

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-4	5	3	23.344	23.517	23.917	0.0	-0.573	-0.700
-6	5	3	30.580	30.668	30.868	0.0	-0.288	-0.352
0	12	0	199.493	204.739	204.739	0.0	-5.246	-1.755 *
-8	5	3	51.290	51.475	51.475	0.0	-0.186	-0.202
-10	5	3	15.104	15.698	15.698	0.0	-0.594	-0.443
-12	5	3	63.270	61.223	61.223	0.0	2.047	1.836
-13	4	3	18.458	17.392	17.392	0.0	1.106	0.879
-9	4	3	11.524	11.566	11.566	0.0	-0.042	-0.026
-7	4	3	3.850	3.515	-3.915	0.0	-0.065	-0.018
-5	4	3	10.832	9.643	9.643	0.0	1.189	0.829
-3	4	3	9.203	8.250	8.250	0.0	0.952	0.664
-1	4	3	11.144	12.769	12.769	0.0	-1.625	-1.203
1	4	3	12.588	11.124	11.124	0.0	1.464	1.119
5	4	3	6.146	9.414	-8.414	0.0	-2.467	-0.926
9	4	3	12.985	13.278	13.278	0.0	-0.293	-0.161
10	3	3	7.860	8.551	8.551	0.0	-0.691	-0.258
8	3	3	11.837	9.405	-9.405	0.0	2.432	1.516
6	3	3	38.060	39.447	-39.447	0.0	-1.387	-1.611
4	3	3	3.858	5.438	5.438	0.0	-1.579	-0.462
2	3	3	59.707	60.261	-60.261	0.0	-0.554	-0.565
0	12	0	198.413	204.739	204.739	0.0	-6.327	-2.129 *
0	3	3	33.222	32.890	32.890	0.0	0.332	0.457
-2	3	3	96.475	95.284	-95.284	0.0	1.191	0.811
-4	3	3	17.730	14.639	14.639	0.0	3.090	3.624
-6	3	3	11.001	12.153	12.153	0.0	-1.152	-0.737
-8	3	3	42.733	44.752	-44.752	0.0	-1.018	-1.171
-10	3	3	14.809	12.868	12.868	0.0	1.940	1.563
-12	3	3	19.553	20.459	-20.459	0.0	-0.906	-0.675
-13	2	3	5.049	5.388	-5.388	0.0	-0.340	-0.091
-11	2	3	5.099	9.152	9.152	0.0	-4.052	-1.212
-9	2	3	27.574	27.915	-27.915	0.0	-0.341	-0.408
-7	2	3	43.852	43.545	43.945	0.0	-0.093	-0.108
-5	2	3	66.157	65.320	-65.320	0.0	0.837	0.793
-3	2	3	87.779	87.170	87.170	0.0	0.609	0.454
1	2	3	8.865	9.853	-9.853	0.0	-0.988	-0.603
3	2	3	46.401	46.384	46.884	0.0	-0.483	-0.572
5	2	3	8.924	5.482	-5.482	0.0	3.442	2.008
7	2	3	25.033	23.660	23.660	0.0	1.373	1.478
9	2	3	23.994	25.181	-25.181	0.0	-1.186	-1.033
10	1	3	6.518	7.520	-7.520	0.0	-1.003	-0.320
0	12	0	198.666	204.739	204.739	0.0	-6.073	-2.044 *
8	1	3	12.875	12.657	12.657	0.0	0.218	0.135
6	1	3	9.203	12.037	-12.037	0.0	-2.835	-1.435
2	1	3	21.048	21.250	-21.250	0.0	-0.202	-0.230
0	1	3	35.713	36.647	36.647	0.0	-0.934	-1.333
-2	1	3	22.897	22.199	-22.199	0.0	0.698	0.950
-4	1	3	25.446	25.787	25.787	0.0	-0.340	-0.453
-6	1	3	6.197	1.657	-1.657	0.0	4.540	1.941
-8	1	3	1.883	1.349	1.349	0.0	0.534	0.118
-13	0	3	12.551	9.002	-9.002	0.0	3.949	2.350
-11	0	3	10.418	9.893	9.893	0.0	0.525	0.276
-9	0	3	14.167	12.325	-12.325	0.0	1.842	1.515
-7	0	3	5.310	6.014	6.014	0.0	-0.703	-0.241

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-5	0	3	9.675	9.569	-9.569	0.0	0.106	0.066
-3	0	3	24.298	24.612	-24.612	0.0	-0.314	-0.465
-1	0	3	6.712	3.335	-3.335	0.0	3.377	1.942
1	0	3	8.595	1.971	1.971	0.0	6.624	4.359
?	0	3	18.456	19.022	-19.022	0.0	-0.566	-0.563
0	12	0	195.637	204.739	204.739	0.0	-5.102	-1.707
5	0	3	8.037	9.606	-9.606	0.0	-1.768	-0.845
7	0	3	10.756	9.663	-9.663	0.0	1.693	1.034
-10	0	4	36.169	36.105	36.105	0.0	0.064	0.070
-8	0	4	22.905	23.549	-23.549	0.0	-0.644	-0.652
-6	0	4	132.635	136.673	136.673	0.0	-4.038	-2.009
-4	0	4	126.101	127.600	127.600	0.0	-1.499	-0.782
-2	0	4	79.049	80.367	-80.367	0.0	-1.317	-1.061
0	0	4	155.169	158.517	158.517	0.0	-3.348	-1.432
2	0	4	4.635	4.518	4.918	0.0	-0.283	-0.093
4	0	4	121.770	124.355	124.355	0.0	-2.586	-1.386
6	0	4	12.597	10.016	10.016	0.0	2.580	1.689
8	0	4	28.570	28.563	28.963	0.0	-0.393	-0.347
7	1	4	19.908	19.592	19.592	0.0	0.316	0.264
5	1	4	8.814	7.197	7.197	0.0	1.617	0.805
3	1	4	76.449	77.573	77.573	0.0	-1.124	-0.918
1	1	4	7.472	2.929	-2.929	0.0	4.543	2.062
-1	1	4	45.971	44.707	-44.707	0.0	1.264	1.482
-3	1	4	123.163	125.562	125.562	0.0	-2.399	-1.286
0	12	0	197.712	204.739	204.739	0.0	-7.027	-2.371
-5	1	4	13.618	13.567	-13.567	0.0	-0.348	-0.253
-7	1	4	74.955	75.720	75.720	0.0	-0.765	-0.634
-9	1	4	17.865	17.211	-17.211	0.0	0.654	0.550
-11	1	4	22.956	25.747	25.747	0.0	-2.791	-2.312
-13	1	4	11.634	6.534	6.984	0.0	4.650	2.481
-12	2	4	5.817	1.196	-1.196	0.0	4.621	1.471
-10	2	4	1.967	5.397	-5.397	0.0	-3.430	-0.684
-6	2	4	8.485	8.425	-8.425	0.0	0.060	0.030
-4	2	4	6.197	5.547	-5.547	0.0	0.650	0.258
-2	2	4	11.845	10.411	-10.411	0.0	1.434	0.976
0	2	4	19.418	18.807	-18.807	0.0	0.611	0.561
2	2	4	13.026	17.267	-17.267	0.0	-4.232	-2.695
6	2	4	8.696	0.990	0.990	0.0	7.706	3.851
7	3	4	13.855	14.720	-14.720	0.0	-0.855	-0.523
5	3	4	21.630	21.472	21.472	0.0	0.158	0.156
3	3	4	38.668	39.735	-39.735	0.0	-1.067	-1.303
1	3	4	11.828	4.985	4.985	0.0	6.843	4.605
0	12	0	198.683	204.739	204.739	0.0	-6.056	-2.038
-1	3	4	42.703	43.822	43.822	0.0	-1.119	-1.352
-3	3	4	70.632	71.656	-71.656	0.0	1.024	-0.899
-5	3	4	38.938	39.603	39.603	0.0	-0.665	-0.788
-7	3	4	20.322	20.800	-20.800	0.0	-0.479	-0.465
-9	3	4	15.923	16.754	16.754	0.0	-0.831	-0.623
-11	3	4	13.559	15.129	-15.129	0.0	-1.570	-0.894
-13	3	4	0.701	4.626	-4.626	0.0	3.925	-0.574
-12	4	4	6.003	10.175	10.175	0.0	-4.173	-1.166
-10	4	4	7.100	5.583	-5.583	0.0	1.517	0.611
-8	4	4	16.607	18.521	18.521	0.0	-1.914	-1.501

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-6	4	4	12.589	15.116	-15.116	0.0	-2.527	-1.663
-2	4	4	43.522	43.655	-43.655	0.0	-0.132	-0.154
0	4	4	53.046	53.362	-53.362	0.0	-0.317	-0.338
2	4	4	66.672	66.742	-66.742	0.0	-0.070	-0.064
4	4	4	13.762	13.930	-13.930	0.0	-0.168	-0.122
6	4	4	13.069	8.953	8.953	0.0	4.116	2.724
8	4	4	8.823	6.142	6.142	0.0	2.681	1.176
7	5	4	10.300	1.420	-1.420	0.0	8.880	4.781
5	5	4	6.940	3.452	-3.452	0.0	3.488	1.440
0	12	0	158.936	204.739	-204.739	0.0	-5.803	-1.947
3	5	4	24.036	23.557	-23.957	0.0	0.079	0.086
-1	5	4	8.392	7.995	7.995	0.0	0.397	0.154
-3	5	4	34.252	33.560	-33.560	0.0	0.292	0.349
-5	5	4	16.143	15.177	-15.177	0.0	0.965	0.828
-7	5	4	7.092	0.609	0.609	0.0	6.483	2.953
-11	5	4	10.038	10.514	-10.914	0.0	-0.375	-0.396
-12	6	4	7.506	1.520	-1.520	0.0	5.985	2.195
-10	6	4	13.280	14.732	-14.732	0.0	-1.452	-0.877
-8	6	4	9.223	11.080	-11.080	0.0	-2.857	-1.267
-6	6	4	3.065	5.119	-5.119	0.0	-2.054	-0.547
-2	6	4	5.834	6.310	6.310	0.0	-0.476	-0.170
0	6	4	11.178	11.474	-11.474	0.0	-0.295	-0.176
4	6	4	7.151	0.456	0.456	0.0	6.695	3.050
6	6	4	13.306	11.635	11.635	0.0	1.671	1.124
8	6	4	14.724	13.566	-13.566	0.0	1.158	0.797
7	7	4	15.678	14.596	-14.996	0.0	0.683	0.490
0	12	0	198.058	204.739	-204.739	0.0	-6.681	-2.255
5	7	4	15.611	16.045	16.045	0.0	-0.435	-0.296
3	7	4	22.432	24.257	-24.257	0.0	-1.824	-1.786
1	7	4	15.214	16.634	-16.634	0.0	-1.420	-1.121
-1	7	4	17.468	15.867	15.867	0.0	1.601	1.415
-3	7	4	16.404	16.583	16.583	0.0	-0.178	-0.145
-5	7	4	19.612	16.671	16.671	0.0	2.942	3.083
-7	7	4	23.125	22.810	-22.810	0.0	0.315	0.316
-9	7	4	32.834	33.326	33.326	0.0	-0.492	-0.535
-11	7	4	15.974	15.551	-15.551	0.0	0.423	0.305
-12	8	4	31.542	30.521	30.921	0.0	0.621	0.541
-10	8	4	39.563	39.304	-39.304	0.0	0.258	0.278
-6	8	4	24.535	25.538	25.538	0.0	-1.404	-1.446
-4	8	4	38.170	38.174	-38.174	0.0	-0.005	-0.006
-2	8	4	6.400	8.126	-8.126	0.0	-1.726	-0.703
0	3	4	15.231	15.355	-15.355	0.0	-0.124	-0.100
2	8	4	47.423	47.293	47.293	0.0	0.130	0.142
4	8	4	64.224	64.120	-64.120	0.0	-0.496	-0.452
6	8	4	25.387	25.255	-25.255	0.0	0.132	0.131
0	12	0	198.911	204.739	-204.739	0.0	-5.828	-1.956
7	9	4	35.113	34.672	-34.672	0.0	1.041	1.063
5	9	4	14.285	13.411	13.411	0.0	0.874	0.595
3	9	4	18.143	18.182	-18.182	0.0	-0.039	-0.032
1	9	4	39.056	38.406	-38.406	0.0	0.550	0.770
-1	9	4	13.745	12.447	12.447	0.0	1.298	1.025
-3	9	4	24.067	22.862	-22.862	0.0	1.225	1.382
-5	9	4	8.899	8.560	8.960	0.0	-0.061	-0.030

*

*

*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-7	9	4	40.128	40.278	-40.278	0.0	-0.149	-0.165
-9	9	4	37.469	38.650	38.650	0.0	-0.581	-0.626
-11	9	4	12.048	10.005	-10.005	0.0	2.043	1.038
-10	10	4	11.702	10.720	10.720	0.0	0.982	0.519
-8	10	4	22.449	22.734	22.734	0.0	-0.285	-0.252
-6	10	4	22.297	23.388	23.388	0.0	-1.091	-1.068
-4	10	4	31.475	32.218	32.218	0.0	-0.744	-0.839
-2	10	4	16.210	14.621	14.621	0.0	1.589	1.437
0	10	4	31.145	32.073	32.073	0.0	-0.928	-1.067
2	10	4	10.461	9.811	9.811	0.0	0.650	0.365
4	10	4	31.559	31.112	31.112	0.0	0.447	0.485
6	10	4	13.694	15.579	15.579	0.0	-1.385	-1.039
7	11	4	45.422	45.552	45.552	0.0	-0.130	-0.122
0	12	0	198.438	204.739	204.739	0.0	-6.301	-2.120
5	11	4	15.999	16.695	16.695	0.0	-0.696	-0.469
3	11	4	62.316	63.524	63.524	0.0	-1.208	-1.126
1	11	4	50.783	51.553	51.553	0.0	-0.770	-0.807
-3	11	4	87.197	87.346	87.346	0.0	-0.150	-0.109
-5	11	4	12.715	12.574	12.974	0.0	-0.259	-0.166
-7	11	4	97.151	99.360	99.360	0.0	-2.210	-1.446
-9	11	4	30.461	30.874	-30.874	0.0	-0.413	-0.429
-11	11	4	27.177	28.537	28.537	0.0	-1.359	-1.193
-10	12	4	39.132	38.819	38.819	0.0	0.313	0.328
-8	12	4	20.896	21.546	-21.946	0.0	-1.050	-0.840
-6	12	4	34.379	32.674	32.674	0.0	1.705	1.941
-4	12	4	83.372	82.891	82.891	0.0	0.481	0.361
-2	12	4	50.454	50.578	-50.978	0.0	-0.525	-0.555
0	12	4	44.139	42.719	42.719	0.0	1.419	1.585
2	12	4	24.957	26.431	-26.481	0.0	-1.524	-1.452
4	12	4	90.489	91.134	91.184	0.0	-0.694	-0.478
6	12	4	31.950	29.295	-29.295	0.0	2.694	2.775
5	13	4	12.394	10.587	-10.587	0.0	1.807	1.034
0	12	0	198.007	204.739	204.739	0.0	-6.732	-2.272
1	13	4	3.158	2.292	-2.292	0.0	0.865	0.218
-1	13	4	32.868	33.690	-33.690	0.0	-0.822	-0.877
-3	13	4	18.363	20.398	20.398	0.0	-2.035	-1.651
-5	13	4	19.536	15.575	-16.575	0.0	2.962	2.924
-7	13	4	41.741	41.623	41.623	0.0	0.118	0.125
-9	13	4	38.170	37.302	-37.302	0.0	0.868	0.878
-10	14	4	2.356	4.137	-4.137	0.0	-1.782	-0.332
-8	14	4	11.752	8.592	8.592	0.0	3.160	1.817
-6	14	4	5.538	7.051	-7.051	0.0	-1.513	-0.487
-4	14	4	5.023	1.129	1.129	0.0	3.894	1.307
-2	14	4	12.200	12.116	12.116	0.0	0.084	0.054
0	14	4	7.801	9.731	-9.731	0.0	-1.930	-0.786
6	14	4	11.440	9.192	9.192	0.0	2.248	1.078
5	15	4	20.887	18.796	18.796	0.0	2.092	1.708
1	15	4	9.439	7.168	-7.168	0.0	2.271	1.080
-1	15	4	21.048	22.654	22.654	0.0	-1.606	-1.378
-3	15	4	16.007	16.534	-16.584	0.0	-0.577	-0.443
0	12	0	198.202	204.739	204.739	0.0	-6.538	-2.200
-5	15	4	19.992	19.073	19.073	0.0	0.920	0.819
-7	15	4	20.659	21.777	-21.777	0.0	-1.117	-0.817

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-9	15	4	24.180	25.840	25.840	0.0	-1.660	-1.294
-8	16	4	7.387	1.039	-1.039	0.0	6.349	2.395
-6	16	4	15.855	15.993	15.993	0.0	-0.138	-0.055
-4	16	4	17.510	17.422	-17.422	0.0	0.088	0.069
-2	16	4	8.519	8.530	-8.530	0.0	-0.011	-0.005
0	16	4	8.054	7.794	-7.794	0.0	0.260	0.109
2	16	4	17.941	19.720	19.720	0.0	-1.779	-1.247
4	16	4	35.958	37.667	-37.667	0.0	-1.710	-1.582
3	17	4	3.267	6.707	6.707	0.0	-3.439	-0.749
1	17	4	14.395	14.591	-14.591	0.0	-0.587	-0.358
-1	17	4	2.896	3.554	3.954	0.0	-1.058	-0.245
-3	17	4	14.614	14.486	14.486	0.0	0.128	0.097
-7	17	4	9.458	8.735	-8.735	0.0	0.763	0.337
-6	18	4	8.856	10.033	10.033	0.0	-1.176	-0.452
-2	18	4	6.258	8.858	8.858	0.0	-2.560	-0.828
0	18	4	2.144	4.578	4.578	0.0	-2.433	-0.486
0	12	0	197.400	204.739	204.739	0.0	-7.340	-2.484
2	18	4	4.728	6.063	6.063	0.0	-1.335	-0.344
1	19	4	8.316	7.734	-7.734	0.0	0.592	0.227
-1	19	4	8.054	4.563	4.963	0.0	3.091	1.204
-3	19	4	21.343	22.673	-22.673	0.0	-1.329	-1.016
-5	19	4	14.167	13.410	13.410	0.0	0.757	0.450
-4	20	4	11.279	11.367	-11.367	0.0	-0.088	-0.039
-2	20	4	12.504	12.556	12.556	0.0	-0.053	-0.028
0	20	4	35.248	34.551	-34.551	0.0	0.687	0.695
-3	18	5	44.004	43.661	-43.661	0.0	0.342	0.335
0	17	5	7.033	0.423	-0.423	0.0	6.610	2.316
-2	17	5	47.212	46.850	46.850	0.0	0.361	0.342
-6	17	5	9.169	8.333	8.333	0.0	0.836	0.342
-7	16	5	4.821	6.452	6.452	0.0	-1.632	-0.397
-5	16	5	26.147	24.859	24.859	0.0	1.288	1.192
-3	16	5	14.218	14.158	14.158	0.0	0.059	0.036
-1	16	5	29.685	29.493	29.493	0.0	0.191	0.183
1	16	5	22.447	21.056	21.056	0.0	1.341	1.088
2	15	5	13.289	11.326	-11.326	0.0	1.963	1.129
0	15	5	19.874	19.237	19.237	0.0	0.507	0.458
0	12	0	196.961	204.739	204.739	0.0	-7.779	-2.640
-2	15	5	20.094	19.609	-19.609	0.0	0.484	0.385
-4	15	5	16.269	15.830	15.830	0.0	0.439	0.285
-6	15	5	15.281	14.448	14.448	0.0	0.833	0.528
-8	15	5	21.056	20.578	-20.578	0.0	0.478	0.350
-7	14	5	23.158	22.402	22.402	0.0	0.757	0.627
-5	14	5	52.016	51.697	-51.697	0.0	0.319	0.317
-3	14	5	28.908	28.422	28.422	0.0	0.485	0.484
-1	14	5	18.388	18.156	-18.156	0.0	0.232	0.179
1	14	5	20.229	15.960	-16.960	0.0	3.269	2.652
3	14	5	4.179	4.860	-4.860	0.0	-0.681	-0.163
4	13	5	14.454	9.749	9.749	0.0	4.705	2.903
2	13	5	4.677	7.586	-7.586	0.0	-2.909	-0.761
0	13	5	20.491	20.569	20.569	0.0	-0.079	-0.063
-2	13	5	17.848	16.517	-16.517	0.0	1.331	1.072
-4	13	5	13.821	11.965	11.965	0.0	1.856	1.175
-6	13	5	5.059	0.478	-0.478	0.0	4.621	1.355

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-8	13	5	10.038	9.253	-9.253	0.0	0.785	0.346
-9	12	5	7.548	9.453	-9.453	0.0	-1.905	-0.660
-7	12	5	9.253	10.671	10.671	0.0	-1.418	-0.627
-5	12	5	1.098	5.719	5.719	0.0	-4.621	-0.810
0	12	0	196.724	204.739	204.739	0.0	-8.015	-2.720 *
-1	12	5	5.682	0.697	0.697	0.0	4.985	1.707
1	12	5	9.988	12.650	12.650	0.0	-2.663	-1.166
3	12	5	4.255	4.591	4.591	0.0	-0.336	-0.084
2	11	5	11.946	10.182	-10.182	0.0	1.765	0.995
-2	11	5	12.149	9.268	-9.268	0.0	2.881	1.875
-4	11	5	8.823	3.459	3.459	0.0	5.363	2.715
-6	11	5	10.157	6.002	-6.002	0.0	4.155	2.140
-8	11	5	5.319	4.841	4.841	0.0	0.479	0.138
-10	11	5	2.204	0.102	0.102	0.0	2.101	0.404
-9	10	5	16.615	15.425	-15.425	0.0	1.191	0.801
-7	10	5	19.469	19.279	19.279	0.0	0.190	0.147
-5	10	5	26.308	27.968	-27.968	0.0	-1.661	-1.613
-3	10	5	26.232	26.083	26.083	0.0	0.148	0.164
-1	10	5	11.693	12.831	-12.831	0.0	-1.137	-0.635
1	10	5	8.662	0.839	-0.839	0.0	7.823	3.893
3	10	5	5.310	1.668	1.668	0.0	3.642	1.160
5	10	5	7.590	5.145	-5.145	0.0	2.445	0.886
0	12	0	198.666	204.739	204.739	0.0	-6.073	-2.044 *
4	9	5	31.753	31.123	31.123	0.0	0.630	0.612
2	9	5	22.635	26.135	-26.135	0.0	-3.500	-2.840
0	9	5	28.925	30.012	30.012	0.0	-1.087	-1.091
-2	9	5	14.116	13.869	-13.869	0.0	0.247	0.172
-4	9	5	14.690	16.482	16.482	0.0	-1.792	-1.256
-8	9	5	19.975	22.203	-22.203	0.0	-2.228	-1.681
-10	9	5	22.930	21.907	21.907	0.0	1.024	0.892
-11	8	5	0.844	0.905	-0.905	0.0	-0.061	-0.010
-5	8	5	9.870	9.509	-9.509	0.0	0.370	0.152
-1	8	5	9.371	12.002	-12.002	0.0	-2.631	-1.262
1	8	5	5.623	1.139	-1.139	0.0	4.484	1.571
5	8	5	10.984	10.880	-10.880	0.0	0.104	0.048
6	7	5	3.301	7.757	7.757	0.0	-4.456	-0.948
4	7	5	45.270	47.258	-47.258	0.0	-1.988	-1.946
2	7	5	51.214	51.727	51.727	0.0	-0.513	-0.524
0	12	0	198.438	204.739	204.739	0.0	-6.301	-2.120 *
0	7	5	16.117	14.219	-14.219	0.0	1.898	1.499
-2	7	5	22.677	23.036	23.036	0.0	-0.359	-0.332
-4	7	5	21.993	22.656	-22.656	0.0	-0.663	-0.600
-6	7	5	9.777	6.788	6.788	0.0	2.988	1.694
-8	7	5	33.028	31.925	31.925	0.0	1.103	1.221
-10	7	5	12.664	10.543	-10.543	0.0	2.121	1.191
-9	6	5	92.845	51.994	91.994	0.0	0.851	0.569
-7	6	5	15.332	14.492	-14.492	0.0	0.840	0.634
-5	6	5	65.127	64.189	64.189	0.0	0.938	0.848
-3	6	5	43.801	43.930	-43.930	0.0	-0.129	-0.144
-1	6	5	116.577	116.243	116.243	0.0	0.335	0.187
1	6	5	34.117	33.150	33.150	0.0	0.967	1.112
3	6	5	11.589	6.122	6.122	0.0	5.867	3.736
5	6	5	40.553	41.518	41.518	0.0	-0.925	-0.891

