786
0	12	0	205.189	211.538	211.538	0.0	-6.349	-2.070 *
-4	4	2	71.654	70.480	-70.480	0.0	1.174	1.060
0	4	2	11.601	12.356	12.356	0.0	-0.756	-1.004
2	4	2	83.808	78.340	78.340	0.0	5.469	4.295
2	4	2	76.772	79.421	79.421	0.0	-2.649	-2.240
4	4	2	80.493	81.540	-81.540	0.0	-1.448	-1.159
6	4	2	69.082	70.417	70.417	0.0	-1.334	-1.155
8	4	2	19.704	19.585	19.585	0.0	0.119	0.117
10	4	2	31.635	32.342	-32.342	0.0	-0.707	-0.744
11	5	2	6.019	6.793	-6.793	0.0	-0.773	-0.242
9	5	2	17.372	14.810	14.810	0.0	2.562	2.262
7	5	2	43.442	42.721	-42.721	0.0	0.721	0.847
5	5	2	7.731	5.977	-5.977	0.0	1.754	0.930
3	5	2	28.625	26.756	26.756	0.0	1.869	2.791
1	5	2	74.449	73.478	-73.478	0.0	0.971	0.844
-1	5	2	48.238	46.786	-46.786	0.0	1.451	1.868
-3	5	2	38.241	35.054	35.054	0.0	3.187	4.701
-5	5	2	17.843	17.328	-17.328	0.0	0.516	0.594
-7	5	2	42.938	43.749	-43.749	0.0	-0.812	-1.002
-9	5	2	39.688	39.025	39.025	0.0	0.664	0.819
-11	5	2	11.121	12.224	-12.224	0.0	-1.103	-0.630
0	12	0	204.742	211.538	211.538	0.0	-6.796	-2.215 *
-12	6	2	3.324	1.687	-1.687	0.0	1.637	0.405
-10	6	2	13.585	14.724	14.724	0.0	-1.139	-0.820
-8	6	2	18.513	18.427	-18.427	0.0	0.086	0.089
-6	6	2	16.008	14.746	14.746	0.0	1.262	1.293
-4	6	2	10.542	11.607	-11.607	0.0	-1.065	-0.937
-2	6	2	8.343	6.193	-6.193	0.0	2.149	1.870
2	6	2	4.035	5.224	5.224	0.0	-1.189	-0.510
4	6	2	6.408	2.033	2.033	0.0	4.375	2.108
6	6	2	14.470	14.419	14.419	0.0	0.051	0.043
8	6	2	21.349	22.702	-22.702	0.0	-1.353	-1.352

H	K	L	F(0BS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
10	6	2	9.550	8.582	8.582	0.0	0.968	0.482
11	7	2	9.955	12.617	-12.617	0.0	-2.662	-1.032
9	7	2	13.692	16.446	16.446	0.0	-2.754	-1.699
7	7	2	5.159	2.380	-2.380	0.0	2.779	1.106
5	7	2	25.334	23.762	23.762	0.0	1.573	1.865
3	7	2	7.483	7.378	-7.378	0.0	0.105	0.057
1	7	2	31.271	32.241	32.241	0.0	-0.970	-1.431
-1	7	2	43.111	41.871	41.871	0.0	1.241	1.686
0	12	0	204.858	211.538	211.538	0.0	-6.680	-2.178
-3	7	2	33.421	33.601	-33.601	0.0	0.420	0.605
-5	7	2	37.324	37.563	37.563	0.0	-0.240	-0.318
-7	7	2	4.763	4.231	4.231	0.0	0.532	0.181
-9	7	2	22.101	21.328	21.328	0.0	0.773	0.858
-11	7	2	15.908	18.710	-18.710	0.0	-2.802	-1.893
-13	7	2	19.902	19.501	19.501	0.0	0.401	0.311
-12	8	2	19.803	19.896	19.896	0.0	-0.093	-0.070
-10	8	2	17.000	15.745	-15.745	0.0	1.255	1.159
-6	8	2	21.961	21.569	-21.569	0.0	-0.008	-0.009
-4	8	2	23.465	22.509	-22.509	0.0	0.557	0.702
-2	8	2	54.869	52.708	52.708	0.0	2.161	2.420
0	8	2	97.021	55.528	-95.528	0.0	1.494	1.009
2	8	2	75.127	75.652	75.652	0.0	-0.535	-0.456
4	8	2	38.076	37.633	-37.633	0.0	0.443	0.553
6	8	2	2.423	4.696	4.695	0.0	-2.273	-0.581
8	8	2	5.867	1.505	-1.505	0.0	4.383	1.779
10	8	2	13.064	11.312	-11.312	0.0	1.752	1.127
9	9	2	8.806	2.646	2.646	0.0	6.760	3.539
7	9	2	34.148	35.716	-35.716	0.0	-1.567	-1.739
0	12	0	205.420	211.538	211.538	0.0	-6.118	-1.989
5	9	2	28.931	28.855	28.855	0.0	0.076	0.098
3	9	2	72.787	74.387	-74.387	0.0	-1.603	-1.382
1	9	2	27.418	26.362	-26.362	0.0	1.056	1.420
-1	9	2	16.041	14.720	14.720	0.0	1.320	1.426
-3	9	2	75.848	80.592	-80.592	0.0	-0.744	-0.600
-5	9	2	22.250	22.563	22.563	0.0	-0.713	-0.798
-7	9	2	44.145	44.127	-44.127	0.0	0.018	0.022
-9	9	2	17.521	17.169	17.169	0.0	0.361	0.333
-11	9	2	11.981	9.013	-9.013	0.0	2.968	1.951
-10	10	2	27.352	26.059	26.059	0.0	1.293	1.408
-8	10	2	34.456	34.826	-34.826	0.0	-0.330	-0.392
-6	10	2	15.751	16.287	16.287	0.0	-0.536	-0.450
-4	10	2	44.451	45.118	45.118	0.0	-0.667	-0.824
-2	10	2	25.723	26.244	26.244	0.0	-0.521	-0.692
0	10	2	51.082	51.793	51.793	0.0	-0.711	-0.811
2	10	2	33.727	34.145	34.145	0.0	-0.418	-0.549
4	10	2	58.978	59.894	59.894	0.0	-0.915	-0.930
6	10	2	13.668	13.246	13.246	0.0	0.421	0.333
8	10	2	13.651	13.666	13.666	0.0	0.586	0.391
0	12	0	204.874	211.538	211.538	0.0	-6.663	-2.172
10	10	2	5.374	8.890	8.890	0.0	-3.516	-1.000
9	11	2	5.657	2.225	2.225	0.0	3.472	1.173
7	11	2	55.134	54.903	54.903	0.0	0.231	0.235
5	11	2	11.559	12.413	-12.413	0.0	-0.853	-0.597

*

*

*

H	%	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
3	11	2	145.433	148.345	148.345	0.0	-2.912	-1.324
1	11	2	87.157	86.236	86.236	0.0	0.921	0.683
-1	11	2	15.966	15.740	15.740	0.0	0.226	0.217
-3	11	2	119.379	120.429	120.429	0.0	-1.049	-0.580
-5	11	2	13.395	12.826	-12.826	0.0	0.569	0.453
-7	11	2	132.261	134.858	134.858	0.0	-2.596	-1.292
-9	11	2	5.589	8.486	8.486	0.0	-2.897	-1.033
-11	11	2	36.985	36.639	36.639	0.0	0.346	0.373
-12	12	2	26.930	28.361	-28.361	0.0	-1.431	-1.210
-10	12	2	16.562	17.226	17.226	0.0	-0.664	-0.515
-8	12	2	20.539	18.210	18.210	0.0	2.329	2.428
-6	12	2	87.157	89.242	89.242	0.0	-2.084	-1.528
-4	12	2	30.535	28.804	28.804	0.0	1.732	2.094
-2	12	2	137.123	139.532	-139.532	0.0	-2.409	-1.161
0	12	2	195.167	198.545	198.545	0.0	-3.377	-1.154
2	12	2	7.359	6.532	-6.532	0.0	0.827	0.380
0	12	0	204.453	211.538	211.538	0.0	-7.085	-2.316
4	12	2	54.141	53.654	53.654	0.0	0.488	0.518
6	12	2	24.632	24.278	-24.278	0.0	0.353	0.365
8	12	2	23.433	23.496	23.496	0.0	-0.064	-0.062
9	13	2	17.711	16.712	-16.712	0.0	0.998	0.755
5	13	2	42.177	42.521	-42.921	0.0	-0.744	-0.865
3	13	2	52.612	54.192	54.192	0.0	-1.580	-1.706
1	13	2	12.618	13.612	-13.612	0.0	-0.995	-0.720
-1	13	2	52.488	53.258	-53.258	0.0	-0.770	-0.839
-3	13	2	34.144	34.671	34.671	0.0	0.073	0.092
-5	13	2	52.653	52.783	-52.783	0.0	-0.130	-0.142
-7	13	2	43.111	43.272	43.272	0.0	-0.160	-0.186
-9	13	2	10.451	10.340	-10.340	0.0	0.111	0.060
-10	14	2	7.417	5.038	-5.038	0.0	2.379	0.979
-8	14	2	8.839	8.138	8.138	0.0	0.651	0.338
-6	14	2	4.324	0.786	-0.786	0.0	3.539	1.169
-2	14	2	11.410	11.655	11.655	0.0	-0.245	-0.171
0	14	2	5.209	4.467	-4.467	0.0	0.742	0.271
0	12	0	205.792	211.538	211.538	0.0	-5.745	-1.868
2	14	2	18.215	17.585	17.585	0.0	0.630	0.663
4	14	2	1.091	3.365	3.365	0.0	-0.442	-0.442
4	14	2	8.177	8.866	8.866	0.0	-2.273	-0.335
8	14	2	2.629	2.812	-2.812	0.0	-0.182	-0.039
7	15	2	21.117	19.565	-19.565	0.0	1.553	1.444
5	15	2	35.008	35.205	35.205	0.0	-0.196	-0.226
3	15	2	21.622	22.148	-22.148	0.0	-0.526	-0.568
1	15	2	6.466	6.765	6.765	0.0	-0.299	-0.137
-1	15	2	29.783	30.280	30.280	0.0	-0.497	-0.620
-3	15	2	28.972	30.374	-30.374	0.0	-1.401	-1.712
-5	15	2	32.379	33.937	33.937	0.0	-1.558	-1.830
-7	15	2	28.526	26.885	-26.885	0.0	1.641	2.026
-9	15	2	22.680	24.818	24.818	0.0	-2.138	-1.847
-8	16	2	5.242	1.535	-1.535	0.0	3.707	1.245
-6	16	2	8.086	7.518	-7.518	0.0	0.568	0.274
-4	16	2	17.959	16.494	-16.494	0.0	1.465	1.452
-2	16	2	14.668	15.157	15.157	0.0	-0.489	-0.417
0	16	2	41.582	43.559	-43.559	0.0	-1.977	-2.299

H	K	L	F(DPS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	12	0	204.756	211.538	211.538	0.0	-6.779	-2.210 *
2	16	2	23.168	23.142	23.142	0.0	0.026	0.028
4	16	2	25.814	25.630	-25.630	0.0	0.184	0.204
6	16	2	5.887	0.179	0.179	0.0	5.709	2.220
7	17	2	7.268	4.299	4.299	0.0	2.968	1.169
5	17	2	3.820	4.176	4.176	0.0	-0.356	-0.101
3	17	2	6.458	4.764	-4.764	0.0	1.694	0.721
-1	17	2	2.348	7.203	7.203	0.0	-4.855	-1.154
-3	17	2	8.698	6.197	-6.197	0.0	2.501	1.369
-5	17	2	2.629	5.414	5.414	0.0	-2.785	-0.671
-7	17	2	4.457	2.262	2.262	0.0	2.194	0.658
-9	17	2	8.475	4.328	4.328	0.0	4.147	1.858
-8	18	2	8.541	4.567	-4.567	0.0	3.974	1.834
-6	18	2	10.327	11.195	11.195	0.0	-0.868	-0.469
-4	18	2	9.327	4.647	4.647	0.0	4.680	2.775
-2	18	2	17.041	16.654	16.654	0.0	0.187	0.162
2	18	2	19.075	15.618	15.618	0.0	2.457	2.584
4	18	2	8.831	8.813	8.813	0.0	0.017	0.008
0	12	0	205.037	211.538	211.538	0.0	-6.531	-2.129 *
6	18	2	17.554	15.307	15.307	0.0	2.247	1.836
5	19	2	10.005	7.239	7.239	0.0	2.765	1.417
3	19	2	8.789	2.766	-2.766	0.0	6.023	3.281
1	19	2	16.189	15.366	-15.366	0.0	0.824	0.701
-3	19	2	14.908	14.763	-14.763	0.0	0.145	0.107
-5	19	2	9.563	7.904	7.904	0.0	2.063	1.102
-7	19	2	28.766	28.765	-28.765	0.0	0.000	0.000
-8	20	2	6.425	0.556	-0.556	0.0	5.868	2.028
-6	20	2	12.568	11.903	11.903	0.0	0.665	0.404
-4	20	2	36.770	37.532	-37.532	0.0	-0.763	-0.846
-2	20	2	8.128	4.950	4.950	0.0	3.178	1.543
0	20	2	30.345	28.045	-28.045	0.0	2.300	2.552
2	20	2	24.723	24.207	24.207	0.0	0.515	0.542
4	20	2	53.521	52.603	-52.603	0.0	0.718	0.700
5	21	2	34.984	36.007	36.007	0.0	-1.024	-0.938
3	21	2	10.550	14.283	14.283	0.0	-3.733	-1.710
1	21	2	8.144	2.590	2.590	0.0	5.555	2.594
-1	21	2	26.351	25.120	25.120	0.0	1.232	1.379
-3	21	2	17.074	17.444	17.444	0.0	-0.369	-0.290
0	12	0	203.915	211.538	211.538	0.0	-7.622	-2.498 *
-5	21	2	25.343	24.478	24.478	0.0	0.865	0.837
-7	21	2	14.370	14.812	-14.812	0.0	-0.441	-0.267
-6	22	2	20.613	20.612	20.612	0.0	0.001	0.001
-4	22	2	31.709	32.330	32.330	0.0	-0.620	-0.610
-2	22	2	10.112	10.218	10.218	0.0	-0.106	-0.052
0	22	2	48.057	48.377	48.377	0.0	-0.280	-0.282
2	22	2	17.198	16.707	16.707	0.0	0.492	0.352
4	22	2	40.036	38.474	38.474	0.0	1.562	1.615
1	23	2	22.561	23.590	23.590	0.0	-1.029	-0.889
-1	23	2	13.552	10.129	-10.129	0.0	3.423	2.214
-3	23	2	25.310	24.528	24.528	0.0	0.381	0.360
-3	22	3	12.105	12.234	12.234	0.0	-0.129	-0.068
-1	22	3	15.181	14.567	-14.567	0.0	0.613	0.417
1	22	3	8.425	5.336	-5.336	0.0	3.090	1.271

H	K	L	F(OR5)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
2	21	3	24.557	25.512	-25.512	0.0	-0.955	-0.813
0	21	3	18.381	20.687	20.687	0.0	-2.307	-1.631
-2	21	3	22.846	22.660	-22.660	0.0	0.185	0.160
-6	21	3	4.382	2.655	2.655	0.0	1.727	0.477
-7	20	3	12.998	10.451	10.451	0.0	2.547	1.613
0	12	0	204.048	211.538	211.538	0.0	-7.490	-2.455
-3	20	3	12.783	13.884	13.884	0.0	-1.101	-0.619
-1	20	3	5.037	2.372	2.372	0.0	6.665	3.430
1	20	3	3.150	6.444	6.444	0.0	-3.294	-0.750
3	20	3	4.845	9.792	9.792	0.0	-4.947	-1.318
4	19	3	35.736	36.492	-36.492	0.0	-0.756	-0.788
2	19	3	25.467	23.580	23.580	0.0	1.487	1.578
0	19	3	12.155	13.445	-13.445	0.0	-1.269	-0.727
-2	19	3	21.109	22.436	22.436	0.0	-1.326	-1.114
-4	19	3	12.626	9.719	-9.719	0.0	2.907	1.964
-8	19	3	5.474	2.377	-2.377	0.0	3.097	0.925
-9	18	3	61.352	62.613	-62.613	0.0	-1.261	-1.097
-7	18	3	57.531	58.633	-58.633	0.0	-0.502	-0.474
-5	18	3	25.715	23.215	23.215	0.0	2.500	2.800
-3	18	3	13.635	14.790	-14.790	0.0	-1.155	-0.732
-1	18	3	67.379	68.069	68.069	0.0	-0.690	-0.609
1	18	3	26.839	27.323	-27.323	0.0	-0.484	-0.496
3	18	3	37.224	37.368	-37.368	0.0	-0.143	-0.151
5	18	3	49.354	49.627	49.627	0.0	-0.273	-0.266
0	12	0	204.659	211.538	211.538	0.0	-6.878	-2.248
6	17	3	57.060	55.731	55.731	0.0	1.329	1.246
4	17	3	35.380	34.272	-34.272	0.0	1.109	1.230
2	17	3	69.777	69.445	69.445	0.0	0.332	0.285
0	17	3	10.236	8.795	-8.795	0.0	1.441	0.838
-2	17	3	94.451	93.380	93.380	0.0	1.111	0.746
-4	17	3	10.732	9.710	9.710	0.0	1.023	0.584
-6	17	3	15.933	15.995	15.995	0.0	-0.062	-0.043
-8	17	3	25.954	25.162	25.162	0.0	0.793	0.786
-9	16	3	26.475	28.277	28.277	0.0	-1.801	-1.492
-7	16	3	6.557	10.663	10.663	0.0	-4.106	-1.595
-5	16	3	46.625	47.540	47.540	0.0	-1.315	-1.432
-3	16	3	30.262	30.268	30.268	0.0	-0.006	-0.007
-1	16	3	49.949	50.043	50.043	0.0	-0.094	-0.102
1	16	3	41.210	40.860	40.860	0.0	0.350	0.403
3	16	3	29.981	29.834	29.834	0.0	0.148	0.167
5	16	3	24.053	25.972	25.972	0.0	-1.579	-1.579
6	15	3	14.908	11.713	-11.713	0.0	3.195	2.415
4	15	3	19.976	20.287	20.287	0.0	-0.311	-0.276
2	15	3	26.608	27.684	-27.684	0.0	-1.076	-1.162
0	15	3	34.115	33.844	33.844	0.0	0.271	0.325
0	12	0	204.860	211.538	211.538	0.0	-6.738	-2.156
-2	15	3	24.185	24.454	-24.454	0.0	-0.269	-0.283
-4	15	3	15.470	13.480	13.480	0.0	1.990	1.616
-6	15	3	10.666	13.498	13.498	0.0	-2.832	-1.522
-8	15	3	8.318	11.710	-11.710	0.0	-3.392	-1.341
-10	15	3	18.009	15.116	15.116	0.0	2.892	2.364
-11	14	3	3.506	9.012	9.012	0.0	-5.507	-1.236
-9	14	3	35.546	35.144	-35.144	0.0	0.402	0.438

*

*

*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-7	14	3	21.498	21.209	21.209	0.0	0.289	0.273
-5	14	3	56.200	55.498	-55.498	0.0	0.702	0.719
-3	14	3	31.031	30.203	30.203	0.0	0.828	1.012
-1	14	3	45.939	46.660	-46.660	0.0	-0.121	-0.136
1	14	3	19.067	19.615	-19.615	0.0	-0.548	-0.502
3	14	3	8.657	7.499	7.499	0.0	1.158	0.645
5	14	3	38.026	37.135	-37.135	0.0	0.291	0.320
7	14	3	13.395	12.373	12.373	0.0	1.022	0.621
8	13	3	9.963	8.970	8.970	0.0	0.993	0.484
6	13	3	8.758	3.184	-8.184	0.0	0.614	0.297
4	13	3	22.225	22.008	-22.008	0.0	0.218	0.219
2	13	3	25.971	26.472	-26.472	0.0	-0.501	-0.571
0	13	3	34.901	35.023	36.023	0.0	-1.122	-1.357
0	12	0	204.915	211.538	211.538	0.0	-6.622	-2.159
0	12	0	9.682	12.149	-12.149	0.0	-2.466	-1.455
-2	13	3	16.892	16.630	16.630	0.0	0.262	0.240
-4	13	3	8.640	4.635	-4.635	0.0	4.005	2.134
-6	13	3	10.716	5.155	5.155	0.0	5.561	3.030
-10	13	3	11.121	10.010	10.010	0.0	1.111	0.567
-11	12	3	4.730	3.024	-3.024	0.0	1.705	0.527
-9	12	3	9.583	11.873	11.873	0.0	-2.290	-1.215
-7	12	3	6.805	2.956	2.956	0.0	3.849	1.854
-5	12	3	6.234	6.584	6.584	0.0	-0.349	-0.149
-3	12	3	13.957	15.187	15.187	0.0	-1.230	-0.953
-1	12	3	18.323	18.721	18.721	0.0	-0.398	-0.412
1	12	3	9.393	6.652	6.652	0.0	2.741	1.564
5	12	3	3.448	4.846	4.846	0.0	-1.398	-0.335
7	12	3	4.151	9.387	9.387	0.0	-5.236	-1.306
8	11	3	21.440	19.897	-19.897	0.0	1.543	1.623
6	11	3	14.238	15.390	-15.390	0.0	-1.152	-0.887
4	11	3	7.028	10.187	-10.187	0.0	-3.159	-1.458
2	11	3	8.285	6.146	6.146	0.0	2.139	1.120
0	11	3	204.130	211.538	211.538	0.0	-7.407	-2.421
0	12	0	35.051	36.475	-36.475	0.0	-1.384	-1.708
-2	11	3	2.770	7.365	7.365	0.0	-4.595	-1.134
-4	11	3	6.970	0.234	-0.234	0.0	6.736	3.325
-6	11	3	7.764	5.505	-5.505	0.0	2.259	1.076
-8	11	3	9.583	5.727	-5.727	0.0	3.856	2.082
-10	11	3	10.542	13.211	-13.211	0.0	-2.669	-1.409
-9	10	3	30.907	30.988	-30.988	0.0	-0.081	-0.100
-7	10	3	56.490	58.215	-58.215	0.0	-1.725	-1.768
-5	10	3	50.942	52.092	-52.092	0.0	-1.150	-1.276
-3	10	3	6.358	5.462	-5.462	0.0	0.897	0.375
-1	10	3	28.237	28.367	-28.367	0.0	-0.130	-0.154
1	10	3	18.604	21.518	21.518	0.0	-2.914	-2.865
3	10	3	2.712	2.601	-2.601	0.0	0.111	0.029
5	10	3	23.515	23.808	-23.808	0.0	-0.292	-0.247
9	10	3	6.267	5.847	5.847	0.0	0.420	0.146
8	9	3	12.841	13.536	-13.536	0.0	-0.695	-0.497
6	9	3	30.221	29.182	29.182	0.0	1.039	1.366
4	9	3	205.255	211.538	211.538	0.0	-6.283	-2.043
2	9	3	24.375	23.952	-23.952	0.0	0.423	0.492
0	9	3	61.525	62.388	62.388	0.0	-0.863	-0.849