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
6	5	5	36.810	37.651	37.051	0.0	-0.241	-0.240
4	5	5	30.748	30.183	-30.183	0.0	0.566	0.603
2	5	5	92.448	93.547	93.547	0.0	-1.099	-0.752
0	5	5	14.825	17.143	17.143	0.0	-2.318	-1.596
-2	5	5	71.611	71.750	71.750	0.0	-0.138	-0.118
0	12	0	198.742	204.739	204.739	0.0	-5.997	-2.012
-6	5	5	26.662	25.693	25.693	0.0	0.969	1.083
-8	5	5	59.927	59.290	59.290	0.0	0.637	0.599
-10	5	5	5.361	3.056	3.056	0.0	2.306	0.691
-12	5	5	36.034	36.429	36.429	0.0	-0.395	-0.371
-11	4	5	4.947	2.781	2.781	0.0	2.167	0.607
-9	4	5	12.006	12.638	12.638	0.0	-0.632	-0.374
-7	4	5	5.961	2.829	2.829	0.0	3.132	1.159
-5	4	5	3.647	7.970	7.870	0.0	-4.223	-1.116
-3	4	5	5.251	1.614	-1.614	0.0	3.638	1.302
-1	4	5	5.522	3.729	3.729	0.0	1.792	0.645
1	4	5	3.343	5.506	5.906	0.0	-2.563	-0.663
3	4	5	11.068	9.876	9.876	0.0	1.193	0.703
5	4	5	6.408	6.762	-6.762	0.0	-0.353	-0.115
6	3	5	20.339	20.123	-20.123	0.0	0.215	0.164
4	3	5	17.738	18.745	18.745	0.0	-1.007	-0.774
2	3	5	43.337	43.416	-43.416	0.0	-0.079	-0.088
0	3	5	16.935	16.086	16.086	0.0	0.748	0.620
-2	3	5	35.367	34.907	-34.907	0.0	0.460	0.539
-4	3	5	9.873	9.189	9.189	0.0	0.689	0.387
0	12	0	199.004	204.739	204.739	0.0	-5.736	-1.924
-6	3	5	7.531	1.702	-1.702	0.0	5.829	2.645
-8	3	5	33.619	34.212	-34.212	0.0	-0.593	-0.645
-10	3	5	26.375	25.359	25.359	0.0	1.016	0.955
-12	3	5	18.540	16.733	-16.733	0.0	1.757	1.156
-11	2	5	12.554	8.841	8.841	0.0	3.714	2.115
-9	2	5	19.570	20.654	-20.654	0.0	-1.083	-0.873
-7	2	5	31.230	30.652	30.652	0.0	0.578	0.658
-5	2	5	46.975	47.756	-47.756	0.0	-0.780	-0.856
-3	2	5	45.827	46.559	46.559	0.0	-0.732	-0.833
-1	2	5	8.156	10.502	-10.502	0.0	-2.346	-1.061
1	2	5	3.318	3.362	3.362	0.0	-0.044	-0.011
3	2	5	5.640	10.011	10.011	0.0	-4.371	-1.377
5	2	5	7.666	0.801	0.801	0.0	6.865	2.775
6	1	5	7.438	11.465	-11.465	0.0	-4.027	-1.321
4	1	5	10.503	9.831	9.831	0.0	0.672	0.329
2	1	5	4.517	6.534	-6.534	0.0	-2.067	-0.615
0	1	5	16.590	18.819	18.819	0.0	-2.230	-1.809
-2	1	5	15.779	12.551	-12.551	0.0	3.228	3.034
-4	1	5	9.616	11.779	11.779	0.0	-2.163	-1.143
-6	1	5	3.436	0.556	0.556	0.0	2.480	0.666
0	12	0	197.889	204.739	204.739	0.0	-6.850	-2.312
-8	1	5	3.455	0.262	0.262	0.0	3.233	0.844
-10	1	5	6.349	4.572	4.572	0.0	1.777	0.600
-12	1	5	8.063	3.085	-3.085	0.0	4.978	1.927
-11	0	5	12.816	11.221	11.221	0.0	1.596	0.896
-9	0	5	10.756	8.600	-8.600	0.0	2.156	1.172
-3	0	5	13.863	13.459	-13.459	0.0	0.404	0.299

*

*

*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-1	0	5	9.295	11.275	-11.275	0.0	-1.979	-0.989
1	0	5	4.120	2.728	2.728	0.0	1.392	0.411
3	0	5	9.414	7.392	-7.392	0.0	2.021	1.010
5	0	5	10.427	5.169	-5.169	0.0	5.258	2.857
-10	0	6	72.228	71.169	71.169	0.0	1.059	0.848
-8	0	6	23.659	24.758	-24.758	0.0	-1.059	-0.847
-6	0	6	15.754	15.965	-15.965	0.0	-0.211	-0.145
-4	0	6	83.819	83.181	83.181	0.0	0.638	0.473
-2	0	6	22.491	21.845	21.845	0.0	0.647	0.563
0	0	6	48.090	48.427	48.427	0.0	-0.337	-0.344
2	0	6	32.049	31.204	-31.204	0.0	0.844	0.885
4	0	6	86.217	85.456	85.456	0.0	0.761	0.530
0	12	0	199.493	204.739	204.739	0.0	-5.246	-1.755
3	1	6	9.498	1.113	1.113	0.0	8.385	3.850
1	1	6	19.199	18.315	18.315	0.0	0.883	0.707
-3	1	6	60.518	60.465	60.465	0.0	0.053	0.049
-5	1	6	13.162	13.013	-13.013	0.0	0.149	0.090
-7	1	6	46.625	46.625	46.625	0.0	-0.367	-0.378
-9	1	6	26.172	25.864	-25.864	0.0	0.308	0.274
-10	2	6	5.116	3.109	-3.109	0.0	2.007	0.542
-8	2	6	7.024	4.591	4.591	0.0	2.433	0.889
-6	2	6	7.320	5.732	-5.732	0.0	1.587	0.621
0	2	6	7.067	5.703	-5.703	0.0	1.364	0.508
2	2	6	11.153	10.164	-10.164	0.0	0.988	0.484
4	2	6	4.669	9.045	-9.045	0.0	-4.376	-1.020
1	3	6	15.231	13.575	-13.575	0.0	1.656	1.102
-1	3	6	18.625	17.860	17.860	0.0	0.765	0.604
-3	3	6	24.526	23.119	-23.119	0.0	1.407	1.450
-5	3	6	22.069	21.195	21.195	0.0	0.874	0.809
0	12	0	199.375	204.739	204.739	0.0	-5.364	-1.795
-7	3	6	24.931	24.092	-24.092	0.0	0.839	0.789
-9	3	6	19.570	19.159	19.159	0.0	0.412	0.292
-10	4	6	29.127	27.295	-27.295	0.0	1.833	1.657
-8	4	6	3.546	4.478	-4.478	0.0	-0.932	-0.216
-6	4	6	17.333	19.910	19.910	0.0	-2.577	-1.775
-4	4	6	8.156	5.283	-5.283	0.0	2.872	1.289
-2	4	6	5.150	2.984	-2.984	0.0	2.166	0.666
0	4	6	5.589	5.492	-5.492	0.0	0.097	0.031
2	4	6	39.056	37.876	37.876	0.0	1.180	1.248
3	5	6	2.296	2.729	2.729	0.0	-0.433	-0.086
1	5	6	19.503	19.734	-19.734	0.0	-0.232	-0.176
-1	5	6	5.302	3.830	3.830	0.0	1.472	0.466
-3	5	6	9.861	6.259	-6.259	0.0	1.913	1.913
-7	5	6	16.582	14.222	-14.222	0.0	2.359	1.694
-9	5	6	19.064	22.485	22.485	0.0	-3.421	-2.356
-4	6	6	8.468	6.505	-6.505	0.0	1.963	0.861
0	12	0	199.105	204.739	204.739	0.0	-5.634	-1.890
-2	6	6	7.945	5.359	5.359	0.0	2.586	1.078
2	6	6	0.794	8.339	-8.339	0.0	-7.544	-1.135
-1	7	6	18.262	18.470	-18.470	0.0	-0.208	-0.154
-3	7	6	17.189	16.446	-16.446	0.0	0.744	0.540
-5	7	6	21.217	20.841	20.841	0.0	0.375	0.313
-7	7	6	6.315	5.528	-5.528	0.0	0.787	0.264

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-8	8	6	15.578	14.446	14.446	0.0	1.232	0.741
-6	8	6	19.933	19.054	-19.054	0.0	0.883	0.672
-2	8	6	15.340	15.701	15.701	0.0	-0.361	-0.219
0	8	6	42.779	42.045	-42.045	0.0	0.734	0.763
2	8	6	29.490	30.717	30.717	0.0	-1.227	-1.118
-1	9	6	13.475	14.203	14.203	0.0	-0.728	-0.399
-3	9	6	44.459	43.724	-43.724	0.0	0.735	0.764
-5	9	6	25.649	27.236	27.236	0.0	-1.587	-1.323
0	12	0	198.767	204.739	204.739	0.0	-5.972	-2.004
-7	9	6	10.511	8.108	-8.108	0.0	2.403	1.143
-8	10	6	11.043	11.342	11.342	0.0	-0.298	-0.129
-6	10	6	3.825	8.781	8.781	0.0	-4.956	-1.116
-4	10	6	20.381	20.119	20.119	0.0	0.262	0.200
-2	10	6	13.914	14.530	14.530	0.0	-0.616	-0.351
0	10	6	16.826	16.467	16.467	0.0	0.359	0.231
1	11	6	16.987	14.022	14.022	0.0	2.965	1.940
-1	11	6	6.467	0.606	0.606	0.0	5.861	1.966
-3	11	6	83.701	82.572	82.572	0.0	1.129	0.820
-5	11	6	12.183	14.775	-14.775	0.0	-2.592	-1.253
-7	11	6	42.298	40.280	40.280	0.0	2.018	2.096
-6	12	6	27.177	26.504	26.504	0.0	0.673	0.582
-4	12	6	39.470	39.113	39.113	0.0	0.357	0.344
-2	12	6	18.025	18.150	-18.150	0.0	-0.125	-0.085
0	12	6	43.362	43.225	43.225	0.0	0.137	0.134
-1	13	6	14.116	13.294	-13.294	0.0	0.822	0.447
-3	13	6	41.808	41.436	41.436	0.0	0.372	0.370
-5	13	6	31.010	30.149	-30.149	0.0	0.861	0.843
0	12	0	157.847	204.739	204.739	0.0	-6.892	-2.326
-4	14	6	5.961	1.612	-1.612	0.0	4.348	1.324
-4	7	7	8.384	1.263	-1.263	0.0	7.120	2.729
-5	6	7	67.593	65.645	65.645	0.0	1.948	1.625
-3	6	7	42.568	40.470	-40.470	0.0	2.098	2.071
-2	5	7	24.779	24.547	24.547	0.0	-0.168	-0.131
-4	5	7	9.878	9.918	9.918	0.0	-0.040	-0.016
-6	5	7	19.900	19.033	19.033	0.0	0.867	0.638
-5	4	7	11.001	7.592	7.592	0.0	3.409	1.634
-1	4	7	6.452	0.534	-0.534	0.0	5.958	1.877
-2	3	7	14.581	13.507	-13.507	0.0	1.074	0.597
-4	3	7	4.238	1.714	-1.714	0.0	2.524	0.643
-6	3	7	3.470	2.601	-2.601	0.0	0.869	0.155
-7	2	7	19.874	20.757	20.757	0.0	-0.883	-0.611
-5	2	7	31.002	31.790	-31.790	0.0	-0.788	-0.753
-3	2	7	22.280	23.530	23.530	0.0	-1.249	-0.919
-1	2	7	10.807	5.508	-5.508	0.0	4.898	2.428
-2	1	7	5.429	6.113	-6.113	0.0	-0.684	-0.187
-4	1	7	10.190	7.696	7.696	0.0	2.495	1.145
0	12	0	197.965	204.739	204.739	0.0	-6.774	-2.286
-6	1	7	7.421	0.371	0.371	0.0	7.050	2.561
-5	0	7	6.982	4.657	4.657	0.0	2.926	1.001
-3	0	7	9.287	2.834	-2.834	0.0	6.453	2.852
-1	0	7	7.894	8.736	-8.736	0.0	-0.842	-0.296

ALL REFLECTIONS

WEIGHTED R	NUMERATOR	DENOMINATOR	NUMBER	R
2682.62	1645273.00		1376	0.040
UNWEIGHTED R	2437.75	51211.17	1376	0.048

RANGES OF F(OBS)

1612.40	12820.66	925	0.126
156.73	10513.64	245	0.019
78.89	5533.74	73	0.014
60.70	3542.61	33	0.017
48.21	2129.87	16	0.023
20.43	657.03	4	0.031
389.62	15540.94	78	0.025
30.83	473.44	2	0.065

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

200.00	5024.59	86	0.040
538.47	15647.50	189	0.027
198.40	5411.50	145	0.037
158.16	4860.96	162	0.041
266.54	4339.90	181	0.061
304.54	3920.24	191	0.078
306.24	3598.79	203	0.077
425.12	4009.73	219	0.106

JNREJECTED REFLECTIONS

WEIGHTED R	2151.36	1173490.00	1190	0.043
UNWEIGHTED R	1861.04	32708.42	1190	0.057

RANGES OF F(OBS)

1473.65	11750.56	852	0.125
180.95	9395.44	220	0.019
71.61	4598.39	66	0.014
54.11	3084.87	29	0.018
39.84	1858.62	14	0.021
20.43	657.03	4	0.031
20.49	964.22	5	0.021
0.0	0.0	0	0.0

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

150.57	3587.90	71	0.038
144.84	4297.31	101	0.034
178.17	5030.27	132	0.035
178.39	4360.52	148	0.041
234.82	4010.64	167	0.059
289.99	3630.60	178	0.080
286.09	3677.73	183	0.078
358.29	3715.41	205	0.107

SUM FCAL 51181.60
STANDARD DEV OF UNIT WEIGHT OBS 1.41

EXTINCTION CORRECTION 0.0
 SCALE FACTOR 1 1.1845 0.0000 1.1845 0.00320 0.00

ATOM 1 O(1) EQUIPOINT FRACTION = 1.0000
 OCCUPANCY SPECIES 1

SPECIES	EQUIPOINT FRACTION	OCCUPANCY	SCALE FACTOR	OLD	CHANGE	NEW	ERROR	SHIFT/ERROR
X	0.1131313	1.00000	1.00000	0.0000023	0.1131290	C.0002165	-0.01	
Y	0.9152495	0.0000010	0.9152485	0.0000010	0.0001121	C.0001121	-0.01	
Z	0.8951893	-0.0000060	0.8951833	0.0000060	C.CCC4257	C.CCC4257	-0.01	
BETA11	0.0033481	0.0000028	0.0033509	0.0000028	0.0002256	C.0002256	0.01	
BETA22	0.0012398	0.0000005	0.0012403	0.0000005	0.0000669	C.0000669	0.01	
BETA33	0.0155448	-0.0000057	0.0155391	0.0000057	0.0008686	C.0008686	-0.01	
BETA12	0.0001643	0.0000001	0.0001642	0.0000001	C.CCC0900	C.CCC0900	-0.00	
BETA13	0.0014186	0.0000025	0.0014211	0.0000025	C.0003550	C.0003550	0.01	
BETA23	-0.0003005	0.0000000	-0.0003005	0.0000000	C.CCC1736	C.CCC1736	0.00	

ATOM 2 O(2) EQUIPOINT FRACTION = 1.0000
 OCCUPANCY SPECIES 1

SPECIES	EQUIPOINT FRACTION	OCCUPANCY	SCALE FACTOR	OLD	CHANGE	NEW	ERROR	SHIFT/ERROR
X	0.1156061	1.00000	1.00000	0.0000035	0.1156096	C.0002181	0.02	
Y	0.8321962	-0.0000005	0.8321557	0.0000005	0.8321557	C.0001230	-0.00	
Z	0.3918404	0.0000078	0.3918481	0.0000078	C.0004225	C.0004225	0.02	
BETA11	0.0038815	-0.0000021	0.0038795	0.0000021	0.0003238	C.CCC2328	-0.01	
BETA22	0.0015976	-0.0000009	0.0015967	0.0000009	0.0000764	C.0000764	-0.01	
BETA33	0.0132803	-0.0000047	0.0132756	0.0000047	0.0008202	C.0008202	-0.01	
BETA12	0.0002310	-0.0000017	0.0002293	0.0000017	C.0000961	C.0000961	-0.02	
BETA13	0.0019557	-0.0000050	0.0010807	0.0000050	C.0003440	C.0003440	-0.01	
BETA23	-0.0004672	-0.0000043	-0.0004715	0.0000043	C.0001156	C.0001156	-0.02	

ATOM 3 F(3) EQUIPOINT FRACTION = 0.500
 OCCUPANCY SPECIES 2

SPECIES	EQUIPOINT FRACTION	OCCUPANCY	SCALE FACTOR	OLD	CHANGE	NEW	ERROR	SHIFT/ERROR
X	0.1031004	1.00000	1.00000	-0.0000001	0.1031003	0.0003165	-0.00	
Y	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Z	0.3915149	0.0000042	0.3915191	0.0000042	C.0005658	C.0005658	0.01	
BETA11	0.0070659	0.0000013	0.0070672	0.0000013	C.0003437	C.0003437	0.00	
BETA22	0.0016697	0.0000001	0.0016698	0.0000001	0.0006676	C.0006676	0.00	
BETA33	0.0268931	0.0000294	0.0269224	0.0000294	0.0012064	C.0012064	0.02	
BETA12	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
BETA13	0.0023467	0.0000087	0.0023554	0.0000087	C.0005185	C.0005185	0.02	
BETA23	0.0	0.0	0.0	0.0	0.0	0.0	0.0	

ATOM 4 O(4) EQUIPOINT FRACTION = 1.000
 OCCUPANCY SPECIES 1

SPECIES	EQUIPOINT FRACTION	OCCUPANCY	SCALE FACTOR	OLD	CHANGE	NEW	ERROR	SHIFT/ERROR
X	0.3618208	1.00000	1.00000	0.0000031	0.3618238	0.0002715	0.01	
Y	0.7534110	0.0000008	0.7534118	0.0000008	0.0001277	0.0001277	0.01	
Z	0.5629370	0.0000087	0.5629457	0.0000087	C.0005225	C.0005225	0.02	
BETA11	0.0079590	-0.0000068	0.0079522	0.0000068	0.0003175	C.0003175	-0.02	
BETA22	0.0012466	-0.0000001	0.0012465	0.0000001	C.0006675	C.0006675	-0.00	
BETA33	0.0229162	0.0000128	0.0229290	0.0000128	C.0011255	C.0011255	0.01	
BETA12	0.0014725	-0.0000010	0.0014714	0.0000010	0.0001127	C.0001127	-0.01	
BETA13	0.0038331	-0.0000028	0.0038303	0.0000028	0.0004755	C.0004755	-0.01	
BETA23	0.00006315	-0.0000019	0.00006297	0.0000019	C.0001973	C.0001973	-0.01	

ATOM 5 O(5) EQUIPOINT FRACTION = 1.000
 OCCUPANCY SPECIES 1

SPECIES	EQUIPOINT FRACTION	OCCUPANCY	SCALE FACTOR	OLD	CHANGE	NEW	ERROR	SHIFT/ERROR
X	0.3460262	1.00000	1.00000	-0.0000015	0.3460247	C.0002447	-0.01	
Y	0.8722616	0.0000016	0.8722633	0.0000016	0.0001325	C.0001325	0.01	
Z	0.2603502	-0.0000016	0.2603486	0.0000016	0.0004540	C.0004540	-0.00	
BETA11	0.0051064	0.0000004	0.0051068	0.0000004	C.0002565	C.0002565	0.00	

ATOM 6		O(6)	EQUIPOINT FRACTION = 1.000	
			OCCUPANCY SPECIES 1	
BETA22	0.0020892	-0.0000009	0.0020883	C.0000766
BETA33	0.0169137	0.0000015	0.0169152	0.0000420
BETA12	0.0002802	-0.0000005	0.0002797	C.0001035
BETA13	0.0024913	-0.0000018	0.0024894	C.0000363
BETA23	0.0023131	-0.0000004	0.0023091	C.0000206

ATOM 6		O(6)	EQUIPOINT FRACTION = 1.000	
			OCCUPANCY SPECIES 1	
X	0.3426499	0.0000028	0.3426527	C.00002471
Y	0.8819098	-0.0000013	C.8919085	C.0001255
Z	0.7606462	0.0000031	C.7606492	0.0000445
BETA11	0.0057536	0.0000022	0.0057558	0.0002672
BETA22	0.0019814	-0.0000013	0.0019801	C.0000763
BETA33	0.0164597	0.0000055	0.0164652	C.0000332
BETA12	0.0000456	-0.0000002	0.0000454	C.0001091
BETA13	0.0038542	0.0000048	0.0038590	C.00003976
BETA23	-0.0022873	0.0000003	-0.0022869	0.00002031

ATOM 7		O(7)	EQUIPOINT FRACTION = 0.500	
			OCCUPANCY SPECIES 1	
X	1.00000	-0.0000005	1.00000	0.0003549
Y	0.3401707	0.0000005	0.3401701	0.0003549
Z	0.0	0.0	0.0	0.0003549
BETA11	0.0440978	-0.0000151	0.0440826	0.0001173
BETA22	0.0059134	-0.0000022	0.0059111	0.0000381
BETA33	0.0007851	0.0000002	0.0007853	0.0000848
BETA12	0.0257670	-0.0000029	0.0257641	0.0016354
BETA13	0.0	0.0	0.0	0.0016354
BETA23	0.0018640	-0.0000048	0.0018591	C.0000262
BETA23	0.0	0.0	0.0	-0.01

ATOM 8		T(1)	EQUIPOINT FRACTION = 1.000	
			OCCUPANCY SPECIES 3	
X	1.00000	0.0000003	1.00000	0.0000902
Y	0.2793508	-0.0000001	0.2793510	C.0000902
Z	0.9160911	-0.0000003	0.9160911	C.0000391
BETA11	0.9856279	-0.0000003	0.9856277	C.0001727
BETA22	0.0032651	-0.0000003	0.0032648	C.0000643
BETA33	0.0008534	0.0000001	0.0008535	0.0000226
BETA12	0.0111149	-0.0000003	0.0111152	0.0000306
BETA13	0.0000994	-0.0000000	0.0000994	0.0000349
BETA23	0.0017996	0.0000004	0.0018000	C.0001258
BETA23	-0.0001255	0.0000006	-0.0001249	C.0000631

ATOM 9		T(2)	EQUIPOINT FRACTION = 1.000	
			OCCUPANCY SPECIES 3	
X	1.00000	-0.0000002	1.00000	0.0000857
Y	0.2868909	-0.0000004	0.2868907	0.0000413
Z	0.8298259	-0.0000000	0.8298254	C.0001767
BETA11	0.4866537	-0.0000000	0.4866537	C.0000882
BETA22	0.0034900	0.0000004	0.0034904	0.0000227
BETA33	0.0010035	-0.0000001	0.0010033	0.0000265
BETA12	0.0109678	-0.0000011	0.0109666	0.0000359
BETA13	0.0003841	-0.0000002	0.0003839	0.00001261
BETA23	0.0017416	-0.0000007	0.0017409	0.00001261
BETA23	0.0002121	-0.0000003	0.0002118	C.0000656

ATOM 10		M(1)	EQUIPOINT FRACTION = 0.500	
			OCCUPANCY SPECIES 4	
X	1.00000	0.0000006	1.00000	0.0000666
Y	0.9104855	0.0000000	0.9104861	0.0000666
Z	0.5000000	-0.0000022	0.5000000	C.00001667
BETA11	0.0044549	0.0000005	0.0044527	C.0000445
BETA22	0.0011576	0.0000005	0.0011581	0.01

BETA33	0.0135132	0.0000038	0.0135170	C.00C5587	0.01
BETA12	0.0	0.0	0.0		
BETA13	0.0018236	0.0000015	0.0018251	C.0002540	0.01
BETA23	0.0	0.0	0.0		

ATOM 11 M(2) EQUIPOINT FRACTION = 0.500

EQUIPOINT FRACTION = 0.500					
OCCUPANCY SPECIES 4					
X	1.00000	1.00000	1.00000		
Y	0.0	0.0	0.0		
Z	0.8196338	0.0000005	0.8196343	C.00C0625	0.01
BETA11	0.0	0.0	0.0		
BETA22	0.0048845	0.0000002	C.0048847	C.00C1725	0.0C
BETA33	0.0013263	0.0030013	0.0013276	C.0000466	0.03
BETA12	0.0150630	-0.0000075	0.0150555	C.00C0C51	-0.01
BETA13	0.0	0.0	0.0		
BETA23	0.0019367	-0.0000009	0.0019357	C.00002541	-0.00
BETA23	0.0	0.0	0.0		

ATOM 12 M(3) EQUIPOINT FRACTION = 0.250

EQUIPOINT FRACTION = 0.250					
OCCUPANCY SPECIES 4					
X	1.00000	1.00000	1.00000		
Y	0.0	0.0	0.0		
Z	0.0	0.0	0.0		
BETA11	0.0050903	-0.0000017	0.0050886	C.0002364	-0.01
BETA22	0.0010885	-0.0000011	0.0010874	C.0000604	-0.02
BETA33	0.0144431	0.0000037	0.0144468	C.00C8397	0.00
BETA12	0.0	0.0	0.0		
BETA13	0.0042415	-0.0000039	0.0042376	C.00003623	-0.01
BETA23	0.0	0.0	0.0		

ATOM 13 M(4) EQUIPOINT FRACTION = 0.500

EQUIPOINT FRACTION = 0.500					
OCCUPANCY SPECIES 5					
OCCUPANCY SPECIES 6					
TOTAL OCCUPANCY (FIXED) = 1.00000					
X	0.0	0.0	0.0		
Y	0.7234545	-0.0000005	0.7234540	C.00C0E22	-0.01
Z	0.5000000	0.5000000	0.5000000		
BETA11	0.0114346	0.0000036	0.0114382	C.0002142	0.02
BETA22	0.0016485	-0.0000011	0.0016475	C.0000440	-0.02
BETA33	0.0228514	-0.0000107	0.0228407	C.00C0E273	-0.02
BETA12	0.0	0.0	0.0		
BETA13	-0.00031089	-0.0000065	-0.00031154	C.00C028C5	-0.02
BETA23	0.0	0.0	0.0		

ATOM 14 A EQUIPOINT FRACTION = 1.000

EQUIPOINT FRACTION = 1.000					
OCCUPANCY SPECIES 6					
X	0.25000	0.0003704	0.25000	C.0016554	0.22
Y	0.9909379	0.0003958	0.9913337	C.00C25714	0.13
Z	0.5474674	0.0006308	0.5480981	C.00C1842	0.20
BETA11	0.0225556	0.0007333	0.0232889	C.00C3035E	0.24
BETA22	0.0074116	0.0002400	0.0076516	C.00014491	C.17
BETA33	0.0574405	-0.0012170	0.0562235	C.0080365	-0.15
BETA12	-0.0055876	-0.0008162	-0.0064039	C.00C29968	-0.27
BETA13	-0.0119834	0.0000918	-0.0118917	C.00C30338	0.03
BETA23	0.0035275	-0.0007066	0.0028209	C.00036243	-0.19

MAXIMUM SHIFT/ERROR = -0.27
 AVERAGE SHIFT/ERROR = 0.02

H	K	L	F(DBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
6	0	0	116.533	117.666	117.666	0.0	0.865	0.464
8	0	0	120.094	126.279	126.279	0.0	-6.184	-3.593
10	0	0	84.192	84.227	34.227	0.0	-0.035	-0.026
12	0	0	23.226	21.839	-21.839	0.0	1.567	1.526
-13	1	0	34.655	34.363	-34.363	0.0	0.292	0.301
-11	1	0	71.557	71.024	71.024	0.0	0.575	0.488
-9	1	0	26.961	26.819	26.819	0.0	0.142	0.186
-7	1	0	77.586	79.272	79.272	0.0	-1.664	-1.592
-5	1	0	110.226	109.485	-109.485	0.0	0.741	0.447
-3	1	0	145.472	153.260	153.260	0.0	-7.789	-3.583
3	1	0	146.523	153.260	153.260	0.0	-6.937	-3.169
5	1	0	110.353	109.485	-109.485	0.0	0.868	0.521
7	1	0	77.259	79.272	79.272	0.0	-2.013	-1.673
9	1	0	26.669	26.819	26.819	0.0	-0.149	-0.194
11	1	0	70.775	71.024	71.024	0.0	-0.249	-0.214
13	1	0	36.090	34.363	-34.363	0.0	1.727	1.751
-12	2	0	11.953	9.103	9.103	0.0	2.849	1.986
-10	2	0	7.448	5.467	-5.467	0.0	1.981	1.040
-8	2	0	17.085	16.225	-16.225	0.0	0.860	0.921
0	2	0	421.553	230.777	230.777	0.0	-9.443	-2.853
-6	2	0	37.195	37.507	-37.507	0.0	-0.312	-0.449
-4	2	0	11.773	12.946	-12.946	0.0	-1.173	-1.725
4	2	0	12.431	12.946	-12.946	0.0	-0.515	-0.802
6	2	0	37.427	37.507	-37.507	0.0	-0.080	-0.116
8	2	0	17.436	16.225	-16.225	0.0	1.211	1.308
10	2	0	7.851	5.467	-5.467	0.0	2.385	1.257
12	2	0	7.356	9.103	9.103	0.0	-1.767	-0.657
-13	3	0	18.161	17.978	17.978	0.0	0.153	0.134
-11	3	0	19.281	18.211	-18.211	0.0	1.070	1.146
-9	3	0	23.577	23.050	23.050	0.0	0.547	0.690
-7	3	0	55.311	55.700	-55.700	0.0	-0.389	-0.427
-5	3	0	62.281	62.208	62.208	0.0	0.075	0.075
-3	3	0	82.922	84.793	-84.793	0.0	-1.872	-1.491
3	3	0	83.587	84.793	-84.793	0.0	-1.207	-0.956
5	3	0	62.378	62.208	62.208	0.0	0.170	0.175
7	3	0	55.458	55.700	-55.700	0.0	-0.262	-0.285
9	3	0	24.596	23.050	23.050	0.0	-0.432	-0.494
11	3	0	18.497	18.211	-18.211	0.0	0.266	0.258
13	3	0	19.483	17.978	17.978	0.0	1.505	1.107
-12	4	0	29.142	28.273	28.273	0.0	0.869	0.938
0	4	0	221.348	230.777	230.777	0.0	-9.428	-2.849
-8	4	0	13.253	14.447	14.447	0.0	-1.194	-0.987
-6	4	0	12.672	11.898	11.898	0.0	0.974	1.026
-4	4	0	19.360	14.104	14.104	0.0	4.256	3.823
-2	4	0	126.922	129.992	129.992	0.0	-3.070	-1.618
2	4	0	126.788	129.992	129.992	0.0	-3.204	-1.689
4	4	0	15.6.8	14.104	14.104	0.0	1.524	2.488
6	4	0	8.016	11.898	11.898	0.0	-3.882	-2.463
8	4	0	16.330	14.447	14.447	0.0	1.884	1.940
10	4	0	5.371	1.553	-1.553	0.0	3.818	1.494
12	4	0	29.351	28.273	28.273	0.0	1.078	1.093
-11	5	0	2.673	23.345	-23.345	0.0	-0.672	-0.677
-7	5	0	10.257	10.201	-10.201	0.0	0.056	0.058

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-5	5	0	14.597	14.670	-14.670	0.0	-0.073	-0.092 *
-3	5	0	77.072	76.887	-76.887	0.0	0.166	0.158 *
-1	5	0	3.817	0.700	0.700	0.0	3.118	1.897 *
1	5	0	5.356	0.700	0.700	0.0	4.657	3.710
3	5	0	76.878	76.887	-76.887	0.0	-0.008	-0.007
5	5	0	14.246	14.670	-14.670	0.0	-0.424	-0.526
7	5	0	222.081	230.777	230.777	0.0	-8.696	-2.622 *
9	5	0	5.839	10.201	-10.201	0.0	-0.363	-0.238
11	5	0	1.912	1.175	-1.175	0.0	0.737	0.183
11	5	0	22.583	23.345	-23.345	0.0	-0.762	-0.708
-12	0	0	4.168	4.740	-4.740	0.0	-0.572	-0.165
-10	0	0	17.443	17.272	17.272	0.0	0.171	0.100
-8	0	0	23.913	23.595	-23.595	0.0	0.318	0.413 *
-4	0	0	5.289	6.321	-6.321	0.0	-1.032	-0.037 *
-2	0	0	11.631	10.273	10.278	0.0	1.354	1.970 *
0	0	0	2.219	1.375	1.375	0.0	0.844	0.364
2	0	0	11.497	10.273	10.278	0.0	1.219	1.755
4	0	0	7.037	6.321	-6.321	0.0	0.716	0.567
6	0	0	2.510	2.013	2.013	0.0	0.497	0.150
8	0	0	21.926	23.595	-23.595	0.0	-1.670	-1.943
10	0	0	18.549	17.272	17.272	0.0	1.277	1.276
12	0	0	0.380	4.740	-4.740	0.0	1.639	0.554
-11	7	0	2.727	0.105	-0.105	0.0	2.622	0.672 *
-9	7	0	35.225	38.444	-38.444	0.0	0.781	0.750
-7	7	0	44.935	45.059	-45.059	0.0	-0.124	-0.151 *
-5	7	0	29.374	29.667	-29.667	0.0	-0.293	-0.441 *
0	12	0	221.959	230.777	230.777	0.0	-8.808	-2.656 *
-3	7	0	6.5977	6.0934	6.0934	0.0	3.023	3.042 *
-1	7	0	10.914	8.776	-8.776	0.0	2.138	2.921 *
1	7	0	11.729	8.776	-8.776	0.0	2.953	4.343
3	7	0	6.070	6.0934	6.0934	0.0	2.716	2.755
5	7	0	29.150	29.667	-29.667	0.0	-0.517	-0.769
7	7	0	45.831	45.059	-45.059	0.0	0.772	0.940
9	7	0	58.680	58.444	-58.444	0.0	0.236	0.237
-12	8	0	4.157	43.663	43.663	0.0	-0.507	-0.522 *
-10	8	0	65.901	69.183	-69.183	0.0	0.718	0.624 *
-8	8	0	9.726	10.273	10.273	0.0	-0.546	-0.358 *
-6	8	0	65.120	65.163	65.163	0.0	-0.044	-0.042 *
-4	8	0	115.186	115.664	-115.664	0.0	-0.477	-0.274 *
2	8	0	44.648	35.737	35.737	0.0	-1.089	-1.777 *
0	8	0	44.344	38.952	38.952	0.0	5.393	7.520
2	8	0	34.192	35.737	35.737	0.0	-1.544	-2.521
4	8	0	114.865	115.664	-115.664	0.0	-0.799	-0.461 *
6	8	0	65.232	65.163	65.163	0.0	0.069	0.066
8	8	0	9.764	10.273	10.273	0.0	-0.509	-0.337
10	8	0	69.699	69.183	-69.183	0.0	0.516	0.449
0	12	0	221.632	230.777	230.777	0.0	-9.144	-2.763 *
12	8	0	4.660	43.663	43.663	0.0	0.016	0.016
-11	9	0	12.014	11.597	-11.597	0.0	0.450	0.280 *
-9	9	0	30.315	30.275	30.275	0.0	0.040	0.051 *
-7	9	0	108.515	109.376	-109.376	0.0	-0.860	-0.519 *
-5	9	0	16.726	16.853	16.853	0.0	-0.126	-0.136 *
-1	9	0	81.114	78.621	-78.621	0.0	2.493	2.023 *

H	K	L	F(ORSS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	9	0	80.725	78.621	-78.621	0.0	2.105	1.708
3	9	0	4.972	7.979	-7.979	0.0	-3.004	-1.641
5	9	0	15.770	16.853	16.853	0.0	-1.083	-1.115
7	9	0	102.251	109.376	-109.376	0.0	-1.144	-0.693
9	9	0	29.643	30.275	30.275	0.0	-0.632	-0.776
11	9	0	11.594	11.557	-11.557	0.0	0.037	0.021
12	10	0	21.323	21.754	21.754	0.0	-0.426	-0.536
10	10	0	32.032	32.579	32.579	0.0	-0.546	-1.082
8	10	0	23.973	23.246	23.246	0.0	0.727	0.892
6	10	0	15.546	15.924	15.924	0.0	-0.378	-0.361
4	10	0	59.473	55.823	55.823	0.0	-0.348	-0.382
2	10	0	32.223	35.503	35.503	0.0	-0.280	-0.425
0	10	0	37.150	37.655	37.655	0.0	-0.505	-0.382
0	12	0	222.514	230.777	230.777	0.0	8.203	-2.486
2	10	0	34.461	35.503	35.503	0.0	-1.042	-1.584
4	10	0	55.438	55.823	55.823	0.0	-0.385	-0.423
6	10	0	19.823	15.924	15.924	0.0	0.900	0.963
8	10	0	21.057	23.246	23.246	0.0	-1.589	-1.662
10	10	0	32.698	32.979	32.979	0.0	-0.281	-0.319
12	10	0	22.337	21.754	21.754	0.0	0.582	0.459
11	11	0	74.891	74.396	74.396	0.0	0.495	0.399
9	11	0	14.612	16.019	16.019	0.0	-1.407	-1.095
7	11	0	152.900	159.977	159.977	0.0	-4.077	-1.732
5	11	0	39.586	41.416	41.416	0.0	-1.830	-2.311
3	11	0	101.971	103.402	103.402	0.0	-1.431	-0.925
1	11	0	133.843	133.631	133.631	0.0	0.216	0.108
1	11	0	133.773	133.631	133.631	0.0	0.141	0.070
3	11	0	101.366	103.402	103.402	0.0	-2.036	-1.323
5	11	0	40.953	41.416	41.416	0.0	-0.463	-0.596
7	11	0	150.910	159.977	159.977	0.0	-3.061	-1.292
9	11	0	17.316	16.019	16.019	0.0	1.297	1.206
11	11	0	75.362	74.396	74.396	0.0	0.965	0.769
10	12	0	80.860	81.359	81.359	0.0	-0.499	-0.380
8	12	0	49.753	49.340	49.340	0.0	0.413	0.465
6	12	0	221.729	230.777	230.777	0.0	-9.047	-2.728
4	12	0	20.200	21.776	21.776	0.0	-1.576	-1.702
2	12	0	54.093	53.185	53.185	0.0	0.908	0.997
0	12	0	42.064	42.129	42.129	0.0	0.535	0.695
0	12	0	221.894	230.777	230.777	0.0	-8.883	-2.678
2	12	0	43.381	42.129	42.129	0.0	1.252	1.627
4	12	0	54.713	53.185	53.185	0.0	1.528	1.663
6	12	0	22.381	21.776	21.776	0.0	0.605	0.786
8	12	0	49.140	49.340	49.340	0.0	-0.200	-0.223
10	12	0	91.277	81.359	81.359	0.0	0.218	0.165
11	13	0	20.783	19.631	19.631	0.0	1.152	1.086
9	13	0	24.129	23.577	23.577	0.0	0.553	0.612
7	13	0	51.150	51.090	51.090	0.0	0.060	0.066
5	13	0	78.619	79.390	79.390	0.0	-0.771	-0.626
3	13	0	16.099	16.040	-16.040	0.0	0.059	0.059
1	13	0	20.895	19.547	19.547	0.0	1.348	1.786
1	13	0	20.798	19.547	19.547	0.0	1.251	1.579
3	13	0	15.426	16.040	-16.040	0.0	-0.613	-0.562
5	13	0	79.381	79.390	-79.390	0.0	-0.009	-0.007

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
7	13	0	51.792	51.090	51.090	0.0	0.702	0.770
9	13	0	23.278	23.577	-23.577	0.0	-0.299	-0.303
0	12	0	221.543	230.777	230.777	0.0	-9.234	-2.790
11	13	0	20.454	19.631	19.631	0.0	0.823	0.653
-10	14	0	8.419	0.761	0.761	0.0	7.659	3.648
-8	14	0	0.402	4.748	4.748	0.0	1.654	0.740
-0	14	0	5.170	7.416	-7.416	0.0	-2.247	-0.892
-2	14	0	32.065	31.370	31.370	0.0	0.715	0.997
0	14	0	13.521	13.866	-13.866	0.0	-0.344	-0.297
2	14	0	30.965	31.370	31.370	0.0	-0.405	-0.554
6	14	0	8.957	7.416	-7.416	0.0	1.541	0.937
10	14	0	2.092	0.761	0.761	0.0	1.331	0.761
-9	15	0	41.356	41.629	41.629	0.0	-0.273	-0.297
-7	15	0	59.524	59.937	-59.937	0.0	-0.412	-0.406
-5	15	0	49.469	49.578	49.578	0.0	-0.109	-0.125
-3	15	0	4.923	7.495	7.495	0.0	-2.572	-1.034
-1	15	0	3.862	3.415	-3.415	0.0	0.448	0.151
1	15	0	0.061	3.415	-3.415	0.0	4.648	2.653
3	15	0	4.393	7.495	7.495	0.0	-3.102	-1.190
5	15	0	50.082	49.578	49.578	0.0	0.503	0.502
0	12	0	222.327	230.777	230.777	0.0	-8.450	-2.542
7	15	0	60.428	59.937	-59.937	0.0	0.492	0.477
9	15	0	41.849	41.629	41.629	0.0	0.220	0.236
-10	16	0	45.363	43.334	-43.334	0.0	2.049	2.143
-8	16	0	4.333	4.496	-4.496	0.0	-0.163	-0.049
-6	16	0	26.677	27.567	27.567	0.0	-0.890	-1.083
-4	16	0	64.963	64.852	-64.852	0.0	0.110	0.103
2	16	0	3.489	1.840	1.840	0.0	1.649	0.550
4	16	0	64.141	64.832	-64.832	0.0	-0.711	-0.675
0	16	0	24.697	27.567	27.567	0.0	-2.869	-3.024
10	16	0	43.334	43.334	-43.334	0.0	-0.043	-0.043
-9	17	0	20.551	19.762	19.762	0.0	0.789	0.682
-7	17	0	20.260	20.657	-20.657	0.0	-0.398	-0.380
-5	17	0	7.635	4.635	-4.635	0.0	3.000	1.510
-3	17	0	25.706	26.696	26.696	0.0	-0.990	-1.262
-1	17	0	14.993	14.657	-14.657	0.0	0.337	0.352
1	17	0	13.506	14.657	-14.657	0.0	-1.050	-0.948
3	17	0	26.774	26.696	26.696	0.0	0.078	0.102
0	12	0	222.006	230.777	230.777	0.0	-8.771	-2.644
5	17	0	3.055	4.635	-4.635	0.0	-1.580	-0.457
7	17	0	19.050	20.657	-20.657	0.0	-1.608	-1.329
9	17	0	20.222	19.762	19.762	0.0	0.461	0.381
-6	18	0	20.775	22.885	22.885	0.0	-2.110	-1.962
-4	18	0	5.797	6.555	6.555	0.0	-0.758	-0.308
-2	18	0	24.720	23.679	23.679	0.0	1.040	1.289
0	18	0	17.219	17.187	17.187	0.0	0.032	0.031
2	18	0	24.100	23.679	23.679	0.0	0.420	0.502
4	18	0	3.182	6.555	6.555	0.0	-3.373	-0.935
6	18	0	23.293	22.885	22.885	0.0	0.407	0.426
8	18	0	6.850	3.876	-3.876	0.0	2.974	1.103
-7	19	0	31.360	29.553	-29.553	0.0	1.815	1.975
-5	19	0	12.745	13.445	13.445	0.0	-0.700	-0.491
-3	19	0	30.644	30.406	-30.406	0.0	0.237	0.289

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-1	15	0	6.656	2.943	2.943	0.0	3.713	1.732 *
1	19	0	4.906	2.943	2.943	0.0	-0.037	-0.010
3	19	0	31.107	30.406	-30.406	0.0	0.701	0.853
5	19	0	14.216	13.445	13.445	0.0	0.772	0.577
7	19	0	31.483	29.553	-29.553	0.0	1.927	2.063
0	12	0	222.133	230.777	230.777	0.0	-3.644	-2.606 *
-6	20	0	8.516	9.142	-9.142	0.0	-0.625	-0.289 *
-4	20	0	47.639	46.931	-46.931	0.0	0.707	0.770 *
-2	20	0	24.652	25.172	25.172	0.0	-0.520	-0.585 *
0	20	0	72.291	72.643	-72.643	0.0	-0.352	-0.300
2	20	0	25.160	25.172	25.172	0.0	-0.012	-0.014
4	20	0	47.579	46.931	-46.931	0.0	0.648	0.599
6	20	0	9.226	9.142	-9.142	0.0	0.084	0.040
-5	21	0	45.196	43.841	-43.841	0.0	1.355	1.499 *
-1	21	0	27.372	27.766	27.766	0.0	-0.395	-0.433 *
1	21	0	28.642	27.766	27.766	0.0	0.875	1.028
5	21	0	44.471	43.841	-43.841	0.0	0.630	0.659 *
-6	22	0	19.587	19.198	-19.198	0.0	0.369	0.328 *
-4	22	0	56.146	56.214	-56.214	0.0	-0.066	-0.064 *
-2	22	0	24.309	24.040	24.040	0.0	0.269	0.275 *
0	22	0	73.337	73.714	73.714	0.0	-0.377	-0.312
2	22	0	22.628	24.040	24.040	0.0	-1.412	-1.252
4	22	0	56.447	56.214	-56.214	0.0	0.233	0.222
6	22	0	20.222	19.198	-19.198	0.0	1.024	0.836
0	22	0	421.573	230.777	230.777	0.0	-9.204	-2.761 *
-3	23	0	51.755	52.970	52.970	0.0	-1.215	-1.232 *
-1	23	0	17.521	18.941	18.941	0.0	-1.610	-1.239 *
1	23	0	19.924	18.941	-18.941	0.0	0.582	0.919
3	23	0	50.881	52.970	52.970	0.0	-2.089	-2.027
-2	24	0	51.479	53.011	-53.011	0.0	-1.532	-1.508 *
0	24	0	108.637	108.760	108.760	0.0	0.076	0.045
2	24	0	53.421	53.011	-53.011	0.0	0.410	0.413
-13	0	1	23.607	41.423	-21.423	0.0	2.184	2.198
-11	0	1	5.595	1.754	-1.754	0.0	3.842	1.558
-9	0	1	18.923	18.543	-18.543	0.0	0.380	0.424
-7	0	1	10.608	11.231	-11.231	0.0	-0.563	-0.426
-5	0	1	10.690	9.751	-9.751	0.0	0.939	1.132
-3	0	1	17.548	18.466	-18.466	0.0	-0.938	-1.609
5	0	1	33.251	33.292	-33.292	0.0	-0.041	-0.071
3	0	1	2.772	5.489	-5.489	0.0	-2.718	-0.952
7	0	1	4.482	3.476	3.476	0.0	1.006	0.378
9	0	1	9.121	11.203	-11.203	0.0	-2.082	-1.171
11	0	1	9.226	8.471	-8.471	0.0	0.755	0.372
0	12	0	421.154	230.777	230.777	0.0	-9.623	-2.914 *
-8	1	1	2.928	5.689	-5.689	0.0	-2.760	-0.805
-6	1	1	8.636	8.828	-8.828	0.0	-0.192	-0.151
-4	1	1	19.729	20.626	-20.626	0.0	-0.897	-1.740
2	1	1	49.985	50.609	-50.609	0.0	-0.625	-0.797
4	1	1	8.703	9.609	-9.609	0.0	-0.906	-0.873
6	1	1	6.036	3.215	-3.215	0.0	2.821	1.430
8	1	1	13.417	15.150	-15.150	0.0	-1.734	-1.517
-13	2	1	18.258	17.220	-17.220	0.0	1.037	0.896
-11	2	1	30.427	30.814	-30.814	0.0	-0.387	-0.451