*

*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-2	9	3	51.272	51.463	-51.463	0.0	-0.191	-0.212
-4	9	3	40.755	41.126	41.126	0.0	-0.371	-0.444
-6	9	3	20.795	21.632	21.632	0.0	-0.837	-0.873
-8	9	3	31.726	31.963	-31.963	0.0	-0.237	-0.276
-10	9	3	21.142	22.449	22.449	0.0	-1.307	-1.255
-12	9	3	17.810	17.829	-17.829	0.0	-0.019	-0.015
-11	8	3	9.137	4.519	-4.519	0.0	4.618	2.428
-9	8	3	14.058	14.017	-14.017	0.0	0.081	0.059
-7	8	3	2.439	0.569	0.569	0.0	1.870	0.493
-5	8	3	14.900	14.506	-14.506	0.0	0.394	0.313
-3	8	3	3.324	2.087	-2.087	0.0	1.237	0.370
-1	8	3	11.658	10.689	-10.689	0.0	0.970	0.702
1	8	3	4.870	1.132	1.132	0.0	3.688	1.344
3	8	3	5.333	1.035	1.035	0.0	4.298	1.650
5	8	3	23.383	24.837	-24.837	0.0	-1.454	-1.557
7	8	3	2.332	2.735	2.735	0.0	-0.404	-0.095
8	7	3	8.996	8.337	8.337	0.0	0.609	0.283
0	12	0	204.676	211.538	211.538	0.0	-6.862	-2.243
6	7	3	38.812	39.693	39.693	0.0	-0.871	-1.003
4	7	3	70.488	71.512	-71.512	0.0	-1.024	-0.904
2	7	3	26.376	25.914	25.914	0.0	0.462	0.570
0	7	3	38.241	38.261	-38.261	0.0	-0.020	-0.025
-2	7	3	95.202	95.181	95.181	0.0	0.022	0.015
-4	7	3	30.565	30.918	-30.918	0.0	-0.333	-0.428
-6	7	3	13.998	15.637	-15.637	0.0	-1.639	-1.270
-8	7	3	22.622	21.224	21.224	0.0	1.399	1.552
-12	7	3	39.043	39.861	39.861	0.0	-0.818	-0.831
-13	6	3	12.651	13.410	13.410	0.0	-0.759	-0.399
-11	6	3	17.851	18.163	18.163	0.0	-0.312	-0.260
-9	6	3	126.085	127.585	127.585	0.0	-1.500	-0.778
-7	6	3	81.378	82.664	-82.664	0.0	-1.287	-1.004
-5	6	3	104.331	104.871	104.871	0.0	-0.540	-0.338
-3	6	3	41.987	41.384	41.384	0.0	0.603	0.759
-1	6	3	193.986	195.364	195.364	0.0	-1.478	-0.509
1	6	3	29.212	30.157	30.157	0.0	-0.944	-1.228
3	6	3	14.568	17.330	-17.330	0.0	-2.712	-2.130
5	6	3	116.113	118.314	118.314	0.0	-2.201	-1.238
0	12	0	205.643	211.538	211.538	0.0	-5.894	-1.916
7	6	3	5.631	0.692	-0.692	0.0	4.938	1.890
9	6	3	77.756	77.667	77.667	0.0	-0.111	-0.085
10	5	3	7.549	7.440	7.440	0.0	0.109	0.039
8	5	3	38.117	38.082	38.082	0.0	0.035	0.038
6	5	3	90.043	90.027	90.026	0.0	0.015	0.011
4	5	3	32.652	33.252	-33.252	0.0	-0.610	-0.776
2	5	3	100.569	102.023	102.023	0.0	-1.454	-0.946
0	5	3	18.827	19.168	19.168	0.0	-0.341	-0.397
-2	5	3	191.752	191.587	191.987	0.0	-0.235	-0.082
-4	5	3	24.904	25.659	25.659	0.0	-0.754	-0.991
-6	5	3	31.933	31.505	31.505	0.0	0.427	0.550
-8	5	3	56.209	56.460	56.460	0.0	-0.252	-0.260
-10	5	3	18.654	16.962	16.962	0.0	1.692	1.637
-12	5	3	70.521	69.595	69.595	0.0	0.926	0.783
-13	4	3	17.132	18.140	18.140	0.0	-1.008	-0.670

*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-11	4	4	6.970	0.011	-0.011	0.0	6.959	2.943
-9	4	3	10.658	10.824	10.824	0.0	-0.166	-0.108
-7	4	3	9.782	5.543	-5.943	0.0	3.839	2.221
-5	4	3	9.955	8.755	8.755	0.0	1.200	0.825
-3	4	3	6.234	6.393	6.393	0.0	-0.159	-0.081
0	12	0	204.990	211.538	211.538	0.0	-6.547	-2.134
-1	4	3	13.544	12.598	12.598	0.0	0.546	0.537
1	4	4	14.313	14.598	14.598	0.0	1.715	1.620
5	4	3	7.516	9.017	-9.017	0.0	-1.501	-0.704
7	4	3	7.516	5.521	5.521	0.0	1.995	0.985
9	4	3	15.528	14.929	14.929	0.0	0.599	0.414
8	3	3	12.320	10.404	-10.404	0.0	1.916	1.259
6	3	3	41.459	41.769	-41.769	0.0	-0.270	-0.323
4	3	3	7.127	4.898	4.898	0.0	2.230	1.070
2	3	3	61.409	61.803	-61.803	0.0	-0.393	-0.393
0	3	3	32.131	31.770	31.770	0.0	0.361	0.514
-2	3	3	99.717	98.468	-98.468	0.0	1.249	0.825
-4	3	3	15.239	13.004	13.004	0.0	2.235	2.252
-6	3	3	11.270	11.703	11.703	0.0	-0.433	-0.306
-8	3	3	46.958	48.920	-48.920	0.0	-1.922	-2.173
-10	3	3	8.624	12.742	12.742	0.0	-4.119	-1.923
-12	3	3	23.805	22.340	-22.340	0.0	1.465	1.406
-13	2	3	2.679	5.238	-5.238	0.0	-2.559	-0.545
0	12	0	4.605	9.324	9.824	0.0	-5.218	-1.458
-9	2	3	204.560	211.538	211.538	0.0	-6.977	-2.281
-7	2	3	26.451	26.209	-26.209	0.0	0.241	0.292
-5	2	3	45.989	46.504	46.504	0.0	-0.516	-0.600
-3	2	3	66.924	66.906	-66.906	0.0	0.019	0.017
1	2	3	92.077	90.612	90.612	0.0	1.465	1.042
3	2	3	9.500	9.599	-9.599	0.0	-0.098	-0.068
5	2	3	46.907	43.613	48.613	0.0	-1.706	-1.984
7	2	3	5.176	3.353	-3.353	0.0	1.823	0.725
9	2	3	27.476	27.371	27.371	0.0	0.105	0.119
10	2	3	24.739	27.002	-27.002	0.0	-2.263	-2.058
8	1	3	8.756	7.417	-7.417	0.0	1.339	0.574
6	1	3	16.008	14.742	-14.742	0.0	1.266	1.086
4	1	3	12.088	12.171	-12.171	0.0	-0.083	-0.059
2	1	3	4.878	3.131	3.131	0.0	1.747	0.622
0	1	3	22.068	21.239	-21.239	0.0	0.829	1.023
-2	1	3	36.571	37.037	37.037	0.0	-0.466	-0.671
-4	1	3	24.003	23.827	-23.827	0.0	0.176	0.251
-8	1	3	25.012	25.116	25.116	0.0	-0.104	-0.143
0	12	0	4.804	0.642	0.642	0.0	4.162	1.468
-10	1	3	204.568	211.538	211.538	0.0	-6.969	-2.278
-12	1	3	8.409	5.802	5.802	0.0	2.607	1.371
-13	1	3	6.689	3.405	-3.405	0.0	3.284	1.281
-11	0	3	9.385	8.648	-8.648	0.0	0.537	0.247
-9	0	3	4.820	9.889	9.889	0.0	-5.069	-1.556
-7	0	3	17.843	14.966	-14.966	0.0	2.877	3.346
-5	0	3	3.927	3.611	3.611	0.0	0.317	0.097
-3	0	3	11.402	10.861	-10.861	0.0	0.541	0.411
1	0	3	24.375	25.800	-25.800	0.0	-1.425	-2.154
0	0	3	7.905	2.203	2.203	0.0	5.702	3.727

*

*

*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
3	0	3	17.959	18.147	-18.147	0.0	-0.188	-0.203
5	0	3	12.031	10.341	-10.341	0.0	1.690	1.336
7	0	3	9.831	9.960	-9.960	0.0	-0.129	-0.076
9	0	3	6.954	4.635	4.635	0.0	2.318	0.907
-12	0	4	5.895	0.545	0.545	0.0	5.350	1.783
-10	0	4	38.208	38.202	38.202	0.0	0.006	0.007
-8	0	4	22.655	23.742	-23.742	0.0	-1.087	-1.143
-6	0	4	142.911	147.703	-147.703	0.0	-4.797	-2.223
-4	0	4	131.501	133.311	-133.311	0.0	-1.811	-0.909
-2	0	4	80.385	81.074	-81.074	0.0	-0.688	-0.548
0	12	0	204.775	211.538	-211.538	0.0	-6.762	-2.204
0	0	4	160.217	164.513	-164.513	0.0	-4.296	-1.779
2	0	4	6.243	8.082	-8.082	0.0	-1.840	-0.737
4	0	4	128.408	131.000	-131.000	0.0	-2.592	-1.323
6	0	4	13.618	12.166	12.166	0.0	1.452	1.051
8	0	4	33.727	33.650	33.650	0.0	0.077	0.076
7	1	4	19.679	21.138	-21.138	0.0	-1.459	-1.169
5	1	4	8.657	7.859	7.859	0.0	0.798	0.396
3	1	4	79.468	81.188	-81.188	0.0	-1.720	-1.369
1	1	4	7.607	3.702	-3.702	0.0	3.905	1.912
-1	1	4	46.477	47.151	-47.151	0.0	-0.674	-0.784
-3	1	4	126.870	129.248	-129.248	0.0	-2.377	-1.239
-5	1	4	9.550	12.917	-12.917	0.0	-3.367	-1.794
-7	1	4	78.219	78.433	-78.433	0.0	-0.214	-0.173
-9	1	4	15.305	18.023	-18.023	0.0	-2.719	-1.957
-11	1	4	24.698	26.515	-26.515	0.0	-2.217	-2.031
-13	2	4	5.589	8.553	-8.553	0.0	-2.963	-0.861
-12	2	4	6.871	2.636	-2.636	0.0	4.235	1.547
-10	2	4	9.413	7.165	-7.165	0.0	2.253	1.216
-8	2	4	7.373	6.899	-6.899	0.0	0.477	0.225
-6	2	4	10.162	10.313	-10.313	0.0	-0.151	-0.089
0	12	0	204.172	211.538	-211.538	0.0	-7.366	-2.408
-4	2	4	6.301	6.720	-6.720	0.0	-0.419	-0.170
-2	2	4	9.811	10.633	-10.633	0.0	-0.818	-0.485
0	2	4	21.184	19.430	-19.430	0.0	1.754	1.877
2	2	4	17.876	18.062	-18.062	0.0	-0.186	-0.181
4	2	4	7.053	3.254	-3.254	0.0	3.799	1.788
8	2	4	3.671	4.172	-4.172	0.0	-0.501	-0.122
7	3	4	15.478	15.743	-15.743	0.0	-0.265	-0.205
5	3	4	21.680	23.451	-23.451	0.0	-1.771	-1.648
3	3	4	40.838	41.750	-41.750	0.0	-0.912	-1.103
1	3	4	8.880	4.682	4.682	0.0	4.199	2.277
-1	3	4	44.492	45.975	-45.975	0.0	-1.482	-1.758
-3	3	4	72.886	73.378	-73.378	0.0	-0.492	-0.422
-5	3	4	40.548	40.287	40.287	0.0	0.262	0.313
-7	3	4	19.728	20.461	-20.461	0.0	-0.732	-0.732
-9	3	4	19.852	17.766	17.766	0.0	2.087	2.086
-11	3	4	16.934	17.026	-17.026	0.0	-0.092	-0.069
-13	3	4	2.803	4.946	-4.946	0.0	-2.143	-0.443
-12	4	4	15.173	12.557	12.557	0.0	2.615	1.719
-10	4	4	7.119	4.970	-4.970	0.0	2.149	0.902
0	12	0	204.337	211.538	-211.538	0.0	-7.201	-2.354
-8	4	4	17.231	18.232	-18.232	0.0	-1.050	-0.895

*

*

*

*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-6	4	4	13.825	14.549	-14.949	0.0	-1.124	-0.872
-4	4	4	13.411	10.463	10.463	0.0	2.949	2.243
-2	4	4	44.914	44.624	44.624	0.0	0.289	0.343
0	4	4	52.967	55.139	-55.139	0.0	-2.172	-2.324
2	4	4	70.257	71.727	-71.727	0.0	-1.471	-1.298
4	4	4	9.533	12.435	-12.435	0.0	-2.901	-1.532
6	4	4	8.971	9.296	9.296	0.0	-0.324	-0.161
8	4	4	0.984	7.409	7.409	0.0	-6.425	-1.064
7	5	4	3.448	1.327	-1.327	0.0	2.121	0.519
3	5	4	26.459	26.152	-26.152	0.0	0.307	0.387
1	5	4	9.575	7.398	-7.398	0.0	2.177	1.330
-1	5	4	6.879	7.484	7.484	0.0	-0.605	-0.261
-3	5	4	36.141	37.466	-37.466	0.0	-1.325	-1.619
-5	5	4	11.435	13.574	13.574	0.0	-2.139	-1.340
-7	5	4	6.954	0.204	0.204	0.0	6.750	3.292
-9	5	4	7.450	2.339	2.339	0.0	5.111	2.424
-11	5	4	14.660	13.815	-13.815	0.0	0.845	0.601
0	12	0	204.692	211.538	211.538	0.0	-6.845	-2.231
-10	6	4	14.999	14.062	14.062	0.0	0.937	0.722
-8	6	4	12.171	11.410	-11.410	0.0	0.761	0.526
-2	6	4	6.747	6.932	6.932	0.0	-0.184	-0.079
0	6	4	13.097	11.719	-11.719	0.0	1.378	1.068
2	6	4	3.084	8.652	-8.652	0.0	-5.568	-1.537
4	6	4	0.620	0.931	0.931	0.0	-0.311	-0.057
6	6	4	10.765	13.365	13.365	0.0	-2.599	-1.349
8	6	4	13.750	13.825	-13.825	0.0	-0.075	-0.044
7	7	4	16.562	16.363	-16.363	0.0	0.199	0.141
5	7	4	20.365	19.838	19.838	0.0	0.527	0.479
3	7	4	24.202	24.553	24.553	0.0	-0.352	-0.397
1	7	4	16.074	17.145	-17.145	0.0	-1.071	-0.932
-1	7	4	17.471	17.283	17.283	0.0	0.188	0.178
-3	7	4	17.810	18.566	18.566	0.0	-0.756	-0.715
-5	7	4	21.250	19.422	19.422	0.0	1.828	2.105
-7	7	4	24.408	24.397	-24.397	0.0	0.011	0.012
-9	7	4	34.355	36.333	36.333	0.0	-1.977	-2.235
-11	7	4	17.471	14.483	-14.483	0.0	2.989	2.459
0	12	0	204.014	211.538	211.538	0.0	-7.523	-2.466
-12	8	4	34.752	34.691	34.691	0.0	0.061	0.060
-10	8	4	43.648	44.898	-44.898	0.0	-1.249	-1.337
-8	8	4	4.151	4.299	4.299	0.0	-0.148	-0.044
-6	8	4	28.113	27.191	27.191	0.0	0.922	1.161
-4	8	4	38.787	39.297	-39.297	0.0	-0.510	-0.624
0	8	4	15.809	15.872	-15.872	0.0	-0.063	-0.056
2	8	4	51.033	51.246	51.246	0.0	-0.213	-0.230
4	8	4	67.677	67.468	-67.468	0.0	0.209	0.165
6	8	4	25.541	26.388	26.388	0.0	-0.847	-0.854
8	8	4	2.571	7.883	7.883	0.0	-5.312	-1.064
7	9	4	38.870	38.498	-38.498	0.0	0.371	0.387
5	9	4	14.106	13.930	13.930	0.0	0.176	0.121
3	9	4	19.406	20.664	-20.664	0.0	-0.659	-0.594
1	9	4	41.755	41.336	-41.336	0.0	0.420	0.503
-1	9	4	10.468	10.644	10.644	0.0	-0.177	-0.115
-3	9	4	26.112	25.250	-25.250	0.0	0.861	0.992

*

*

H	K	L	F(DBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-5	9	4	10.947	7.049	7.049	0.0	3.898	2.619
-7	9	4	44.037	44.351	-44.351	0.0	-0.314	-0.348
-9	9	4	39.110	38.620	38.620	0.0	0.490	0.554
0	12	0	204.486	211.538	211.538	0.0	-7.052	-2.305
-11	9	4	11.948	11.809	-11.809	0.0	0.139	0.071
-10	10	4	12.403	13.170	13.170	0.0	-0.767	-0.440
-8	10	4	22.093	22.865	22.865	0.0	-0.771	-0.735
-6	10	4	24.483	24.942	24.942	0.0	-0.459	-0.487
-4	10	4	35.091	33.510	33.910	0.0	1.181	1.472
-2	10	4	14.627	15.237	15.237	0.0	-0.610	-0.509
0	10	4	33.710	34.322	34.322	0.0	-0.612	-0.771
2	10	4	12.345	8.975	8.975	0.0	3.369	2.383
4	10	4	33.735	33.775	33.775	0.0	-0.040	-0.046
6	10	4	19.017	18.491	18.491	0.0	0.527	0.430
7	11	4	52.728	52.435	52.435	0.0	0.292	0.280
5	11	4	16.710	17.967	17.967	0.0	-1.257	-0.932
3	11	4	68.570	68.556	68.556	0.0	0.014	0.012
1	11	4	54.629	54.541	54.541	0.0	0.088	0.090
-3	11	4	94.458	93.721	93.721	0.0	0.737	0.501
-5	11	4	13.585	14.732	14.732	0.0	-1.147	-0.802
-7	11	4	108.093	108.663	108.663	0.0	-0.570	-0.340
-9	11	4	31.565	31.282	-31.282	0.0	0.303	0.330
-11	11	4	30.758	29.851	29.851	0.0	0.908	0.900
0	12	0	203.866	211.538	211.538	0.0	-7.672	-2.515
-10	12	4	43.178	42.667	42.667	0.0	0.511	0.537
-8	12	4	26.302	25.505	-25.505	0.0	0.797	0.868
-6	12	4	38.440	37.631	37.631	0.0	0.809	0.950
-4	12	4	90.101	89.343	89.343	0.0	0.757	0.532
-2	12	4	53.472	53.576	-53.576	0.0	-0.105	-0.109
0	12	4	44.219	44.094	44.094	0.0	0.125	0.140
2	12	4	25.500	25.432	-25.432	0.0	0.068	0.073
4	12	4	98.766	99.441	99.441	0.0	-0.675	-0.432
6	12	4	32.429	31.278	-31.278	0.0	1.151	1.221
5	13	4	5.879	10.356	-10.356	0.0	-4.487	-1.314
3	13	4	8.070	5.567	5.567	0.0	2.103	0.925
1	13	4	4.920	2.083	-2.083	0.0	2.837	1.024
-1	13	4	36.174	36.233	-36.233	0.0	-0.059	-0.068
-3	13	4	20.224	20.078	20.078	0.0	0.146	0.142
-5	13	4	13.950	15.743	-15.743	0.0	-1.753	-1.165
-7	13	4	43.144	44.581	44.581	0.0	-1.437	-1.551
-9	13	4	42.185	41.626	-41.626	0.0	0.559	0.583
-10	14	4	9.269	5.709	-5.709	0.0	3.560	1.601
-8	14	4	10.799	10.668	10.668	0.0	0.131	0.069
-6	14	4	10.294	6.625	-6.625	0.0	3.669	2.175
0	12	0	204.097	211.538	211.538	0.0	-7.440	-2.439
-4	14	4	7.772	1.949	1.949	0.0	5.824	2.817
-2	14	4	14.023	13.636	13.636	0.0	0.187	0.148
0	14	4	11.617	10.690	-10.690	0.0	0.927	0.590
2	14	4	7.177	7.291	7.291	0.0	-0.114	-0.046
6	14	4	11.377	11.107	11.107	0.0	0.271	0.142
5	15	4	22.746	22.065	-22.065	0.0	0.682	0.557
1	15	4	9.881	8.771	-8.771	0.0	1.110	0.608
-1	15	4	23.573	24.494	24.494	0.0	-0.921	-0.920

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-3	15	4	16.558	16.406	-16.406	0.0	0.552	0.481
-5	15	4	22.730	21.203	21.203	0.0	1.527	1.552
-7	15	4	24.516	24.710	-24.710	0.0	-0.195	-0.190
-9	15	4	27.767	28.859	28.859	0.0	-1.152	-0.955
-6	16	4	17.752	17.022	17.022	0.0	0.730	0.605
-4	16	4	19.885	19.450	-19.450	0.0	0.435	0.405
-2	16	4	11.931	11.153	-11.153	0.0	0.778	0.480
0	16	4	10.311	9.676	-8.676	0.0	1.535	0.924
2	16	4	21.217	21.624	21.624	0.0	-0.407	-0.354
0	12	0	203.924	211.538	211.538	0.0	-7.614	-2.496
4	16	4	42.748	41.161	-41.161	0.0	1.587	1.658
3	17	4	7.111	8.213	8.213	0.0	-1.107	-0.397
1	17	4	16.082	15.080	-16.080	0.0	0.002	0.001
-1	17	4	3.216	4.021	4.021	0.0	-0.804	-0.204
-3	17	4	15.966	15.056	15.056	0.0	0.910	0.734
-5	17	4	5.027	5.533	-5.533	0.0	-0.906	-0.280
-7	17	4	9.591	9.107	-9.107	0.0	0.484	0.227
-6	18	4	13.974	11.224	11.224	0.0	2.750	1.760
-4	18	4	0.893	1.398	1.398	0.0	-0.505	-0.087
-2	18	4	10.460	11.210	11.210	0.0	-0.750	-0.376
0	18	4	11.328	5.508	5.508	0.0	5.820	3.666
2	18	4	8.326	6.592	6.592	0.0	1.344	0.570
1	19	4	7.921	7.803	-7.803	0.0	0.118	0.044
-1	19	4	9.360	5.534	5.534	0.0	3.376	1.673
-3	19	4	25.713	24.789	-24.789	0.0	0.985	0.976
-5	19	4	14.709	14.206	14.206	0.0	0.503	0.324
-4	20	4	15.462	12.911	-12.911	0.0	2.551	1.753
-2	20	4	13.726	12.237	12.237	0.0	1.488	0.968
0	20	4	39.498	39.582	-39.582	0.0	-0.084	-0.083
-3	16	5	49.553	43.163	-48.163	0.0	1.339	1.355
0	12	0	203.890	211.538	211.538	0.0	-7.647	-2.506
0	17	5	7.880	0.785	0.785	0.0	7.094	2.948
-2	17	5	51.553	52.298	52.298	0.0	-0.744	-0.703
-4	17	5	9.021	7.627	-7.627	0.0	1.394	0.600
-6	17	5	4.498	9.239	9.239	0.0	-4.741	-1.149
-7	16	5	3.803	8.223	8.223	0.0	-4.419	-1.026
-5	16	5	29.882	28.966	28.966	0.0	0.916	0.923
-3	16	5	12.758	14.868	14.868	0.0	-2.110	-1.114
-1	16	5	31.974	33.154	33.154	0.0	-1.180	-1.142
1	16	5	21.680	24.411	24.411	0.0	-2.731	-1.943
2	15	5	10.617	11.713	-11.713	0.0	-1.096	-0.455
0	15	5	19.844	18.898	18.898	0.0	0.947	0.806
-4	15	5	23.011	23.894	-21.894	0.0	1.117	1.032
-2	15	5	16.206	16.722	16.722	0.0	-0.516	-0.345
-6	15	5	13.899	14.215	14.215	0.0	-0.316	-0.190
-8	15	5	24.607	23.502	-23.902	0.0	0.705	0.627
-7	14	5	24.251	23.340	23.340	0.0	0.911	0.810
-5	14	5	57.955	57.701	-57.701	0.0	0.294	0.278
-3	14	5	28.361	28.890	28.890	0.0	-0.530	-0.543
-1	14	5	17.496	18.694	-18.694	0.0	-1.198	-0.873
1	14	5	19.927	19.563	-19.563	0.0	0.364	0.291
0	12	0	203.700	211.538	211.538	0.0	-7.837	-2.569
3	14	5	3.886	6.010	-6.010	0.0	-2.124	-0.511