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-9	2	1	22.777	22.743	-22.743	0.0	0.034	0.045
-7	2	1	54.534	54.785	54.785	0.0	-0.251	-0.280
-5	2	1	46.076	46.207	-46.207	0.0	-0.129	-0.171
-3	2	1	131.487	138.391	138.391	0.0	-6.904	-3.514
1	2	1	8.867	7.584	-7.584	0.0	1.283	1.466
3	2	1	113.035	114.379	114.379	0.0	-1.344	-0.793
5	2	1	27.222	26.151	-26.151	0.0	1.072	1.068
7	2	1	47.923	48.580	48.580	0.0	-0.657	-0.772
9	2	1	22.105	22.063	-22.063	0.0	0.042	0.046
0	12	0	222.125	230.777	230.777	0.0	-8.651	-2.608
11	2	1	45.064	43.585	-43.585	0.0	1.499	1.632
-12	2	1	49.865	50.655	-50.655	0.0	-0.790	-0.826
-10	2	1	7.272	5.751	-5.751	0.0	1.622	0.852
-8	2	1	31.488	31.031	-31.031	0.0	0.437	0.573
-6	2	1	6.925	6.542	-6.542	0.0	-0.017	-0.011
-4	2	1	26.819	25.312	-25.312	0.0	1.506	2.800
-2	2	1	141.079	145.249	-145.249	0.0	-4.171	-1.980
2	2	1	117.263	121.930	121.930	0.0	-4.547	-2.579
4	2	1	26.823	27.392	-27.392	0.0	1.425	4.432
6	2	1	31.249	31.556	-31.556	0.0	-0.709	-1.010
8	2	1	18.066	18.217	-18.217	0.0	-0.131	-0.133
10	2	1	10.162	8.271	-8.271	0.0	1.911	1.152
-12	2	1	42.678	41.358	-41.358	0.0	1.281	1.371
-13	2	1	23.995	22.211	-22.211	0.0	1.734	1.731
-11	2	1	19.924	21.795	-21.795	0.0	-1.872	-1.693
-9	2	1	6.372	4.612	-4.612	0.0	1.760	0.896
-7	2	1	3.944	7.227	7.227	0.0	-3.282	-1.144
-5	2	1	21.291	21.441	-21.441	0.0	-0.150	-0.245
-1	2	1	9.024	9.822	-9.822	0.0	-0.798	-0.897
1	12	0	221.659	230.777	230.777	0.0	-9.928	-2.692
1	4	1	3.755	3.098	-3.098	0.0	0.697	0.411
3	4	1	5.057	2.664	-2.664	0.0	2.393	1.760
5	4	1	5.555	6.715	6.715	0.0	-1.120	-0.577
7	4	1	12.152	12.846	12.846	0.0	-0.714	-0.546
9	4	1	15.546	18.369	18.369	0.0	-2.823	-2.256
11	4	1	23.442	22.839	-22.839	0.0	0.602	0.594
-12	4	1	103.908	107.972	107.972	0.0	1.014	0.598
-10	4	1	7.224	5.496	-5.496	0.0	1.728	0.880
-8	4	1	31.159	30.872	-30.872	0.0	0.287	0.385
-6	4	1	99.058	102.155	102.155	0.0	-3.097	-2.052
-4	4	1	102.965	101.856	-101.856	0.0	1.109	0.714
-2	4	1	206.064	219.343	219.343	0.0	-13.279	-4.314
0	4	1	77.418	75.104	-75.104	0.0	2.312	1.972
2	4	1	136.447	142.150	142.150	0.0	-5.703	-2.786
4	4	1	24.324	23.256	-23.256	0.0	1.068	1.787
6	4	1	145.046	149.116	149.116	0.0	-4.070	-1.866
8	4	1	56.940	56.078	-56.078	0.0	0.862	0.901
10	4	1	18.833	17.392	-17.392	0.0	1.441	1.439
12	4	1	68.026	67.445	-67.445	0.0	0.581	0.495
-13	4	1	37.272	35.428	-35.428	0.0	1.945	1.859
0	12	0	421.685	230.777	230.777	0.0	-9.092	-2.747
-11	6	1	16.838	16.300	-16.300	0.0	0.538	0.490
-9	6	1	121.502	125.048	125.048	0.0	-3.146	-1.658

*

*

*

H	K	L	FICRS)	FICALC)	AICALC)	BICALC)	DELTA F	DELTA/SIGMA
-7	0	1	103.114	105.649	-105.649	0.0	-2.534	-1.608
-5	0	1	202.814	215.792	215.792	0.0	-12.977	-4.279
-3	6	1	170.759	171.620	171.620	0.0	-0.861	-0.337
-1	6	1	141.333	144.337	144.337	0.0	-3.004	-1.421
1	6	1	57.731	46.967	-46.967	0.0	10.764	12.008
3	6	1	53.124	53.640	53.640	0.0	1.584	1.898
5	6	1	402.899	278.808	278.808	0.0	-15.909	-4.056
7	6	1	40.983	41.619	-41.619	0.0	-0.637	-0.812
9	6	1	89.174	89.862	89.862	0.0	-0.688	-0.493
11	6	1	11.041	13.097	-13.097	0.0	-2.056	-1.063
-12	7	1	65.217	64.748	64.748	0.0	0.469	0.418
-10	7	1	53.378	52.047	-32.047	0.0	1.331	1.649
-8	7	1	26.849	28.214	-28.214	0.0	-1.365	-1.810
-6	7	1	52.033	51.471	51.471	0.0	0.562	0.792
-4	7	1	13.663	12.047	12.047	0.0	1.616	2.041
-2	7	1	73.524	72.631	72.631	0.0	0.893	0.797
0	7	1	134.363	135.384	-135.384	0.0	-1.021	-0.508
2	7	1	50.868	50.173	50.173	0.0	0.695	1.163
4	7	1	221.558	230.777	230.777	0.0	-9.219	-2.786
6	7	1	48.625	47.794	-47.794	0.0	0.831	1.021
8	7	1	61.459	62.085	62.085	0.0	-0.626	-0.625
10	7	1	5.775	6.076	6.076	0.0	-0.302	-0.127
-11	8	1	43.470	42.117	-42.117	0.0	1.353	1.548
-9	8	1	19.774	20.197	-20.197	0.0	-0.423	-0.402
-7	8	1	18.698	18.895	-18.895	0.0	-0.196	-0.199
-5	8	1	9.304	9.186	9.186	0.0	0.123	0.078
-3	8	1	19.229	17.952	-17.952	0.0	1.277	1.709
-1	8	1	13.073	12.140	-12.140	0.0	0.933	1.314
1	8	1	10.877	10.625	-10.625	0.0	0.252	0.286
3	8	1	8.382	8.503	8.503	0.0	-0.581	-0.450
5	8	1	22.262	23.125	-23.125	0.0	-0.863	-1.080
7	8	1	41.896	42.486	42.486	0.0	-0.590	-0.731
9	8	1	8.143	8.132	-8.132	0.0	0.011	0.006
11	8	1	21.074	19.843	-19.843	0.0	1.231	1.091
-12	9	1	31.099	31.351	-31.351	0.0	-0.251	-0.263
-10	9	1	21.679	20.732	20.732	0.0	0.948	1.048
-8	9	1	25.631	26.044	26.044	0.0	-0.413	-0.542
-6	9	1	421.080	230.777	230.777	0.0	-9.697	-2.937
0	9	1	22.374	21.672	21.672	0.0	0.702	0.990
-2	9	1	53.272	52.142	-52.142	0.0	1.130	1.327
0	9	1	106.102	105.984	105.984	0.0	0.118	0.074
2	9	1	60.421	59.217	-59.217	0.0	1.204	1.269
4	9	1	35.582	35.256	35.256	0.0	0.326	0.450
10	9	1	32.511	31.915	31.915	0.0	0.590	0.665
-11	10	1	24.832	24.197	24.197	0.0	0.634	0.702
-9	10	1	27.521	26.851	-26.851	0.0	0.670	0.838
-7	10	1	15.162	18.553	-18.553	0.0	0.598	0.709
-5	10	1	27.350	28.585	-28.585	0.0	-0.735	-0.974
-3	10	1	59.315	58.797	58.797	0.0	0.518	0.546
-1	10	1	43.650	43.442	-43.442	0.0	0.207	0.280
1	10	1	6.417	8.350	-8.350	0.0	-2.533	-1.514
3	10	1	56.476	56.125	56.125	0.0	0.352	0.386
5	10	1	44.240	43.332	-43.332	0.0	0.908	1.115

H	K	L	F(UBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
7	10	1	22.605	23.193	-23.193	0.0	-0.587	-0.672
9	10	1	16.136	15.078	-15.078	0.0	1.058	0.896
11	10	1	21.179	21.764	-21.764	0.0	-0.586	-0.470
0	12	0	222.193	230.777	230.777	0.0	-8.584	-2.588 *
-12	11	1	9.136	8.588	-8.588	0.0	0.549	0.259
-10	11	1	18.213	18.544	-18.544	0.0	-0.272	-0.258
-8	11	1	7.082	6.775	-6.775	0.0	0.307	0.155
-6	11	1	18.713	19.931	-19.931	0.0	-1.218	-1.325
-4	11	1	17.615	17.314	-17.314	0.0	0.301	0.336
-2	11	1	22.688	22.282	-22.282	0.0	0.406	0.578
0	11	1	1.233	4.383	-4.383	0.0	-3.151	-0.808
2	11	1	57.276	56.037	-56.037	0.0	1.239	1.556
4	11	1	10.421	9.548	-9.548	0.0	0.873	0.625
8	11	1	7.314	4.299	-4.299	0.0	3.014	1.534
10	11	1	19.533	19.684	-19.684	0.0	-0.149	-0.127
-11	12	1	12.020	11.553	-11.553	0.0	0.466	0.279
-9	12	1	5.498	5.730	-5.730	0.0	-0.232	-0.091
-7	12	1	13.932	18.451	-18.451	0.0	0.502	0.551
-5	12	1	17.705	17.487	-17.487	0.0	0.218	0.224
-3	12	1	12.199	14.642	-14.642	0.0	-2.442	-1.912
-1	12	1	20.155	20.553	-20.553	0.0	-0.398	-0.508
1	12	1	20.028	20.412	-20.412	0.0	-0.384	-0.472
3	12	1	10.220	11.246	-11.246	0.0	-1.026	-0.712
5	12	0	221.772	230.777	230.777	0.0	-9.005	-2.730 *
7	12	1	13.126	13.344	-13.344	0.0	0.484	0.447
-10	13	1	17.301	17.230	-17.230	0.0	0.071	0.069
-8	13	1	9.278	12.593	-12.593	0.0	-3.315	-1.551
-6	13	1	7.866	6.555	-6.555	0.0	1.312	0.714
-4	13	1	7.709	10.346	-10.346	0.0	-2.636	-1.440
-2	13	1	43.493	44.654	-44.654	0.0	-0.561	-0.669
0	13	1	41.595	42.767	-42.767	0.0	-1.171	-1.493
2	13	1	52.196	52.526	-52.526	0.0	-1.130	-1.293
4	13	1	19.453	19.444	-19.444	0.0	-0.003	-0.006
6	13	1	18.975	18.534	-18.534	0.0	0.441	0.522
8	13	1	6.522	1.679	-1.679	0.0	4.843	2.340
-11	14	1	230.200	22.646	-22.646	0.0	-2.446	-2.140
-9	14	1	6.566	3.600	-3.600	0.0	2.966	1.135
-7	14	1	35.021	35.147	-35.147	0.0	-0.126	-0.149
-5	14	1	28.836	28.785	-28.785	0.0	0.051	0.064
-3	14	1	108.246	101.750	-101.750	0.0	-1.504	-0.977
-1	14	1	42.372	43.564	-43.564	0.0	-1.192	-1.519
1	14	1	33.863	34.589	-34.589	0.0	-0.725	-0.952
3	14	0	421.556	230.777	230.777	0.0	-9.421	-2.847
5	14	1	70.110	72.045	-72.045	0.0	-1.936	-1.739
7	14	1	18.751	20.469	-20.469	0.0	-1.718	-1.933
9	14	1	46.249	46.865	-46.865	0.0	-0.616	-0.723
-10	15	1	11.138	7.708	-7.708	0.0	3.431	2.404
-8	15	1	54.198	53.804	-53.804	0.0	0.334	0.331
-6	15	1	10.459	10.303	-10.303	0.0	0.155	0.085
-4	15	1	22.665	22.389	-22.389	0.0	0.276	0.306
-2	15	1	21.029	20.775	-20.775	0.0	0.255	0.286
1	15	1	18.803	17.673	-17.673	0.0	1.130	1.304
-2	15	1	67.555	67.734	-67.734	0.0	-0.179	-0.166

H	K	L	FUBS)	FICALC)	AICALC)	BICALC)	DELTA F	DELTA/SIGMA
0	15	1	50.889	50.891	50.891	0.0	-0.002	-0.003
2	15	1	22.267	23.896	-23.896	0.0	0.529	-0.668
4	15	1	8.457	5.150	-5.150	0.0	3.527	2.052
6	15	1	14.029	13.494	-13.494	0.0	0.535	0.426
8	15	1	7.231	10.987	10.987	0.0	-0.750	-1.397
-9	16	1	47.542	47.577	47.577	0.0	0.164	0.169
-7	16	1	23.629	24.841	24.841	0.0	-1.212	-1.309
-5	16	1	74.226	73.085	73.085	0.0	0.541	0.455
-3	16	1	47.594	47.587	47.587	0.0	0.007	0.008
-1	16	1	60.407	68.322	68.322	0.0	0.084	0.077
0	12	0	220.945	230.777	230.777	0.0	-9.832	-2.978
1	16	1	54.163	54.710	54.710	0.0	-0.527	-0.569
2	16	1	37.773	37.392	37.392	0.0	0.385	0.491
3	16	1	65.979	67.205	67.205	0.0	-1.286	-1.179
7	16	1	33.340	33.457	33.457	0.0	-0.116	-0.133
9	16	1	50.261	49.619	49.619	0.0	0.642	0.652
-8	17	1	32.974	32.578	32.578	0.0	0.397	0.402
-6	17	1	26.461	25.797	25.797	0.0	0.665	0.685
-4	17	1	25.063	25.135	25.135	0.0	-0.072	-0.087
-2	17	1	143.902	146.740	146.740	0.0	-2.778	-1.273
0	17	1	47.758	49.138	49.138	0.0	-1.379	-1.592
2	17	1	88.375	87.752	87.752	0.0	0.623	0.453
4	17	1	11.400	12.564	12.564	0.0	-1.165	-0.795
6	17	1	97.153	97.873	97.873	0.0	-0.721	-0.473
8	17	1	23.106	23.751	23.751	0.0	-0.645	-0.572
-9	18	1	37.561	37.335	37.335	0.0	0.227	0.251
-7	18	1	105.729	107.216	107.216	0.0	-1.489	-0.902
-5	18	1	101.075	102.466	102.466	0.0	-1.392	-0.887
-3	18	1	8.083	6.929	6.929	0.0	1.154	0.654
1	18	1	26.287	26.268	26.268	0.0	0.319	0.395
0	14	0	221.214	230.777	230.777	0.0	-9.563	-2.890
2	18	1	19.535	19.816	19.816	0.0	-0.281	-0.285
3	18	1	87.628	88.229	88.229	0.0	-0.601	-0.433
5	18	1	53.107	53.813	53.813	0.0	-0.711	-0.710
7	18	1	4.129	3.075	-3.075	0.0	1.654	0.497
-8	19	1	7.724	9.616	-9.616	0.0	-1.892	-0.904
-4	19	1	30.769	50.770	50.770	0.0	-0.001	-0.001
-2	19	1	44.539	44.101	-44.101	0.0	0.438	0.514
0	19	1	1.315	1.719	-1.719	0.0	-0.404	-0.087
2	19	1	9.554	8.970	-8.970	0.0	0.416	-0.212
4	19	1	41.274	41.114	41.114	0.0	0.160	0.174
6	19	1	27.222	27.435	27.435	0.0	-0.212	-0.214
-7	20	1	8.352	4.690	-4.690	0.0	3.662	1.843
-5	20	1	21.209	20.504	0.504	0.0	0.797	0.867
-3	20	1	0.844	0.564	0.564	0.0	-0.280	0.054
-1	20	1	8.225	8.707	8.707	0.0	-0.482	-0.237
1	20	1	17.944	17.774	17.774	0.0	0.170	0.153
3	20	1	14.812	13.891	-13.891	0.0	-1.080	-0.642
5	20	1	30.683	29.228	29.228	0.0	1.655	1.744
7	20	1	5.110	7.801	7.801	0.0	-2.692	-0.810
-6	21	0	222.006	230.777	230.777	0.0	-8.771	-2.644
0	12	0	11.519	14.649	14.649	0.0	-3.129	-1.813
-4	21	1	53.794	53.411	-53.411	0.0	0.383	0.395

H	K	L	F (DBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA
0	21	1	40.359	40.113	40.113	0.0	0.280	0.331
2	21	1	27.073	25.736	-25.736	0.0	1.337	1.455
4	21	1	6.492	0.308	0.308	0.0	6.184	2.352
6	21	1	10.864	13.378	-13.378	0.0	-2.516	-1.207
-5	22	1	42.425	42.124	-42.124	0.0	0.300	0.329
-3	22	1	17.884	18.139	-18.139	0.0	-0.255	-0.198
-1	22	1	4.305	4.369	-4.369	0.0	-0.066	-0.020
4	22	1	34.999	35.075	-35.075	0.0	-0.076	-0.082
3	22	1	10.324	5.804	5.804	0.0	4.520	2.564
5	22	1	4.523	4.742	-3.742	0.0	0.591	0.161
-4	23	1	21.791	21.673	21.673	0.0	0.119	0.104
-2	23	1	8.232	6.831	-6.831	0.0	1.401	0.619
0	23	1	18.071	18.172	-18.172	0.0	-0.102	-0.085
2	23	1	19.789	20.923	20.923	0.0	-1.133	-0.898
4	23	1	7.866	0.889	0.889	0.0	6.977	2.883
-3	24	1	10.272	8.251	8.251	0.0	2.021	1.013
1	24	1	9.487	2.630	2.630	0.0	6.857	3.387
0	24	1	22.1393	23.0777	23.0777	0.0	-9.364	-2.835
-12	0	2	51.629	109.598	-51.858	0.0	0.771	0.800
-10	0	2	109.591	109.432	109.432	0.0	0.159	0.094
-8	0	2	71.537	73.371	73.371	0.0	-1.834	-1.615
-6	0	2	128.613	132.561	132.561	0.0	-4.545	-2.245
-4	0	2	170.557	180.723	180.723	0.0	-10.166	-3.991
-2	0	2	113.642	112.193	-112.193	0.0	3.444	1.987
0	0	2	249.772	278.140	278.140	0.0	-48.266	-7.809
2	0	2	142.468	141.588	141.588	0.0	0.501	0.234
4	0	2	208.462	217.070	217.070	0.0	-8.609	-2.763
6	0	2	43.112	44.526	-44.526	0.0	-1.414	-1.785
8	0	2	63.029	63.629	63.629	0.0	-0.601	-0.579
10	0	2	119.497	120.074	120.074	0.0	-0.577	-0.314
-13	1	2	8.935	12.107	12.107	0.0	-3.173	-1.370
-11	1	2	25.571	24.722	24.722	0.0	0.849	1.093
-9	1	2	26.968	28.575	-28.575	0.0	-1.606	-2.068
-7	1	2	179.477	187.639	187.639	0.0	-8.162	-3.025
-5	1	2	32.302	32.773	-32.773	0.0	-0.471	-0.742
-3	1	2	9.649	0.581	-0.581	0.0	6.068	3.309
1	1	2	118.287	116.248	116.248	0.0	2.039	1.147
3	1	2	241.580	230.777	230.777	0.0	-9.197	-2.779
5	1	2	83.751	84.969	84.969	0.0	-1.218	-0.954
7	1	2	47.325	48.540	-48.540	0.0	-1.215	-1.466
9	1	2	69.863	70.043	70.043	0.0	-0.180	-0.161
11	1	2	35.430	33.751	-33.751	0.0	-0.320	-0.380
-12	1	2	67.637	68.352	-68.352	0.0	-0.715	-0.614
-10	1	2	6.459	9.078	-9.078	0.0	-2.579	-0.970
-8	1	2	8.890	5.362	-5.362	0.0	3.528	2.176
-6	1	2	2.682	1.742	1.742	0.0	0.940	0.261
-4	1	2	33.505	33.614	-33.614	0.0	-0.311	-0.453
-2	1	2	23.786	23.823	-23.823	0.0	-0.038	-0.065
0	1	2	20.768	20.760	-20.760	0.0	0.007	0.014
2	1	2	48.985	49.250	-29.250	0.0	-0.265	-0.473
4	1	2	8.507	6.243	-6.243	0.0	2.064	1.932
6	1	2	3.997	6.504	6.504	0.0	-2.508	-0.970
8	1	2	12.080	14.016	-14.016	0.0	-1.936	-1.473

H	K	L	F(UBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
8	2	2	22.097	21.320	-21.320	0.0	0.778	0.913
10	2	2	19.035	19.244	-15.844	0.0	-0.810	-0.653
-13	3	2	26.610	27.047	-27.047	0.0	-0.437	-0.440
-9	2	2	70.703	72.243	-72.243	0.0	-1.535	-1.352
0	12	0	221.789	230.777	-230.777	0.0	-8.988	-2.710
-7	2	2	95.076	97.810	-97.810	0.0	-2.724	-1.677
-5	2	2	24.316	26.725	-26.725	0.0	-2.409	-3.706
-3	2	2	24.174	20.100	20.100	0.0	4.014	7.300
-1	3	2	4.994	3.785	3.785	0.0	0.809	0.523
1	3	2	78.215	75.256	-75.256	0.0	2.959	2.491
3	3	2	7.127	0.875	0.875	0.0	6.452	4.755
5	2	2	55.040	56.928	-56.928	0.0	-1.288	-1.402
7	2	2	80.103	80.702	-80.702	0.0	-0.515	-0.410
9	3	2	30.009	37.577	-37.577	0.0	0.433	0.513
11	3	2	10.554	15.310	-15.310	0.0	1.244	0.952
-12	4	2	60.077	59.538	59.538	0.0	0.109	0.104
-10	4	2	54.400	54.274	-54.274	0.0	0.125	0.133
-8	4	2	22.450	20.472	20.472	0.0	1.984	2.505
-6	4	2	92.165	92.864	-92.864	0.0	-0.679	-0.481
-4	4	2	71.380	69.448	-69.448	0.0	1.932	1.759
-2	4	2	14.522	15.942	-15.942	0.0	-1.419	-2.289
0	4	2	89.735	84.076	84.076	0.0	5.658	4.162
2	4	2	84.319	87.440	-87.440	0.0	-3.121	-2.429
4	4	2	86.134	87.120	-87.120	0.0	-0.986	-0.745
6	4	2	73.432	78.662	-78.662	0.0	-0.230	-0.187
8	4	2	221.580	230.777	-230.777	0.0	-9.197	-2.779
10	4	2	33.938	33.373	33.373	0.0	0.565	0.742
-11	5	2	40.313	39.919	-39.919	0.0	0.399	0.434
-9	5	2	15.852	17.037	-17.037	0.0	-1.185	-0.985
-7	5	2	39.294	39.455	-39.455	0.0	-0.160	-0.203
-5	5	2	50.948	52.588	-52.588	0.0	-1.640	-1.876
-3	5	2	23.995	22.320	-22.320	0.0	1.675	2.491
-1	5	2	32.725	27.551	27.551	0.0	4.764	7.906
1	5	2	53.936	52.659	-52.659	0.0	1.273	1.500
3	5	2	71.737	74.774	-74.774	0.0	2.964	2.495
5	5	2	28.943	28.772	28.772	0.0	2.175	3.346
7	5	2	7.747	7.625	-7.625	0.0	0.122	0.067
9	5	2	53.035	53.642	-53.642	0.0	-0.607	-0.640
11	5	2	16.487	14.169	14.169	0.0	2.298	2.166
-12	6	2	10.361	7.423	7.423	0.0	2.938	1.530
-10	6	2	10.376	6.144	-6.144	0.0	4.232	2.672
-8	6	2	13.910	13.117	13.117	0.0	0.793	0.672
-6	6	2	14.176	19.753	-19.753	0.0	-1.578	-1.600
-4	6	2	10.309	9.856	9.856	0.0	0.453	0.337
0	12	0	13.521	12.712	-12.712	0.0	0.840	0.986
-2	6	2	221.458	230.777	-230.777	0.0	-9.339	-2.822
0	6	2	5.954	5.511	-5.511	0.0	0.442	0.299
2	6	2	5.364	3.495	3.495	0.0	1.868	1.191
6	6	2	8.613	7.034	7.034	0.0	1.579	1.355
8	6	2	14.440	13.454	13.454	0.0	0.987	0.964
10	6	2	20.353	27.144	-27.144	0.0	-0.811	-0.935
-13	7	2	10.152	7.237	7.237	0.0	2.915	1.647
-13	7	2	21.536	27.046	-27.046	0.0	-0.110	-0.108