*

*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
4	13	5	13.229	11.086	11.086	0.0	2.143	1.217
2	13	5	5.044	6.574	-6.574	0.0	-1.530	-0.443
0	13	5	25.062	23.113	23.113	0.0	1.948	2.162
-2	13	5	19.017	18.112	-18.112	0.0	0.905	0.771
-4	13	5	13.684	13.824	13.824	0.0	-0.140	-0.090
-6	13	5	7.822	1.486	1.486	0.0	6.336	2.727
-8	13	5	4.407	10.375	-10.375	0.0	-0.792	-0.342
-9	12	5	13.296	10.048	-10.048	0.0	-5.641	-1.401
-7	12	5	6.540	11.453	11.453	0.0	1.842	1.185
-3	12	5	11.212	0.198	0.198	0.0	6.342	2.451
1	12	5	6.615	13.752	13.752	0.0	-2.540	-1.371
3	12	5	4.870	7.075	7.075	0.0	-0.460	-0.159
4	11	5	12.386	0.951	0.951	0.0	3.919	1.150
2	11	5	12.146	12.070	-12.070	0.0	0.315	0.154
-2	11	5	5.317	10.349	-10.349	0.0	1.797	1.162
-4	11	5	20.5.337	1.406	1.406	0.0	3.910	1.351
0	12	0	13.436	211.538	211.538	0.0	-6.200	-2.016
-6	11	5	4.804	8.059	-8.059	0.0	5.377	4.014
-8	11	5	5.135	4.366	4.366	0.0	0.438	0.124
-10	11	5	16.843	0.376	-0.376	0.0	4.759	1.370
-9	10	5	20.109	16.647	-16.647	0.0	0.195	0.145
-5	10	5	29.874	20.181	20.181	0.0	-0.072	-0.062
-3	10	5	26.657	30.587	-30.587	0.0	-0.714	-0.778
-1	10	5	15.801	27.016	27.016	0.0	-0.358	-0.398
3	10	5	6.797	13.716	-13.716	0.0	2.085	1.776
5	10	5	6.739	0.952	0.952	0.0	5.845	2.303
4	9	5	34.140	5.186	-5.186	0.0	1.553	0.530
2	9	5	25.491	34.196	34.196	0.0	-0.056	-0.058
0	9	5	31.784	27.162	-27.162	0.0	-1.670	-1.643
-2	9	5	12.957	32.553	32.553	0.0	-0.769	-0.869
-4	9	5	16.330	14.640	-14.640	0.0	-1.084	-0.732
-6	9	5	3.936	17.903	17.903	0.0	-1.573	-1.243
-8	9	5	22.440	6.257	6.257	0.0	-2.321	-0.647
-10	9	5	25.822	23.818	-23.818	0.0	-1.377	-1.198
-11	8	5	7.235	24.790	24.790	0.0	1.032	0.953
0	12	0	204.304	1.644	-1.644	0.0	5.391	1.964
-9	8	5	6.549	211.538	211.538	0.0	-7.234	-2.365
-5	8	5	10.162	0.748	-0.748	0.0	5.801	2.113
-1	8	5	13.643	10.934	-10.934	0.0	-0.772	-0.408
3	8	5	7.838	12.655	12.655	0.0	0.988	0.703
5	8	5	10.235	5.757	5.757	0.0	2.082	0.915
6	7	5	10.443	12.544	-12.544	0.0	-2.308	-1.030
4	7	5	50.793	7.553	7.553	0.0	2.890	1.432
2	7	5	54.770	50.645	-50.645	0.0	0.148	0.148
0	7	5	14.048	55.103	55.103	0.0	-0.333	-0.330
-2	7	5	24.516	14.807	-14.807	0.0	-0.759	-0.543
-4	7	5	26.368	23.346	23.346	0.0	1.170	1.263
-6	7	5	6.185	24.383	-24.383	0.0	1.985	2.265
-8	7	5	33.644	5.390	5.390	0.0	0.795	0.312
-10	7	5	10.972	34.046	34.046	0.0	-0.402	-0.438
-11	6	5	8.376	10.737	-10.737	0.0	0.235	0.117
-9	6	5	102.900	10.674	-10.674	0.0	-2.298	-0.842
				101.855	101.855	0.0	1.045	0.648

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-7	6	5	11.501	12.524	-12.524	0.0	-1.023	-0.583
0	12	0	205.238	211.538	211.538	0.0	-6.299	-2.054 *
-5	6	5	67.256	66.789	66.789	0.0	0.508	0.452
-3	6	5	46.353	45.751	-45.751	0.0	0.602	0.668
-1	6	5	125.977	125.891	125.891	0.0	0.087	0.045
1	6	5	38.407	36.846	36.846	0.0	1.561	1.815
3	6	5	8.136	5.943	5.943	0.0	2.193	1.012
5	6	5	47.477	47.801	47.801	0.0	-0.324	-0.318
6	5	5	39.779	39.773	39.773	0.0	0.006	0.006
4	5	5	33.107	32.088	-32.088	0.0	1.018	1.151
2	5	5	100.230	100.806	100.806	0.0	-0.577	-0.369
0	5	5	18.133	18.405	18.405	0.0	-0.272	-0.246
-2	5	5	75.400	75.955	75.955	0.0	-0.555	-0.457
-6	5	5	26.740	27.415	27.415	0.0	-0.675	-0.704
-8	5	5	66.561	66.742	66.742	0.0	-0.181	-0.161
-10	5	5	2.919	4.081	4.081	0.0	-1.162	-0.256
-12	5	5	41.441	41.241	41.241	0.0	0.200	0.195
-9	4	5	12.295	12.113	12.113	0.0	0.182	0.110
-5	4	5	7.020	8.577	8.577	0.0	-1.557	-0.685
0	12	0	204.221	211.538	211.538	0.0	-7.316	-2.392 *
-1	4	5	4.870	2.562	2.562	0.0	2.308	0.807
1	4	5	10.030	6.247	6.247	0.0	3.782	2.310
3	4	5	10.823	11.108	11.108	0.0	-0.284	-0.164
5	4	5	2.356	6.696	-6.696	0.0	-4.340	-0.897
6	3	5	23.970	22.403	-22.403	0.0	1.567	1.425
4	3	5	16.710	18.991	18.991	0.0	-2.281	-1.662
2	3	5	46.659	45.750	-45.750	0.0	0.908	1.027
0	3	5	16.330	16.152	16.152	0.0	0.178	0.151
-2	3	5	38.200	37.253	-37.253	0.0	0.947	1.145
-6	3	5	8.227	2.478	-2.478	0.0	5.749	3.104
-8	3	5	36.836	37.251	-37.251	0.0	-0.415	-0.470
-10	3	5	25.880	26.310	26.310	0.0	-0.430	-0.413
-12	3	5	18.571	19.257	-19.257	0.0	-0.687	-0.480
-11	2	5	10.319	8.678	8.678	0.0	1.641	0.788
-9	2	5	20.117	20.309	-20.309	0.0	-0.192	-0.166
-7	2	5	33.189	33.821	33.821	0.0	-0.631	-0.688
-5	2	5	49.610	49.692	-49.692	0.0	-0.081	-0.085
-3	2	5	48.701	49.497	49.497	0.0	-0.796	-0.859
0	12	0	204.411	211.538	211.538	0.0	-7.126	-2.329 *
-1	2	5	9.393	8.800	-8.800	0.0	0.593	0.332
3	2	5	11.940	11.347	11.347	0.0	0.592	0.365
5	2	5	3.208	1.835	1.835	0.0	1.373	0.331
6	1	5	12.254	12.521	-12.521	0.0	-0.268	-0.135
4	1	5	12.105	10.888	10.888	0.0	1.217	0.787
2	1	5	6.185	7.150	-7.150	0.0	-0.965	-0.372
0	1	5	16.950	19.204	-19.204	0.0	-2.254	-1.933
-2	1	5	15.760	14.092	-14.092	0.0	1.667	1.653
-4	1	5	13.097	12.546	12.546	0.0	0.551	0.430
-6	1	5	8.351	1.404	1.404	0.0	6.947	3.802
-8	1	5	8.583	1.125	-1.125	0.0	7.458	4.045
-10	1	5	6.515	5.760	-5.760	0.0	0.756	0.216
-12	1	5	7.805	3.339	-3.339	0.0	4.467	1.783
-11	0	5	10.765	10.622	10.622	0.0	0.143	0.070

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-9	0	5	12.833	10.562	-10.562	0.0	2.271	1.526
-7	0	5	8.120	4.882	4.882	0.0	3.237	1.673
-3	0	5	15.793	15.029	-15.029	0.0	0.763	0.664
-1	0	5	12.634	13.977	-13.977	0.0	-1.343	-0.944
0	12	0	204.130	211.538	211.538	0.0	-7.407	-2.421 *
3	0	5	5.408	6.818	-6.818	0.0	-1.411	-0.496
5	0	5	2.803	6.381	-6.381	0.0	-3.573	-0.820
-10	0	6	80.989	81.321	81.321	0.0	-0.332	-0.246
-8	0	6	28.576	29.236	-29.236	0.0	-0.660	-0.639
-6	0	6	18.323	19.067	19.067	0.0	-0.745	-0.634
-4	0	6	92.242	92.872	92.872	0.0	-0.630	-0.430
-2	0	6	23.755	25.120	25.120	0.0	-1.365	-1.260
0	0	6	52.008	51.652	51.652	0.0	0.356	0.359
2	0	6	31.064	31.703	-31.703	0.0	-0.639	-0.655
4	0	6	97.220	95.862	95.862	0.0	1.358	0.869
3	1	6	6.416	1.098	1.098	0.0	5.318	1.832
1	1	6	20.646	19.597	19.597	0.0	1.049	0.983
-1	1	6	3.547	3.920	-3.920	0.0	-0.373	-0.096
-3	1	6	65.378	65.132	65.132	0.0	0.247	0.222
-5	1	6	15.578	13.916	-13.916	0.0	1.662	1.314
-7	1	6	49.751	50.083	50.083	0.0	-0.332	-0.335
-9	1	6	28.625	28.310	-28.310	0.0	0.316	0.303
-10	2	6	6.334	4.439	-4.439	0.0	1.894	0.603
0	12	0	204.279	211.538	211.538	0.0	-7.259	-2.373 *
-6	2	6	6.367	7.425	-7.425	0.0	-1.058	-0.381
-4	2	6	8.616	2.509	-2.509	0.0	6.106	3.156
-2	2	6	7.069	1.042	-1.042	0.0	6.028	2.540
2	2	6	8.492	11.873	-11.873	0.0	-3.381	-1.323
4	2	6	7.392	10.311	-10.311	0.0	-2.919	-0.973
3	3	6	5.110	2.550	2.550	0.0	2.560	0.763
1	3	6	13.147	14.659	-14.659	0.0	-1.512	-0.859
-1	3	6	21.084	19.724	19.724	0.0	1.361	1.210
-3	3	6	24.789	23.581	-23.581	0.0	1.207	1.292
-5	3	6	23.788	22.763	22.763	0.0	1.025	1.016
-7	3	6	28.700	26.202	-26.202	0.0	2.498	2.674
-9	3	6	19.910	20.874	20.874	0.0	-0.963	-0.693
-10	4	6	29.791	30.845	-30.845	0.0	-1.054	-0.966
-8	4	6	8.525	5.559	5.559	0.0	2.966	1.272
-6	4	6	20.737	21.507	21.507	0.0	-0.770	-0.670
-4	4	6	4.663	4.563	-4.563	0.0	0.101	0.031
-2	4	6	8.029	2.621	-2.621	0.0	5.408	2.565
0	4	6	7.756	5.579	-5.579	0.0	2.177	0.947
2	4	6	42.591	42.284	42.284	0.0	0.307	0.320
0	12	0	205.031	211.538	211.538	0.0	-6.506	-2.121 *
1	5	6	24.127	22.149	-22.149	0.0	1.978	1.883
-1	5	6	4.572	3.156	3.156	0.0	1.416	0.440
-7	5	6	17.835	17.290	-17.290	0.0	0.545	0.405
-9	5	6	24.483	23.283	23.283	0.0	1.195	1.156
-6	6	6	4.341	3.389	3.389	0.0	0.952	0.267
-4	6	6	7.797	8.684	-8.684	0.0	-0.887	-0.375
0	6	6	5.722	1.982	1.982	0.0	3.740	1.300
2	6	6	12.725	9.130	-9.130	0.0	3.595	2.312
1	7	6	6.515	6.302	6.302	0.0	0.214	0.075

H	K	L	F(10BS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-1	7	6	19.555	21.599	21.599	0.0	-2.044	-1.585
-3	7	6	19.588	17.814	-17.814	0.0	1.774	1.638
-5	7	6	22.598	22.539	22.939	0.0	-0.341	-0.315
0	12	0	204.593	211.538	211.538	0.0	-6.944	-2.270
-9	7	6	3.374	6.283	6.283	0.0	-2.909	-0.650
-8	8	6	17.190	14.481	14.481	0.0	2.709	1.974
-6	8	6	22.622	21.488	-21.488	0.0	1.135	1.024
-2	8	6	19.108	17.576	17.076	0.0	2.033	1.684
0	8	6	45.518	46.301	-46.301	0.0	-0.777	-0.777
2	8	6	34.471	34.457	34.457	0.0	0.014	0.014
-1	9	6	12.312	14.289	14.289	0.0	-1.977	-1.013
-3	9	6	47.882	48.642	-48.042	0.0	-0.160	-0.161
-5	9	6	26.525	26.842	26.842	0.0	-0.317	-0.286
-7	9	6	11.493	9.675	-9.075	0.0	2.418	1.250
-9	9	6	5.184	1.853	-1.853	0.0	3.331	0.950
-8	10	6	12.841	12.044	12.044	0.0	0.797	0.430
-6	10	6	6.168	10.304	10.304	0.0	-4.136	-1.211
-4	10	6	22.225	21.021	21.021	0.0	1.204	1.048
-2	10	6	15.503	15.719	15.719	0.0	-0.216	-0.140
0	10	6	19.001	19.514	19.514	0.0	-0.514	-0.374
1	11	6	16.636	15.711	15.711	0.0	0.925	0.625
0	12	0	204.800	211.538	211.538	0.0	-6.738	-2.156
-3	11	6	94.805	92.618	92.618	0.0	2.188	1.438
-5	11	6	11.567	14.458	-14.458	0.0	-2.890	-1.355
-7	11	6	44.071	43.870	43.870	0.0	0.200	0.199
-6	12	6	30.643	29.968	29.968	0.0	0.675	0.658
-4	12	6	44.840	43.770	43.770	0.0	1.070	1.087
-2	12	6	18.819	18.573	-18.573	0.0	0.246	0.180
0	12	6	45.269	46.523	46.523	0.0	-1.254	-1.194
-1	13	6	17.818	14.729	-14.729	0.0	3.089	2.292
-3	13	6	44.914	45.373	45.373	0.0	-0.459	-0.459
-5	13	6	31.924	31.543	-31.943	0.0	-0.019	-0.019
-2	14	6	4.754	6.670	6.070	0.0	-1.316	-0.349
-5	6	7	76.177	72.844	72.844	0.0	3.333	2.584
-3	6	7	45.121	44.733	-44.733	0.0	0.387	0.384
-2	5	7	25.940	27.860	27.860	0.0	2.080	2.029
-4	5	7	14.554	12.357	12.357	0.0	2.237	1.439
-6	5	7	23.325	22.079	22.079	0.0	1.246	1.077
-5	4	7	7.326	8.205	8.205	0.0	-0.879	-0.287
0	12	0	204.395	211.538	211.538	0.0	-7.143	-2.335
-3	4	7	3.704	0.592	0.592	0.0	3.112	0.747
-2	3	7	15.578	15.116	-15.116	0.0	0.461	0.305
-7	2	7	23.954	23.867	23.867	0.0	0.086	0.069
-5	2	7	33.363	34.209	-34.209	0.0	-0.846	-0.839
-3	2	7	24.417	25.821	25.821	0.0	-1.405	-1.148
-1	2	7	5.143	4.837	-4.837	0.0	0.306	0.088
-4	1	7	9.815	8.108	8.108	0.0	1.707	0.803
-6	1	7	4.647	0.365	0.365	0.0	4.281	1.143
-3	0	7	5.862	2.776	-2.776	0.0	3.086	0.977
-1	0	7	11.055	11.775	-11.775	0.0	-0.720	-0.329

RESULTS OF STRUCTURE FACTOR CALCULATIONS

VA RICHTERITE 600 C, JUNE, 1973

ALL REFLECTIONS

WEIGHTED R	NUMERATOR	DENOMINATOR	NUMBER	R
2871.08	1771911.00		1375	0.040
UNWEIGHTED R	2451.68	53235.33	1375	0.047
RANGES OF F(OBS)				
	1548.78	12661.55	900	0.122
	203.21	11626.37	265	0.017
	80.51	5490.97	71	0.015
	48.56	3217.67	31	0.015
	63.85	3168.42	24	0.020
	20.56	640.11	4	0.032
	489.41	15550.10	78	0.031
	36.87	480.91	2	0.077

RANGES OF (SIN(THETA)/LAMBDA)**2

	215.57	5102.25	88	0.042
	613.62	19548.73	185	0.031
	234.32	5627.27	150	0.042
	196.49	5122.02	157	0.038
	247.44	4472.11	179	0.055
	278.97	4343.47	195	0.064
	345.54	4343.06	212	0.080
	359.24	4278.23	209	0.084

INREJECTED REFLECTIONS

WEIGHTED R	2231.87	1285720.00	1191	0.042
UNWEIGHTED R	1834.09	34189.18	1191	0.054

RANGES OF F(OBS)

	1441.27	11645.75	832	0.124
	180.29	10337.54	237	0.017
	72.46	4936.73	64	0.015
	45.14	3002.97	29	0.015
	51.19	2641.64	20	0.019
	20.56	640.11	4	0.032
	23.23	585.15	5	0.024
	0.0	0.0	0	0.0

RANGES OF (SIN(THETA)/LAMBDA)**2

	162.90	4057.09	73	0.040
	125.03	4195.23	99	0.030
	206.74	5220.50	137	0.040
	182.81	4605.15	143	0.040
	223.44	4131.86	165	0.054
	267.82	4014.03	181	0.067
	324.82	4051.87	198	0.080
	340.65	3915.31	195	0.087

SUM FCAL 53398.27
STANDARD DEV OF UNIT WEIGHT OBS 1.43

EXTINCTION CORRECTION 0.0

SCALE FACTOR 1 1.2094

0.0000

0.0

1.2094

0.00323

0.00

ATOM 1	O(1)	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 1	1.00000	1.00000	0.0002017	0.00
X		0.1130942	0.0000001	0.1130943	0.0001030	0.0001030	0.00
Y		0.9155793	0.0000000	0.9155793	0.0003920	0.0003920	0.00
Z		0.8953556	0.0000000	0.8953558	0.0002113	0.0002113	-0.00
BETA11		0.0029788	-0.0000000	0.0029788	0.0000553	0.0000553	0.00
BETA22		0.0009836	0.0000000	0.0009836	0.0007815	0.0007815	0.00
BETA33		0.0126202	0.0000002	0.0126203	0.0000825	0.0000825	0.00
BETA12		0.0002007	0.0000000	0.0002007	0.0003266	0.0003266	-0.00
BETA13		0.0016263	-0.0000000	0.0016263	0.0001561	0.0001561	0.00
BETA23		-0.0001944	0.0000000	-0.0001944			0.00

ATOM 2	O(2)	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 1	1.00000	1.00000	0.0002029	-0.00
X		0.1191316	-0.0000000	0.1191315	0.0001153	0.0001153	0.00
Y		0.8323335	0.0000001	0.8323336	0.0003928	0.0003928	-0.00
Z		0.3921707	-0.0000003	0.3921704	0.0002115	0.0002115	-0.00
BETA11		0.0033007	0.0000001	0.0033007	0.0000635	0.0000635	0.00
BETA22		0.0013889	0.0000000	0.0013889	0.0007668	0.0007668	-0.00
BETA33		0.0116666	-0.0000000	0.0116666	0.0000566	0.0000566	0.00
BETA12		0.0001813	0.0000000	0.0001814	0.0002187	0.0002187	-0.00
BETA13		0.0012578	-0.0000000	0.0012577	0.0001701	0.0001701	0.00
BETA23		-0.00004905	0.0000001	-0.00004904			0.00

ATOM 3	F(3)	EQUIPOINT FRACTION = 0.500	OCCUPANCY SPECIES 2	1.00000	1.00000	0.0002732	0.00
X		0.1033006	0.0000000	0.1033006	0.0005078	0.0005078	0.00
Y		0.0	0.0000002	0.3908777	0.0002938	0.0002938	0.00
Z		0.3908776	0.0000001	0.3908777	0.0000755	0.0000755	-0.00
BETA11		0.0055290	-0.0000000	0.0055291	0.0001077	0.0001077	-0.00
BETA22		0.0012604	0.0000004	0.0012603	0.0004516	0.0004516	0.00
BETA33		0.0180947	0.0000000	0.0180943			0.00
BETA12		0.0	0.0000000	0.0			0.00
BETA13		0.0020441	0.0000000	0.0020442			0.00
BETA23		0.0	0.0000000	0.0			0.00

ATOM 4	O(4)	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 1	1.00000	1.00000	0.0002470	0.00
X		0.3619478	0.0000001	0.3619479	0.0001192	0.0001192	0.00
Y		0.7526363	0.0000000	0.7526363	0.0004656	0.0004656	0.00
Z		0.5641311	0.0000001	0.5641312	0.0002680	0.0002680	-0.00
BETA11		0.0064533	-0.0000000	0.0064533	0.0000627	0.0000627	0.00
BETA22		0.0011420	0.0000000	0.0011420	0.0005626	0.0005626	-0.00
BETA33		0.0176704	-0.0000002	0.0176702	0.0001068	0.0001068	0.00
BETA12		0.0011317	0.0000000	0.0011317	0.0004672	0.0004672	-0.00
BETA13		0.0029567	-0.0000001	0.0029566	0.0001762	0.0001762	-0.00
BETA23		0.0005710	-0.0000000	0.0005709			0.00

ATOM 5	O(5)	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 1	1.00000	1.00000	0.0002166	-0.00
X		0.3472323	-0.0000000	0.3472323	0.0001230	0.0001230	-0.00
Y		0.8716962	0.0000000	0.8716962	0.0004165	0.0004165	0.00
Z		0.2603095	0.0000000	0.2603095	0.0002271	0.0002271	0.00
BETA11		0.0041155	0.0000001	0.0041156			0.00

ATOM 6	T(1)	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 1	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 1	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 1	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 1
BETA22		0.0017358	-0.0006690	0.0017358	0.0006690	0.0017358	0.0006690	0.0017358	0.0006690
BETA33		0.0144261	0.0000002	0.0144263	0.0000002	0.0144263	0.0000002	0.0144263	0.0000002
BETA12		0.0001361	0.0000000	0.0001361	0.0000000	0.0001361	0.0000000	0.0001361	0.0000000
BETA13		0.0024528	0.0000001	0.0024529	0.0000001	0.0024529	0.0000001	0.0024529	0.0000001
BETA23		0.0021144	0.0000001	0.0021145	0.0000001	0.0021145	0.0000001	0.0021145	0.0000001

ATOM 6	T(2)	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 1	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 1	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 1	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 1
BETA22		0.0016955	0.0000000	0.0016955	0.0000000	0.0016955	0.0000000	0.0016955	0.0000000
BETA33		0.0142728	0.0000000	0.0142728	0.0000000	0.0142728	0.0000000	0.0142728	0.0000000
BETA12		-0.0000374	0.0000000	-0.0000374	0.0000000	-0.0000374	0.0000000	-0.0000374	0.0000000
BETA13		0.0028563	-0.0000000	0.0028563	-0.0000000	0.0028563	-0.0000000	0.0028563	-0.0000000
BETA23		-0.0020368	-0.0000000	-0.0020368	-0.0000000	-0.0020368	-0.0000000	-0.0020368	-0.0000000

ATOM 7	T(1)	EQUIPOINT FRACTION = 0.500	OCCUPANCY SPECIES 1	EQUIPOINT FRACTION = 0.500	OCCUPANCY SPECIES 1	EQUIPOINT FRACTION = 0.500	OCCUPANCY SPECIES 1	EQUIPOINT FRACTION = 0.500	OCCUPANCY SPECIES 1
BETA22		0.0456916	0.0000002	0.0456918	0.0006566	0.0456918	0.0006566	0.0456918	0.0006566
BETA11		0.0046903	-0.0000000	0.0046903	0.0003319	0.0046903	0.0003319	0.0046903	0.0003319
BETA22		0.0006796	0.0000000	0.0006796	0.0006796	0.0006796	0.0006796	0.0006796	0.0006796
BETA33		0.0267549	0.0000000	0.0267549	0.0014724	0.0267549	0.0014724	0.0267549	0.0014724
BETA12		0.0	0.0000000	0.0	0.0000000	0.0	0.0000000	0.0	0.0000000
BETA13		0.0015578	0.0000001	0.0015579	0.0005544	0.0015579	0.0005544	0.0015579	0.0005544
BETA23		0.0	0.0000000	0.0	0.0000000	0.0	0.0000000	0.0	0.0000000

ATOM 8	T(1)	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 3	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 3	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 3	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 3
BETA22		0.0007364	-0.0000000	0.0007364	0.0002012	0.0007364	0.0002012	0.0007364	0.0002012
BETA33		0.0089389	-0.0000000	0.0089388	0.0002806	0.0089388	0.0002806	0.0089388	0.0002806
BETA12		0.0000925	-0.0000000	0.0000925	0.0000328	0.0000925	0.0000328	0.0000925	0.0000328
BETA13		0.0015669	0.0000000	0.0015669	0.0001177	0.0015669	0.0001177	0.0015669	0.0001177
BETA23		-0.0000632	-0.0000000	-0.0000632	0.0000565	-0.0000632	0.0000565	-0.0000632	0.0000565

ATOM 9	T(2)	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 3	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 3	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 3	EQUIPOINT FRACTION = 1.000	OCCUPANCY SPECIES 3
BETA22		0.0008551	-0.0000000	0.0008551	0.0000210	0.0008551	0.0000210	0.0008551	0.0000210
BETA33		0.0053079	-0.0000000	0.0053078	0.0002727	0.0053078	0.0002727	0.0053078	0.0002727
BETA12		0.0002451	0.0000000	0.0002451	0.0000332	0.0002451	0.0000332	0.0002451	0.0000332
BETA13		0.0013680	-0.0000000	0.0013680	0.0001123	0.0013680	0.0001123	0.0013680	0.0001123
BETA23		0.0000955	-0.0000000	0.0000955	0.0000596	0.0000955	0.0000596	0.0000955	0.0000596