*

*

*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-11	7	2	10.063	13.010	-18.010	0.0	0.053	0.043
-9	7	2	32.078	32.252	32.252	0.0	-0.174	-0.218
-7	7	2	9.047	11.762	11.762	0.0	-2.716	-1.540
-5	7	2	42.417	41.580	41.580	0.0	0.837	1.110
-3	7	2	36.463	35.100	-35.100	0.0	1.363	2.027
-1	7	2	50.141	48.822	48.822	0.0	1.320	1.021
5	7	2	32.745	33.109	33.109	0.0	-0.366	-0.569
7	7	2	12.774	11.672	-11.673	0.0	1.101	1.053
9	7	2	5.476	32.660	32.660	0.0	1.256	1.716
11	7	2	21.104	21.631	-2.123	0.0	3.352	1.411
12	7	2	13.566	11.203	-11.263	0.0	-0.527	-0.518
0	0	0	221.602	230.777	230.777	0.0	2.303	1.427
-12	8	2	30.517	29.724	29.724	0.0	-9.174	-2.772
-10	8	2	21.903	20.242	-20.242	0.0	0.793	0.849
-8	8	2	0.873	3.197	3.197	0.0	1.861	2.021
-6	8	2	19.610	20.894	-20.894	0.0	3.676	1.937
-4	8	2	16.943	15.147	-15.147	0.0	-1.284	-1.304
-2	8	2	54.925	53.007	53.007	0.0	1.796	2.425
0	8	2	102.292	100.606	-100.606	0.0	1.916	2.192
2	8	2	88.915	88.384	88.384	0.0	1.657	1.091
4	8	2	39.145	38.795	-38.795	0.0	0.529	0.369
6	8	2	0.904	2.142	2.142	0.0	0.352	0.458
8	8	2	8.262	4.095	4.095	0.0	-1.239	-0.264
10	8	2	11.930	13.342	-13.345	0.0	4.168	2.354
-11	9	2	22.239	20.426	-20.428	0.0	-1.415	-0.783
-9	9	2	13.701	13.114	13.114	0.0	1.812	2.004
-7	9	2	51.030	52.443	-52.443	0.0	0.646	0.527
-5	9	2	13.447	12.122	12.122	0.0	-1.412	-1.589
-3	9	2	92.367	92.518	-92.518	0.0	1.325	1.207
-1	9	2	14.186	12.567	12.567	0.0	-0.131	-0.093
1	9	2	33.729	32.797	-32.797	0.0	1.619	1.776
3	9	2	62.742	64.466	-84.466	0.0	0.932	1.357
0	12	0	221.304	230.777	230.777	0.0	-1.724	-1.349
5	9	2	26.475	26.577	26.577	0.0	-9.473	-2.662
7	9	2	43.137	46.350	-46.350	0.0	-0.502	-0.566
9	9	2	7.074	4.589	-4.589	0.0	-0.413	-0.476
-12	10	2	9.955	1.928	1.928	0.0	2.485	1.073
-10	10	2	36.269	36.001	36.001	0.0	8.068	4.779
-8	10	2	36.045	36.394	36.394	0.0	0.268	0.323
-6	10	2	18.811	19.941	19.941	0.0	-0.349	-0.441
-4	10	2	47.758	47.376	47.376	0.0	-1.130	-1.182
-2	10	2	23.293	23.491	23.491	0.0	0.381	0.459
0	10	2	53.038	53.338	53.338	0.0	-0.198	-0.276
2	10	2	33.072	33.458	33.458	0.0	-0.501	-0.532
4	10	2	64.574	65.882	65.882	0.0	-0.387	-0.529
6	10	2	15.912	16.129	16.129	0.0	-1.308	-1.250
8	10	2	13.073	13.952	13.952	0.0	-0.217	-0.211
10	10	2	16.308	14.790	14.790	0.0	0.879	-0.636
-11	11	2	54.153	54.792	54.792	0.0	1.513	1.129
-9	11	2	20.977	20.024	20.024	0.0	-0.639	-0.639
-7	11	2	155.706	159.337	159.337	0.0	0.953	1.046
-5	11	2	7.949	9.433	-9.433	0.0	-3.631	-1.543
							-1.485	-0.805

*

*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-3	11	2	133.346	140.430	140.430	0.0	-1.084	-0.517
0	12	0	220.975	230.777	230.777	0.0	-9.802	-2.969 *
-1	11	2	14.717	15.358	15.358	0.0	-0.642	-0.627
1	11	2	92.257	91.404	91.404	0.0	0.853	0.567
3	11	2	167.524	171.179	171.179	0.0	-3.655	-1.452
5	11	2	11.702	10.802	-10.802	0.0	0.904	0.766
7	11	2	69.169	69.396	69.396	0.0	-0.228	-0.200
9	11	2	5.043	6.117	6.117	0.0	-1.075	-0.542
-12	12	2	40.960	39.216	-39.216	0.0	1.744	1.698
-10	12	2	19.968	18.550	18.550	0.0	1.418	1.449
-8	12	2	24.242	23.856	23.856	0.0	0.385	0.453
-6	12	2	103.172	109.773	109.773	0.0	-1.602	-0.970
-4	12	2	29.501	28.564	28.564	0.0	0.937	1.194
-2	12	2	147.414	149.037	-149.037	0.0	-1.623	-0.732
0	12	2	210.411	220.396	220.396	0.0	-4.485	-1.387
2	12	2	9.156	2.001	2.081	0.0	4.074	1.881
4	12	2	61.086	60.626	60.626	0.0	0.460	0.456
6	12	2	25.825	25.825	-25.825	0.0	-0.141	-0.164
8	12	2	33.594	31.750	31.750	0.0	1.844	2.265
-9	13	2	11.333	11.688	-11.688	0.0	-0.355	-0.424
-7	13	2	46.018	46.687	46.687	0.0	-0.669	-0.766
0	12	0	221.528	230.777	230.777	0.0	-9.249	-2.795
-5	13	2	57.268	58.238	-58.238	0.0	-0.969	-1.014
-3	13	2	27.797	28.077	28.077	0.0	-0.279	-0.370
-1	13	2	59.273	59.485	-59.485	0.0	-0.205	-0.203
1	13	2	10.982	10.807	-10.807	0.0	0.114	0.089
3	13	2	59.487	60.876	60.876	0.0	-1.389	-1.408
5	13	2	50.687	51.270	-51.270	0.0	-0.583	-0.640
7	13	2	11.564	13.332	-13.332	0.0	-1.768	-1.122
9	13	2	42.105	41.077	-41.077	0.0	1.028	0.912
-6	14	2	14.216	15.402	15.402	0.0	-1.186	-0.939
-4	14	2	3.399	2.554	-2.554	0.0	0.845	0.261
-2	14	2	0.499	4.166	-4.166	0.0	2.334	1.192
0	14	2	13.474	18.974	18.974	0.0	-0.500	-0.548
2	14	2	10.638	9.712	-9.712	0.0	0.926	0.666
4	14	2	23.308	23.840	23.840	0.0	-0.532	-0.672
6	14	2	3.035	5.051	5.051	0.0	-0.019	-0.006
-9	15	2	13.985	12.512	12.512	0.0	1.473	1.224
-7	15	2	35.963	35.810	-35.810	0.0	0.153	0.176
-1	15	2	29.986	29.582	-29.582	0.0	0.404	0.501
1	15	2	38.346	38.880	38.880	0.0	-0.534	-0.688
3	15	2	4.557	5.727	5.727	0.0	-1.170	-0.455
5	15	2	27.065	27.510	-27.510	0.0	-0.444	-0.551
7	15	2	46.324	46.885	46.885	0.0	-0.561	-0.648
-10	16	2	21.537	22.063	-22.063	0.0	-0.466	-0.431
-8	16	2	12.214	9.740	-9.740	0.0	2.474	1.526
-6	16	2	8.337	9.658	-9.658	0.0	-1.321	-0.614
-4	16	2	13.081	12.899	-12.899	0.0	0.182	0.147
0	16	2	19.752	19.291	-19.291	0.0	0.460	0.497
2	16	2	11.460	9.232	9.232	0.0	2.228	1.765
4	16	2	51.284	50.873	-50.873	0.0	0.411	0.459
6	16	2	26.781	27.143	27.143	0.0	-0.362	-0.440
8	16	2	32.265	31.497	-31.497	0.0	0.768	0.569

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA
6	16	2	2.255	5.994	-5.994	0.0	-3.640	-0.826
-7	17	2	1.442	6.590	6.590	0.0	-5.148	-1.000
0	12	0	221.005	230.777	230.777	0.0	-9.772	-2.959 *
-3	17	2	11.714	11.149	-11.149	0.0	0.565	0.435
-1	17	2	6.260	7.091	7.091	0.0	-0.831	-0.361
1	17	2	4.765	2.814	-2.814	0.0	1.953	0.726
3	17	2	9.950	5.805	-5.805	0.0	4.129	2.820
7	17	2	2.353	3.116	3.116	0.0	-0.763	-0.163
-6	18	2	18.975	17.551	-17.551	0.0	1.424	1.444
-4	18	2	9.242	8.756	-8.756	0.0	0.567	0.346
-2	18	2	21.829	21.694	-21.694	0.0	0.135	0.149
0	18	2	9.243	6.063	-6.063	0.0	3.185	2.040
2	18	2	24.070	24.806	24.806	0.0	-0.736	-0.801
4	18	2	13.733	13.757	13.757	0.0	-0.019	-0.014
6	18	2	19.289	20.350	20.350	0.0	-1.041	-0.806
-7	19	2	39.758	40.430	-40.430	0.0	-0.675	-0.738
-5	19	2	15.680	13.954	-13.954	0.0	1.726	1.583
-3	19	2	16.123	16.821	-16.821	0.0	-0.693	-0.580
-1	19	2	9.365	1.811	-1.811	0.0	4.554	4.060
1	19	2	20.110	19.047	-19.047	0.0	1.064	1.087
3	19	2	2.615	3.923	-3.923	0.0	-1.308	-0.310
0	12	0	221.894	230.777	230.777	0.0	-8.883	-2.678 *
5	19	2	16.138	16.539	-16.539	0.0	-0.351	-0.257
-6	20	2	4.759	8.231	8.231	0.0	-3.472	-1.024
-4	20	2	5.675	5.820	-5.820	0.0	-0.145	-0.148
-2	20	2	5.782	0.482	-0.482	0.0	5.300	2.016
0	20	2	40.848	39.299	-39.299	0.0	1.549	1.819
2	20	2	27.083	26.508	-26.508	0.0	0.580	0.658
4	20	2	72.366	72.745	-72.745	0.0	-0.379	-0.313
-7	21	2	16.955	16.579	-16.579	0.0	0.417	0.312
-5	21	2	26.293	28.730	28.730	0.0	-0.432	-0.441
-3	21	2	22.060	21.162	-21.162	0.0	0.899	0.940
-1	21	2	29.120	28.230	-28.230	0.0	0.889	0.976
1	21	2	6.880	3.631	-3.631	0.0	3.250	1.358
3	21	2	18.170	18.143	-18.143	0.0	0.032	0.026
-4	22	2	48.573	48.128	-48.128	0.0	0.444	0.468
-2	22	2	15.830	15.532	-15.532	0.0	0.298	0.214
0	22	2	65.554	67.596	67.596	0.0	-0.842	-0.742
2	22	2	20.648	20.606	-20.606	0.0	0.042	0.036
-3	23	2	35.955	36.205	36.205	0.0	-0.250	-0.277
-1	23	2	10.615	11.666	-11.666	0.0	1.050	-0.515
1	23	2	34.242	34.166	-34.166	0.0	0.176	0.199
0	12	0	221.558	230.777	230.777	0.0	-9.219	-2.786 *
-13	0	0	11.744	12.106	-12.106	0.0	-0.363	-0.207
-11	0	0	1.285	4.024	-4.024	0.0	-2.739	-0.574
-9	0	0	26.386	25.571	-25.571	0.0	0.814	1.069
-7	0	0	3.788	4.881	-4.881	0.0	-1.094	-0.347
-5	0	0	15.882	16.712	-16.712	0.0	-0.830	-0.881
-3	0	0	25.993	26.251	-26.251	0.0	-0.261	-0.416
1	0	0	2.592	0.500	-0.500	0.0	2.093	0.682
3	0	0	16.510	16.844	-16.844	0.0	-0.335	-0.342
5	0	0	13.058	13.229	-13.229	0.0	-0.171	-0.149
7	0	0	12.199	11.440	-11.440	0.0	0.759	0.558

H	K	L	F(DBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
9	0	3	5.342	6.764	6.764	0.0	-0.422	-0.159
-12	1	3	7.814	1.732	-1.732	0.0	6.082	2.929
-10	1	3	13.200	11.387	11.387	0.0	1.813	1.489
-6	1	3	2.488	0.606	0.606	0.0	1.882	0.521
-4	1	3	26.774	26.570	26.570	0.0	0.204	0.311
-2	1	3	29.420	28.356	-28.356	0.0	1.078	1.677
0	1	3	50.620	37.139	37.139	0.0	-0.519	-0.755
2	1	3	21.709	21.172	-21.172	0.0	0.537	0.725
4	1	3	421.924	430.777	430.777	0.0	-8.853	-2.609
6	1	3	11.400	13.846	-13.846	0.0	-2.446	-1.637
8	1	3	13.258	19.059	19.059	0.0	-0.802	-0.756
-12	2	3	6.459	1.900	-1.900	0.0	4.599	1.710
-11	2	3	13.798	13.824	-13.824	0.0	-0.026	-0.021
-9	2	3	13.422	18.758	18.758	0.0	-0.336	-0.354
-7	2	3	57.298	57.805	57.805	0.0	-0.507	-0.530
-5	2	3	70.655	70.882	-70.882	0.0	-0.227	-0.206
-3	2	3	103.503	102.065	102.065	0.0	1.438	0.917
-1	2	3	10.742	10.295	10.295	0.0	0.447	0.437
1	2	3	3.830	9.608	-9.608	0.0	-0.778	-0.563
3	2	3	50.620	51.851	51.851	0.0	-1.232	-1.409
7	2	3	38.749	38.051	38.051	0.0	0.698	0.881
9	2	3	31.712	32.618	-32.618	0.0	-0.906	-0.986
-12	3	3	23.253	29.049	-29.049	0.0	-0.790	-0.832
-10	3	3	9.358	11.563	11.563	0.0	-2.163	-1.164
-8	3	3	61.063	62.037	-62.037	0.0	-0.974	-0.975
-6	3	3	3.586	8.518	8.518	0.0	-4.932	-1.546
-4	3	3	221.376	230.777	230.777	0.0	-9.398	-2.840
-2	3	3	11.519	10.992	10.992	0.0	0.527	0.455
0	3	3	110.077	107.984	-107.984	0.0	2.013	1.255
2	3	3	27.251	27.150	27.150	0.0	0.402	0.604
4	3	3	65.620	65.714	-65.714	0.0	-0.094	-0.090
6	3	3	50.993	52.163	-52.163	0.0	-1.170	-1.284
8	3	3	13.036	13.089	-13.089	0.0	-0.052	-0.039
10	3	3	13.484	10.638	10.638	0.0	2.846	1.915
-13	4	3	19.998	19.029	19.029	0.0	0.969	0.827
-11	4	3	0.143	3.647	-3.647	0.0	4.501	1.021
-7	4	3	14.664	14.224	-14.224	0.0	0.441	0.361
-5	4	3	11.242	7.300	7.300	0.0	3.943	3.273
-1	4	3	15.695	14.462	14.462	0.0	1.233	1.543
1	4	3	14.179	13.851	13.851	0.0	0.328	0.340
5	4	3	11.071	9.148	-9.148	0.0	1.923	1.514
7	4	3	3.167	5.339	5.339	0.0	-2.171	-0.625
9	4	3	19.692	19.807	19.807	0.0	-0.115	-0.097
0	4	3	220.355	230.777	230.777	0.0	-10.422	-3.163
-12	5	3	97.220	97.726	97.726	0.0	-0.506	-0.330
-10	5	3	24.593	23.354	23.354	0.0	1.239	1.442
-8	5	3	74.503	75.403	75.403	0.0	-0.901	-0.763
-6	5	3	35.216	35.347	35.347	0.0	-0.131	-0.173
-4	5	3	30.016	30.283	30.283	0.0	-0.267	-0.388
-2	5	3	201.873	203.134	203.134	0.0	-1.261	-0.418
0	5	3	19.729	19.214	19.214	0.0	0.515	0.657
2	5	3	110.353	111.090	111.090	0.0	-0.737	-0.440
4	5	3	37.123	37.587	-37.587	0.0	-0.459	-0.597

H	K	L	F(UBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
6	5	3	102.091	103.114	103.114	0.0	-1.023	-0.649
8	5	3	94.213	94.757	94.757	0.0	-0.545	-0.556
10	5	3	11.467	10.973	10.973	0.0	0.494	0.269
-13	6	3	16.383	16.566	16.566	0.0	-0.183	-0.129
-11	6	3	34.476	34.733	34.733	0.0	-0.257	-0.297
-9	6	3	149.782	154.748	154.748	0.0	-4.966	-2.194
-7	6	3	60.231	67.151	67.151	0.0	-0.920	-0.688
-5	6	3	110.314	117.517	117.517	0.0	-1.203	-0.632
-3	6	3	52.293	51.499	51.499	0.0	0.794	0.908
-1	6	3	215.170	216.285	216.285	0.0	-1.116	-0.347
0	6	3	35.499	36.736	36.736	0.0	-1.236	-1.689
0	12	0	221.169	230.777	230.777	0.0	-9.603	-2.910
3	6	3	17.062	17.841	17.841	0.0	-0.779	-0.827
3	6	3	139.010	142.261	142.261	0.0	-3.271	-1.553
7	6	3	8.933	4.793	4.793	0.0	2.140	1.030
9	6	3	104.765	104.142	104.142	0.0	0.623	0.381
-12	7	3	48.797	49.159	49.159	0.0	-0.362	-0.370
-8	7	3	20.066	19.434	19.434	0.0	0.631	0.755
-6	7	3	23.950	25.417	25.417	0.0	-1.467	-1.769
-4	7	3	35.156	34.759	34.759	0.0	0.397	0.542
-2	7	3	100.776	99.771	99.771	0.0	1.005	0.656
0	7	3	39.100	38.588	38.588	0.0	0.513	0.686
2	7	3	22.232	21.808	21.808	0.0	0.424	0.511
4	7	3	80.561	81.457	81.457	0.0	-0.896	-0.714
6	7	3	45.428	45.652	45.652	0.0	-0.224	-0.261
8	7	3	11.026	12.584	12.584	0.0	-1.553	-0.684
-11	8	3	7.919	7.552	7.552	0.0	0.367	0.165
-9	8	3	21.067	22.354	22.354	0.0	-1.287	-1.346
-5	8	3	20.708	19.175	19.175	0.0	1.533	1.739
-3	8	3	6.686	2.162	2.162	0.0	4.524	2.338
0	12	0	220.777	230.777	230.777	0.0	-10.056	-3.045
-1	8	3	14.575	12.323	12.323	0.0	2.252	2.266
1	8	3	4.303	0.979	0.979	0.0	3.324	1.229
5	8	3	29.404	29.774	29.774	0.0	-0.371	-0.482
7	8	3	8.748	3.959	3.959	0.0	4.789	2.811
9	8	3	4.266	7.192	7.192	0.0	-2.927	-0.798
-12	9	3	16.263	14.838	14.838	0.0	1.425	1.129
-10	9	3	35.109	33.549	33.549	0.0	-0.441	-0.508
-8	9	3	36.934	37.101	37.101	0.0	-0.168	-0.214
-6	9	3	31.383	32.896	32.896	0.0	-1.512	-1.965
-4	9	3	50.672	50.851	50.851	0.0	-0.179	-0.205
-2	9	3	59.883	60.116	60.116	0.0	-0.233	-0.240
0	9	3	65.844	66.696	66.696	0.0	-0.852	-0.808
2	9	3	20.227	21.100	21.100	0.0	-0.873	-0.870
4	9	3	30.801	31.347	31.347	0.0	-0.547	-0.711
6	9	3	19.901	19.307	19.307	0.0	0.594	0.607
8	9	3	14.829	13.636	13.636	0.0	1.192	0.907
-11	10	3	7.366	1.990	1.990	0.0	5.475	2.403
-9	10	3	10.571	11.773	11.773	0.0	-1.203	-0.732
-7	10	3	34.969	35.112	35.112	0.0	-0.143	-0.184
0	12	0	221.670	230.777	230.777	0.0	-9.107	-2.752
-5	10	3	70.297	71.037	71.037	0.0	-0.740	-0.661
-3	10	3	55.535	56.549	56.549	0.0	-1.014	-1.095

H	K	L	FIBRS)	FICALC)	AICALC)	BICALC)	DELTA F	DELTA/SIGMA
-1	10	3	7.989	4.664	4.664	0.0	3.322	1.861
1	10	3	33.057	33.520	-33.520	0.0	-0.464	-0.609
3	10	3	16.825	18.425	16.425	0.0	-1.602	-1.715
5	10	3	2.286	5.218	5.218	0.0	-2.932	-0.736
7	10	3	9.921	9.855	9.855	0.0	0.066	0.039
9	10	3	36.075	35.310	-35.310	0.0	0.759	0.788
-12	11	3	8.255	5.519	5.519	0.0	2.736	1.259
-10	11	3	0.406	9.378	-3.878	0.0	-1.633	-0.826
-8	11	3	16.455	17.599	-17.599	0.0	1.164	-1.039
-6	11	3	10.058	7.678	-7.678	0.0	2.960	2.291
-4	11	3	3.040	6.688	6.688	0.0	-2.848	-0.939
-2	11	3	42.952	42.897	-42.897	0.0	0.030	0.044
0	11	3	5.282	1.402	-1.402	0.0	3.880	1.593
2	11	3	11.422	10.452	-10.452	0.0	1.179	1.018
4	11	3	22.105	22.550	-22.550	0.0	-0.845	-0.943
6	11	3	29.015	27.977	-27.977	0.0	1.038	1.241
8	11	3	10.655	12.058	12.058	0.0	-1.408	-0.735
-11	12	3	16.674	15.195	15.195	0.0	1.481	1.120
0	12	0	221.431	230.777	230.777	0.0	-9.346	-2.824
-7	12	3	13.805	14.470	14.470	0.0	-0.664	-0.514
-5	12	3	6.200	5.159	5.159	0.0	1.041	0.472
-3	12	3	9.099	9.820	9.820	0.0	-0.721	-0.457
-1	12	3	19.991	20.316	20.316	0.0	-0.325	-0.372
1	12	3	23.054	22.399	22.399	0.0	0.655	0.851
3	12	3	3.414	4.787	4.787	0.0	-1.373	-0.417
5	12	3	10.698	7.254	7.254	0.0	3.464	2.466
7	12	3	12.386	10.568	10.568	0.0	1.418	0.949
-10	13	3	15.860	13.860	13.860	0.0	2.000	1.625
-8	13	3	7.814	3.325	3.325	0.0	4.489	2.366
-6	13	3	3.250	1.863	1.863	0.0	1.587	0.595
-4	13	3	20.656	19.763	19.763	0.0	0.893	1.013
-2	13	3	8.359	10.267	-10.267	0.0	-1.907	-1.082
0	13	3	46.018	46.434	46.434	0.0	-0.416	-0.495
2	13	3	29.205	30.612	-30.612	0.0	-1.402	-1.707
4	13	3	27.528	27.526	27.526	0.0	0.002	0.003
6	13	3	2.907	5.867	-5.867	0.0	-3.260	-0.771
8	13	3	14.246	12.453	12.453	0.0	1.793	1.237
-11	14	3	9.697	7.435	7.435	0.0	2.261	1.142
0	14	0	221.177	230.777	230.777	0.0	-9.600	-2.907
-9	14	3	47.504	47.700	-47.700	0.0	-0.196	-0.210
-7	14	3	17.802	17.301	17.301	0.0	0.501	0.462
-5	14	3	58.205	68.042	-68.042	0.0	0.163	0.147
-3	14	3	34.132	33.762	33.762	0.0	0.370	0.481
-1	14	3	57.395	57.275	-57.275	0.0	0.120	0.122
1	14	3	25.026	23.796	-23.796	0.0	1.230	1.599
3	14	3	8.188	10.264	10.264	0.0	-2.076	-1.049
5	14	3	51.830	50.822	-50.822	0.0	1.008	1.071
7	14	3	10.660	14.830	14.830	0.0	-4.170	-2.015
-10	15	3	12.759	13.321	13.321	0.0	-0.562	-0.336
-8	15	3	16.136	17.252	-17.252	0.0	-1.116	-0.816
-6	15	3	8.696	9.221	9.221	0.0	-0.287	-0.287
-4	15	3	11.011	7.690	7.690	0.0	3.321	2.456
-2	15	3	29.277	29.071	-29.071	0.0	0.205	0.269