ATOM 10	M(1)	EQUIPOINT FRACTION = 0.500	OCCUPANCY SPECIES 4	EQUIPOINT FRACTION = 0.500	OCCUPANCY SPECIES 4	EQUIPOINT FRACTION = 0.500	OCCUPANCY SPECIES 4	EQUIPOINT FRACTION = 0.500	OCCUPANCY SPECIES 4
BETA22		0.0010004	0.0000000	0.0010004	0.0000401	0.0010004	0.0000401	0.0010004	0.0000401
BETA11		0.0038712	0.0000000	0.0038713	0.0001518	0.0038713	0.0001518	0.0038713	0.0001518
BETA22		0.5000000	0.0000000	0.5000000	0.0000000	0.5000000	0.0000000	0.5000000	0.0000000
BETA11		0.9107487	0.0000000	0.9107487	0.0000749	0.9107487	0.0000749	0.9107487	0.0000749

BETA33 0.017342 -0.0000001 0.0107341 C.0005369 -0.00
 BETA12 0.0 0.0000000 0.0 C.0017655 0.00
 BETA13 0.0017655 0.0000000 C.0017655 C.0002271 0.00
 BETA23 0.0 0.0

ATOM 11 M(2) EQUIPOINT FRACTION = 0.500
 OCCUPANCY SPECIES 4

X 1.00000 1.00000
 Y 0.0 0.0
 Z 0.8201517 0.0000000 0.8201517 C.CCCCT750 0.00
 BETA11 0.0039756 0.0000000 0.0039756 0.0001539 0.00
 BETA22 0.0010734 -0.0000000 0.0010734 0.0000424 -0.00
 BETA33 0.0132369 0.0000002 0.0132370 0.0005556 0.00
 BETA12 0.0 0.0
 BETA13 0.0017188 -0.0000000 0.0017188 0.0002288 -0.00
 BETA23 0.0 0.0

ATOM 12 M(3) EQUIPOINT FRACTION = 0.250
 OCCUPANCY SPECIES 4

X 1.00000 1.00000
 Y 0.0 0.0
 Z 0.0 0.0
 BETA11 0.0039248 0.0000000 0.0039248 C.CC02076 0.00
 BETA22 0.0007985 0.0000000 0.0007985 0.0000034 0.00
 BETA33 0.0117142 -0.0000001 0.0117141 0.0007536 -0.00
 BETA12 0.0 0.0
 BETA13 0.0029037 0.0000000 0.0029038 C.0003177 0.00
 BETA23 0.0 0.0

ATOM 13 M(4) EQUIPOINT FRACTION = 0.500
 OCCUPANCY SPECIES 5
 OCCUPANCY SPECIES 6
 TOTAL OCCUPANCY (FIXED) = 1.00000

X 0.0 0.0
 Y 0.7235966 0.0000000 0.7235966 0.0000741 0.00
 Z 0.5000000 0.5000000 0.5000000 C.CC00741 0.00
 BETA11 0.0093963 -0.0000001 0.0093962 0.0001753 -0.00
 BETA22 0.0014130 0.0000000 0.0014130 0.0000369 0.00
 BETA33 0.0184079 0.0000002 0.0184081 0.0005352 0.00
 BETA12 0.0 0.0
 BETA13 -0.0023699 0.0000000 -0.0023699 C.0002270 0.00
 BETA23 0.0 0.0

ATOM 14 A EQUIPOINT FRACTION = 1.000
 OCCUPANCY SPECIES 6

X 0.25000 0.25000
 Y 0.4700820 -0.0000073 0.4700747 0.0016239 -0.00
 Z 0.9884678 -0.0000046 0.9884632 0.0017301 -0.00
 BETA11 0.5426709 -0.0000146 0.5426563 0.0003288 -0.00
 BETA22 0.0197838 -0.0000088 0.0197751 C.C025373 -0.00
 BETA33 0.0046588 -0.0000032 0.0046556 0.0010806 -0.00
 BETA12 0.0525466 0.0000300 0.0525766 0.0074056 0.00
 BETA13 -0.0029775 0.0000061 -0.0029714 0.0014031 0.00
 BETA23 -0.0130069 -0.0000053 -0.0130122 0.0025510 -0.00
 BETA33 0.0024320 0.0000050 0.0024370 C.00020203 0.00

MAXIMUM SHIFT/ERROR = -0.00
 AVERAGE SHIFT/ERROR = 0.00

H	K	L	F(CBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
4	0	0	24.963	36.601	36.601	0.0	-11.638	-12.705 *
6	0	0	117.405	114.077	114.077	0.0	3.327	1.754
8	0	0	129.456	135.190	135.190	0.0	-5.693	-2.752
10	0	0	81.683	79.854	79.854	0.0	1.789	1.180
12	0	0	5.085	1.773	-1.773	0.0	7.312	2.322
-13	1	0	42.288	42.793	-42.793	0.0	-0.505	-0.302 *
-11	1	0	69.900	71.336	71.336	0.0	-1.436	-0.976 *
-9	1	0	26.767	25.579	25.579	0.0	0.788	0.667 *
-7	1	0	71.785	73.315	73.315	0.0	-1.530	-1.177 *
-5	1	0	125.238	123.639	-123.639	0.0	1.599	0.824 *
-3	1	0	140.556	139.529	139.929	0.0	0.667	0.313 *
3	1	0	140.483	139.529	139.929	0.0	0.554	0.260
5	1	0	128.506	123.639	-123.639	0.0	2.867	1.460
7	1	0	72.126	73.315	73.315	0.0	-1.188	-0.892
9	1	0	28.701	25.579	25.579	0.0	2.722	2.363
11	1	0	71.785	71.336	71.336	0.0	0.449	0.302
13	1	0	42.150	42.793	-42.793	0.0	-0.603	-0.386
-12	2	0	15.757	17.061	17.061	0.0	-1.264	-0.506 *
-8	2	0	14.172	14.504	-14.904	0.0	-0.732	-0.328 *
0	12	0	328.845	234.171	234.171	0.0	-5.326	-1.538 *
-6	2	0	34.536	34.003	-34.003	0.0	0.533	0.514 *
-4	2	0	2.145	1.570	1.970	0.0	0.175	0.041
6	2	0	34.373	34.003	-34.003	0.0	0.370	0.347
8	2	0	13.059	14.504	-14.504	0.0	-1.805	-0.773
12	2	0	18.657	17.061	17.061	0.0	1.596	0.777
-13	3	0	26.913	25.692	25.692	0.0	1.222	0.677 *
-11	3	0	24.817	24.032	-24.032	0.0	0.785	0.444 *
-9	3	0	19.031	20.174	20.174	0.0	-1.143	-0.671 *
-7	3	0	58.666	60.582	-60.582	0.0	-1.896	-1.553 *
-5	3	0	56.866	56.334	56.334	0.0	0.532	0.457 *
-3	3	0	89.646	94.303	-94.303	0.0	-4.657	-3.259 *
3	3	0	91.678	94.303	-94.303	0.0	-2.625	-1.822
5	3	0	58.702	56.334	56.334	0.0	2.368	2.203
7	3	0	60.831	60.582	-60.582	0.0	0.249	0.209
9	3	0	20.006	20.174	-20.174	0.0	-0.168	-0.102
11	3	0	26.003	24.032	-24.032	0.0	1.971	1.207
13	3	0	23.152	25.692	25.692	0.0	-2.500	-1.108
-12	4	0	23.950	20.684	20.684	0.0	3.207	1.758 *
0	12	0	229.950	234.171	234.171	0.0	-4.221	-1.213 *
-10	4	0	9.182	7.940	7.940	0.0	1.243	0.375 *
-8	4	0	14.757	14.349	14.349	0.0	0.408	0.209 *
-6	4	0	19.389	22.943	22.943	0.0	-3.554	-2.263 *
-4	4	0	19.242	17.321	17.321	0.0	1.921	1.653 *
2	4	0	138.467	144.305	144.305	0.0	-5.838	-2.780 *
4	4	0	140.223	144.305	144.305	0.0	-4.083	-1.920
6	4	0	18.674	17.321	17.321	0.0	1.352	1.145
8	4	0	22.395	22.943	22.943	0.0	-0.548	-0.427
10	4	0	15.212	14.349	14.349	0.0	0.863	0.443
12	4	0	19.389	20.684	20.684	0.0	-1.295	-0.516 *
-13	5	0	20.900	24.240	24.240	0.0	-3.340	-1.385 *
-11	5	0	31.009	28.621	28.621	0.0	2.388	1.859 *
-9	5	0	12.530	9.331	9.331	0.0	3.199	1.684 *
-7	5	0	11.555	12.927	-12.927	0.0	-1.371	-0.547 *

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-5	5	0	26.652	26.168	-26.168	0.0	-0.116	-0.166
-3	5	0	85.778	87.179	-87.079	0.0	-1.301	-0.947
-1	5	0	12.555	16.308	-16.308	0.0	-3.712	-2.559
1	5	0	11.019	16.308	-16.308	0.0	-5.289	-3.106
3	5	0	87.679	87.679	-87.679	0.0	0.340	0.244
0	12	0	228.292	234.171	-234.171	0.0	-5.878	-1.701
5	5	0	26.036	26.168	-26.168	0.0	-0.133	-0.145
7	5	0	13.717	12.927	-12.927	0.0	0.790	0.371
9	5	0	5.264	9.331	-9.331	0.0	-0.067	-0.023
11	5	0	25.824	28.621	-28.621	0.0	-2.797	-1.455
13	5	0	24.257	24.240	-24.240	0.0	0.057	0.034
-12	6	0	8.110	9.313	-9.313	0.0	-1.203	-0.278
-10	6	0	26.621	30.194	-30.194	0.0	-3.573	-2.215
-8	6	0	25.174	27.787	-27.787	0.0	-2.613	-1.762
-6	6	0	9.264	14.571	-14.571	0.0	-5.307	-1.688
-2	6	0	18.300	23.243	-23.243	0.0	-4.943	-4.438
0	6	0	11.003	17.188	-17.188	0.0	-6.186	-3.531
2	6	0	20.136	23.243	-23.243	0.0	-3.107	-3.016
4	6	0	15.156	14.571	-14.571	0.0	0.625	0.334
6	6	0	26.897	27.787	-27.787	0.0	-0.890	-0.692
8	6	0	29.367	30.194	-30.194	0.0	-0.827	-0.592
-11	7	0	11.954	10.578	-10.578	0.0	1.416	0.468
-9	7	0	59.954	60.401	-60.401	0.0	-0.447	-0.334
0	12	0	229.820	234.171	-234.171	0.0	-4.351	-1.251
-7	7	0	41.946	43.509	-43.509	0.0	-1.662	-1.440
-5	7	0	16.073	13.232	-13.232	0.0	2.842	1.871
-3	7	0	60.604	57.092	-57.092	0.0	3.512	3.238
-1	7	0	15.876	18.814	-18.814	0.0	1.063	1.048
1	7	0	19.714	18.814	-18.814	0.0	0.900	0.913
3	7	0	61.059	57.092	-57.092	0.0	3.967	3.610
5	7	0	13.083	13.232	-13.232	0.0	-0.149	-0.073
7	7	0	45.116	43.609	-43.609	0.0	1.507	1.389
9	7	0	60.051	60.401	-60.401	0.0	-0.350	-0.261
11	7	0	8.581	10.578	-10.578	0.0	-1.997	-0.480
-12	8	0	45.508	47.957	-47.957	0.0	-2.451	-1.639
-10	8	0	60.588	60.340	-60.340	0.0	0.247	0.181
-6	8	0	79.391	80.018	-80.018	0.0	-0.627	-0.443
-4	8	0	106.370	106.404	-106.404	0.0	-0.035	-0.020
-2	8	0	39.014	39.914	-39.914	0.0	-3.899	-4.216
0	8	0	52.169	49.120	-49.120	0.0	3.049	3.109
2	8	0	36.573	39.914	-39.914	0.0	-2.941	-3.287
4	8	0	108.677	106.404	-106.404	0.0	-2.273	-1.313
6	8	0	80.561	80.018	-80.018	0.0	0.543	0.383
0	12	0	229.316	234.171	-234.171	0.0	-4.854	-1.359
8	8	0	5.152	1.536	-1.536	0.0	-3.616	-0.885
10	8	0	58.946	60.340	-60.340	0.0	-1.394	-1.032
12	8	0	46.205	47.957	-47.957	0.0	-1.752	-1.215
-11	9	0	20.494	21.574	-21.574	0.0	-1.080	-0.481
-9	9	0	32.459	31.252	-31.252	0.0	1.187	0.855
-7	9	0	111.066	112.104	-112.104	0.0	-1.038	-0.567
-3	9	0	5.564	13.825	-13.825	0.0	-7.860	-2.264
-1	9	0	86.802	88.598	-88.598	0.0	-1.796	-1.271
1	9	0	89.240	88.598	-88.598	0.0	0.642	0.446

H	K	L	F(UBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
3	5	0	11.003	13.625	-13.825	0.0	-2.822	-1.494
5	9	0	3.640	0.514	0.514	0.0	3.127	0.671
7	9	0	111.830	112.104	-112.104	0.0	-0.274	-0.149
9	9	0	27.531	31.252	31.252	0.0	-3.721	-2.179
11	9	0	23.565	21.574	-21.574	0.0	1.592	1.067
-12	10	0	27.661	30.513	30.513	0.0	-2.852	-1.243
-10	10	0	35.216	38.139	38.139	0.0	1.077	0.791
-8	10	0	33.089	31.675	31.675	0.0	1.414	1.159
-6	10	0	20.104	19.977	19.977	0.0	0.127	0.080
-4	10	0	71.086	72.260	72.260	0.0	-1.173	-0.905
0	12	0	229.495	234.171	234.171	0.0	-4.676	-1.347
-2	10	0	45.059	46.778	46.778	0.0	-1.678	-1.670
0	10	0	106.890	109.628	109.628	0.0	-2.738	-1.615
0	10	0	43.562	46.778	46.778	0.0	-2.816	-2.593
2	10	0	72.387	72.260	72.260	0.0	0.127	0.058
4	10	0	20.608	19.977	19.977	0.0	0.630	0.435
6	10	0	34.308	31.675	31.675	0.0	2.633	2.312
8	10	0	40.289	38.139	38.139	0.0	2.150	1.681
10	10	0	33.073	30.513	30.513	0.0	2.560	1.739
-11	11	0	82.365	82.432	82.432	0.0	-0.066	-0.039
-9	11	0	11.929	9.581	9.581	0.0	1.948	0.738
-7	11	0	150.582	154.582	154.582	0.0	-4.830	-2.027
-5	11	0	46.123	48.109	48.109	0.0	-1.986	-1.753
-3	11	0	67.680	89.693	89.693	0.0	-2.013	-1.365
-1	11	0	129.366	128.158	128.158	0.0	1.208	0.598
1	11	0	130.666	143.158	128.158	0.0	2.508	1.231
3	11	0	89.516	69.693	89.693	0.0	-0.177	-0.118
5	11	0	47.757	48.109	48.109	0.0	-0.312	-0.289
7	11	0	154.671	154.582	154.582	0.0	-0.312	-0.128
9	11	0	14.562	9.581	9.581	0.0	4.581	2.371
11	11	0	81.293	82.432	82.432	0.0	-1.139	-0.679
0	12	0	229.560	234.171	234.171	0.0	-4.611	-1.327
-10	12	0	73.784	73.922	73.922	0.0	-0.137	-0.088
-8	12	0	62.099	63.628	63.628	0.0	-1.529	-1.120
-6	12	0	33.073	32.479	32.479	0.0	0.594	0.479
-4	12	0	63.757	63.734	63.734	0.0	0.022	0.018
-2	12	0	38.225	35.939	35.939	0.0	2.286	2.185
0	12	0	228.542	234.171	234.171	0.0	-5.228	-1.509
2	12	0	38.371	35.939	35.939	0.0	2.432	2.258
4	12	0	64.147	63.734	63.734	0.0	0.412	0.323
6	12	0	31.318	32.479	32.479	0.0	-1.161	-0.820
8	12	0	63.887	63.628	63.628	0.0	0.259	0.194
10	12	0	73.979	73.922	73.922	0.0	0.058	0.037
-11	13	0	24.752	23.688	23.688	0.0	1.064	0.668
-9	13	0	25.174	30.388	30.388	0.0	-5.214	-2.335
-7	13	0	38.972	40.397	40.397	0.0	-1.424	-1.165
-5	13	0	78.070	79.016	79.016	0.0	-0.747	-0.521
-3	13	0	28.067	27.168	27.168	0.0	0.900	0.758
-1	13	0	9.312	9.403	9.403	0.0	-0.090	-0.032
1	13	0	9.719	9.403	9.403	0.0	0.316	0.119
3	13	0	25.581	27.168	27.168	0.0	-1.587	-1.204
5	13	0	73.514	79.016	79.016	0.0	-0.503	-0.354
0	12	0	229.186	234.171	234.171	0.0	-4.985	-1.437

H	K	L	F(JBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
7	13	0	39.200	40.397	40.397	0.0	-1.197	-0.338
9	13	0	28.279	30.388	-30.388	0.0	-2.109	-1.287
11	13	0	22.834	23.688	23.688	0.0	-0.853	-0.446
-8	14	0	5.818	1.659	1.659	0.0	4.159	1.052
-2	14	0	14.351	14.273	14.273	0.0	0.077	0.038
-4	14	0	44.466	43.829	43.829	0.0	0.637	0.582
0	14	0	7.703	7.448	-7.448	0.0	0.255	0.077
2	14	0	41.459	43.829	43.829	0.0	-2.370	-1.977
4	14	0	11.360	14.273	14.273	0.0	-2.913	-1.072
6	14	0	5.656	1.659	1.659	0.0	3.996	1.133
-9	15	0	40.435	42.536	42.536	0.0	-2.101	-1.389
-7	15	0	65.869	64.525	-64.526	0.0	0.940	-0.940
-5	15	0	36.323	36.654	36.654	0.0	-0.331	-0.247
-1	15	0	13.863	15.504	-15.904	0.0	-2.041	-0.944
1	15	0	18.040	15.504	-15.904	0.0	-2.135	-1.465
0	12	0	229.219	234.171	234.171	0.0	-4.952	-1.428
3	15	0	9.442	0.508	-0.508	0.0	8.935	3.675
5	15	0	38.436	36.654	36.654	0.0	1.782	1.530
7	15	0	65.252	64.525	-64.526	0.0	0.726	0.523
9	15	0	41.865	42.536	42.536	0.0	-0.671	-0.472
-10	16	0	35.259	36.888	-36.888	0.0	-1.589	-0.957
-8	16	0	4.924	13.729	-13.729	0.0	-6.805	-1.575
-6	16	0	37.315	40.026	40.026	0.0	-2.711	-2.087
4	16	0	55.742	61.251	-61.251	0.0	-1.509	-1.122
-2	16	0	4.291	5.688	5.688	0.0	-1.398	-0.251
0	16	0	6.550	9.353	9.353	0.0	-2.804	-0.753
2	16	0	6.485	5.688	5.688	0.0	0.796	0.226
4	16	0	61.579	61.251	-61.251	0.0	0.328	0.255
6	16	0	40.143	40.026	40.026	0.0	0.117	0.090
8	16	0	15.017	13.729	-13.729	0.0	1.288	0.580
10	16	0	36.827	36.888	-36.888	0.0	-0.061	-0.042
-9	17	0	21.875	21.235	-21.235	0.0	0.640	0.333
-7	17	0	16.450	16.108	-18.108	0.0	-1.613	-0.669
-5	17	0	11.750	12.550	-12.950	0.0	-1.200	-0.443
-3	17	0	25.386	26.028	26.028	0.0	-0.642	-0.450
-1	17	0	20.201	19.348	-19.348	0.0	0.854	0.548
0	12	0	229.641	234.171	234.171	0.0	-4.529	-1.304
1	17	0	18.771	19.348	-19.348	0.0	-0.577	-0.327
3	17	0	23.240	26.028	26.028	0.0	-2.787	-1.768
5	17	0	12.124	12.950	-12.950	0.0	-0.826	-0.281
7	17	0	20.445	18.108	-18.108	0.0	2.337	1.402
9	17	0	17.357	21.235	21.235	0.0	-3.878	-1.391
-8	18	0	6.826	5.128	-5.128	0.0	1.698	0.404
-6	18	0	32.468	32.857	32.857	0.0	-0.370	-0.243
-4	18	0	6.485	13.921	13.921	0.0	-7.437	-1.549
-2	18	0	35.673	33.639	33.639	0.0	2.034	1.801
0	18	0	27.970	26.789	26.789	0.0	1.680	1.356
4	18	0	15.878	13.921	13.921	0.0	1.957	1.028
6	18	0	32.959	32.657	32.657	0.0	0.102	0.066
8	18	0	2.633	5.128	-5.128	0.0	-2.495	-0.367
-7	19	0	34.926	34.192	-34.192	0.0	0.734	-0.511
-3	19	0	37.412	39.162	-39.162	0.0	-1.750	-1.247
-1	19	0	9.861	7.473	-7.473	0.0	2.409	0.851

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	19	0	4.583	7.473	-7.473	0.0	-2.890	-0.571
3	19	0	39.281	39.162	-39.162	0.0	0.119	0.089
0	12	0	228.455	234.171	234.171	0.0	-5.710	-1.654
5	19	0	5.916	3.750	3.750	0.0	2.166	0.538
7	19	0	35.766	34.192	-34.192	0.0	1.514	1.063
-6	20	0	8.467	4.259	-4.259	0.0	4.208	1.236
-4	20	0	41.345	40.563	-40.563	0.0	0.382	0.257
-2	20	0	32.488	31.312	-31.312	0.0	1.176	0.829
0	20	0	63.627	65.492	65.492	0.0	-1.866	-1.536
2	20	0	32.564	31.312	-31.312	0.0	1.192	0.791
4	20	0	42.011	40.563	-40.563	0.0	1.048	0.819
6	20	0	5.686	4.259	-4.259	0.0	5.427	1.749
-7	21	0	4.464	4.092	-4.092	0.0	0.312	0.055
-5	21	0	40.289	40.490	40.490	0.0	-0.201	-0.143
-3	21	0	5.564	4.916	4.916	0.0	1.049	0.234
-1	21	0	26.735	26.710	26.710	0.0	0.025	0.016
1	21	0	27.255	26.710	26.710	0.0	0.545	0.328
3	21	0	2.487	4.516	4.516	0.0	-2.429	-0.380
5	21	0	41.686	40.490	-40.490	0.0	1.197	0.914
-6	22	0	20.153	17.794	17.794	0.0	2.359	1.162
-4	22	0	63.220	63.666	63.666	0.0	0.154	0.100
-2	22	0	26.637	25.749	25.749	0.0	0.388	0.569
0	22	0	229.105	234.171	234.171	0.0	-5.066	-1.461
0	22	0	66.851	66.263	66.263	0.0	0.588	0.360
2	22	0	20.621	25.749	25.749	0.0	0.872	0.470
4	22	0	64.439	63.666	63.666	0.0	1.373	0.942
6	22	0	15.066	17.794	17.794	0.0	-2.728	-0.853
-5	23	0	61.059	62.526	62.526	0.0	-1.867	-1.107
-3	23	0	40.614	43.147	43.147	0.0	-2.533	-1.680
-1	23	0	14.562	12.363	12.363	0.0	2.198	0.859
1	23	0	8.402	12.363	12.363	0.0	-3.961	-0.971
3	23	0	43.063	43.147	43.147	0.0	-0.144	-0.101
5	23	0	61.920	62.926	62.926	0.0	-1.006	-0.612
-2	24	0	47.757	48.941	48.941	0.0	-1.144	-0.854
0	24	0	112.952	112.361	112.361	0.0	0.590	0.256
2	24	0	47.325	48.941	48.941	0.0	-1.615	-1.102
-13	0	1	22.915	22.600	-22.600	0.0	0.056	0.029
-9	0	1	20.123	16.822	-16.822	0.0	3.298	2.377
-3	0	1	11.913	9.694	-9.694	0.0	2.219	1.443
3	0	1	27.888	26.164	-26.164	0.0	1.724	1.948
0	12	0	229.455	234.171	234.171	0.0	-4.676	-1.347
5	0	1	4.827	1.164	1.164	0.0	3.663	1.002
7	0	1	9.150	5.735	5.735	0.0	3.415	1.353
-12	1	1	6.290	5.616	-5.616	0.0	0.673	0.155
-10	1	1	4.258	10.227	10.227	0.0	-5.969	-1.161
-8	1	1	6.420	5.476	-5.476	0.0	0.944	0.256
-6	1	1	7.492	2.404	-2.404	0.0	5.088	2.036
-4	1	1	12.449	14.658	14.658	0.0	-2.209	-1.361
2	1	1	55.723	68.308	68.308	0.0	-2.584	-2.353
4	1	1	4.274	8.324	8.324	0.0	-4.050	-1.058
6	1	1	10.450	12.529	12.529	0.0	-2.079	-0.752
8	1	1	15.699	14.097	-14.097	0.0	1.602	0.969
10	1	1	11.815	13.214	-13.214	0.0	-1.399	-0.458