H	K	L	F (UBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA
0	15	3	33.389	33.087	33.687	0.0	-0.302	-0.574
4	15	3	38.816	38.916	-38.916	0.0	-0.100	-0.123
4	15	3	19.921	18.882	18.882	0.0	1.039	1.033
6	15	3	13.267	14.124	-14.124	0.0	-0.855	-0.536
-9	16	3	42.290	41.574	41.574	0.0	0.716	0.779
-7	16	3	15.449	15.228	15.228	0.0	0.221	0.175
0	12	0	221.774	230.777	230.777	0.0	-9.003	-2.714
-5	10	3	64.141	64.649	64.649	0.0	-0.508	-0.476
-3	16	3	32.915	33.545	33.545	0.0	-1.030	-1.242
-1	16	3	62.976	62.571	62.971	0.0	0.004	0.004
1	16	3	49.081	50.434	50.434	0.0	-1.353	-1.473
5	16	3	34.590	35.701	35.701	0.0	-1.106	-1.333
5	16	3	38.568	38.536	38.536	0.0	0.032	0.030
-8	17	3	37.681	38.926	38.926	0.0	-1.245	-1.344
-6	17	3	22.628	23.044	23.044	0.0	-0.416	-0.425
-4	17	3	19.707	20.104	20.104	0.0	-0.397	-0.399
-2	17	3	112.661	113.043	113.043	0.0	-0.381	-0.220
0	17	3	6.006	8.293	-8.293	0.0	-2.292	-0.900
2	17	3	95.930	95.905	95.905	0.0	-0.209	-0.180
4	17	3	43.545	42.682	-42.682	0.0	0.863	0.955
6	17	3	71.903	71.651	71.651	0.0	0.252	0.207
-7	18	3	75.920	74.223	-74.223	0.0	0.787	0.639
-5	18	3	13.520	16.386	16.386	0.0	-3.066	-1.900
-3	18	3	16.622	10.144	-16.144	0.0	0.478	0.435
-1	18	3	93.470	93.176	93.176	0.0	0.294	0.201
1	18	3	38.600	37.561	-37.561	0.0	1.038	1.241
3	18	3	55.647	55.289	-55.289	0.0	0.353	0.353
0	12	0	221.767	230.777	230.777	0.0	-9.010	-2.716
5	18	3	72.067	71.778	71.778	0.0	0.289	0.239
-2	19	3	11.400	10.826	-10.826	0.0	0.574	0.320
-2	19	3	25.452	25.250	25.250	0.0	0.202	0.219
0	19	3	13.895	14.916	-14.916	0.0	-1.021	-0.759
2	19	3	26.774	27.121	27.121	0.0	-0.347	-0.354
4	19	3	45.749	46.555	-46.555	0.0	-0.806	-0.856
-7	20	3	21.873	19.158	19.158	0.0	2.716	2.653
-5	20	3	5.244	9.990	-9.990	0.0	-4.746	-1.428
-3	20	3	23.039	22.776	22.776	0.0	0.263	0.262
1	20	3	10.474	11.038	11.038	0.0	-0.564	-0.305
3	20	3	14.209	14.677	14.677	0.0	-0.468	-0.297
-6	21	3	2.129	3.796	3.796	0.0	-1.667	-0.343
-4	21	3	4.139	6.558	6.558	0.0	-2.419	-0.682
-2	21	3	28.530	28.886	-28.886	0.0	-0.350	-0.364
0	21	3	24.990	26.387	26.387	0.0	-1.391	-1.302
2	21	3	34.700	34.571	-34.571	0.0	0.129	0.135
-3	22	3	12.364	11.337	11.337	0.0	1.027	0.608
0	12	0	221.993	230.777	230.777	0.0	-8.778	-2.647
-1	22	3	24.443	25.054	-25.054	0.0	-0.611	-0.606
1	22	3	7.911	8.244	-8.244	0.0	-0.333	-0.132
-12	0	4	11.841	10.836	10.836	0.0	1.005	0.582
-10	0	4	51.225	52.239	52.239	0.0	-1.014	-1.086
-8	0	4	21.642	22.063	-22.063	0.0	-0.421	-0.485
-6	0	4	170.415	178.469	178.469	0.0	-8.054	-3.143
-4	0	4	148.228	151.754	151.754	0.0	-3.526	-1.579

H	K	L	FIBRS1	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-2	0	0	78.507	80.663	-20.663	0.0	-2.156	-1.760
0	0	4	176.937	181.506	181.506	0.0	-4.570	-1.723
2	0	4	18.450	17.450	17.450	0.0	1.000	1.068
4	0	4	152.987	155.032	155.032	0.0	-2.046	-0.886
6	0	4	20.940	21.119	21.119	0.0	-0.179	-0.179
8	0	4	48.610	48.709	48.709	0.0	-0.099	-0.100
-13	1	4	16.435	14.364	14.364	0.0	2.071	1.557
-11	1	4	30.390	31.310	31.310	0.0	-0.921	-1.002
-9	1	4	20.886	19.320	-19.320	0.0	1.366	1.550
-7	1	4	86.029	86.731	86.731	0.0	-0.701	-0.524
-5	1	4	8.920	10.954	-10.954	0.0	-2.035	-1.125
-3	1	4	130.612	130.824	130.824	0.0	-2.212	-1.073
-1	1	4	54.377	54.790	-54.790	0.0	-0.413	-0.453
0	1	4	221.423	230.777	230.777	0.0	-9.354	-2.826
1	1	4	6.335	7.479	-7.479	0.0	1.144	-0.516
3	1	4	91.617	93.155	93.155	0.0	-1.538	-1.084
5	1	4	10.160	10.958	10.958	0.0	-0.799	-0.475
7	1	4	24.991	24.588	24.588	0.0	0.402	0.402
-12	2	4	11.295	12.975	-12.975	0.0	-1.679	-0.855
-10	2	4	10.061	15.731	-15.731	0.0	0.330	-0.269
-8	2	4	2.786	1.718	1.718	0.0	1.069	0.294
-6	2	4	10.965	17.417	-17.417	0.0	-0.451	-0.454
-4	2	4	13.917	12.397	-12.397	0.0	1.520	1.348
-2	2	4	13.394	14.364	-14.364	0.0	-0.970	-0.792
0	2	4	23.084	22.929	-22.929	0.0	0.155	0.188
2	2	4	10.637	18.379	-18.379	0.0	-1.742	-1.754
4	2	4	3.728	4.553	-4.553	0.0	-0.825	-0.247
6	2	4	10.922	7.946	-7.946	0.0	2.976	1.786
-13	3	4	1.255	4.810	-4.810	0.0	-3.555	-0.632
-11	3	4	23.105	22.802	-22.802	0.0	1.103	1.119
-9	3	4	24.279	24.165	-24.165	0.0	0.114	0.131
-7	3	4	13.905	15.243	-15.243	0.0	0.661	0.661
-5	3	4	40.460	41.528	41.528	0.0	-1.468	-1.803
0	3	4	222.110	230.777	230.777	0.0	-8.666	-2.613
-3	3	4	32.600	32.041	-32.041	0.0	0.560	0.436
-1	3	4	53.406	54.519	-54.519	0.0	-1.113	-1.231
1	3	4	3.341	1.532	1.532	0.0	3.809	1.478
3	3	4	51.008	51.371	-51.371	0.0	-0.363	-0.408
5	3	4	30.449	30.127	-30.127	0.0	0.322	0.411
7	3	4	17.593	18.345	-18.345	0.0	-0.752	-0.645
-12	4	4	24.764	24.560	-24.560	0.0	0.204	0.191
-10	4	4	3.078	0.192	0.192	0.0	2.886	0.777
-8	4	4	10.002	18.198	-18.198	0.0	-2.197	-1.885
-6	4	4	9.674	11.711	-11.711	0.0	-2.037	-1.280
-4	4	4	27.416	27.048	-27.048	0.0	0.368	0.457
-2	4	4	46.130	46.041	-46.041	0.0	0.089	0.108
0	4	4	60.466	61.874	-61.874	0.0	-1.408	-1.417
2	4	4	87.735	89.577	-89.577	0.0	-1.822	-1.340
4	4	4	5.468	7.757	-7.757	0.0	-2.288	-0.885
6	4	4	10.431	8.725	8.725	0.0	1.756	1.153
8	4	4	15.598	14.830	14.830	0.0	0.769	0.585
-11	5	4	27.917	26.572	-26.572	0.0	1.345	1.526
-9	5	4	2.846	3.060	-3.060	0.0	-0.214	-0.056

II	K	L	F(UBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	12	0	221.259	230.777	230.777	0.0	-9.516	-2.676 *
-9	5	4	5.050	6.607	6.607	0.0	-1.557	-0.615
-3	5	4	45.360	46.124	-46.124	0.0	-0.763	-0.912
-1	5	4	7.560	6.908	6.908	0.0	0.652	0.328
1	5	4	11.960	12.190	-12.190	0.0	-0.230	-0.175
3	5	4	33.146	35.507	-35.507	0.0	-0.821	-1.047
5	5	4	3.310	2.339	-2.339	0.0	1.471	0.480
7	5	4	6.163	5.846	-5.846	0.0	2.317	0.899
-12	6	4	9.794	7.709	-7.709	0.0	2.084	1.049
-10	6	4	11.406	9.700	-9.700	0.0	1.506	0.933
-8	6	4	15.299	15.298	-15.298	0.0	0.002	0.001
-6	6	4	6.664	1.772	1.772	0.0	4.892	2.462
-2	6	4	8.315	4.298	4.298	0.0	4.016	2.203
0	6	4	13.073	12.260	-12.260	0.0	0.813	0.676
2	6	4	6.156	7.792	-7.792	0.0	-1.637	-0.750
4	6	4	4.490	2.626	2.626	0.0	1.864	0.663
4	6	4	16.002	16.543	16.543	0.0	-0.942	-0.778
6	6	4	16.779	15.244	-15.244	0.0	1.535	1.167
8	6	4	6.865	9.003	-9.003	0.0	-2.138	-0.797
-11	7	4	48.401	48.747	48.747	0.0	-0.346	-0.583
-9	7	4	23.560	24.838	24.838	0.0	-1.478	-1.815
0	7	4	23.009	20.731	20.731	0.0	2.273	2.850
-7	7	4	19.274	19.651	-19.651	0.0	-0.377	-0.417
-5	7	4	26.729	27.408	27.408	0.0	-0.678	-0.841
0	7	4	31.025	31.065	31.065	0.0	-0.040	-0.049
7	7	4	24.361	21.939	-21.939	0.0	2.422	2.593
-12	8	4	49.850	47.821	47.821	0.0	2.029	2.106
-10	8	4	61.093	60.562	-60.562	0.0	0.531	0.504
-8	8	4	6.634	8.392	8.392	0.0	-1.758	-0.738
-6	8	4	29.971	31.687	31.687	0.0	-1.715	-2.126
-4	8	4	42.701	41.313	-41.313	0.0	1.588	1.737
0	8	4	18.594	17.424	-17.424	0.0	1.170	1.516
2	8	4	63.252	63.231	63.231	0.0	0.021	0.020
4	8	4	78.520	77.155	-77.155	0.0	1.165	0.933
6	8	4	31.234	31.726	31.726	0.0	-0.493	-0.549
-11	9	4	22.060	20.662	-20.662	0.0	1.398	1.282
-9	9	4	36.224	37.008	37.008	0.0	-0.784	-0.897
0	9	4	221.901	230.777	230.777	0.0	-8.876	-2.676 *
-7	9	4	57.948	58.144	-58.144	0.0	-0.196	-0.197
-5	9	4	3.832	2.278	2.278	0.0	1.554	0.514
-2	9	4	36.573	35.302	-35.302	0.0	1.273	1.639
1	9	4	50.911	51.230	-51.230	0.0	-0.319	-0.355
3	9	4	25.370	26.083	-26.083	0.0	-0.714	-0.810
5	9	4	14.627	13.207	13.207	0.0	1.421	1.204
7	9	4	53.143	54.133	-54.133	0.0	-1.003	-1.000
-10	10	4	21.365	21.631	21.631	0.0	0.103	0.101
-6	10	4	25.116	24.045	24.045	0.0	1.070	1.204
-4	10	4	28.724	28.531	28.531	0.0	0.192	0.228
-2	10	4	38.398	37.950	37.950	0.0	0.448	0.565
-2	10	4	18.444	16.327	16.327	0.0	2.117	2.443

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	10	4	39.922	39.800	39.800	0.0	0.122	0.152
2	10	4	12.229	7.504	7.504	0.0	4.925	4.044
4	10	4	43.485	43.520	43.520	0.0	-0.035	-0.041
6	10	4	27.611	23.688	23.688	0.0	1.923	2.163
-11	11	4	39.603	39.922	39.922	0.0	-0.314	-0.339
-9	11	4	27.924	28.492	28.492	0.0	-0.568	-0.608
-7	11	4	140.175	140.929	140.929	0.0	-0.754	-0.834
0	12	0	421.152	430.777	430.777	0.0	-9.625	-4.921
-5	11	4	19.541	19.895	19.895	0.0	-0.354	-0.554
-3	11	4	14.656	14.670	14.670	0.0	-0.014	-0.008
-1	11	4	1.853	2.421	2.421	0.0	-0.568	-0.137
1	11	4	62.931	63.699	63.699	0.0	-0.768	-0.729
3	11	4	82.839	83.840	83.840	0.0	-1.000	-0.761
5	11	4	27.304	26.636	26.636	0.0	0.669	0.734
7	11	4	76.176	76.663	76.663	0.0	-0.487	-0.381
-10	12	4	57.649	56.807	56.807	0.0	0.843	0.812
-8	12	4	41.080	41.352	41.352	0.0	-0.272	-0.306
-6	12	4	51.777	50.825	50.825	0.0	0.953	1.028
-4	12	4	113.169	111.969	111.969	0.0	1.201	0.693
-2	12	4	83.304	64.067	64.067	0.0	-0.763	-0.724
0	12	4	47.788	48.406	46.406	0.0	1.382	1.595
2	12	4	21.246	19.539	19.539	0.0	1.707	1.904
4	12	4	128.063	127.084	127.084	0.0	-1.021	-0.528
6	12	4	40.012	40.056	40.056	0.0	-0.044	-0.048
-9	13	4	53.675	54.654	54.654	0.0	-1.179	-1.169
-7	13	4	54.101	53.193	53.193	0.0	0.903	0.950
-5	13	4	19.348	19.206	19.206	0.0	0.142	0.140
-3	13	4	14.754	15.861	15.861	0.0	-1.107	-0.866
0	13	0	221.476	230.777	230.777	0.0	-9.301	-2.811
-1	13	4	49.149	42.145	42.145	0.0	1.004	1.200
1	13	4	7.993	6.902	6.902	0.0	1.091	0.584
3	13	4	7.448	6.049	6.049	0.0	1.399	0.662
5	13	4	4.706	9.430	9.430	0.0	-4.724	-1.304
-10	14	4	6.469	8.331	8.331	0.0	-1.862	-0.631
-8	14	4	20.043	19.763	19.763	0.0	0.280	0.257
-6	14	4	6.918	5.172	5.172	0.0	1.746	0.784
-2	14	4	16.704	17.413	17.413	0.0	-0.709	-0.612
0	14	4	15.312	13.387	13.387	0.0	-0.075	-0.056
2	14	4	15.090	14.670	14.670	0.0	1.020	0.664
-9	15	4	41.580	42.419	42.419	0.0	-0.839	-0.921
-7	15	4	28.298	29.423	29.423	0.0	-1.125	-1.195
-5	15	4	29.321	28.069	28.069	0.0	1.252	1.510
-3	15	4	16.756	17.122	17.122	0.0	-0.366	-0.306
-1	15	4	32.758	32.782	32.782	0.0	-0.024	-0.030
1	15	4	12.214	12.332	12.332	0.0	-0.118	-0.077
3	15	4	5.707	3.057	3.057	0.0	2.650	1.008
5	15	4	32.384	33.107	33.107	0.0	-0.722	-0.761
0	12	0	220.938	230.777	230.777	0.0	-9.839	-2.960
-8	16	4	7.254	7.195	7.195	0.0	0.059	0.022
-6	16	4	15.053	17.512	17.512	0.0	-2.459	-1.680
-4	16	4	26.164	27.462	27.462	0.0	-1.298	-1.391
-2	16	4	20.544	19.398	19.398	0.0	1.146	1.198
0	16	4	13.858	11.928	11.928	0.0	1.929	1.476

H	K	L	F(UBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
2	10	4	26.583	25.024	25.024	0.0	1.550	1.760
4	10	4	53.047	52.711	-52.711	0.0	0.336	0.333
-7	17	4	10.780	11.121	-11.121	0.0	-0.341	-0.179
-5	17	4	6.186	6.665	-6.665	0.0	-0.480	-0.181
-3	17	4	16.308	16.765	-16.765	0.0	-0.597	-0.322
1	17	4	19.655	19.745	-19.745	0.0	-0.091	-0.081
3	17	4	11.033	11.898	-11.898	0.0	-0.005	-0.038
-0	18	4	17.090	17.518	-17.518	0.0	0.172	0.133
-4	19	4	7.149	7.664	-7.664	0.0	-0.515	-0.203
-2	19	4	19.289	18.799	18.799	0.0	0.469	0.420
2	19	4	13.357	11.307	11.307	0.0	2.050	1.365
-3	19	4	17.466	18.801	-18.801	0.0	-1.335	-0.982
-3	19	4	33.736	33.191	-33.191	0.0	0.546	0.594
0	12	0	220.639	230.777	230.777	0.0	-10.138	-3.077
-1	19	4	12.050	11.648	11.648	0.0	0.402	0.234
1	19	4	11.123	9.861	-9.861	0.0	1.262	0.716
-4	20	4	17.391	17.944	-17.944	0.0	-0.553	-0.409
-2	20	4	8.376	6.902	6.982	0.0	1.594	0.751
0	20	4	59.838	60.010	-60.010	0.0	-0.172	-0.159
-11	0	5	6.619	7.440	-7.440	0.0	-0.821	-0.294
-9	0	5	18.840	18.725	-18.725	0.0	0.116	0.108
-7	0	5	4.520	2.747	-2.747	0.0	1.773	0.624
-5	0	5	9.547	9.069	-9.069	0.0	0.478	0.305
-3	0	5	22.450	22.576	-22.576	0.0	-0.120	-0.140
-1	0	5	13.402	15.266	-15.266	0.0	-1.864	-1.426
1	0	5	3.167	2.189	2.189	0.0	0.978	0.275
3	0	5	7.769	6.523	-6.523	0.0	1.247	0.625
5	0	5	5.252	9.331	-9.331	0.0	-4.129	-1.313
-12	1	5	5.311	4.190	-4.190	0.0	1.121	0.346
-10	1	5	12.558	11.802	-11.802	0.0	0.756	0.479
-8	1	5	4.093	1.378	-1.378	0.0	3.515	1.238
-4	1	5	15.068	15.341	-15.341	0.0	-0.273	-0.243
-2	1	5	16.734	15.848	-15.848	0.0	0.886	0.853
0	12	0	220.213	230.777	230.777	0.0	-10.564	-3.207
0	1	5	19.326	20.814	-20.814	0.0	-1.483	-1.606
2	1	5	2.959	5.833	-5.833	0.0	-1.873	-0.567
4	1	5	10.466	11.901	-11.901	0.0	-1.434	-0.803
6	1	5	19.311	18.456	-18.456	0.0	0.855	0.711
-11	2	5	13.312	10.832	-10.832	0.0	2.480	1.643
-9	2	5	15.135	15.128	-15.128	0.0	0.007	0.006
-7	2	5	47.183	47.443	-47.443	0.0	-0.260	-0.293
-5	2	5	50.917	55.504	-55.504	0.0	1.413	1.466
-3	2	5	58.934	58.242	-58.242	0.0	0.692	0.707
1	2	5	11.250	10.642	10.642	0.0	0.609	0.420
3	2	5	15.023	14.503	14.503	0.0	0.520	0.446
5	2	5	6.504	5.973	5.973	0.0	0.631	0.251
-12	3	5	27.372	27.315	-27.315	0.0	0.057	0.056
-10	3	5	29.986	30.068	-30.068	0.0	-0.681	-0.742
-8	3	5	49.305	50.091	-50.091	0.0	-0.786	-0.870
-6	3	5	5.580	6.144	-6.144	0.0	-0.564	-0.214
-4	3	5	5.222	5.180	-5.180	0.0	0.042	0.017
-2	3	5	45.552	46.070	-46.070	0.0	-0.478	-0.571
0	3	5	16.502	15.802	-15.802	0.0	0.700	0.689