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
12	1	1	6.550	7.921	7.931	0.0	-1.382	-0.303
-13	2	1	20.104	20.874	-20.874	0.0	-0.771	-0.343
-11	2	1	38.257	35.330	35.330	0.0	2.927	2.495
-9	2	1	19.746	19.752	-19.752	0.0	-0.005	-0.004
-7	2	1	62.213	62.072	62.072	0.0	0.141	0.119
-5	2	1	38.485	38.730	-38.730	0.0	-0.245	-0.257
0	12	0	229.284	234.171	234.171	0.0	-4.887	-1.409
-3	2	1	145.488	148.715	148.715	0.0	-3.227	-1.462
3	2	1	10.548	14.802	14.802	0.0	-4.255	-2.513
3	2	1	121.289	121.327	121.327	0.0	-0.038	-0.020
3	2	1	20.022	15.782	-19.782	0.0	0.240	0.177
5	2	1	53.940	53.893	53.893	0.0	0.047	0.040
7	2	1	15.959	16.551	-16.951	0.0	-0.992	-0.472
9	2	1	48.561	49.892	49.892	0.0	-0.930	-0.643
11	2	1	50.853	52.230	-52.230	0.0	-1.377	-0.959
-6	3	1	37.217	35.372	-35.372	0.0	1.846	1.644
-6	3	1	10.450	14.009	-14.609	0.0	-4.158	-1.748
-4	3	1	35.104	34.763	-34.763	0.0	0.342	0.358
-2	3	1	151.485	156.278	-156.278	0.0	-4.792	-2.093
2	3	1	136.317	140.908	-140.908	0.0	-4.521	-2.176
4	3	1	25.237	30.076	-30.076	0.0	-0.839	-0.842
6	3	1	42.239	42.586	-42.986	0.0	-0.747	-0.659
8	3	1	23.452	21.484	-21.484	0.0	1.967	1.256
10	3	1	9.052	4.284	4.284	0.0	4.708	1.528
12	3	1	40.224	41.619	-41.619	0.0	-1.395	-0.881
-13	4	1	26.328	28.293	28.293	0.0	-1.965	-1.010
0	12	0	229.251	234.171	234.171	0.0	-4.919	-1.419
-11	4	1	28.083	25.605	-25.605	0.0	5.616	2.478
-9	4	1	6.225	0.609	-0.609	0.0	1.374	1.604
-7	4	1	14.253	15.627	15.627	0.0	-1.374	-0.721
-5	4	1	26.474	29.176	29.176	0.0	-0.702	-0.691
-3	4	1	15.342	15.300	15.300	0.0	0.042	0.037
-1	4	1	20.949	24.564	24.564	0.0	-3.615	-3.519
1	4	1	14.318	16.143	16.143	0.0	-1.825	-1.375
7	4	1	25.954	26.807	26.807	0.0	-0.853	-0.643
9	4	1	23.842	24.733	24.733	0.0	-0.892	-0.528
11	4	1	25.922	26.643	-26.643	0.0	-0.721	-0.385
-12	5	1	103.217	103.531	103.531	0.0	-0.314	-0.167
-10	5	1	14.887	12.256	12.256	0.0	2.630	1.539
-8	5	1	16.951	16.108	16.108	0.0	0.843	0.535
-6	5	1	102.339	105.126	105.126	0.0	-2.787	-1.673
-4	5	1	95.627	95.271	95.271	0.0	0.356	0.233
-2	5	1	208.652	211.586	211.586	0.0	-3.293	-1.050
0	5	1	85.502	86.182	-86.182	0.0	-0.680	-0.503
2	5	1	129.756	128.691	128.691	0.0	1.066	0.535
0	12	0	225.885	234.171	234.171	0.0	-4.286	-1.232
4	5	1	7.330	9.570	9.570	0.0	-2.240	-0.760
6	5	1	159.416	163.821	163.821	0.0	-4.404	-1.781
8	5	1	36.145	37.383	37.383	0.0	-1.238	-0.921
12	5	1	58.052	58.426	58.426	0.0	-0.374	-0.244
-11	6	1	71.086	70.571	70.571	0.0	0.516	0.331
-9	6	1	126.577	128.086	128.086	0.0	-1.431	-0.423
							-1.109	-0.537

H	K	L	F(UBSI)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
-7	6	1	94.766	57.451	-97.451	0.0	-2.686	-1.656
-5	6	1	213.828	221.072	221.072	0.0	-7.244	-2.239
-3	6	1	180.901	179.840	179.840	0.0	1.061	0.587
-1	6	1	149.657	154.573	154.573	0.0	-4.876	-2.144
1	6	1	57.548	44.256	-44.256	0.0	13.293	13.045
3	6	1	74.564	74.585	74.585	0.0	-0.021	-0.017
5	6	1	262.681	269.834	269.834	0.0	-7.153	-1.806
7	6	1	30.521	29.113	-29.113	0.0	1.409	1.089
9	6	1	101.008	102.742	102.742	0.0	-1.134	-0.624
11	6	1	26.605	25.072	-25.072	0.0	1.532	1.089
-12	7	1	56.086	54.581	54.581	0.0	1.505	1.015
-10	7	1	27.856	27.569	-27.569	0.0	0.287	0.178
0	12	C	228.585	234.171	234.171	0.0	-5.586	-1.615
-8	7	1	41.426	41.363	-41.363	0.0	0.064	0.056
-6	7	1	30.115	28.563	28.563	0.0	1.152	0.970
-2	7	1	58.686	57.398	57.398	0.0	1.288	1.247
0	7	1	140.027	141.585	-141.585	0.0	-1.558	-0.728
2	7	1	17.048	12.482	12.482	0.0	4.567	3.877
4	7	1	66.635	65.545	-65.545	0.0	0.688	0.575
6	7	1	66.227	68.174	68.174	0.0	-1.947	-1.493
8	7	1	11.084	12.304	-12.304	0.0	-1.221	-0.457
10	7	1	33.869	34.681	-34.681	0.0	-1.011	-0.621
12	7	1	14.009	11.444	11.444	0.0	2.565	0.972
-11	8	1	22.525	20.887	-20.887	0.0	1.638	0.879
-9	8	1	19.755	17.033	-17.033	0.0	2.762	1.954
-7	8	1	22.152	22.070	22.070	0.0	0.082	0.056
-5	8	1	15.439	13.313	-13.313	0.0	2.127	1.357
-3	8	1	14.952	15.456	15.456	0.0	-0.504	-0.341
-1	8	1	4.226	0.104	-0.104	0.0	4.122	1.221
3	8	1	7.687	4.351	4.351	0.0	3.336	1.311
5	8	1	22.477	24.167	-24.167	0.0	-1.690	-1.148
7	8	1	229.365	234.171	234.171	0.0	-4.806	-1.385
9	8	1	32.732	35.582	35.582	0.0	-2.851	-2.212
11	8	1	18.787	19.379	-19.379	0.0	-0.592	-0.288
12	8	1	31.269	31.245	-31.245	0.0	0.024	0.015
-10	9	1	18.316	19.622	19.622	0.0	-0.306	-0.164
-8	9	1	9.247	1.820	1.820	0.0	7.428	2.356
-6	9	1	15.862	17.358	17.358	0.0	-1.496	-0.749
-4	9	1	17.422	15.861	15.861	0.0	1.562	1.025
-2	9	1	62.254	63.074	-63.074	0.0	-0.780	-0.686
0	9	1	99.040	97.100	97.100	0.0	1.940	1.225
2	9	1	73.183	73.671	-73.671	0.0	-0.488	-0.385
4	9	1	35.852	35.017	35.017	0.0	0.835	0.789
6	9	1	15.147	10.762	-10.762	0.0	4.384	3.351
8	9	1	2.763	1.821	1.821	0.0	0.942	0.164
10	9	1	29.627	27.904	27.904	0.0	1.724	1.156
-11	10	1	22.769	27.856	27.856	0.0	-5.086	-2.250
-9	10	1	24.020	24.566	-24.566	0.0	-0.946	-0.557
-7	10	1	18.040	20.689	20.689	0.0	-2.649	-1.476
-5	10	1	23.647	25.608	-25.608	0.0	-1.961	-1.330
-3	10	1	64.244	64.239	64.239	0.0	0.005	0.005
0	12	C	229.609	234.171	234.171	0.0	-4.562	-1.313
-1	10	1	41.556	38.211	-38.211	0.0	3.346	3.478

H	K	L	F(OBS)	F(CALC)	A(CALC)	F(CALC)	DELTA F	DELTA/SIGMA
1	10	1	9.637	3.166	3.166	0.0	6.472	3.147
3	10	1	55.176	57.358	57.358	0.0	-2.183	-1.872
5	10	1	36.518	36.581	-36.581	0.0	-0.463	-0.353
7	10	1	27.450	26.271	26.271	0.0	1.119	0.770
9	10	1	11.344	13.536	-13.536	0.0	-2.192	-0.701
11	10	1	25.629	24.991	24.991	0.0	0.638	0.366
12	11	1	8.792	4.045	-4.045	0.0	4.747	1.484
12	11	1	24.833	25.564	-25.564	0.0	-0.731	-0.354
12	11	1	28.864	29.318	-29.318	0.0	-0.455	-0.381
12	11	1	23.549	22.785	22.785	0.0	0.764	0.535
12	11	1	31.334	31.375	-31.375	0.0	-0.041	-0.037
12	11	1	8.655	14.264	-14.264	0.0	-5.559	-1.895
12	11	1	66.991	67.312	-67.312	0.0	-0.322	-0.263
12	11	1	13.522	11.704	-11.704	0.0	1.818	0.938
12	11	1	18.430	19.866	-19.866	0.0	-1.436	-0.845
12	11	1	11.718	9.063	-6.063	0.0	5.654	2.344
12	11	1	29.530	27.100	-27.100	0.0	2.430	1.783
12	11	1	15.716	14.152	14.152	0.0	1.564	0.643
12	12	0	230.941	234.171	234.171	0.0	-3.229	-0.924
12	12	0	26.426	26.312	26.312	0.0	0.113	0.084
12	12	1	27.823	26.572	26.572	0.0	0.851	0.708
12	12	1	25.434	26.495	-26.495	0.0	-1.060	-0.783
12	12	1	35.738	37.332	37.332	0.0	-1.594	-1.406
12	12	1	20.348	20.524	20.524	0.0	-0.177	-0.111
12	12	1	23.289	24.710	24.710	0.0	-1.420	-0.939
12	12	1	25.483	24.709	24.709	0.0	0.775	0.517
12	12	1	15.976	18.101	18.101	0.0	-2.125	-0.871
12	12	1	14.026	9.032	9.032	0.0	4.994	2.089
12	12	1	7.590	6.875	-6.875	0.0	-1.285	-0.329
12	12	1	36.876	37.530	37.530	0.0	-0.549	-0.478
12	12	1	51.958	52.507	-52.507	0.0	0.549	0.478
12	12	1	43.539	43.456	43.456	0.0	0.083	0.073
12	12	1	33.447	33.880	-33.880	0.0	-0.433	-0.396
12	12	1	11.635	14.573	-14.573	0.0	-2.893	-1.034
12	12	1	16.252	10.879	10.879	0.0	5.373	3.140
12	12	1	17.845	20.628	-20.628	0.0	-2.783	-1.101
12	12	0	230.243	234.171	234.171	0.0	-3.928	-1.128
12	12	0	13.847	7.555	-7.555	0.0	5.892	2.458
12	12	1	8.695	3.579	-3.579	0.0	4.716	1.360
12	12	1	33.674	36.130	-36.130	0.0	-2.456	-1.461
12	12	1	34.844	33.297	33.297	0.0	1.548	1.148
12	12	1	94.157	96.101	-96.101	0.0	-1.904	-1.177
12	12	1	46.367	47.535	-47.535	0.0	-1.168	-0.952
12	12	1	32.975	32.644	-32.644	0.0	0.332	0.272
12	12	1	60.393	60.309	-60.309	0.0	0.084	0.068
12	12	1	22.764	25.226	-25.226	0.0	-2.522	-1.678
12	12	1	41.638	43.363	-43.363	0.0	-1.725	-1.321
12	12	1	4.112	8.597	-8.597	0.0	-4.885	-0.910
12	12	1	48.265	48.320	-48.320	0.0	-0.056	-0.024
12	12	1	12.855	11.332	-11.332	0.0	1.523	0.582
12	12	1	23.630	23.553	-23.553	0.0	0.078	0.048
12	12	1	17.162	17.905	-17.905	0.0	-0.743	-0.367
12	12	1	11.701	12.653	-12.653	0.0	-0.951	-0.356

H	K	L	F(OBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
-2	15	1	60.032	67.635	-67.635	0.0	-1.603	-1.220
0	15	1	43.799	43.710	43.710	0.0	0.089	0.077
2	15	1	31.431	31.683	-31.683	0.0	-0.251	-0.205
4	15	1	11.214	9.889	-9.889	0.0	1.325	0.571
0	12	0	228.747	234.171	234.171	0.0	-5.423	-1.567
6	15	1	8.516	13.897	-13.897	0.0	-5.381	-1.340
8	15	1	16.289	9.074	9.074	0.0	7.211	4.561
-9	10	1	52.864	52.395	52.395	0.0	0.489	0.354
-7	10	1	29.107	29.693	-29.693	0.0	-0.585	-0.373
-5	10	1	83.129	85.170	-85.170	0.0	-2.041	-1.293
-3	16	1	57.126	58.865	-58.865	0.0	-1.739	-1.351
-1	16	1	75.732	80.563	-80.563	0.0	-0.831	-0.571
3	16	1	62.278	62.389	62.389	0.0	-0.111	-0.087
5	16	1	49.017	50.204	50.204	0.0	-0.586	-0.474
7	16	1	75.954	75.353	75.354	0.0	0.641	0.446
9	16	1	45.229	44.008	44.008	0.0	1.221	0.892
-6	17	1	58.475	59.209	-59.209	0.0	-0.734	-0.473
-4	17	1	17.975	17.881	-17.881	0.0	2.670	0.812
-2	17	1	10.434	7.163	-7.163	0.0	1.914	1.024
0	17	1	138.061	138.054	138.054	0.0	0.007	0.003
2	17	1	63.269	63.306	-63.306	0.0	-0.037	-0.028
4	17	1	75.666	77.337	-77.337	0.0	-1.652	-1.056
6	17	1	10.613	1.739	-1.739	0.0	8.873	3.977
8	17	1	40.224	39.636	39.636	0.0	-5.862	-1.697
-9	18	1	228.309	234.171	-234.171	0.0	-1.194	-0.658
-7	18	1	102.095	103.289	-103.289	0.0	0.588	0.396
-5	18	1	8.565	5.019	-5.019	0.0	3.546	0.966
-3	18	1	14.611	11.515	-11.515	0.0	0.966	0.396
-1	18	1	6.875	7.820	-7.820	0.0	3.096	1.744
3	18	1	26.578	25.331	-25.331	0.0	-0.946	-0.233
5	18	1	12.458	9.974	-9.974	0.0	1.647	1.272
7	18	1	83.438	82.023	-82.023	0.0	2.524	1.114
-8	18	1	41.940	43.390	-43.390	0.0	1.415	0.895
-6	19	1	10.873	7.114	-7.114	0.0	-1.443	-0.910
-4	19	1	3.900	8.282	-8.282	0.0	3.758	1.314
-2	19	1	14.074	14.730	-14.730	0.0	-4.381	-0.730
0	19	1	41.686	41.936	41.936	0.0	-0.650	-0.287
2	19	1	45.408	42.860	-42.860	0.0	-0.250	-0.203
4	19	1	6.875	7.629	-7.629	0.0	2.548	2.067
6	19	1	19.194	14.971	-14.971	0.0	-0.755	-0.214
-7	20	1	40.208	40.092	40.092	0.0	4.223	2.753
-5	20	1	36.242	35.112	35.112	0.0	0.116	0.081
-3	20	1	228.731	234.171	-234.171	0.0	1.130	0.705
-1	20	1	6.712	4.679	-4.679	0.0	-5.440	-1.572
3	20	1	26.605	25.401	25.401	0.0	1.834	0.450
5	20	1	8.191	5.711	-5.711	0.0	1.204	0.652
7	20	1	16.415	17.706	-17.706	0.0	2.480	0.710
9	20	1	24.849	24.281	24.281	0.0	-1.291	-0.567
5	20	1	14.334	14.828	-14.828	0.0	0.569	0.359
							-0.493	-0.155

*

*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
7	20	1	39.574	37.328	37.328	0.0	2.245	1.446
-0	21	1	4.177	-2.277	-2.277	0.0	1.900	0.348
-4	21	1	12.750	8.394	8.394	0.0	4.396	2.175
-2	21	1	63.703	-63.278	-63.278	0.0	0.430	0.288
0	21	1	31.464	32.270	32.270	0.0	-0.806	-0.544
2	21	1	40.973	38.570	-38.570	0.0	-2.353	1.838
4	21	1	6.306	-4.060	-4.060	0.0	2.246	0.524
0	21	1	26.231	23.852	-23.852	0.0	2.379	1.356
-5	22	1	36.437	37.395	-37.395	0.0	-0.958	-0.655
-3	22	1	22.135	23.123	23.123	0.0	-0.987	-0.514
-1	22	1	3.413	0.445	0.445	0.0	2.568	0.535
1	22	1	28.685	-26.020	-26.020	0.0	2.665	1.968
3	22	1	13.343	12.311	12.311	0.0	1.032	0.375
5	22	1	9.751	1.807	1.807	0.0	7.944	2.634
0	22	0	228.812	234.171	234.171	0.0	-5.358	-1.547
-4	23	1	21.754	23.085	23.085	0.0	-1.291	-0.636
-2	23	1	1.853	7.017	-7.017	0.0	-5.164	-0.681
0	23	1	19.746	19.319	19.319	0.0	0.427	0.236
2	23	1	10.332	16.960	16.960	0.0	1.372	0.612
4	23	1	9.247	2.075	2.075	0.0	7.173	2.270
-1	24	1	8.857	8.287	8.287	0.0	0.571	0.152
-12	0	2	53.063	51.567	-51.567	0.0	1.496	1.110
-10	0	2	108.109	107.307	107.307	0.0	6.802	0.438
-8	0	2	85.372	87.780	87.780	0.0	-2.408	-1.614
-6	0	2	133.283	134.640	134.640	0.0	-1.357	-0.652
-4	0	2	181.633	183.474	183.474	0.0	-1.841	-0.669
-2	0	2	105.833	58.781	-98.781	0.0	7.052	4.285
0	0	2	284.768	287.205	287.205	0.0	-2.437	-0.572
2	0	2	154.069	151.592	151.592	0.0	2.477	1.053
4	0	2	230.714	237.471	237.471	0.0	-6.757	-1.938
6	0	2	54.136	56.622	56.622	0.0	-2.487	-2.029
8	0	2	90.475	91.258	91.258	0.0	-0.783	-0.453
10	0	2	103.623	104.283	104.283	0.0	-0.660	-0.354
0	0	0	228.829	234.171	234.171	0.0	-5.342	-1.543
-11	1	2	29.416	29.166	29.166	0.0	0.250	0.117
-9	1	2	32.244	33.936	-33.936	0.0	-1.692	-1.263
-7	1	2	178.919	182.097	182.097	0.0	-3.178	-1.158
-5	1	2	35.915	39.770	-39.770	0.0	0.145	0.152
-3	1	2	13.635	6.651	-6.651	0.0	6.984	5.304
-1	1	2	21.826	23.323	-23.323	0.0	-1.496	-1.602
1	1	2	120.801	112.885	112.885	0.0	7.917	4.244
3	1	2	69.234	68.836	68.836	0.0	0.398	0.328
5	1	2	37.737	39.520	-39.520	0.0	-1.783	-1.544
7	1	2	57.240	56.825	56.825	0.0	0.414	0.337
9	1	2	42.629	42.033	-42.033	0.0	0.576	0.452
-11	1	2	71.834	73.702	73.702	0.0	-1.868	-1.210
-12	2	2	8.224	6.361	-6.361	0.0	1.863	0.507
-6	2	2	29.676	30.675	-30.675	0.0	-0.999	-0.916
-4	2	2	12.482	15.079	-15.079	0.0	-2.598	-1.455
-2	2	2	11.669	9.048	-9.048	0.0	2.621	1.652
0	2	2	22.282	20.619	-20.619	0.0	1.662	1.562
0	2	2	228.617	234.171	234.171	0.0	-5.553	-1.605
2	2	2	4.811	2.353	-2.353	0.0	2.457	0.747

H	K	L	F(UBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
4	2	2	16.772	18.664	13.664	0.0	-1.892	-1.070
6	2	2	10.239	5.583	-5.583	0.0	4.656	1.920
8	2	2	22.184	21.411	-21.411	0.0	0.773	0.530
10	2	2	20.250	21.023	-21.023	0.0	-0.773	-0.365
-13	3	2	23.565	22.120	-22.120	0.0	1.445	0.775
-11	3	2	6.656	9.484	-9.484	0.0	-2.788	-0.637
-5	3	2	71.021	72.162	72.162	0.0	-1.141	-0.818
-7	3	2	59.455	101.071	-101.071	0.0	-1.576	-0.959
-5	3	2	17.958	21.924	-21.924	0.0	-3.965	-2.667
-3	3	2	14.026	10.957	10.957	0.0	3.028	1.952
-1	3	2	9.150	10.123	-10.123	0.0	-0.974	-0.487
1	3	2	84.949	83.536	-83.536	0.0	1.414	1.028
3	3	2	10.020	0.443	0.443	0.0	3.585	1.047
3	3	2	37.120	30.352	36.352	0.0	0.768	0.642
7	3	2	31.276	62.080	-62.080	0.0	-0.804	-0.545
9	3	2	45.554	45.459	-45.459	0.0	0.056	0.074
11	3	2	30.156	32.135	-32.135	0.0	-1.938	-0.999
-12	4	2	62.001	61.989	-61.989	0.0	0.012	0.009
-10	4	2	46.741	47.560	-47.560	0.0	-0.819	-0.660
0	4	2	229.007	234.171	-234.171	0.0	-5.163	-1.490
0	4	2	20.396	16.458	16.458	0.0	-3.898	-2.679
-6	4	2	99.430	99.869	99.869	0.0	-0.439	-0.271
-4	4	2	64.391	63.972	-63.972	0.0	0.418	0.367
-2	4	2	23.562	29.441	-29.441	0.0	-5.859	-5.359
0	4	2	104.728	99.172	99.172	0.0	5.550	3.389
2	4	2	77.343	80.486	80.486	0.0	-3.142	-2.433
4	4	2	81.455	80.558	-80.558	0.0	0.498	0.359
6	4	2	103.330	104.024	104.024	0.0	-0.694	-0.406
8	4	2	15.779	17.158	17.158	0.0	2.621	1.586
10	4	2	28.157	27.490	-27.490	0.0	0.707	0.472
-11	5	2	24.898	25.812	-25.812	0.0	-0.914	-0.556
-5	5	2	38.241	36.209	36.209	0.0	2.032	1.734
-7	5	2	55.809	57.413	-57.413	0.0	-1.604	-1.359
-3	5	2	30.684	30.550	-30.550	0.0	0.125	0.112
-1	5	2	21.193	17.706	17.706	0.0	3.486	3.079
1	5	2	69.356	70.721	-70.721	0.0	-1.325	-1.120
3	5	2	84.316	83.967	-83.967	0.0	0.348	0.251
5	5	2	33.203	30.234	30.234	0.0	2.969	2.967
7	5	2	35.283	34.779	-34.779	0.0	0.505	0.424
9	5	2	228.601	234.171	234.171	0.0	-5.570	-1.610
-10	6	2	54.258	53.480	-53.480	0.0	0.818	0.659
-8	6	2	14.074	14.146	-14.146	0.0	-0.072	-0.027
-6	6	2	19.502	19.390	-19.390	0.0	4.809	3.201
-2	6	2	8.906	9.530	-9.530	0.0	-1.023	-0.293
0	6	2	23.159	20.591	20.591	0.0	2.168	1.455
2	6	2	16.285	21.056	-21.056	0.0	-4.811	-2.333
4	6	2	19.502	18.030	18.030	0.0	1.473	1.029
6	6	2	5.136	6.157	-6.157	0.0	-1.021	-0.324
8	6	2	6.465	9.893	-9.893	0.0	-3.408	-1.227
4	6	2	11.945	11.595	-11.595	0.0	-0.050	-0.028
6	6	2	8.240	15.314	-15.314	0.0	-7.074	-2.146
8	6	2	27.612	27.398	-27.398	0.0	0.214	0.197
8	6	2	30.278	33.135	-33.135	0.0	-2.857	-2.082

*

*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
10	6	2	15.567	20.235	20.235	0.0	-C.668	-0.313
-13	7	2	34.406	33.450	33.450	0.0	C.955	C.604
-11	7	2	21.155	19.872	-19.872	0.0	1.321	C.795
-7	7	2	25.075	29.670	29.670	0.0	-0.595	-0.425
-7	7	2	9.702	9.163	9.163	0.0	0.539	C.158
-5	7	2	35.958	36.112	36.112	0.0	-0.113	-0.102
0	12	0	227.918	234.171	234.171	0.0	-6.252	-1.812
-3	7	2	44.653	42.889	-42.889	0.0	1.804	1.871
-1	7	2	46.708	45.018	45.018	0.0	1.690	1.662
1	7	2	18.186	18.297	18.297	0.0	-0.111	-0.079
3	7	2	9.231	11.122	-11.122	0.0	1.891	-0.652
3	7	2	23.013	21.529	21.529	0.0	1.484	1.085
5	7	2	19.535	16.737	16.737	0.0	2.798	1.830
9	7	2	18.959	14.252	-14.252	0.0	4.746	2.519
11	7	2	23.858	25.607	-25.607	0.0	-1.749	-0.861
-12	8	2	18.495	15.605	-15.605	0.0	2.890	1.660
-10	8	2	7.232	5.894	5.894	0.0	1.338	0.398
-8	8	2	18.446	19.682	-19.682	0.0	-0.636	-0.368
-6	8	2	11.181	8.313	-8.313	0.0	2.868	1.250
-4	8	2	56.573	56.289	-56.289	0.0	C.284	C.264
-2	8	2	92.409	85.664	-85.664	0.0	2.745	1.820
0	8	2	57.073	57.830	97.830	0.0	-0.757	-0.475
2	8	2	44.352	41.768	-41.768	0.0	2.583	2.354
4	8	2	15.878	15.632	15.632	0.0	0.246	0.129
6	8	2	7.411	2.450	2.450	0.0	4.961	1.362
8	8	2	5.753	4.461	-4.461	0.0	1.292	0.282
10	8	2	229.966	234.171	234.171	0.0	-4.204	-1.209
-11	9	2	20.738	20.078	-20.078	0.0	0.659	C.301
-9	9	2	5.134	7.894	7.894	0.0	1.239	0.410
-7	9	2	55.956	55.370	-55.370	0.0	C.586	0.488
-3	9	2	58.032	99.518	-99.518	0.0	-1.886	-1.178
-1	9	2	11.799	4.238	4.238	0.0	7.561	3.950
1	9	2	48.789	48.075	-48.075	0.0	C.713	C.672
3	9	2	83.405	85.616	-85.616	0.0	-2.210	-1.525
5	9	2	15.179	18.743	18.743	0.0	-3.563	-1.627
7	9	2	53.778	53.450	-53.450	0.0	0.328	0.256
9	9	2	9.134	3.712	-8.772	0.0	0.361	0.104
-12	10	2	6.858	4.065	4.065	0.0	2.793	0.650
-10	10	2	40.711	35.827	35.827	0.0	C.864	0.654
-8	10	2	42.613	44.202	44.202	0.0	-1.589	-1.272
-6	10	2	20.215	27.430	27.430	0.0	-1.216	-0.819
-4	10	2	57.825	57.983	57.983	0.0	-0.159	-0.134
-2	10	2	32.439	31.681	31.681	0.0	0.758	0.686
0	10	2	74.028	74.476	74.476	0.0	-0.448	-0.344
2	10	2	42.364	42.394	42.394	0.0	0.170	0.156
4	10	2	83.649	84.880	84.880	0.0	-1.231	-0.822
6	10	2	228.130	234.171	234.171	0.0	-6.041	-1.749
8	10	2	20.348	22.308	22.308	0.0	-1.960	-1.048
10	10	2	19.804	20.730	20.730	0.0	-1.976	-1.001
10	10	2	13.977	15.824	15.824	0.0	-1.847	-0.667
-11	11	2	55.517	54.507	54.507	0.0	1.010	0.721
-9	11	2	22.444	17.595	17.595	0.0	4.449	3.117
-7	11	2	155.053	159.764	159.764	0.0	-4.671	-1.903

H	K	L	F(0BS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-5	11	2	13.099	16.964	-16.964	0.0	-3.865	-1.710
-3	11	2	134.177	134.721	134.721	0.0	-0.544	-0.258
-1	11	2	5.654	6.915	-6.915	0.0	2.739	1.111
1	11	2	100.616	98.666	98.666	0.0	1.950	1.176
3	11	2	159.189	160.470	160.470	0.0	-1.281	-0.517
5	11	2	18.349	15.797	-15.797	0.0	2.552	1.621
7	11	2	60.880	60.711	60.711	0.0	0.169	0.124
-12	12	2	37.802	35.063	-35.063	0.0	2.759	1.868
-10	12	2	11.116	14.611	-14.611	0.0	-3.495	-1.002
-8	12	2	30.976	27.910	-27.910	0.0	3.066	2.383
-6	12	2	106.987	109.362	109.362	0.0	-2.375	-1.324
-4	12	2	29.457	26.548	-26.548	0.0	2.949	2.578
0	12	0	135.249	137.290	-137.290	0.0	-2.040	-0.957
0	12	0	228.130	234.171	234.171	0.0	-6.041	-1.750
0	12	0	220.540	224.307	224.307	0.0	-3.767	-1.123
2	12	2	1.706	5.276	-5.276	0.0	-3.570	-0.550
4	12	2	79.602	80.549	80.549	0.0	-0.947	-0.645
6	12	2	27.053	28.006	-28.006	0.0	-0.373	-0.250
8	12	2	37.786	39.628	-39.628	0.0	-1.842	-1.169
10	12	2	25.727	24.240	24.240	0.0	1.487	0.886
-9	13	2	10.590	12.212	-12.212	0.0	-1.615	-0.550
-7	13	2	40.077	38.562	-38.562	0.0	1.515	1.265
-5	13	2	59.401	61.471	-61.471	0.0	-2.070	-1.608
-3	13	2	23.175	23.858	-23.858	0.0	-0.723	-0.532
-1	13	2	73.183	75.346	-75.346	0.0	-2.163	-1.586
1	13	2	9.159	12.481	-12.481	0.0	-0.319	-0.177
3	13	2	48.447	48.765	48.765	0.0	0.319	-0.274
5	13	2	55.712	54.191	-54.191	0.0	1.521	1.177
7	13	2	22.021	22.707	-22.707	0.0	-0.686	-0.352
9	13	2	18.982	20.733	-20.733	0.0	-1.751	-0.717
-10	14	2	7.460	1.033	1.033	0.0	6.426	1.742
-8	14	2	18.154	18.583	18.583	0.0	-0.429	-0.219
-6	14	2	227.621	234.171	234.171	0.0	-6.350	-1.841
-2	14	2	33.707	32.694	-32.694	0.0	1.013	0.880
2	14	2	33.073	31.721	-31.721	0.0	1.352	1.113
4	14	2	14.432	14.119	14.119	0.0	0.313	0.138
6	14	2	26.101	26.643	26.643	0.0	-0.542	-0.332
-9	15	2	31.318	32.138	-32.138	0.0	-0.820	-0.514
-7	15	2	34.503	35.266	-35.266	0.0	-0.763	-0.506
-5	15	2	33.650	33.541	-33.541	0.0	0.150	0.109
-3	15	2	43.799	43.542	-43.542	0.0	0.257	0.203
-1	15	2	31.773	32.263	-32.263	0.0	-0.490	-0.389
1	15	2	5.329	9.718	-9.718	0.0	-0.389	-0.122
3	15	2	33.252	33.049	-33.049	0.0	0.203	0.144
5	15	2	33.530	35.036	-35.036	0.0	-1.609	-1.063
7	15	2	30.310	27.420	-27.420	0.0	2.891	2.111
-10	16	2	4.323	6.824	-6.824	0.0	-2.501	-0.420
-8	16	2	11.376	12.787	-12.787	0.0	1.410	0.464
-6	16	2	10.775	5.437	-5.437	0.0	1.338	0.501
-4	16	2	14.383	16.102	-16.102	0.0	-1.719	-0.754
0	16	0	229.722	234.171	234.171	0.0	-4.448	-1.280
-2	16	2	18.430	12.241	12.241	0.0	6.189	4.885
0	16	2	43.913	44.631	-44.631	0.0	-0.718	-0.610

H	K	L	F(UBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
4	16	2	33.767	33.717	33.717	0.0	-0.010	-0.008
4	16	2	32.147	32.271	-32.271	0.0	-0.124	-0.092
6	16	2	5.461	3.650	3.650	0.0	1.811	0.361
6	16	2	13.684	7.011	-7.011	0.0	6.674	3.348
7	17	2	8.337	5.959	5.959	0.0	2.379	0.662
5	17	2	6.322	0.285	0.285	0.0	6.037	1.518
3	17	2	13.392	13.135	-13.135	0.0	0.209	0.084
1	17	2	7.037	3.972	3.972	0.0	3.065	0.874
1	17	2	6.749	4.341	-4.341	0.0	2.404	0.649
3	17	2	2.633	4.509	-4.509	0.0	-1.877	-0.311
3	17	2	2.503	5.085	-5.085	0.0	-2.583	-0.370
2	17	2	25.012	23.829	23.829	0.0	1.183	0.723
6	16	2	17.566	14.247	14.247	0.0	3.321	1.743
4	16	2	25.167	29.344	29.344	0.0	-0.536	-0.389
2	18	2	15.911	15.693	15.693	0.0	0.218	0.094
0	12	2	229.430	234.171	234.171	0.0	-4.741	-1.365
2	18	2	33.759	32.321	32.321	0.0	1.435	1.200
2	18	2	20.998	20.618	20.618	0.0	0.380	0.232
4	16	2	32.845	32.208	32.208	0.0	0.637	0.416
6	16	2	45.034	44.558	-44.558	0.0	0.476	0.322
7	19	2	5.672	6.642	6.642	0.0	-0.970	-0.190
5	19	2	24.833	25.353	-25.353	0.0	-0.530	-0.297
3	19	2	13.310	9.665	-9.665	0.0	3.645	1.545
1	19	2	32.455	31.052	-31.052	0.0	1.404	0.979
3	19	2	5.249	5.876	-5.876	0.0	-0.627	-0.128
3	20	2	11.328	3.542	-3.542	0.0	7.786	2.818
0	20	2	4.973	10.140	10.140	0.0	-5.167	-0.851
4	20	2	49.374	49.214	-49.214	0.0	0.160	0.117
2	20	2	29.042	28.924	-28.924	0.0	0.119	0.074
2	20	2	26.763	26.612	-26.612	0.0	0.172	0.100
4	20	2	68.194	68.126	-68.126	0.0	0.068	0.045
7	21	2	8.265	12.263	-12.263	0.0	-4.023	-0.919
5	21	2	27.458	27.427	27.427	0.0	0.071	0.041
3	21	2	24.232	23.326	23.326	0.0	0.906	0.595
0	12	0	229.544	234.171	234.171	0.0	-4.627	-1.332
1	21	2	25.694	23.881	23.881	0.0	1.813	1.117
3	21	2	26.605	24.179	24.179	0.0	2.426	1.555
5	21	2	37.071	35.973	35.973	0.0	1.097	0.721
4	22	2	50.653	51.280	51.280	0.0	-0.623	-0.414
2	22	2	14.578	15.705	15.705	0.0	-1.127	-0.396
0	22	2	74.321	75.684	75.684	0.0	-1.563	-0.965
2	22	2	23.370	22.655	22.655	0.0	0.715	0.376
3	23	2	25.451	28.906	28.906	0.0	-3.455	-1.610
1	23	2	27.267	25.179	-25.179	0.0	2.108	1.210
1	23	2	30.651	33.937	33.937	0.0	-3.286	-1.656
1	23	2	18.917	16.126	-16.126	0.0	2.791	1.463
9	0	3	22.087	26.028	-26.028	0.0	-3.942	-2.526
7	0	3	3.397	2.289	-2.289	0.0	1.107	0.231
5	0	3	8.597	12.601	-12.601	0.0	-4.004	-1.286
3	0	3	18.641	18.975	-18.975	0.0	-0.334	-0.247
1	0	3	14.448	13.924	-13.924	0.0	0.524	0.285
3	0	3	14.302	14.749	-14.749	0.0	-0.447	-0.214
0	12	0	229.414	234.171	234.171	0.0	-4.757	-1.371

*

H	K	L	F(COBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
7	0	3	12.027	13.534	-13.334	0.0	-1.307	-0.464
9	0	3	23.663	15.452	19.852	0.0	3.011	2.750
-12	1	3	9.784	1.110	-1.110	0.0	8.674	3.125
-10	1	3	7.005	7.169	7.169	0.0	-0.164	-0.043
-8	1	3	7.980	4.305	-4.385	0.0	3.595	1.285
-4	1	3	11.571	15.422	15.422	0.0	-3.851	-1.508
-2	1	3	31.301	31.773	-31.773	0.0	-0.471	-0.448
0	1	3	30.403	30.519	30.519	0.0	-0.111	-0.055
2	1	3	33.203	33.645	-33.645	0.0	-0.442	-0.384
6	1	3	21.144	20.088	-20.088	0.0	1.056	0.556
8	1	3	18.170	17.884	17.884	0.0	0.286	0.167
10	1	3	21.566	19.576	-19.576	0.0	1.590	0.819
-11	1	3	19.697	16.303	16.303	0.0	3.395	1.938
-9	1	3	16.171	17.677	-17.077	0.0	-0.906	-0.451
-7	1	3	59.372	59.839	-59.839	0.0	0.034	0.028
-5	1	3	63.253	62.800	-62.800	0.0	0.453	0.378
0	1	3	229.137	234.171	234.171	0.0	-5.035	-1.452
-3	1	3	114.561	115.335	115.335	0.0	-0.775	-0.427
-1	1	3	6.663	3.275	3.275	0.0	3.388	1.203
1	2	3	10.206	7.797	7.797	0.0	2.410	1.047
3	2	3	56.541	56.298	56.298	0.0	0.243	0.209
5	2	3	13.148	13.184	13.184	0.0	-0.036	-0.017
7	2	3	34.438	36.634	36.634	0.0	-2.196	-1.441
9	2	3	26.458	24.721	-24.721	0.0	1.737	1.151
-12	3	3	33.414	31.722	-31.722	0.0	1.592	1.240
-1	3	3	64.492	64.642	-64.642	0.0	0.350	0.270
-4	3	3	9.085	4.407	-4.407	0.0	4.678	2.043
-2	3	3	110.335	110.540	-110.940	0.0	-0.605	-0.346
0	3	3	26.881	23.497	23.497	0.0	3.384	3.054
2	3	3	80.155	80.499	-80.499	0.0	-0.344	-0.245
0	3	3	61.156	60.844	-60.844	0.0	0.312	0.235
3	3	3	16.456	14.711	-14.711	0.0	1.784	0.852
10	3	3	9.085	0.790	0.790	0.0	8.294	2.525
-13	4	3	23.338	23.897	23.897	0.0	-0.559	-0.327
0	4	3	228.374	234.171	234.171	0.0	-5.797	-1.677
-11	4	3	3.689	4.239	-4.239	0.0	-0.549	-0.057
-9	4	3	13.132	6.401	6.401	0.0	6.730	3.621
-7	4	3	10.434	11.333	-11.333	0.0	-0.899	-0.332
-5	4	3	12.173	13.318	13.318	0.0	-1.145	-0.500
-3	4	3	11.766	9.566	9.566	0.0	0.701	1.081
-1	4	3	24.882	24.181	24.181	0.0	0.701	0.588
3	4	3	20.071	21.740	-21.740	0.0	-1.669	-1.119
5	4	3	12.985	13.229	13.229	0.0	-0.244	-0.110
7	4	3	12.270	13.912	-13.912	0.0	1.641	-0.692
9	4	3	11.193	14.521	14.521	0.0	-3.323	-1.067
-10	5	3	28.669	29.367	29.367	0.0	-0.699	-0.358
-12	5	3	56.537	56.316	56.316	0.0	0.221	0.124
-8	5	3	25.792	26.604	26.604	0.0	-0.812	-0.451
-6	5	3	70.713	71.610	71.610	0.0	-0.897	-0.658
-4	5	3	25.757	28.415	28.415	0.0	1.342	1.031
-2	5	3	26.555	28.506	28.506	0.0	-1.511	-1.304
0	5	3	192.489	153.244	193.244	0.0	-0.755	-0.258
5	5	3	22.834	22.910	22.910	0.0	-0.076	-0.054

H	K	L	F(0BS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
2	5	3	106.743	104.812	1.931	0.0	1.117	
0	5	3	53.2C9	-53.917	-0.591	0.0	-0.591	
0	12	0	229.202	234.171	-4.968	0.0	-1.432	
6	5	3	116.673	116.251	0.423	0.0	0.418	
8	5	3	33.479	34.511	-1.032	0.0	-0.704	
10	5	3	26.475	26.377	0.097	0.0	0.056	
-15	6	3	23.370	23.545	-0.175	0.0	-0.085	
-11	6	3	31.984	33.450	-1.466	0.0	-0.934	
-9	6	3	150.315	154.443	-4.128	0.0	-1.723	
-7	6	3	82.904	85.566	-2.792	0.0	-1.857	
-5	6	3	121.159	122.356	-1.197	0.0	-0.620	
-3	6	3	51.470	52.247	-0.777	0.0	-0.704	
-1	6	3	230.324	231.534	-1.210	0.0	-0.347	
1	6	3	25.857	28.749	-2.892	0.0	-2.047	
3	6	3	10.856	11.165	-0.328	0.0	-0.125	
5	6	3	125.027	125.473	-0.446	0.0	-0.220	
7	6	3	18.636	18.083	0.753	0.0	0.362	
9	6	3	114.544	115.231	-0.686	0.0	-0.344	
-12	7	3	47.855	45.020	2.874	0.0	2.048	
-10	7	3	9.036	5.434	3.602	0.0	1.158	
-8	7	3	14.318	13.007	1.311	0.0	0.716	
-6	7	3	31.854	31.234	0.620	0.0	0.562	
-4	7	3	39.704	40.357	-0.653	0.0	-0.635	
0	12	0	228.942	234.171	-5.228	0.0	-1.509	
-2	7	3	83.465	83.254	0.151	0.0	0.107	
0	7	3	41.020	39.133	1.887	0.0	1.754	
2	7	3	13.440	11.448	1.992	0.0	0.995	
4	7	3	95.204	95.639	-0.435	0.0	-0.269	
6	7	3	48.171	48.377	-0.206	0.0	-0.159	
8	7	3	11.636	8.447	3.190	0.0	1.150	
-11	8	3	15.033	8.338	6.695	0.0	3.157	
-9	8	3	23.988	21.063	2.925	0.0	2.213	
-7	8	3	2.909	5.973	-3.064	0.0	-0.543	
-5	8	3	12.173	13.948	-1.775	0.0	-0.768	
-3	8	3	11.198	10.419	0.779	0.0	0.332	
-1	8	3	12.173	8.217	3.956	0.0	1.895	
1	8	3	12.758	13.939	-1.182	0.0	-0.505	
3	8	3	6.728	15.563	-8.834	0.0	-2.114	
5	8	3	32.000	32.207	-0.207	0.0	-0.163	
7	8	3	17.057	14.076	3.021	0.0	1.695	
9	8	3	8.126	13.355	-5.229	0.0	-1.182	
-12	9	3	17.893	16.198	1.656	0.0	0.851	
-10	9	3	31.301	32.648	-1.347	0.0	-0.820	
-3	9	3	36.176	36.158	0.018	0.0	0.014	
0	12	0	428.817	234.171	-5.553	0.0	-1.605	
-6	9	3	28.506	31.569	-3.063	0.0	-2.119	
-4	9	3	38.939	39.829	-0.890	0.0	-0.656	
-2	9	3	62.847	63.542	-0.695	0.0	-0.567	
0	9	3	60.961	62.954	-1.993	0.0	-1.602	
2	9	3	33.772	35.567	-1.795	0.0	-1.406	
4	9	3	32.285	31.516	1.069	0.0	0.929	
6	9	3	28.669	28.161	0.507	0.0	0.336	
8	9	3	14.659	12.880	1.779	0.0	0.757	

*

*

H	K	L	F(UBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
-9	10	3	4.484	13.206	-13.206	0.0	-4.723	-1.254
-7	10	3	34.530	34.783	34.783	0.0	-0.247	-0.199
-5	10	3	63.529	67.556	-37.556	0.0	-4.027	-3.045
1	10	3	20.543	22.340	-22.340	0.0	-1.197	-1.159
3	10	3	19.951	22.365	22.365	0.0	-2.813	-1.481
5	10	3	13.847	12.969	12.969	0.0	0.878	0.405
7	10	3	12.027	5.191	5.191	0.0	6.875	3.000
9	10	3	24.979	27.446	-27.446	0.0	-2.467	-1.159
-12	11	3	4.876	3.699	3.699	0.0	1.177	0.219
0	12	0	229.365	234.171	234.171	0.0	-4.806	-1.385
-10	11	3	17.422	14.543	-14.543	0.0	2.874	1.685
-8	11	3	16.625	15.765	-15.765	0.0	0.861	0.393
-6	11	3	13.245	12.515	-12.915	0.0	0.331	0.137
-4	11	3	7.947	3.938	-3.938	0.0	4.009	1.276
-2	11	3	45.376	47.586	-47.586	0.0	-2.211	-1.875
0	11	3	11.019	4.766	-4.766	0.0	6.253	3.043
2	11	3	26.218	22.265	-22.265	0.0	-2.047	-1.230
4	11	3	29.627	30.803	-30.803	0.0	-1.176	-0.826
6	11	3	27.385	31.486	-31.486	0.0	-4.101	-2.342
-11	12	3	20.234	18.704	18.704	0.0	1.529	0.757
-7	12	3	21.160	19.692	19.692	0.0	1.468	0.752
-5	12	3	7.362	11.508	11.508	0.0	-4.146	-1.051
-3	12	3	20.608	20.787	20.787	0.0	-0.179	-0.115
-1	12	3	24.069	24.877	24.877	0.0	-0.808	-0.582
1	12	3	36.210	36.950	36.950	0.0	-0.341	-0.274
3	12	3	16.382	12.879	12.879	0.0	2.503	2.386
5	12	3	18.901	13.210	13.210	0.0	0.591	0.307
7	12	3	12.985	12.347	12.347	0.0	0.639	0.230
0	12	0	228.585	234.171	234.171	0.0	-5.586	-1.615
-10	13	3	12.514	12.066	12.066	0.0	0.449	0.159
-8	13	3	3.250	0.102	-0.102	0.0	3.148	0.533
-4	13	3	12.769	12.487	-12.487	0.0	0.222	0.104
-2	13	3	10.531	14.228	-14.228	0.0	-3.697	-1.292
0	13	3	38.615	37.249	37.249	0.0	1.366	1.141
2	13	3	43.653	41.128	-41.128	0.0	2.525	2.090
4	13	3	25.158	25.291	25.291	0.0	-0.133	-0.080
6	13	3	16.268	15.501	-15.501	0.0	0.767	0.292
8	13	3	11.880	10.574	10.574	0.0	1.206	0.393
-9	14	3	48.512	47.110	-47.110	0.0	1.402	0.955
-7	14	3	17.658	16.140	16.140	0.0	1.559	0.791
-5	14	3	63.480	64.582	-64.582	0.0	-1.102	-0.818
-3	14	3	39.167	39.548	39.548	0.0	-0.380	-0.286
-1	14	3	55.89	60.600	-60.600	0.0	-0.712	-0.560
1	14	3	8.191	10.468	-10.468	0.0	-2.277	-0.658
3	14	3	2.909	8.451	8.451	0.0	-5.542	-0.927
5	14	3	44.888	43.199	-43.199	0.0	1.689	1.269
7	14	3	13.944	15.931	15.931	0.0	-1.987	-0.635
0	12	0	229.885	234.171	234.171	0.0	-4.286	-1.232
-10	15	3	15.959	12.840	12.840	0.0	3.120	1.345
-8	15	3	16.561	17.126	-17.126	0.0	-1.165	-0.489
-6	15	3	11.539	10.547	10.547	0.0	0.992	0.365
-2	15	3	27.238	26.462	-26.462	0.0	0.776	0.545
0	15	3	29.562	28.649	28.649	0.0	0.913	0.720