*

*

H	K	L	FI(BS)	FI(CALC)	AI(CALC)	BI(CALC)	DELTA F	DELTA/SIGMA
0	2	2	421.027	230.777	430.777	0.0	-9.750	-2.953 *
2	2	3	54.885	54.429	-54.429	0.0	0.456	0.477
4	2	5	19.737	18.146	18.146	0.0	1.591	1.601
6	3	5	32.780	32.455	-32.455	0.0	0.327	0.344
-11	4	5	1.803	1.002	1.002	0.0	0.806	0.155
-9	4	5	6.843	8.255	8.255	0.0	-1.412	-0.568
-7	4	5	5.132	6.218	-6.218	0.0	-1.086	-0.591
-5	4	5	1.957	3.075	3.675	0.0	-1.717	-0.598
-2	4	5	8.225	8.272	-8.272	0.0	-0.048	-0.026
-1	4	5	4.154	1.349	1.349	0.0	2.805	0.970
1	4	5	5.633	5.883	5.883	0.0	-0.251	-0.098
2	4	5	13.113	13.157	13.157	0.0	-0.039	-0.029
5	4	5	9.077	7.509	-7.509	0.0	1.507	0.761
-10	5	5	13.260	11.717	11.717	0.0	1.543	1.033
-6	5	5	87.852	88.465	88.465	0.0	-0.613	-0.441
-6	5	5	35.387	35.110	35.110	0.0	0.277	0.347
-4	5	5	12.984	12.431	12.431	0.0	0.552	0.425
-2	5	5	80.971	69.593	80.593	0.0	0.377	0.278
0	5	5	22.405	22.091	22.091	0.0	0.314	0.014
2	5	5	124.467	125.817	125.817	0.0	-1.329	-0.698
4	5	5	40.768	39.299	-39.299	0.0	1.467	1.707
0	12	5	222.068	230.777	230.777	0.0	-8.689	-2.620
0	5	5	47.751	47.256	47.256	0.0	0.493	0.508
-11	6	5	9.689	9.251	-9.251	0.0	0.433	0.206
-9	6	5	130.080	132.066	132.066	0.0	-1.406	-0.702
-7	6	5	5.991	1.141	-1.141	0.0	4.850	1.986
-5	6	5	75.914	75.264	75.264	0.0	0.650	0.534
-3	6	5	53.877	53.312	-53.312	0.0	0.565	0.605
-1	6	5	156.565	158.454	158.454	0.0	-1.889	-0.798
1	6	5	51.362	51.066	51.066	0.0	0.314	0.339
3	6	5	2.674	4.490	4.490	0.0	-1.815	-0.448
5	6	5	68.892	67.970	67.970	0.0	0.914	0.795
-10	7	5	14.717	13.076	-13.076	0.0	1.641	1.200
-8	7	5	37.636	36.933	36.933	0.0	0.703	0.791
-6	7	5	4.281	2.011	-2.011	0.0	2.270	0.750
-4	7	5	29.643	28.619	-28.619	0.0	0.824	1.012
-2	7	5	21.231	22.454	22.454	0.0	-1.223	-1.231
0	7	5	18.811	18.666	-18.666	0.0	0.144	0.142
2	7	5	65.710	66.006	66.006	0.0	-0.297	-0.270
4	7	5	64.201	63.689	-63.689	0.0	0.512	0.463
0	12	0	421.924	230.777	230.777	0.0	-8.953	-2.669
-9	8	5	4.056	4.610	-4.610	0.0	-0.754	-0.212
-7	8	5	6.962	3.903	-3.903	0.0	3.060	1.393
-5	8	5	18.975	17.924	-17.924	0.0	1.051	1.005
-1	8	5	16.652	15.919	-15.919	0.0	0.732	0.726
3	8	5	9.622	6.709	6.709	0.0	2.913	1.773
5	8	5	17.406	16.900	-16.900	0.0	0.506	0.416
-10	9	5	38.898	38.722	-38.722	0.0	0.176	0.190
-8	9	5	25.116	25.335	-25.335	0.0	-0.219	-0.235
-6	9	5	13.970	13.551	-13.551	0.0	0.418	0.333
-4	9	5	23.734	24.551	-24.551	0.0	-0.817	-0.855
-2	9	5	12.416	12.929	-12.929	0.0	-0.513	-0.342
0	9	5	40.116	40.177	40.177	0.0	-0.061	-0.072

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
2	9	5	21.981	31.104	-31.104	0.00	0.877	1.012
4	9	5	45.151	44.494	44.494	0.00	0.657	0.727
-9	10	3	18.878	19.133	-19.133	0.00	-0.255	-0.207
-7	10	5	23.778	22.555	22.555	0.00	1.223	1.310
-5	10	5	27.703	38.040	-38.040	0.00	-0.537	-0.406
-3	10	5	28.724	29.776	29.776	0.00	-1.052	-1.247
0	12	0	220.601	230.777	230.777	0.00	-10.175	-3.089
-1	10	5	13.775	13.906	-13.906	0.00	-0.130	-0.092
3	10	5	3.299	1.246	1.246	0.00	2.153	0.568
-10	11	5	4.004	4.148	-4.148	0.00	-0.144	-0.039
-6	11	5	15.210	16.021	-16.021	0.00	-0.811	-0.617
-4	11	5	4.774	6.232	-6.232	0.00	-1.459	-0.487
-2	11	5	12.612	14.560	-14.560	0.00	-1.749	-1.194
0	11	5	5.364	2.540	-2.940	0.00	2.925	1.208
2	11	5	17.204	18.693	-16.693	0.00	0.512	0.439
-7	11	5	6.073	4.999	-4.999	0.00	1.075	0.386
4	12	5	15.494	15.643	15.643	0.00	-0.149	-0.112
-5	12	3	8.180	8.246	8.246	0.00	-0.066	-0.032
-3	12	5	4.662	2.097	2.097	0.00	2.565	0.854
-1	12	5	2.961	3.457	2.057	0.00	0.854	0.125
1	12	5	19.206	17.689	17.689	0.00	-0.477	-0.125
3	12	5	11.602	13.761	13.761	0.00	1.517	1.461
-8	13	5	14.635	13.614	-13.614	0.00	-2.160	-1.225
0	14	0	221.027	230.777	230.777	0.00	1.020	0.686
-6	13	5	6.292	9.240	-9.240	0.00	-5.750	-2.953
-4	13	5	23.420	24.377	24.377	0.00	-2.943	-1.013
-2	13	5	23.846	22.475	-22.475	0.00	-0.957	-0.949
0	13	5	30.629	30.758	30.758	0.00	1.370	1.529
2	13	5	5.551	1.038	-1.038	0.00	-0.129	-0.145
-7	14	5	29.605	29.797	29.797	0.00	4.742	1.545
-5	14	5	83.504	82.997	-82.997	0.00	-0.192	-0.201
-3	14	5	29.575	28.553	28.553	0.00	3.508	0.378
-1	14	5	18.146	18.192	-18.192	0.00	1.023	1.160
1	14	5	28.089	27.347	-27.347	0.00	-0.046	-0.039
3	14	5	15.016	15.008	-15.008	0.00	0.742	0.782
-6	15	5	11.833	10.691	10.691	0.00	0.007	0.005
-4	15	5	18.960	19.856	19.856	0.00	1.142	0.642
-2	15	3	31.968	31.821	-31.821	0.00	-0.686	-0.745
0	15	5	15.778	15.342	15.342	0.00	0.567	0.403
2	15	5	12.498	13.590	-13.590	0.00	0.436	0.314
-7	16	5	18.667	14.434	-14.434	0.00	-1.092	-0.617
-3	16	3	49.734	45.371	45.371	0.00	2.232	1.789
-1	16	5	16.794	17.608	17.608	0.00	0.563	0.386
0	16	5	46.384	48.861	48.861	0.00	-0.815	-0.583
0	12	0	221.184	230.777	230.777	0.00	-0.477	-0.491
1	16	5	36.254	35.555	35.555	0.00	-9.593	-2.905
-4	17	5	6.589	6.788	-6.788	0.00	0.699	0.735
-2	17	5	72.881	71.909	71.909	0.00	-0.200	-0.070
0	17	5	7.530	5.820	5.820	0.00	0.972	0.799
-10	0	6	120.528	121.514	121.514	0.00	1.910	0.817
-8	0	6	40.437	40.615	-40.615	0.00	-0.986	-0.528
-6	0	6	28.851	28.935	-28.935	0.00	-0.178	-0.190
-4	0	6	125.077	127.197	127.197	0.00	-0.084	-0.096
							-2.119	-1.108

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-2	0	6	58.030	37.925	27.925	0.0	0.707	0.838
0	0	6	59.246	58.977	58.977	0.0	0.271	0.261
2	0	6	31.226	31.153	-31.153	0.0	0.073	0.073
4	0	3	132.480	132.452	132.452	0.0	-0.272	-0.272
-9	1	6	33.535	34.794	-34.794	0.0	-1.260	-1.297
-7	1	6	62.811	63.521	63.521	0.0	-0.709	-0.659
-5	1	6	17.884	17.390	-17.390	0.0	0.494	0.469
-3	1	6	76.161	76.962	76.962	0.0	-0.801	-0.650
-1	1	6	6.350	0.277	0.277	0.0	6.073	2.589
1	1	6	21.477	21.184	41.184	0.0	0.294	0.275
3	1	5	4.520	2.946	-2.946	0.0	1.574	0.462
-10	2	0	13.947	13.778	-13.778	0.0	0.170	0.102
0	12	0	221.057	230.777	230.777	0.0	-9.720	-2.944
-0	0	6	15.120	15.047	-15.047	0.0	0.072	0.055
-4	2	6	10.137	7.786	-7.786	0.0	2.351	1.485
-2	2	6	9.652	5.394	-5.394	0.0	3.758	2.197
0	2	6	10.122	10.289	-10.289	0.0	-0.166	-0.091
2	2	6	10.823	15.966	-15.966	0.0	0.856	0.671
4	2	6	15.464	16.008	-16.008	0.0	-1.144	-0.754
-9	3	6	27.379	26.036	26.686	0.0	0.693	0.725
-7	3	6	31.045	30.421	-30.421	0.0	1.224	1.450
-5	3	6	32.765	31.148	31.148	0.0	1.617	1.950
-3	3	6	26.139	26.051	-26.091	0.0	0.048	0.054
-1	3	6	29.892	29.553	29.553	0.0	0.339	0.382
1	3	6	20.529	19.842	-19.842	0.0	0.687	0.652
-10	4	6	36.000	37.744	-37.744	0.0	0.855	0.924
-8	4	6	14.433	11.103	11.103	0.0	3.330	2.436
-6	4	6	29.202	28.158	28.158	0.0	1.044	1.237
-2	4	6	8.539	1.348	1.348	0.0	7.190	3.913
0	4	6	4.079	5.060	-5.060	0.0	-0.981	-0.286
0	12	0	220.721	230.777	230.777	0.0	-10.056	-3.045
2	4	6	53.794	55.527	55.527	0.0	-1.542	-1.529
-9	5	6	20.940	21.617	21.617	0.0	-0.678	-0.556
-7	5	6	28.619	26.215	-26.215	0.0	2.404	2.823
-5	5	6	4.923	6.734	-6.734	0.0	-1.611	-0.596
-3	5	6	2.780	4.891	4.891	0.0	-2.104	-0.528
-1	5	6	2.443	0.370	-0.370	0.0	2.073	0.499
1	5	6	30.240	30.004	-30.004	0.0	0.244	0.261
3	5	6	3.877	0.135	-0.135	0.0	3.743	1.010
-3	6	6	8.038	8.712	-8.712	0.0	-0.674	-0.273
-6	6	6	7.934	0.519	-0.519	0.0	7.415	3.520
-4	6	6	13.066	11.856	-11.856	0.0	1.830	1.331
-2	6	6	5.262	5.313	5.313	0.0	-0.032	-0.011
0	6	6	3.459	1.070	1.070	0.0	2.389	0.631
2	6	6	11.004	12.587	-12.587	0.0	-1.585	-0.865
-9	7	6	13.148	10.817	10.817	0.0	2.331	1.479
-7	7	6	8.008	4.545	4.545	0.0	3.464	1.505
-5	7	6	21.383	31.664	31.664	0.0	-0.301	-0.353
-3	7	6	16.891	18.908	-18.908	0.0	-2.017	-1.452
-1	7	6	35.522	34.603	34.603	0.0	0.719	0.802
1	7	6	13.006	10.993	10.993	0.0	2.013	1.514
0	12	0	220.594	230.777	230.777	0.0	-10.183	-3.091
3	7	6	7.441	5.622	-5.622	0.0	1.819	0.690

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-3	3	6	15.537	12.314	12.314	0.0	3.022	2.260
-3	3	6	30.581	30.502	-30.502	0.0	0.179	0.167
-4	3	6	13.357	13.534	13.534	0.0	-0.177	-0.116
-2	6	6	21.069	20.775	20.775	0.0	0.214	0.290
0	3	6	63.558	63.940	-63.940	0.0	-0.382	-0.348
2	3	6	43.363	49.407	49.407	0.0	-1.044	-1.083
-7	9	6	10.010	12.915	-12.915	0.0	-2.903	-1.513
-5	9	6	23.850	23.490	23.490	0.0	0.400	0.372
-3	9	6	65.605	66.019	-66.019	0.0	-0.414	-0.389
-1	9	6	18.220	19.504	16.504	0.0	1.717	1.512
1	9	6	11.744	8.614	-8.614	0.0	3.129	1.921
-1	9	6	14.921	12.795	12.795	0.0	1.528	1.033
-3	10	6	16.780	14.847	14.847	0.0	1.939	1.536
-4	10	6	25.437	25.432	25.432	0.0	0.005	0.005
-2	10	6	16.652	17.843	17.843	0.0	-1.192	-0.853
0	10	6	26.792	26.884	26.884	0.0	-0.133	-0.134
-7	11	6	61.063	60.769	60.769	0.0	0.294	0.270
-5	11	6	12.363	12.094	-12.094	0.0	0.292	0.174
-3	11	6	127.349	127.349	127.349	0.0	-0.045	-0.023
0	12	6	220.766	230.777	230.777	0.0	-10.071	-3.050
-1	11	6	2.921	8.359	8.359	0.0	-5.438	-1.184
1	11	6	20.999	21.931	21.931	0.0	-0.932	-0.758
-6	12	6	36.881	38.448	38.448	0.0	-1.567	-1.639
-4	12	6	37.814	37.735	37.735	0.0	0.073	0.074
-2	12	6	15.023	13.208	-13.208	0.0	-3.135	-2.021
0	12	6	58.902	56.946	56.946	0.0	0.016	0.016
-5	13	6	38.896	37.645	-37.645	0.0	1.253	1.364
-3	13	6	55.221	54.657	-54.657	0.0	0.565	0.548
-1	13	6	21.209	21.895	-21.895	0.0	-0.686	-0.540
-5	0	7	4.505	2.253	-2.253	0.0	2.251	0.651
-3	0	7	6.925	9.080	-9.080	0.0	-2.155	-0.744
-1	0	7	18.138	17.755	-17.755	0.0	0.383	0.304
-6	1	7	4.676	2.630	-2.630	0.0	2.046	0.584
-4	1	7	13.494	12.951	-12.951	0.0	0.504	0.312
-2	1	7	5.528	9.011	-9.011	0.0	-3.483	-1.064
-7	2	7	42.036	40.933	-40.933	0.0	1.103	1.181
-5	2	7	40.161	39.560	-39.560	0.0	0.601	0.665
-3	2	7	29.217	31.032	-31.032	0.0	-1.815	-1.724
0	12	0	220.751	230.777	230.777	0.0	-10.026	-3.036
-6	3	7	3.504	1.960	-1.960	0.0	1.544	0.372
-4	3	7	9.174	3.889	-3.889	0.0	5.285	2.545
-2	3	7	20.969	21.749	-21.749	0.0	-0.780	-0.648
-3	4	7	2.996	5.279	-5.279	0.0	-2.283	-0.495
-6	5	7	32.683	33.171	-33.171	0.0	-0.488	-0.491
-4	5	7	24.077	23.301	-23.301	0.0	0.776	0.716
-2	5	7	38.241	38.167	-38.167	0.0	0.074	0.078
-5	6	7	99.887	99.033	-99.033	0.0	0.854	0.539
-3	6	7	59.838	58.794	-58.794	0.0	1.044	0.971

ALL REFLECTIONS

WEIGHTED R	UNWEIGHTED R	NUMERATOR	DENOMINATOR	NUMBER	R
2711.40	2342.78	2135999.00	60265.19	1373	0.036
				1373	0.039

RANGES OF F(OBS)

1151.98	13587.32	863	0.085
156.03	13135.34	272	0.015
82.55	6600.40	83	0.012
78.19	5428.38	48	0.014
69.24	3455.23	24	0.020
35.47	1035.67	6	0.034
685.11	16530.89	75	0.041
44.27	512.37	2	0.086

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

225.49	5305.55	66	0.043
798.44	20716.77	182	0.039
204.84	6414.38	148	0.032
161.63	5022.26	151	0.029
167.65	5253.01	179	0.036
432.72	5585.09	205	0.042
250.73	5467.22	200	0.046
281.20	5924.41	222	0.047

UNREJECTED REFLECTIONS

WEIGHTED R	UNWEIGHTED R				
1733.53	1488.87	1618293.00	39743.02	1190	0.033
				1190	0.037

RANGES OF F(OBS)

1079.68	12508.91	799	0.086
166.43	11736.31	244	0.014
73.25	5905.86	74	0.012
71.61	4865.57	43	0.015
57.16	3020.01	21	0.019
25.30	865.11	5	0.029
15.47	841.92	4	0.018
0.0	0.0	0	0.0

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

131.51	3777.04	67	0.035
121.11	4375.99	100	0.028
194.80	5948.70	134	0.032
149.67	5040.53	139	0.030
170.80	4880.71	164	0.035
219.89	5109.54	190	0.043
237.33	5158.14	188	0.046
263.87	5453.97	208	0.048

SUM F-CAL 60837.85
 STANDARD DEV OF UNIT WEIGHT OBS 1.26

NA-K1 CHTERITE 24C, 3/6/75
ATOM

PARAMETER

OLD

CHANGE

NEW

ERROR

SHIFT/ERROR

EXTINCTION CORRECTION 0.0

0.0

SCALE FACTOR 1 1.3386

0.0000

1.3386

0.00254

0.00

ATOM 1 U(1)

EQUIPOINT FRACTION = 1.000
OCCUPANCY SPECIES 1

1.00000 0.1131974 0.9157349 0.8951383 0.0013354 0.0003991 0.0061600 0.0000090 0.0006888 0.0000294

1.00000 0.1131974 0.9157349 0.8951381 0.0013373 0.0003592 0.0005141 0.0000552 0.0002196 0.0001039

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

ATOM 2 Q(2)

EQUIPOINT FRACTION = 1.000
OCCUPANCY SPECIES 1

1.00000 0.1188345 0.8323570 0.3922273 0.0014991 0.0005516 0.0000256 0.0007084 0.00002813

1.00000 0.1188344 0.8323570 0.3922272 0.0014991 0.0005517 0.0000256 0.0007084 0.00002813

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

ATOM 3 F(3)

EQUIPOINT FRACTION = 0.500
OCCUPANCY SPECIES 2

1.00000 0.1030566 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

1.00000 0.1030566 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

ATOM 4 Q(4)

EQUIPOINT FRACTION = 1.000
OCCUPANCY SPECIES 1

1.00000 0.3613016 0.7509876 0.5677693 0.0026763 0.0005383 0.0070212 0.0004355 0.0012775 0.0002628

1.00000 0.3613017 0.7509876 0.5677693 0.0026763 0.0005383 0.0070215 0.0004356 0.0012776 0.0002628

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

ATOM 5 O(5)

EQUIPOINT FRACTION = 1.000
OCCUPANCY SPECIES 1

1.00000 0.3492101 0.8654186 0.2584964

1.00000 0.3492101 0.8654186 0.2584964

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

BETA33 0.0048766 0.0000000 0.0048766 0.0003552 0.00
 BETA12 0.0 0.0000000 0.0 0.0003552 0.00
 BETA13 0.0009569 0.0000000 0.0009569 0.0001491 0.00
 BETA23 0.0 0.0 0.0 0.0 0.00

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

X 1.00000 1.00000
 Y 0.8211948 0.0000001 0.0 0.8211948 C.0000515 0.00
 Z 0.0 0.0000000 0.0 0.0 0.00
 BETA11 0.0015852 0.0000000 0.0015852 C.0000961 0.00
 BETA22 0.0004393 0.0000000 0.0004393 0.0000275 0.00
 BETA33 0.0058957 -0.0000002 0.0058955 0.0003555 -0.00
 BETA12 0.0 0.0000000 0.0 0.0003555 -0.00
 BETA13 0.0006563 -0.0000000 0.0006563 C.0001474 -0.00
 BETA23 0.0 0.0 0.0 0.0 0.00

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

X 1.00000 1.00000
 Y 0.0 0.0 0.0 0.0
 Z 0.0 0.0 0.0 0.0
 BETA11 0.0015677 0.0000000 0.0015677 C.0001310 0.00
 BETA22 0.0003087 -0.0000000 0.0003087 0.0000362 -0.00
 BETA33 0.0045020 -0.0000002 0.0045077 0.0004348 -0.00
 BETA12 0.0 0.0 0.0 0.0 0.00
 BETA13 0.0009506 -0.0000000 0.0009506 0.0002061 -0.00
 BETA23 0.0 0.0 0.0 0.0 0.00

ATOM 13 M(4) EQUIPOINT FRACTION = 0.500
 OCCUPANCY SPECIES 5

OCCUPANCY SPECIES 5 0.50000 0.50000 0.50000
 OCCUPANCY SPECIES 6 0.50000 0.50000
 TOTAL OCCUPANCY (FIXED) = 1.00000
 X 0.0 0.0
 Y 0.7243279 -0.0000000 0.0 0.7243273 0.0000451 -0.00
 Z 0.5000000 0.5000000 0.5000000 0.5000000
 BETA11 0.0034049 0.0000000 0.0034049 C.0000360 0.00
 BETA22 0.0006098 0.0000000 0.0006098 0.0000225 0.00
 BETA33 0.0063870 -0.0000002 0.0063868 C.0002905 -0.00
 BETA12 0.0 0.0 0.0 0.0 0.00
 BETA13 -0.0006421 -0.0000000 -0.0006421 0.0001236 -0.00
 BETA23 0.0 0.0 0.0 0.0 0.00

ATOM 14 A EQUIPOINT FRACTION = 1.000
 OCCUPANCY SPECIES 6

X 0.25000 0.25000
 Y 0.4756150 0.0000049 0.4756193 0.00009165 0.01
 Z 0.9868482 0.0000000 0.9868491 0.0004047 0.00
 0.5365365 0.0000072 0.5365435 0.0016748 0.00
 BETA11 0.0116684 0.0000052 0.0116736 0.0011653 0.00
 BETA22 0.0023222 0.0000009 0.0023231 C.0003400 0.00
 BETA33 0.0231661 -0.0000127 0.0231534 0.0032444 -0.00
 BETA12 -0.0022351 -0.0000025 -0.0022376 0.0004358 -0.01
 BETA13 -0.00084632 0.0000013 -0.00084669 0.0010718 0.00
 BETA23 0.0010077 -0.0000031 0.0010046 0.00006417 -0.00

MAXIMUM SHIFT/ERROR = -0.01
 AVERAGE SHIFT/ERROR = 0.00

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	12	0	203.519	196.774	196.774	0.0	6.745	2.215 *
4	0	0	0.715	13.476	13.476	0.0	-12.761	-3.317 *
6	0	0	94.792	89.775	89.775	0.0	5.018	3.446
8	0	0	90.848	91.053	91.053	0.0	-0.205	-0.144
10	0	0	55.894	54.566	54.566	0.0	1.328	1.255
12	0	0	18.505	18.052	18.052	0.0	0.453	0.293
13	1	0	22.988	21.324	-21.324	0.0	1.664	1.123
11	1	0	47.758	47.231	47.231	0.0	0.527	0.514
9	1	0	19.096	17.413	17.413	0.0	1.683	1.603
7	1	0	75.405	74.785	74.785	0.0	0.620	0.517
5	1	0	105.655	101.456	-101.456	0.0	4.200	2.615
3	1	0	146.786	150.622	150.622	0.0	-3.836	-1.746
-3	1	0	149.566	150.622	150.622	0.0	-1.056	-0.471 *
-5	1	0	107.058	101.456	-101.456	0.0	5.603	3.451 *
-7	1	0	75.343	74.785	74.785	0.0	0.558	0.465 *
-9	1	0	18.108	17.413	17.413	0.0	0.695	0.592 *
-11	1	0	49.055	47.231	47.231	0.0	1.824	1.782 *
-13	1	0	25.582	21.324	-21.324	0.0	4.259	3.601 *
-12	2	0	2.974	9.750	9.750	0.0	-6.776	-1.371 *
-8	2	0	8.877	8.749	-8.749	0.0	0.128	0.060 *
0	12	0	204.128	196.774	196.774	0.0	7.354	2.409 *
-6	2	0	30.780	30.161	-30.161	0.0	0.618	0.825 *
-4	2	0	10.254	10.226	-10.226	0.0	0.028	0.029 *
4	2	0	8.772	10.226	-10.226	0.0	-1.454	-1.268
6	2	0	29.218	30.161	-30.161	0.0	-0.943	-1.273
8	2	0	11.225	8.749	-8.749	0.0	2.476	1.439
12	2	0	13.237	9.750	9.750	0.0	3.486	1.975
13	3	0	14.454	9.701	9.701	0.0	4.754	2.529
11	3	0	17.243	14.171	-14.171	0.0	3.072	2.321
9	3	0	17.658	15.010	15.010	0.0	2.648	2.308
7	3	0	48.173	49.578	-49.578	0.0	-1.405	-1.546
5	3	0	59.468	60.513	60.513	0.0	-1.045	-1.096
3	3	0	73.940	78.712	-78.712	0.0	-4.772	-4.225
-3	3	0	77.161	78.712	78.712	0.0	-1.551	-1.312 *
-5	3	0	61.657	60.513	60.513	0.0	1.144	1.168 *
-7	3	0	50.520	49.578	-49.578	0.0	0.942	1.027 *
-9	3	0	14.507	15.010	15.010	0.0	-0.502	-0.345 *
-11	3	0	16.881	14.171	-14.171	0.0	2.711	2.133 *
-13	3	0	11.948	9.701	9.701	0.0	2.247	1.027 *
-12	4	0	13.978	14.118	14.118	0.0	-0.140	-0.073 *
0	12	0	203.298	196.774	196.774	0.0	6.524	2.143 *
-10	4	0	8.401	4.867	-4.867	0.0	3.534	1.628 *
-8	4	0	8.855	4.938	4.938	0.0	3.957	1.900 *
-6	4	0	8.039	4.097	4.097	0.0	3.942	2.097 *
-4	4	0	5.674	4.582	4.582	0.0	0.692	0.433 *
-2	4	0	117.595	128.580	128.580	0.0	-10.986	-6.225 *
2	4	0	109.715	128.580	128.580	0.0	-18.866	-11.433 *
4	4	0	5.555	4.982	4.982	0.0	0.613	0.375
6	4	0	0.891	4.097	4.097	0.0	-3.206	-0.625
8	4	0	8.763	4.938	4.938	0.0	3.824	1.844
12	4	0	12.504	14.118	14.118	0.0	-1.614	-0.723
13	5	0	17.799	15.802	15.802	0.0	-1.997	-1.223
11	5	0	13.881	13.555	-13.955	0.0	-0.074	-0.043