*

*

*

H	K	L	F(ODS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
2	15	3	43.117	43.786	-43.786	0.0	-0.669	-0.488
4	15	3	16.902	16.420	16.420	0.0	0.482	0.217
6	15	3	20.851	20.334	-20.334	0.0	0.518	0.275
-9	16	3	47.147	47.383	47.383	0.0	-0.236	-0.151
-7	16	3	17.780	16.020	16.020	0.0	1.759	0.912
-5	16	3	70.145	71.639	71.639	0.0	-0.894	-0.610
-3	16	3	39.054	39.276	39.276	0.0	-0.223	-0.173
-1	16	3	77.132	77.469	77.469	0.0	-0.336	-0.217
1	16	3	55.322	56.847	56.847	0.0	-1.525	-1.084
3	16	3	48.106	48.759	48.759	0.0	-0.653	-0.487
5	16	3	40.012	39.138	39.138	0.0	0.875	0.585
7	16	3	32.975	32.904	32.904	0.0	0.071	0.043
-8	17	3	32.147	33.760	33.760	0.0	-1.014	-0.891
-6	17	3	13.830	14.364	14.364	0.0	-0.533	-0.158
0	17	0	225.430	234.171	234.171	0.0	-4.741	-1.366
-4	17	3	13.855	15.527	15.527	0.0	-1.631	-0.681
-2	17	3	103.119	103.815	103.815	0.0	-0.696	-0.385
0	17	3	14.188	10.406	-10.406	0.0	3.782	1.762
2	17	3	84.478	85.787	85.787	0.0	-1.289	-0.781
4	17	3	62.635	61.167	-61.167	0.0	1.409	1.028
0	17	3	80.545	81.218	81.218	0.0	-0.673	-0.400
-7	18	3	75.881	74.282	-74.282	0.0	1.599	1.054
-5	18	3	18.901	17.701	-17.701	0.0	1.200	0.542
-3	18	3	12.238	15.117	-15.117	0.0	-2.879	-0.962
-1	18	3	95.676	98.187	98.187	0.0	-2.512	-1.449
1	18	3	43.474	44.307	-44.307	0.0	-0.833	-0.575
3	18	3	30.953	32.359	-32.359	0.0	-1.366	-0.788
5	18	3	58.003	58.209	58.209	0.0	-0.205	-0.133
-6	19	3	7.736	2.015	-2.015	0.0	5.721	1.654
-4	19	3	11.718	6.876	-6.876	0.0	4.842	1.989
-2	19	3	15.179	16.061	16.061	0.0	-0.881	-0.521
0	19	3	6.452	8.158	-8.158	0.0	-2.306	-0.450
2	19	3	17.853	20.386	-20.386	0.0	-2.493	-0.965
4	19	3	51.990	53.443	-53.443	0.0	-1.453	-0.935
0	12	0	230.259	234.171	234.171	0.0	-3.912	-1.123
-7	20	3	26.328	23.639	23.639	0.0	-2.689	-2.039
-3	20	3	27.173	27.887	27.887	0.0	-0.714	-0.402
-1	20	3	5.217	1.116	-1.116	0.0	4.101	0.849
1	20	3	17.061	18.356	18.356	0.0	-1.315	-0.493
3	20	3	24.152	23.937	-23.937	0.0	0.814	0.423
-6	21	3	8.224	0.662	-0.662	0.0	7.561	2.071
-4	21	3	3.722	0.655	-0.655	0.0	3.067	0.552
-2	21	3	36.762	35.231	-35.231	0.0	1.532	0.957
0	21	3	20.331	18.181	-18.181	0.0	2.150	1.259
2	21	3	45.571	45.683	-45.683	0.0	-0.113	-0.075
-3	22	3	16.545	14.948	-14.948	0.0	1.597	0.729
-1	22	3	21.371	23.381	-23.381	0.0	-2.009	-0.932
1	22	3	5.152	1.403	-1.403	0.0	3.749	0.712
-12	0	4	13.570	12.608	-12.608	0.0	0.962	0.353
-10	0	4	48.902	49.779	49.779	0.0	-0.876	-0.612
-8	0	4	20.754	19.763	-19.763	0.0	0.991	0.684
-6	0	4	184.331	190.135	-190.135	0.0	-5.805	-2.042
-4	0	4	135.461	136.677	-136.677	0.0	-1.217	-0.568

*

*

H	K	L	F(ORBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-2	0	4	53.615	53.547	-53.547	0.0	0.068	0.059
0	12	0	230.113	234.171	234.171	0.0	-4.058	-1.165
0	0	4	186.247	186.400	186.400	0.0	1.847	0.659
0	0	4	7.183	7.140	7.140	0.0	0.043	0.012
4	0	4	172.954	175.710	175.710	0.0	-2.755	-1.022
0	0	4	25.077	24.924	24.924	0.0	0.153	0.089
0	0	4	65.951	66.376	66.376	0.0	-0.426	-0.276
8	0	4	8.922	11.051	11.051	0.0	-2.129	-0.527
-13	1	4	30.603	25.560	29.560	0.0	1.042	0.666
-11	1	4	21.469	20.106	-20.166	0.0	1.303	0.820
-9	1	4	79.342	78.799	78.759	0.0	0.544	0.373
-7	1	4	10.954	11.805	-11.805	0.0	-0.851	-0.321
-5	1	4	139.361	141.805	141.805	0.0	-2.443	-1.115
-3	1	4	79.570	80.736	-80.736	0.0	-1.166	-0.824
-1	1	4	2.162	2.616	-2.616	0.0	-0.454	-0.074
1	1	4	76.076	77.651	77.651	0.0	-1.575	-1.112
3	1	4	11.230	12.590	12.590	0.0	-1.359	-0.447
5	1	4	12.140	14.051	14.051	0.0	-1.911	-0.635
7	1	4	30.651	29.559	-29.559	0.0	1.092	0.604
9	1	4	14.253	12.785	-12.785	0.0	1.468	0.563
-12	2	4	13.522	15.457	-15.457	0.0	-1.976	-0.686
-10	2	4	2.698	3.839	3.839	0.0	-1.141	-0.203
-8	2	4	229.219	234.171	234.171	0.0	-4.952	-1.428
0	2	4	11.620	15.122	-15.122	0.0	-3.502	-1.362
-4	2	4	5.764	9.550	-9.550	0.0	-3.846	-0.970
0	2	4	18.166	16.826	-16.826	0.0	1.360	0.856
2	2	4	20.526	17.791	-17.791	0.0	2.736	2.063
6	2	4	21.583	16.633	-16.633	0.0	4.949	4.280
-11	3	4	20.022	20.466	-20.466	0.0	-0.443	-0.202
-9	3	4	24.086	22.665	-22.665	0.0	1.421	0.821
-7	3	4	14.513	17.306	-17.306	0.0	-2.792	-1.255
-2	3	4	35.517	36.455	36.455	0.0	-0.538	-0.473
-3	3	4	83.925	85.375	-85.375	0.0	-1.450	-0.985
-1	3	4	56.378	57.340	57.340	0.0	-0.962	-0.800
1	3	4	21.323	18.048	-18.048	0.0	3.274	2.570
3	3	4	46.432	46.652	-46.652	0.0	-0.220	-0.176
5	3	4	23.679	22.369	-22.369	0.0	1.310	0.833
7	3	4	22.558	23.526	-23.526	0.0	-1.368	-0.689
-12	4	4	25.109	22.497	-22.497	0.0	2.613	1.424
0	12	0	228.731	234.171	234.171	0.0	-5.440	-1.571
-10	4	4	3.202	1.509	1.509	0.0	1.693	0.304
-8	4	4	21.501	20.191	20.191	0.0	1.311	0.927
-4	4	4	36.056	35.102	35.102	0.0	0.994	0.759
-2	4	4	38.712	39.167	39.167	0.0	-0.455	-0.395
0	4	4	46.725	47.305	-47.305	0.0	-0.581	-0.513
2	4	4	99.934	99.826	99.826	0.0	0.108	0.064
4	4	4	15.943	14.557	-14.557	0.0	0.986	0.469
4	4	4	21.250	21.450	21.450	0.0	-0.192	-0.107
6	4	4	13.560	16.141	16.141	0.0	-2.180	-0.719
-11	4	4	25.353	29.056	-29.056	0.0	-3.703	-1.753
-7	5	4	5.621	4.721	-4.721	0.0	4.900	2.087
-5	5	4	5.834	1.858	-1.858	0.0	3.936	1.082
-3	5	4	48.805	50.636	-50.636	0.0	-1.831	-1.525

H	K	L	F (UBSI)	F (CALC)	Δ (CALC)	B (CALC)	DELTA F	DELTA/SIGMA
1	5	4	30.560	31.646	-31.848	0.0	-0.663	-0.690
3	5	4	32.537	31.380	-31.380	0.0	1.150	0.365
5	5	4	18.917	15.524	-15.524	0.0	3.393	2.385
7	5	4	7.573	6.394	-6.394	0.0	1.179	0.305
0	12	0	229.836	234.171	234.171	0.0	-4.334	-1.247
-12	6	4	13.895	9.692	-9.692	0.0	4.203	2.013
-10	6	4	13.115	11.769	-11.769	0.0	1.346	0.533
-6	6	4	17.043	15.566	-15.566	0.0	1.482	0.992
-6	6	4	6.111	5.139	-5.139	0.0	0.972	0.244
-4	6	4	2.763	1.846	-1.846	0.0	0.917	0.176
-2	6	4	9.914	7.469	-7.469	0.0	2.445	0.892
2	6	4	10.726	7.650	-7.650	0.0	3.076	1.413
4	6	4	8.987	9.049	9.049	0.0	-0.062	-0.019
6	6	4	29.270	28.712	-28.712	0.0	0.557	0.385
6	6	4	13.669	18.368	-18.368	0.0	-4.700	-1.329
-11	7	4	5.452	10.261	-10.261	0.0	-2.809	-0.790
-9	7	4	43.252	48.120	48.120	0.0	0.133	0.055
-7	7	4	26.492	26.259	-26.259	0.0	-1.767	-0.583
-5	7	4	31.269	29.021	-29.021	0.0	2.243	1.762
-3	7	4	17.032	15.616	-15.616	0.0	-2.584	-1.366
-1	7	4	15.147	13.406	-13.406	0.0	1.741	0.890
1	7	4	27.807	28.204	-28.204	0.0	-0.396	-0.292
3	7	4	39.956	37.855	-37.855	0.0	2.141	1.816
5	7	4	14.724	8.331	-8.331	0.0	6.593	3.481
7	7	4	228.292	234.171	234.171	0.0	-5.878	-1.701
7	7	4	20.526	15.640	-15.640	0.0	0.886	0.451
-12	8	4	47.115	46.566	-46.566	0.0	0.148	0.056
-10	8	4	63.123	60.730	-60.730	0.0	2.393	1.718
-8	8	4	12.092	14.053	14.053	0.0	-1.961	-0.668
-6	8	4	76.686	29.495	-29.495	0.0	-2.809	-1.661
-4	8	4	40.191	39.448	-39.448	0.0	0.743	0.628
-2	8	4	3.884	4.621	-4.621	0.0	-0.737	-0.154
2	8	4	56.281	56.582	56.582	0.0	-0.301	-0.229
4	8	4	76.385	76.659	-76.659	0.0	-0.274	-0.182
4	8	4	55.809	54.392	-54.392	0.0	1.418	1.018
6	8	4	4.144	2.829	-2.829	0.0	1.315	0.238
8	8	4	18.722	18.929	-18.929	0.0	-0.207	-0.073
-11	9	4	34.178	33.061	-33.061	0.0	1.117	0.738
-9	9	4	61.410	60.783	-60.783	0.0	0.633	0.462
-7	9	4	39.216	37.682	-37.682	0.0	1.534	1.306
-3	9	4	8.207	6.352	-6.352	0.0	1.856	0.611
-1	9	4	61.026	62.625	-62.625	0.0	-0.999	-0.754
1	9	4	20.201	19.686	-19.686	0.0	0.515	0.293
3	9	4	225.072	234.171	234.171	0.0	-5.098	-1.470
5	9	4	7.163	4.504	-4.504	0.0	2.679	0.673
7	9	4	56.850	57.573	-57.573	0.0	-1.123	-0.740
-10	10	4	16.447	22.563	22.563	0.0	-6.516	-2.170
-8	10	4	26.068	26.190	-26.190	0.0	-0.122	-0.077
-6	10	4	35.251	35.684	-35.684	0.0	-0.433	-0.319
-4	10	4	42.905	43.773	-43.773	0.0	-0.872	-0.706
-2	10	4	24.638	26.114	-26.114	0.0	-1.476	-0.897
0	10	4	50.544	48.404	-48.404	0.0	2.140	1.846
2	10	4	11.158	10.297	-10.297	0.0	0.901	0.329

I	K	L	F (UBS)	F (CALC)	A (CALC)	E (CALC)	DELTA F	DELTA/SIGMA
4	10	4	57.818	57.285	57.286	0.0	0.522	0.384
8	10	4	34.082	36.226	36.226	0.0	-1.544	-0.993
-11	11	4	35.655	38.935	38.935	0.0	0.722	0.437
-9	11	4	29.189	30.252	-30.252	0.0	-1.004	-0.612
-7	11	4	135.802	138.444	138.444	0.0	-2.642	-1.188
-5	11	4	13.603	15.844	15.844	0.0	-2.241	-0.961
-3	11	4	119.046	119.016	119.016	0.0	0.030	0.016
-1	11	4	11.535	14.509	-14.509	0.0	-2.970	-1.009
1	11	4	87.170	68.342	68.342	0.0	-1.172	-0.828
3	11	4	64.927	65.025	65.025	0.0	-0.098	-0.072
5	11	4	36.327	38.793	38.793	0.0	-0.406	-0.287
0	12	0	228.666	234.171	234.171	0.0	-5.505	-1.591
7	12	4	64.467	64.617	64.617	0.0	-0.410	-0.264
-10	12	4	53.827	52.539	52.539	0.0	1.233	0.989
-8	12	4	44.027	43.647	-43.647	0.0	0.380	0.276
-6	12	4	58.948	57.899	57.899	0.0	1.047	0.766
-4	12	4	104.111	102.884	102.884	0.0	1.227	0.691
-2	12	4	53.980	54.530	-54.530	0.0	-0.349	-0.641
0	12	4	46.042	44.611	44.611	0.0	1.451	1.127
2	12	4	12.124	15.694	-15.694	0.0	-3.570	-1.134
4	12	4	135.103	133.756	133.756	0.0	1.547	0.806
6	12	4	46.855	47.126	-47.126	0.0	-0.274	-0.180
-9	13	4	51.015	53.013	-53.013	0.0	-1.993	-1.422
-7	13	4	47.521	48.480	48.480	0.0	1.041	0.781
-5	13	4	24.411	23.549	-23.549	0.0	0.861	0.528
-3	13	4	17.747	16.772	16.772	0.0	0.975	0.558
-1	13	4	51.568	50.207	-50.207	0.0	1.361	1.064
1	13	4	14.568	9.470	-9.470	0.0	5.493	3.324
3	13	4	16.100	11.075	-11.075	0.0	5.031	2.822
-10	14	4	6.777	6.191	-6.191	0.0	0.626	0.128
-8	14	4	25.900	23.644	23.644	0.0	2.261	1.469
0	14	0	229.121	234.171	234.171	0.0	-5.049	-1.456
-6	14	4	2.389	3.188	-3.188	0.0	-0.799	-0.117
-4	14	4	9.670	6.326	6.326	0.0	3.344	1.141
-2	14	4	27.900	25.930	25.930	0.0	1.975	1.462
0	14	4	7.963	5.151	-5.151	0.0	2.813	0.840
2	14	4	18.349	20.272	20.272	0.0	-1.923	-0.764
4	14	4	7.395	2.495	2.495	0.0	4.899	1.340
6	14	4	32.179	23.045	23.045	0.0	-0.868	-0.460
-9	15	4	41.020	41.011	41.011	0.0	0.009	0.006
-7	15	4	33.804	34.358	-34.358	0.0	-0.554	-0.319
-5	15	4	25.597	24.562	24.562	0.0	0.635	0.390
-3	15	4	21.956	23.426	-23.426	0.0	-1.409	-0.699
-1	15	4	26.086	26.500	-26.500	0.0	-0.214	-0.148
1	15	4	24.000	24.517	-24.517	0.0	0.088	0.050
3	15	4	11.718	1.266	1.266	0.0	10.452	4.216
5	15	4	11.393	14.258	14.258	0.0	-2.866	-0.843
-3	16	4	12.027	8.896	-8.896	0.0	3.131	1.181
-0	16	4	15.179	16.757	16.757	0.0	-1.617	-0.936
-4	16	4	24.862	29.335	-29.335	0.0	-4.453	-2.497
-2	16	4	19.405	18.120	-18.120	0.0	1.234	0.765
0	16	4	2.649	2.003	-2.003	0.0	0.646	0.105
0	16	0	229.836	234.171	234.171	0.0	-4.334	-1.246

*

*

*

*

H	K	L	F(OBS)	F(CALC)	A(CALC)	F(CALC)	DELTA F	DELTA/SIGMA
2	16	4	22.379	19.957	19.957	0.0	2.422	1.346
4	16	4	53.339	52.530	-52.530	0.0	1.009	0.713
-7	17	4	15.957	15.200	-15.200	0.0	4.753	-4.258
-3	17	4	14.513	18.042	18.042	0.0	-3.529	-1.256
-1	17	4	1.836	6.715	-6.715	0.0	-4.879	-0.685
1	17	4	26.345	24.856	-24.856	0.0	1.446	0.892
3	17	4	18.105	19.490	19.490	0.0	-1.385	-0.666
-6	18	4	20.958	20.072	20.072	0.0	0.926	0.472
-4	18	4	11.149	11.258	11.258	0.0	-0.110	-0.032
-2	18	4	21.989	22.517	22.517	0.0	-0.528	-0.286
0	18	4	19.470	17.065	17.065	0.0	2.404	1.418
2	18	4	15.309	14.063	14.063	0.0	1.247	0.484
-2	18	4	13.148	14.213	14.213	0.0	-1.065	-0.359
-3	19	4	42.467	41.410	-41.410	0.0	1.057	0.731
-1	19	4	0.530	10.316	10.316	0.0	-3.783	-0.756
1	19	4	23.403	22.882	-22.882	0.0	0.521	0.253
-4	20	4	13.424	11.778	-11.778	0.0	1.646	0.558
0	20	4	51.746	50.844	-50.844	0.0	0.903	0.607
0	20	3	229.316	234.171	234.171	0.0	-4.854	-1.399
-9	0	5	23.614	20.890	-20.890	0.0	2.724	1.774
-5	0	5	13.180	9.175	-9.175	0.0	4.005	2.172
-3	0	5	17.433	17.375	-17.375	0.0	0.064	0.037
-1	0	5	17.951	17.308	-17.308	0.0	0.683	0.379
1	0	5	7.297	7.514	7.514	0.0	-0.217	-0.052
3	0	5	7.931	4.118	-4.118	0.0	3.813	1.127
5	0	5	9.654	0.692	-0.692	0.0	8.962	2.867
7	0	5	24.264	24.782	-24.782	0.0	-0.518	-0.256
-10	1	5	9.946	8.707	8.707	0.0	1.239	0.342
-8	1	5	4.778	4.523	-4.523	0.0	0.255	0.052
-2	1	5	13.213	17.125	17.125	0.0	-3.916	-1.525
0	1	5	15.033	15.140	15.140	0.0	-0.106	-0.048
2	1	5	16.723	11.616	-11.616	0.0	5.107	2.963
4	1	5	9.101	3.777	3.777	0.0	5.324	1.462
6	1	5	21.306	21.159	-21.159	0.0	0.148	0.069
0	12	3	230.064	234.171	234.171	0.0	-4.107	-1.180
-11	2	5	11.469	10.554	10.554	0.0	0.455	0.141
-9	2	5	11.425	10.735	-10.735	0.0	0.691	0.232
-7	2	5	44.319	43.634	-43.634	0.0	0.685	0.521
-5	2	5	52.933	51.594	-51.594	0.0	1.339	1.070
-3	2	5	70.404	70.543	70.543	0.0	-0.139	-0.101
-1	2	5	9.134	7.289	-7.289	0.0	1.845	0.611
1	2	5	24.102	22.959	-22.959	0.0	1.143	0.718
3	2	5	14.139	13.554	-13.554	0.0	0.585	0.261
5	2	5	22.038	20.812	-20.812	0.0	1.226	0.678
-12	3	5	34.048	34.253	-34.253	0.0	-0.205	-0.114
-10	3	5	25.256	26.403	26.403	0.0	-1.147	-0.566
-8	3	5	29.449	28.323	-28.323	0.0	1.126	0.665
-4	3	5	53.908	53.878	-53.878	0.0	0.030	0.023
-4	3	5	7.525	7.531	-7.531	0.0	-0.006	-0.002
-2	3	5	46.383	46.392	-46.392	0.0	-0.009	-0.007
4	3	5	64.147	62.594	-62.594	0.0	1.553	1.159
4	3	5	17.350	16.060	-16.060	0.0	1.329	0.599
6	3	5	43.490	41.674	-41.674	0.0	1.816	1.333

*

*

STRUCTURE FACTORS

II	R	L	F(UBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
0	12	0	229.527	234.171	234.171	C.0	-4.645	-1.337 *
-9	4	5	6.241	10.271	10.271	0.0	-4.030	-0.803
-2	4	5	5.524	7.601	7.601	0.0	-1.923	0.643
1	4	5	12.027	10.442	10.442	0.0	1.584	0.985
3	4	5	20.881	28.499	28.499	0.0	-1.618	-0.943
5	4	5	10.060	11.225	-11.325	0.0	-1.265	-0.340
-10	5	5	8.126	10.906	10.906	0.0	-2.780	-0.666
-3	5	5	92.247	93.039	93.039	0.0	-C.788	-0.467
-0	5	5	25.052	28.156	28.156	0.0	-1.536	-0.355
-4	5	5	10.041	16.635	16.635	0.0	-0.594	-0.269
-2	5	5	71.184	70.655	70.655	0.0	0.489	0.355
0	5	5	32.975	31.661	31.661	0.0	0.489	0.355
2	5	5	118.266	120.524	120.524	0.0	-2.458	-0.951
4	5	5	49.471	45.745	-45.745	0.0	-0.274	-1.128
6	5	5	51.825	58.729	58.729	0.0	-C.904	-0.183
-11	6	5	11.576	5.330	-5.330	0.0	6.648	-0.560
-9	6	5	129.610	128.812	128.812	0.0	C.798	2.633
0	12	0	228.244	234.171	234.171	0.0	-5.927	0.368
-7	0	5	9.685	0.564	0.564	0.0	9.301	-1.716 *
-5	0	5	79.554	76.159	76.159	0.0	-0.164	3.114
-3	0	5	50.853	51.725	-51.725	0.0	-C.872	-0.109
-1	0	5	167.770	165.657	169.657	0.0	-1.687	-C.681
1	0	5	36.811	33.647	33.647	0.0	3.163	-0.714
3	0	5	41.054	41.534	41.534	0.0	0.120	2.544
5	0	5	50.755	52.841	52.841	0.0	-2.086	C.065
-10	0	5	16.456	16.201	-16.201	0.0	C.295	-1.328
-6	0	5	37.705	36.610	36.610	0.0	C.894	0.117
-4	0	5	31.722	7.290	-7.290	0.0	-3.569	-0.609
-2	0	5	23.701	23.190	-23.190	0.0	C.512	0.366
0	0	5	4.339	3.265	3.285	0.0	1.054	C.211
2	0	5	14.903	11.027	-11.027	0.0	3.070	1.429
4	0	5	57.142	56.311	56.311	0.0	C.831	0.619
6	0	5	72.110	75.050	-75.050	0.0	-2.940	-1.321
-11	0	5	10.515	7.492	7.492	0.0	3.023	0.898
-9	0	5	6.680	1.421	-1.421	0.0	5.259	1.160
-7	0	5	1.528	4.272	-4.272	0.0	-2.745	-0.366
-5	0	5	3.234	1.668	-1.668	0.0	1.566	0.273
0	0	5	17.081	14.680	-14.680	0.0	2.201	1.073
3	0	5	228.666	234.171	234.171	0.0	-5.505	-1.550 *
-1	0	5	9.914	7.721	7.721	0.0	-2.193	0.788
1	0	5	13.538	16.217	-16.217	0.0	-2.679	-C.986
3	0	5	8.354	7.088	7.088	0.0	1.266	-0.442
5	0	5	12.514	20.219	20.219	0.0	-7.705	-2.020
-10	0	5	15.781	15.770	-15.770	0.0	0.011	0.005
-8	0	5	41.373	37.515	37.515	0.0	3.463	2.257
-6	0	5	26.751	28.601	-28.601	0.0	-1.850	-1.057
-4	0	5	15.585	18.040	18.040	0.0	-2.454	-0.551
0	0	5	20.071	16.312	16.312	0.0	3.759	2.322
-2	0	5	15.757	12.760	-12.780	0.0	3.017	1.554
0	0	5	34.154	35.265	-35.265	0.0	-1.071	-0.859
2	0	5	40.289	38.448	-38.448	0.0	1.840	1.392
4	0	5	43.734	44.272	44.272	0.0	-0.538	-0.553
-9	10	5	15.912	19.627	-19.627	0.0	-5.715	-1.822

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-7	10	5	18.797	19.256	19.256	0.0	-0.509	-0.221
-5	10	5	37.753	38.100	-38.100	0.0	-0.346	-0.242
-3	10	5	34.563	34.818	34.818	0.0	-0.250	-0.153
-1	10	5	18.074	19.373	-19.373	0.0	-0.699	-0.350
1	10	5	14.562	10.592	10.592	0.0	3.970	1.507
0	10	5	228.910	234.171	234.171	0.0	-5.261	-1.519
5	10	5	8.643	5.493	5.493	0.0	3.153	0.750
-10	11	5	9.550	8.959	-8.959	0.0	6.597	0.183
-8	11	5	4.466	1.275	-1.275	0.0	3.213	0.591
-6	11	5	14.383	10.227	-16.227	0.0	-1.844	-0.677
-4	11	5	16.008	15.622	-13.622	0.0	4.388	1.183
-2	11	5	14.919	17.510	-17.510	0.0	-2.590	-1.072
0	11	5	7.102	10.039	-10.039	0.0	2.957	-0.645
2	11	5	22.233	21.018	-21.018	0.0	1.215	0.642
4	11	5	13.180	12.374	-12.374	0.0	6.807	0.254
-9	12	5	8.809	7.506	-7.566	0.0	1.242	0.308
-7	12	5	15.456	17.468	-17.468	0.0	-2.012	-0.746
-5	12	5	13.034	10.588	-10.588	0.0	2.046	0.823
-1	12	5	27.710	27.469	27.469	0.0	0.241	0.143
3	12	5	15.163	17.893	-17.853	0.0	-2.750	-0.891
-6	13	5	19.154	17.090	-17.090	0.0	2.104	1.249
-4	13	5	15.439	11.549	-11.949	0.0	3.491	1.255
-2	13	5	15.553	14.307	-14.307	0.0	1.246	0.561
0	13	5	14.432	20.493	-20.493	0.0	-6.007	-1.802
0	13	5	229.957	234.171	234.171	0.0	-4.773	-1.376
0	13	5	20.572	26.350	26.350	0.0	0.214	0.123
4	13	5	11.425	10.513	10.513	0.0	0.913	0.313
-7	14	5	19.177	21.662	-21.662	0.0	-2.485	-1.008
-5	14	5	79.879	81.136	-81.136	0.0	-1.259	-0.766
-3	14	5	40.451	38.027	38.027	0.0	2.424	1.870
-1	14	5	28.148	27.674	-27.674	0.0	6.475	0.295
1	14	5	16.512	20.502	-20.502	0.0	-3.990	-1.455
3	14	5	14.139	13.590	-13.590	0.0	6.549	0.202
-6	15	5	18.836	17.436	-17.436	0.0	1.400	0.734
-4	15	5	7.006	10.286	-10.286	0.0	-2.660	-0.588
-2	15	5	32.325	30.521	-30.521	0.0	1.804	1.204
0	15	5	15.161	17.490	-17.490	0.0	1.672	0.761
2	15	5	15.488	16.719	-16.719	0.0	-1.230	-0.469
-7	16	5	19.502	16.044	-16.044	0.0	3.458	1.735
-5	16	5	49.357	45.757	-45.757	0.0	-0.439	-0.293
-3	16	5	20.006	19.047	-19.047	0.0	0.959	0.530
-1	16	5	56.752	55.598	-55.598	0.0	1.154	0.758
1	16	5	37.331	37.707	37.707	0.0	-0.376	-0.220
0	16	5	429.869	234.171	234.171	0.0	-4.302	-1.237
-2	17	5	57.110	57.668	57.668	0.0	-0.558	-0.372
-3	18	5	13.700	8.056	8.056	0.0	5.604	2.767
-10	0	6	69.382	69.459	-69.459	0.0	-4.077	-2.375
-8	0	6	121.939	120.702	-120.702	0.0	1.237	0.581
-6	0	6	49.942	49.485	-49.485	0.0	0.428	0.340
-4	0	6	44.453	40.664	-46.664	0.0	-2.166	-1.324
-2	0	6	113.862	114.771	-114.771	0.0	-0.909	-0.465
0	0	6	52.445	50.831	-50.831	0.0	1.614	1.179
0	0	6	57.971	57.429	-57.429	0.0	0.542	0.388

*

*

*

STRUCTURE FACTORS

H	N	L	F (UBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA
2	0	0	17.747	15.586	-15.586	0.0	1.761	0.820
4	0	0	134.973	133.187	-133.187	0.0	1.786	0.780
-7	1	0	28.457	28.614	-28.614	0.0	-0.157	-0.683
-7	1	0	56.850	56.146	-56.146	0.0	0.703	0.475
-5	1	0	22.598	23.605	-23.605	0.0	-0.717	-0.394
-3	1	0	79.277	81.913	-81.913	0.0	-2.636	-1.652
-1	1	0	10.629	7.222	-7.222	0.0	3.407	1.169
1	1	0	26.572	24.454	-24.454	0.0	2.078	1.207
-10	1	0	21.875	23.268	-23.268	0.0	-1.393	-0.647
0	2	0	15.163	13.899	-13.899	0.0	1.204	0.473
-8	2	0	3.835	2.177	-2.177	0.0	1.698	0.280
0	2	0	230.658	234.171	-234.171	0.0	-3.473	-0.280
-4	2	0	14.172	13.619	-13.619	0.0	0.552	0.213
0	2	0	11.425	9.672	-9.672	0.0	0.552	0.213
0	2	0	7.765	4.448	-4.448	0.0	3.337	0.832
2	2	0	7.768	13.338	-13.338	0.0	-5.569	-1.250
4	2	0	13.343	18.884	-18.884	0.0	-5.541	-1.725
-9	3	0	23.127	24.502	-24.502	0.0	-1.375	-0.708
-7	3	0	33.255	30.720	-30.720	0.0	2.516	1.545
-5	3	0	28.004	30.501	-30.501	0.0	-2.297	-1.286
-3	3	0	25.545	22.602	-22.602	0.0	-2.337	-1.172
-1	3	0	22.602	23.280	-23.280	0.0	-0.479	-0.291
1	3	0	30.749	30.019	-30.019	0.0	0.730	0.436
-1	3	0	13.229	13.366	-13.366	0.0	-0.136	-0.046
-10	3	0	41.313	40.504	-40.504	0.0	0.809	0.520
-8	4	0	19.755	17.543	-17.543	0.0	2.252	1.351
0	4	0	24.801	25.672	-25.672	0.0	-0.871	-0.453
-4	4	0	5.932	1.595	-1.595	0.0	3.937	0.954
0	4	0	6.430	10.618	-10.618	0.0	-4.182	-0.927
2	4	0	49.601	49.301	-49.301	0.0	0.300	0.210
0	4	0	230.600	234.171	-234.171	0.0	-3.571	-1.024
4	4	0	30.570	31.697	-31.697	0.0	-1.127	-0.608
-9	5	0	19.226	19.218	-19.218	0.0	0.008	0.003
-7	5	0	30.668	32.269	-32.269	0.0	-1.602	-0.986
-5	5	0	12.920	9.540	-9.540	0.0	3.372	1.654
-3	5	0	5.932	2.055	-2.055	0.0	3.877	0.840
1	5	0	41.053	39.706	-39.706	0.0	1.347	0.948
3	5	0	8.388	7.270	-7.270	0.0	1.116	0.270
0	6	0	12.238	10.923	-10.923	0.0	1.315	0.445
0	6	0	9.329	15.391	-15.391	0.0	-6.062	-1.394
-9	6	0	12.052	10.294	-10.294	0.0	1.797	0.528
-5	6	0	26.019	26.561	-26.561	0.0	-0.541	-0.266
-3	6	0	20.786	20.189	-20.189	0.0	0.617	0.300
-1	6	0	36.161	37.541	-37.541	0.0	-1.761	-1.015
1	6	0	2.113	3.299	-3.299	0.0	-1.187	-0.414
0	6	0	229.103	234.171	-234.171	0.0	-5.066	-1.461
-8	6	0	14.269	13.349	-13.349	0.0	0.920	0.326
-6	6	0	30.603	31.266	-31.266	0.0	-0.664	-0.412
-4	6	0	23.549	24.033	-24.033	0.0	-0.484	-0.258
-2	6	0	7.768	5.587	-5.587	0.0	2.182	0.524
0	6	0	52.283	51.794	-51.794	0.0	0.489	0.342
2	6	0	55.791	57.597	-57.597	0.0	2.194	1.359
-7	6	0	14.578	11.251	-11.251	0.0	3.327	1.559

STRUCTURE FACTORS

H	F	L	F (GROSS)	F (CALC)	A (CALC)	E (CALC)	DELTA F	DELTA/SIGMA
-9	9	6	10,140	14,959	14,595	0.0	2.071	0.863
-5	9	6	64,066	64,643	-64,843	0.0	-0.777	-0.919
-1	9	6	21,040	20,509	20,569	0.0	0.470	0.259
1	9	6	25,077	25,438	-25,438	0.0	-0.362	-0.188
-8	10	6	14,117	11,212	11,212	0.0	2.895	1.058
-0	10	6	23,419	20,092	20,092	0.0	3.327	2.126
-4	10	6	24,248	29,665	25,665	0.0	-1.417	-0.712
-2	10	6	25,357	25,665	25,665	0.0	-0.502	-0.241
0	10	6	35,641	33,993	33,993	0.0	1.688	1.092
-7	11	6	94,266	92,255	92,255	0.0	1.911	1.311
-5	11	6	4,329	11,009	-11,009	0.0	-6.669	-1.018
0	12	6	229,074	234,171	234,171	0.0	-4.497	-1.294
-9	11	6	134,664	134,395	134,395	0.0	0.269	0.119
-1	11	6	9,247	7,459	-7,459	0.0	1.768	0.489
1	11	6	34,022	33,594	33,594	0.0	0.436	0.220
-6	12	6	45,603	67,794	47,794	0.0	-2.191	-1.256
-4	12	6	35,603	27,516	37,516	0.0	-1.715	-0.920
0	12	6	56,261	55,450	55,450	0.0	0.790	0.464
-5	13	6	35,949	30,557	-36,657	0.0	-0.708	-0.431
-3	13	6	59,403	55,760	55,760	0.0	-0.376	-0.256
-1	13	6	30,213	32,044	-32,044	0.0	1.891	-1.015
-7	0	7	6,826	6,102	-6,102	0.0	0.824	0.168
-5	0	7	9,426	5,622	-3,622	0.0	5.804	1.719
-3	0	7	4,421	8,590	-8,590	0.0	-4.169	-0.717
-6	1	7	10,661	9,666	9,666	0.0	4.995	1.564
-4	1	7	7,752	4,085	4,085	0.0	3.687	0.844
-7	1	7	12,985	7,551	-7,551	0.0	5.434	2.437
-7	2	7	30,424	34,273	34,273	0.0	-3.849	-1.876
-5	2	7	39,427	38,905	-38,905	0.0	0.525	0.345
-3	2	7	41,183	39,900	39,900	0.0	1.282	0.841
1	2	7	228,959	234,171	234,171	0.0	-5.212	-1.505
-1	3	7	2,942	3,054	-3,054	0.0	-0.112	-0.016
-1	3	7	17,048	13,036	-13,036	0.0	4.013	1.914
-2	3	7	18,892	21,334	-21,334	0.0	-2.481	-0.983
-5	4	7	9,052	7,157	7,157	0.0	1.855	0.478
-3	4	7	10,171	1,501	-1,501	0.0	8.673	2.819
-1	4	7	7,470	4,667	-4,667	0.0	2.009	0.725
-0	5	7	20,410	27,563	27,563	0.0	-1.155	-0.564
-4	5	7	36,811	35,809	35,809	0.0	1.002	0.668
-2	5	7	19,945	21,349	21,349	0.0	-5.405	-1.580
-5	6	7	92,568	94,114	94,114	0.0	-1.526	-0.831
-3	6	7	57,906	56,806	-56,806	0.0	1.106	0.733

ALL REFLECTIONS

RESULTS OF STRUCTURE FACTOR CALCULATIONS

WEIGHTED R	NUMERATOR	DENOMINATOR	NUMBER	R
2467.66	1450325.00		1367	C.041
2787.64	63715.20		1367	C.044

RANGES OF F(OBS)

1850.22	15704.66		867	C.118
311.67	14137.77		275	C.022
114.86	7663.75		67	C.015
72.55	5307.46		42	C.014
35.64	1870.30		12	G.021
25.03	1529.04		8	G.016
563.93	16555.39		14	C.021
5.59	547.45		2	C.018

RANGES OF (SIN(THETA)/LAMBDA)**2

233.89	5584.44		64	C.042
575.93	22066.45		134	C.026
240.69	6499.38		145	C.034
250.77	6102.72		156	C.041
295.10	9524.75		168	C.053
350.85	9719.57		199	C.061
400.42	6066.12		208	C.067
460.25	6205.13		223	C.074

UNWEIGHTED REFLECTIONS

WEIGHTED R	UNWEIGHTED R			
1774.49	2159.27	1024513.38	1182	C.042
		42945.16	1182	C.051

RANGES OF F(OBS)

1693.61	14333.09		759	C.118
426.86	12528.01		244	G.021
103.49	6893.68		78	C.015
62.20	4662.73		37	C.013
34.81	1720.15		11	C.020
25.03	1529.04		8	C.016
11.73	681.58		3	G.017
5.59	547.45		2	C.018

RANGES OF (SIN(THETA)/LAMBDA)**2

173.34	4609.78		68	G.038
195.20	5203.70		101	C.038
206.66	5501.43		131	C.035
231.65	5517.79		143	C.042
261.94	5092.68		153	C.051
332.15	5241.56		186	C.064
361.12	5602.54		192	G.064
436.61	5656.77		208	G.077

SUM FCAL 63859.39
 STANDARD DEV OF UNIT WEIGHT CBS 1.28

K-ALUMINIUM 240, 1/15/73

ATOM 1

PARAMETER

GLD

CHANGE

NEW

ERRR

SHIFT/ERRDR

EXTINCTIEN CORRECTIEN

0.0

0.0

SCALE FACTR 1

0.e153

0.C000

0.e153

0.C016C

0.00

ATOM 1 0(1)

EQUIPUNT FRACTIEN = 1.000
OCCUPANCY SPECIES 1

X	1.C0000	0.0000017	0.1112329	1.C0000	0.0002141	0.01
Y	0.1112312	0.C000003	0.C0145715	0.C0145715	0.C001116	0.C0
Z	0.8918610	0.C000008	0.C8918618	0.C0011530	0.C004236	0.00
DETAIL1	0.0011524	0.C000009	0.C0011530	0.C002807	0.C000000	0.00
DETAIL2	0.0004072	0.C000001	0.C0004071	0.C0005584	0.C000000	0.00
BETA22	0.0001303	0.C000010	0.C001303	0.C0007577	0.C000000	0.00
BETA33	0.C001458	0.C000011	0.C001469	0.C0006859	0.C000000	0.00
BETA12	0.0000000	0.C000011	0.C000000	0.C0003240	0.C000000	0.00
BETA15	0.0000000	0.C000024	0.C000000	0.C000000	0.C000000	0.00
BETA23	-0.00000715	0.C000024	-0.C000000	-0.C000000	0.C0001623	0.01

ATOM 2 0(2)

EQUIPUNT FRACTIEN = 1.000
OCCUPANCY SPECIES 1

X	1.C0000	-0.C000019	0.1175913	1.C0000	0.1175913	0.01
Y	0.8313561	0.C000007	0.C013568	0.C013568	0.C0001179	0.01
Z	0.3518321	-0.C000019	0.3518320	0.3518320	0.C0004221	-0.03
DETAIL1	0.0013103	-0.C000009	0.0013058	0.C0002089	0.C000000	-0.02
DETAIL2	0.0000000	0.C000002	0.C000000	0.C000000	0.C000000	0.00
BETA22	0.0000000	0.C000002	0.C000000	0.C000000	0.C000000	0.00
BETA33	-0.0000000	-0.C000002	-0.C000000	-0.C000000	0.C000000	0.00
BETA12	0.C000000	-0.C000003	0.C000000	0.C000000	0.C000000	0.00
BETA15	0.C000000	0.C000009	0.C000000	0.C000000	0.C000000	0.00
BETA23	-0.0000000	0.C000009	-0.C000000	-0.C000000	0.C0001704	-0.01

ATOM 3 F(3)

EQUIPUNT FRACTIEN = 0.500
OCCUPANCY SPECIES 2

X	1.C0000	-0.0000002	0.1014631	1.C0000	0.1014631	0.00
Y	0.1014633	0.0	0.0	0.0	0.C0002685	-0.00
Z	0.3874525	0.C000003	0.3874567	0.3874567	0.C000000	0.01
DETAIL1	0.0000000	0.C000004	0.0000000	0.C000000	0.C0002572	0.02
DETAIL2	0.0000000	-0.C000000	0.0000000	0.C000000	0.C000000	-0.00
BETA33	0.C000000	-0.C0000149	0.C000000	0.C000000	0.C000000	-0.00
BETA12	0.0	0.0	0.0	0.0	0.C000000	-0.02
BETA15	-0.C000000	0.C000009	-0.C000000	-0.C000000	0.C000000	0.02
BETA23	0.0	-0.C000009	0.0	-0.C000000	0.C000000	0.02

ATOM 4 0(4)

EQUIPUNT FRACTIEN = 1.000
OCCUPANCY SPECIES 1

X	1.C0000	0.0000005	1.00000	1.C0000	0.0002386	0.00
Y	0.3605945	-0.C000002	0.3605950	0.3605950	0.C0001238	0.00
Z	0.7514645	-0.C000014	0.7514643	0.7514643	0.C0004733	-0.00
DETAIL1	0.5041114	-0.0000004	0.5041100	0.5041100	0.C0002227	-0.00
DETAIL2	0.0000000	0.C000004	0.0000000	0.0000000	0.C000000	0.01
BETA22	0.0000000	0.C000004	0.0000000	0.0000000	0.C000000	0.01
BETA33	0.0000000	-0.C0000151	0.0000000	0.0000000	0.C0008664	-0.02
BETA12	0.0000000	0.C000010	0.0000000	0.0000000	0.C000000	-0.01
BETA15	0.0000000	0.C000020	0.0000000	0.0000000	0.C000000	0.01
BETA23	-0.0000000	0.C000007	-0.C000000	-0.C000000	0.C0001723	0.00

ATOM 5 C(5)

EQUIPUNT FRACTIEN = 1.000
OCCUPANCY SPECIES 1

X	1.C0000	-0.C000005	1.C0000	1.C0000	0.0002263	-0.00
Y	0.3453760	0.C000001	0.3453755	0.3453755	0.C0001229	-0.00
Z	0.8657052	0.C000005	0.8697051	0.8697051	0.C0004376	0.01
DETAIL1	0.2456031	0.C000004	0.2496035	0.2496035	0.C000000	0.01
DETAIL2	0.0015273	0.C000004	0.0015273	0.0015273	0.C000000	0.01

ALUM 6 U(6) EQUIPINT FRACTION = 1.000
 OCCUPANCY SPECIES 1

BETA22	0.0006533	0.0000003	0.0000537	0.0000036	0.00
BETA23	0.0058013	0.0000094	0.0058057	0.0000076	0.01
BETA12	-0.0000083	0.0000000	-0.0000033	0.0000094	0.00
BETA13	0.00000549	0.0000021	0.0000070	0.0000094	0.01
BETA23	0.00005494	0.0000009	0.00005503	0.00001760	0.00

ALUM 7 U(7) EQUIPINT FRACTION = 0.500
 OCCUPANCY SPECIES 1

BETA22	0.0000000	-0.0000028	0.0000000	0.00002241	-0.01
BETA23	0.5417631	0.0000000	0.3417603	0.00002241	0.01
BETA12	0.8845921	0.0000000	0.8825928	0.00001228	0.01
BETA13	0.7486595	-0.0000010	0.7486649	0.00004357	-0.02
BETA22	0.0015084	0.0000007	0.0015091	0.00002149	0.00
BETA23	0.0000000	-0.0000003	0.0000004	0.00000633	-0.00
BETA12	0.0000000	0.0000000	0.0000000	0.0000000	0.00
BETA13	-0.0000000	0.0000000	0.0000000	0.0000000	0.00
BETA23	-0.0000000	-0.0000000	-0.0000000	0.0000000	0.00

ALUM 8 U(8) EQUIPINT FRACTION = 1.000
 OCCUPANCY SPECIES 3

BETA22	0.0000000	0.0000011	0.0000000	0.00003561	0.00
BETA23	0.2771781	0.0000003	0.2771766	0.0000000	0.02
BETA12	0.9151640	-0.0000000	0.9151637	0.00000424	-0.01
BETA13	0.5768894	-0.0000000	0.5768885	0.00001729	-0.01
BETA22	0.0010930	0.0000000	0.0010950	0.00000788	0.02
BETA23	0.0000000	-0.0000000	0.0000000	0.0000000	-0.00
BETA12	0.0042498	0.0000000	0.0042418	0.00003014	-0.03
BETA13	0.0000000	0.0000000	0.0000000	0.0000000	0.01
BETA23	0.0000000	-0.0000000	0.0000000	0.0000000	0.00

ALUM 9 U(9) EQUIPINT FRACTION = 1.000
 OCCUPANCY SPECIES 3

BETA22	0.2857828	0.0000000	0.2857828	0.0000000	0.00
BETA23	0.8284900	-0.0000000	0.8284958	0.00000428	-0.00
BETA12	0.4804572	0.0000000	0.4804579	0.00001687	0.00
BETA13	0.0010206	-0.0000000	0.0010269	0.00000787	-0.02
BETA22	0.0000000	0.0000000	0.0000000	0.0000000	0.01
BETA23	0.0051563	0.0000000	0.0051573	0.00000287	0.00
BETA12	0.0000000	-0.0000000	0.0000000	0.0000000	0.00
BETA13	0.0000000	-0.0000000	0.0000000	0.0000000	-0.01
BETA23	0.0000000	-0.0000000	0.0000000	0.0000000	-0.01

ALUM 10 U(10) EQUIPINT FRACTION = 0.500
 OCCUPANCY SPECIES 4

BETA22	0.0000000	0.0000000	0.0000000	0.0000000	0.01
BETA23	0.9106601	0.0000000	0.9106607	0.0000000	0.01
BETA12	0.5000000	-0.0000000	0.5000000	0.0000000	-0.00
BETA13	0.0014735	0.0000000	0.0014732	0.0000000	0.01
BETA23	0.0000000	0.0000000	0.0000000	0.0000000	0.01

BETA33 0.0033520
 BETA12 0.0
 BETA13 0.0000266
 BETA23 0.0

-C.0000000
 -0.0000002
 C.0033421
 C.0008264
 C.0002171

-0.02
 -0.00

ATOM 11 M(2)
 EQUIPPOINT FRACTION = C.900
 OCCUPANCY SPECIES 4

X 1.00000
 Y 0.0
 Z 0.8209632

0.0
 0.0
 0.0016773
 0.0003642
 0.0000004
 0.0000136
 0.0000025
 0.0

-0.0000005
 C.0000000
 -0.0000004
 0.0000136
 -0.0000025
 C.0003781
 C.0000000

C.0000000
 C.8209627
 C.0
 C.0010773
 0.0003639
 C.0006817
 C.0003781
 C.0000000

C.0000764
 C.0001472
 C.0000422
 C.0005602
 C.0002251

-0.01
 0.00
 -0.01
 0.02
 -0.01

ATOM 12 M(3)
 EQUIPPOINT FRACTION = C.250
 OCCUPANCY SPECIES 4

X 1.00000
 Y 0.0
 Z 0.0

0.0014908
 0.00002964
 0.00058017
 0.0
 0.0003719
 0.0

-C.0000001
 0.0000002
 0.0000093
 0.0
 0.0000041
 0.0

C.0014907
 C.0002965
 C.0058111
 0.0
 0.0003760
 0.0

C.0002026
 C.0000555
 C.0007636
 C.0003175

-0.00
 0.00
 0.01
 0.01
 0.01

ATOM 13 M(4)
 EQUIPPOINT FRACTION = 0.500
 OCCUPANCY SPECIES 5
 OCCUPANCY SPECIES 6
 TOTAL OCCUPANCY (FIXED) =

X 1.00000
 Y 0.0
 Z 0.7227494

0.50000
 C.50000
 1.00000

0.50000
 0.50000
 0.0031277
 0.0004417
 0.0052215
 0.0
 -0.0000001
 0.0000152
 0.0

-0.0000008
 -0.0000020
 -0.0000001
 0.0000152
 0.0
 -0.0000001
 0.0052215
 0.0

0.7227486
 C.5000000
 C.0031257
 0.0004416
 0.0052215
 0.0
 -0.0000001
 0.0052215
 0.0

C.0000676
 C.0001287
 C.0000324
 C.0004308
 C.0001828

-0.01
 -0.02
 -0.00
 C.04
 -0.02

ATOM 14 A
 EQUIPPOINT FRACTION = 1.000
 OCCUPANCY SPECIES 7

X 0.25000
 Y 0.4870853
 Z 0.0

0.25000
 0.4870853
 0.0

0.5154589
 0.0129226
 0.0020964
 0.0246585
 0.0
 -0.0116506
 0.0

-0.0071292
 -0.0011382
 -0.0000001
 0.0046877
 0.0
 -0.0013566
 0.0

0.5083297
 C.0117843
 0.0020963
 0.0333462
 0.0
 -0.0130132
 C.0040323

C.0066533
 C.0161876
 C.0035870
 C.0000738
 C.0108912
 C.0040323

-0.29
 -0.44
 -0.29
 -0.00
 0.43
 -0.34

MAXIMUM SHIFT/ERROR = -C.44
 AVERAGE SHIFT/ERROR = C.03