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
7	5	0	10.066	4.480	-4.480	0.0	5.606	3.209
5	5	0	2.030	2.413	-2.413	0.0	-0.383	-0.105
3	5	0	59.283	67.201	-67.201	0.0	-7.918	-8.546
-3	5	0	63.271	67.201	-67.201	0.0	-3.976	*
0	12	0	202.548	196.774	196.774	0.0	5.774	1.902
-7	5	0	5.330	4.480	-4.480	0.0	0.850	0.285
-11	5	0	13.819	13.555	-13.955	0.0	-0.136	-0.078
-13	5	0	17.022	15.802	15.802	0.0	1.220	0.678
-10	6	0	5.859	3.208	-3.308	0.0	2.551	0.743
-12	6	0	17.322	15.147	15.147	0.0	2.175	1.724
-8	6	0	22.414	20.241	-20.241	0.0	2.173	2.345
-6	6	0	6.389	7.936	7.936	0.0	-1.547	-0.654
-4	6	0	2.321	6.413	-6.413	0.0	-4.092	-1.240
-2	6	0	10.854	6.563	6.963	0.0	3.891	4.366
0	6	0	7.501	2.393	-2.393	0.0	5.108	4.134
2	6	0	10.166	6.563	6.963	0.0	3.203	3.424
6	6	0	8.163	7.936	7.936	0.0	0.226	0.113
8	6	0	16.131	20.241	-20.241	0.0	-4.110	-2.911
10	6	0	14.728	15.147	15.147	0.0	-0.419	-0.271
12	6	0	9.601	3.308	-3.308	0.0	6.293	2.775
11	7	0	13.201	12.478	-12.478	0.0	0.723	0.420
9	7	0	39.084	39.667	39.667	0.0	-0.584	-0.649
0	12	0	203.395	196.774	196.774	0.0	6.621	2.175
7	7	0	32.077	34.663	-34.663	0.0	-2.586	-2.990
5	7	0	15.125	16.376	16.376	0.0	-1.251	-1.153
3	7	0	50.855	55.917	55.917	0.0	-5.061	-6.102
1	7	0	7.007	4.236	-4.236	0.0	2.770	2.136
-1	7	0	5.515	4.236	-4.236	0.0	1.279	0.801
-3	7	0	54.138	55.917	55.917	0.0	-1.779	-2.015
-5	7	0	16.546	16.376	16.376	0.0	0.170	0.170
-7	7	0	34.358	34.663	-34.663	0.0	-0.307	-0.307
-9	7	0	42.102	39.667	39.667	0.0	2.434	2.678
-11	7	0	13.765	12.478	-12.478	0.0	1.288	0.806
-12	8	0	29.933	26.518	26.518	0.0	3.414	3.046
-10	8	0	45.693	42.870	-42.870	0.0	2.823	2.990
-6	8	0	54.712	54.621	54.621	0.0	0.090	0.095
-4	8	0	97.140	104.728	-104.728	0.0	-7.589	-5.089
-2	8	0	26.262	26.885	26.885	0.0	-0.625	-1.012
0	8	0	38.258	33.118	33.118	0.0	5.180	7.623
2	8	0	26.041	26.886	26.886	0.0	-0.846	-1.389
4	8	0	90.301	104.728	-104.728	0.0	-14.428	-10.414
6	8	0	50.926	54.621	54.621	0.0	-3.695	-4.027
0	12	0	203.377	156.774	156.774	0.0	6.604	2.169
8	8	0	6.760	3.172	-3.172	0.0	3.587	1.489
10	8	0	43.690	42.870	-42.870	0.0	0.820	0.837
12	8	0	26.668	26.518	26.518	0.0	0.149	0.111
11	9	0	9.186	9.889	-5.889	0.0	3.297	1.364
9	9	0	28.062	29.238	29.238	0.0	-1.176	-1.149
7	9	0	76.332	81.216	-81.216	0.0	-4.884	-3.982
5	9	0	20.835	24.209	24.209	0.0	-3.375	-3.445
1	9	0	72.193	67.631	-67.631	0.0	4.562	4.070
-1	9	0	73.878	67.631	-67.631	0.0	6.247	5.446
-5	9	0	21.620	24.209	24.209	0.0	-2.589	-2.692

H	K	L	F(BOBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-7	9	0	80.303	81.216	-81.216	0.0	-0.913	-0.709 *
-9	9	0	31.503	29.238	29.238	0.0	2.265	2.593 *
-11	9	0	4.112	5.889	-5.889	0.0	-1.777	-0.426 *
-12	10	0	15.469	13.825	13.825	0.0	1.644	0.913 *
-10	10	0	15.919	17.154	17.154	0.0	-1.235	-0.773 *
-8	10	0	22.767	22.406	22.406	0.0	0.361	0.335 *
-6	10	0	16.299	14.062	14.062	0.0	2.237	1.935 *
-4	10	0	45.075	46.319	46.319	0.0	-1.244	-1.468 *
0	12	0	202.839	196.774	196.774	0.0	6.065	1.998 *
-2	10	0	37.636	36.913	36.913	0.0	0.723	0.976 *
0	10	0	86.603	81.580	81.580	0.0	5.023	3.770 *
2	10	0	37.089	36.913	36.913	0.0	-0.176	0.244 *
4	10	0	42.066	46.319	46.319	0.0	-4.253	-5.127 *
6	10	0	11.392	14.062	14.062	0.0	-2.669	-1.505 *
8	10	0	20.790	22.406	22.406	0.0	-1.616	-1.477 *
10	10	0	13.607	17.154	17.154	0.0	-3.547	-1.923 *
12	10	0	14.066	13.825	13.825	0.0	0.241	0.114 *
11	11	0	43.249	42.911	42.911	0.0	0.338	0.314 *
9	11	0	3.318	2.824	2.824	0.0	0.494	0.118 *
7	11	0	103.008	115.670	115.670	0.0	-12.662	-7.884 *
5	11	0	31.742	35.076	-35.076	0.0	-3.335	-3.779 *
3	11	0	80.241	85.052	85.052	0.0	-4.811	-3.813 *
1	11	0	124.301	122.455	122.455	0.0	1.846	0.982 *
-1	11	0	126.075	122.455	122.455	0.0	3.620	1.899 *
-3	11	0	82.526	85.052	85.052	0.0	-2.526	-1.947 *
-5	11	0	33.798	35.076	-35.076	0.0	-1.278	-1.509 *
-7	11	0	112.662	115.670	115.670	0.0	-3.008	-1.731 *
-9	11	0	2.453	2.824	2.824	0.0	-0.371	-0.081 *
-11	11	0	45.905	42.911	42.911	0.0	2.994	2.828 *
0	12	0	203.307	156.774	196.774	0.0	6.533	2.146 *
-10	12	0	49.214	48.426	48.426	0.0	0.788	0.745 *
-8	12	0	35.686	36.424	36.424	0.0	-0.738	-0.796 *
-6	12	0	21.505	23.604	-23.604	0.0	-2.099	-1.949 *
-4	12	0	46.487	44.501	44.501	0.0	1.986	2.229 *
-2	12	0	47.829	46.356	-46.356	0.0	1.472	1.685 *
0	12	0	203.007	156.774	196.774	0.0	6.233	2.047 *
2	12	0	48.146	46.356	-46.356	0.0	1.790	2.070 *
4	12	0	42.640	44.501	44.501	0.0	-1.861	-2.130 *
6	12	0	21.038	23.604	-23.604	0.0	-2.566	-2.507 *
8	12	0	31.715	36.424	36.424	0.0	-4.709	-4.941 *
10	12	0	46.743	48.426	48.426	0.0	-1.682	-1.629 *
11	13	0	17.640	16.469	16.469	0.0	1.171	0.741 *
9	13	0	18.081	20.533	-20.533	0.0	-2.852	-2.045 *
7	13	0	38.881	42.243	42.243	0.0	-3.363	-3.664 *
5	13	0	56.627	61.172	-61.172	0.0	-4.545	-4.640 *
3	13	0	7.960	6.440	-6.440	0.0	0.691	0.691 *
1	13	0	8.842	11.426	11.426	0.0	-2.584	-1.313 *
-1	13	0	11.507	11.426	11.426	0.0	0.081	0.055 *
-3	13	0	6.248	6.440	-6.440	0.0	-0.193	-0.073 *
-5	13	0	59.521	61.172	-61.172	0.0	-1.651	-1.585 *
0	12	0	203.475	196.774	196.774	0.0	6.701	2.201 *
-7	13	0	41.193	42.243	42.243	0.0	-1.051	-1.092 *
-9	13	0	19.087	20.533	-20.933	0.0	-1.846	-1.385 *

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-11	13	0	13.554	16.469	16.469	0.0	-2.915	-1.371 *
-8	14	0	5.162	0.723	-0.723	0.0	4.440	1.356 *
-6	14	0	4.774	7.110	-7.110	0.0	-2.336	-0.710 *
-2	14	0	22.714	19.027	19.027	0.0	3.687	4.017 *
0	14	0	9.928	10.821	-10.821	0.0	-0.894	-0.482
2	14	0	20.217	19.027	19.027	0.0	1.190	1.105
4	14	0	3.565	4.725	4.725	0.0	-1.160	-0.314
6	14	0	4.068	7.110	-7.110	0.0	-3.042	-0.855
10	14	0	8.983	1.523	-1.523	0.0	7.460	2.935
9	15	0	22.838	25.356	25.356	0.0	-2.519	-2.053
7	15	0	35.757	40.419	-40.419	0.0	-4.663	-5.130
5	15	0	30.806	32.389	32.389	0.0	-1.583	-1.794
3	15	0	6.477	3.822	3.822	0.0	2.656	1.106
-1	15	0	2.594	1.532	1.532	0.0	1.062	0.241 *
0	12	0	203.554	196.774	196.774	0.0	6.780	2.221 *
-5	15	0	33.517	32.389	32.389	0.0	1.188	1.373 *
-7	15	0	39.198	40.419	-40.419	0.0	-1.221	-1.258 *
-9	15	0	24.859	25.356	25.356	0.0	-0.498	-0.412 *
-10	16	0	23.049	19.691	-19.691	0.0	3.358	2.643 *
-6	16	0	22.044	24.444	24.444	0.0	-2.400	-2.076 *
-4	16	0	44.687	45.162	-45.162	0.0	-0.474	-0.512 *
-2	16	0	5.824	4.725	4.725	0.0	1.099	0.415 *
2	16	0	5.162	4.725	4.725	0.0	0.437	0.149
4	16	0	43.302	45.162	-45.162	0.0	-1.860	-2.027
6	16	0	19.026	24.444	24.444	0.0	-5.418	-4.121
8	16	0	5.771	2.760	-2.760	0.0	3.011	0.945
10	16	0	20.879	19.691	-19.691	0.0	1.187	0.862
9	17	0	9.054	12.140	-12.140	0.0	-3.087	-1.182
7	17	0	13.316	14.381	-14.381	0.0	-1.065	-0.607
5	17	0	5.974	0.726	0.726	0.0	5.248	1.830
3	17	0	24.047	24.205	24.205	0.0	-0.158	-0.160
1	17	0	13.025	12.814	-12.814	0.0	0.211	0.147
0	12	0	203.422	196.774	196.774	0.0	6.648	2.184 *
-1	17	0	12.557	12.814	-12.814	0.0	-0.256	-0.172 *
-3	17	0	23.420	24.205	24.205	0.0	-0.785	-0.780 *
-7	17	0	12.160	14.381	-14.381	0.0	-2.221	-1.155 *
-9	17	0	11.225	12.140	-12.140	0.0	-0.916	-0.407 *
-8	18	0	5.718	7.734	-7.734	0.0	-2.016	-0.570 *
-6	18	0	14.278	15.372	15.372	0.0	-1.094	-0.652 *
-4	18	0	5.555	0.362	-0.362	0.0	5.233	1.776 *
-2	18	0	13.607	12.767	12.767	0.0	0.841	0.523 *
0	18	0	12.072	10.800	10.800	0.0	1.272	0.801
2	18	0	16.016	12.767	12.767	0.0	3.250	2.505
4	18	0	4.227	0.362	-0.362	0.0	3.865	1.076
6	18	0	15.637	15.372	15.372	0.0	0.265	0.183
8	18	0	4.783	7.734	-7.734	0.0	-2.951	-0.724
7	19	0	20.437	18.943	-18.943	0.0	2.394	1.858
5	19	0	6.601	5.781	5.781	0.0	0.820	0.286
3	19	0	20.190	20.709	-20.709	0.0	-0.518	-0.466
-1	19	0	3.609	0.750	0.750	0.0	2.859	0.753 *
-3	19	0	20.332	20.709	-20.709	0.0	-0.377	-0.314 *
0	12	0	203.289	196.774	196.774	0.0	6.515	2.140 *
-5	19	0	7.421	5.781	5.781	0.0	1.640	0.618 *

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-7	19	0	17.940	18.043	-18.043	0.0	-0.103	-0.065 *
-6	20	0	3.874	1.842	1.842	0.0	2.032	0.470 *
-4	20	0	30.171	28.417	-28.417	0.0	1.754	1.774 *
-2	20	0	23.158	23.158	23.158	0.0	0.332	0.294 *
0	20	0	51.579	47.002	-47.002	0.0	4.577	4.715
2	20	0	24.682	23.158	23.158	0.0	1.524	1.476
4	20	0	28.635	28.417	-28.417	0.0	0.218	0.217
6	20	0	1.077	1.842	1.842	0.0	-0.766	-0.123
8	20	0	8.136	1.647	-1.647	0.0	6.489	2.228
7	21	0	6.062	7.177	-7.177	0.0	-1.114	-0.305
5	21	0	34.036	32.548	32.548	0.0	1.488	1.454
3	21	0	7.121	3.020	3.020	0.0	4.101	1.549
1	21	0	21.417	21.187	21.187	0.0	0.230	0.190
-1	21	0	18.681	21.187	21.187	0.0	-2.506	-1.701 *
-5	21	0	35.748	32.548	32.548	0.0	3.200	3.073 *
0	12	0	203.236	156.774	196.774	0.0	6.463	2.123 *
-4	22	0	33.304	30.625	30.625	0.0	2.679	2.468 *
-2	22	0	17.058	15.647	15.647	0.0	1.411	0.919 *
0	22	0	46.037	42.093	42.093	0.0	3.944	3.921
2	22	0	17.720	15.647	15.647	0.0	2.073	1.441
4	22	0	33.392	30.625	30.625	0.0	2.767	2.751
6	22	0	10.836	7.216	7.216	0.0	3.621	1.566
5	23	0	34.918	32.553	-32.553	0.0	2.065	1.918
3	23	0	29.730	28.017	28.017	0.0	1.713	1.471
1	23	0	13.060	10.095	10.095	0.0	2.965	1.600
-1	23	0	12.619	10.095	10.095	0.0	2.524	1.306 *
-3	23	0	31.300	28.017	28.017	0.0	3.284	3.025 *
-5	23	0	35.518	32.553	-32.553	0.0	2.665	2.517 *
-2	24	0	38.775	36.664	-36.664	0.0	2.710	2.603 *
0	24	0	71.813	65.672	65.672	0.0	5.541	4.453
2	24	0	36.295	36.664	-36.664	0.0	0.231	0.201
1	25	0	3.380	0.312	-0.312	0.0	3.068	0.611
0	12	0	203.369	196.774	196.774	0.0	6.595	2.166 *
4	23	1	5.806	0.303	-0.303	0.0	5.503	1.510
2	23	1	5.868	7.114	7.114	0.0	-1.246	-0.339
0	23	1	14.419	14.890	14.890	0.0	-0.471	-0.248
-5	22	1	22.361	20.246	-20.246	0.0	2.115	1.619
-3	22	1	16.272	14.667	14.667	0.0	1.605	1.076
-1	22	1	9.368	5.500	-5.500	0.0	3.898	1.732
3	22	1	17.190	15.504	-15.504	0.0	1.686	1.151
1	22	1	11.278	9.931	9.931	0.0	1.347	0.641
5	22	1	6.512	7.381	-7.381	0.0	-0.868	-0.239
4	21	1	5.012	4.664	4.664	0.0	0.348	0.092
2	21	1	24.866	21.170	-21.170	0.0	3.636	3.552
0	21	1	27.629	26.544	26.544	0.0	0.686	0.626
-2	21	1	34.433	31.211	-31.211	0.0	3.222	3.380
-4	21	1	11.145	10.863	10.863	0.0	0.283	0.136
-7	20	1	12.407	12.145	12.145	0.0	0.262	0.127
-5	20	1	4.695	2.791	-2.791	0.0	1.904	0.541
0	12	0	203.174	156.774	196.774	0.0	6.401	2.102 *
-3	20	1	8.507	9.788	9.788	0.0	-1.281	-0.534
-1	20	1	7.068	0.744	0.744	0.0	6.324	2.463
1	20	1	10.951	4.734	4.734	0.0	6.217	3.488

H	K	L	F(0BS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
3	20	1	9.036	9.690	9.690	0.0	-0.654	-0.278
5	20	1	7.598	8.364	-8.364	0.0	-0.766	-0.266
7	20	1	11.136	11.449	11.449	0.0	-0.313	-0.131
6	19	1	21.779	22.127	22.127	0.0	-0.349	-0.278
4	19	1	16.052	15.351	-15.351	0.0	0.701	0.487
2	19	1	9.839	10.514	10.514	0.0	-0.675	-0.316
0	19	1	35.757	33.574	-33.974	0.0	1.783	1.962
-2	19	1	31.345	34.575	34.575	0.0	2.770	2.961
-4	19	1	15.522	12.826	-12.826	0.0	2.696	2.023
-9	18	1	29.941	31.981	31.981	0.0	-2.040	-1.725
-7	18	1	69.828	67.767	-67.767	0.0	2.061	1.692
-5	18	1	71.893	67.768	67.768	0.0	4.125	3.412
-3	18	1	3.362	0.504	0.504	0.0	2.858	0.716
-1	18	1	4.924	5.137	5.137	0.0	-0.213	-0.065
1	18	1	22.308	22.709	-22.709	0.0	-0.401	-0.379
0	12	0	203.907	196.774	196.774	0.0	7.133	2.336
3	18	1	17.119	18.970	-18.970	0.0	-1.851	-1.353
5	18	1	56.159	61.129	61.129	0.0	-4.970	-4.655
7	18	1	32.024	36.148	-36.148	0.0	-4.124	-3.863
6	17	1	55.700	61.062	61.062	0.0	-5.362	-5.193
4	17	1	2.294	4.001	4.001	0.0	-1.707	-0.360
2	17	1	66.386	64.546	64.546	0.0	1.840	1.655
0	17	1	43.866	41.826	-41.826	0.0	2.040	2.336
-2	17	1	109.988	103.540	103.540	0.0	6.448	3.786
-4	17	1	16.555	16.494	16.494	0.0	0.061	0.043
-6	17	1	41.607	39.210	39.210	0.0	2.397	2.539
-8	17	1	9.301	8.835	8.835	0.0	0.466	0.191
-10	17	1	5.992	4.943	-4.943	0.0	1.049	0.293
-9	16	1	25.529	26.606	26.606	0.0	-1.076	-0.865
-7	16	1	18.981	17.490	17.490	0.0	1.491	1.243
-5	16	1	49.646	48.418	48.418	0.0	1.228	1.277
-3	16	1	45.128	42.229	42.229	0.0	2.900	3.286
-1	16	1	52.382	50.061	50.061	0.0	2.321	2.413
1	16	1	41.422	40.125	40.125	0.0	1.297	1.484
3	16	1	32.571	32.012	32.012	0.0	0.559	0.627
0	12	0	203.545	156.774	196.774	0.0	6.771	2.224
5	16	1	36.180	41.849	41.849	0.0	-5.669	-6.118
7	16	1	18.849	21.648	21.648	0.0	-2.799	-1.982
9	16	1	23.376	24.728	24.728	0.0	-1.352	-0.995
10	15	1	13.272	12.416	12.416	0.0	0.856	0.404
2	15	1	20.473	21.522	-21.522	0.0	-1.050	-1.008
0	15	1	57.456	56.020	56.020	0.0	1.436	1.428
-2	15	1	50.661	47.255	-47.255	0.0	3.406	3.607
-4	15	1	17.746	17.126	17.126	0.0	0.620	0.541
-6	15	1	17.358	18.880	18.880	0.0	-1.522	-1.078
-8	15	1	8.895	7.505	-7.505	0.0	1.390	0.623
-10	15	1	16.978	12.423	12.423	0.0	4.555	3.309
-9	14	1	22.335	24.525	-24.525	0.0	-2.191	-1.633
-7	14	1	26.544	26.278	26.278	0.0	0.266	0.262
-5	14	1	71.743	70.580	-70.580	0.0	1.163	0.991
-3	14	1	34.627	35.624	35.624	0.0	-0.997	-1.129
-1	14	1	35.227	35.535	-35.535	0.0	-0.308	-0.360
0	12	0	202.636	196.774	196.774	0.0	5.862	1.931

*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	14	1	50.335	52.638	-52.638	0.0	-2.303	-2.462
3	14	1	17.693	20.032	20.032	0.0	-2.339	-2.023
5	14	1	34.971	40.773	-40.773	0.0	-5.801	-6.848
7	14	1	10.951	10.143	10.143	0.0	0.808	0.449
9	14	1	23.791	27.381	-27.381	0.0	-3.590	-2.694
8	13	1	9.601	8.903	8.903	0.0	0.698	0.316
4	13	1	14.649	18.144	18.144	0.0	-3.495	-2.401
2	13	1	23.447	23.549	-23.549	0.0	-0.102	-0.103
0	13	1	39.357	39.981	39.981	0.0	-0.624	-0.761
-2	13	1	33.904	32.105	-32.105	0.0	1.798	2.191
-4	13	1	34.954	32.212	32.212	0.0	2.742	3.139
-8	13	1	3.592	3.876	-3.876	0.0	-0.285	-0.072
-11	12	1	15.037	9.197	9.197	0.0	5.840	4.136
-9	12	1	7.130	4.737	-4.737	0.0	2.393	0.968
-7	12	1	9.239	11.536	11.536	0.0	-2.296	-1.141
-5	12	1	14.560	11.239	11.239	0.0	3.321	2.444
0	12	0	203.210	156.774	196.774	0.0	6.436	2.114
-3	12	1	6.239	7.666	7.666	0.0	-1.427	-0.548
-1	12	1	17.446	15.191	15.191	0.0	2.255	2.130
1	12	1	15.593	16.489	16.489	0.0	-0.896	-0.725
3	12	1	6.389	6.031	6.031	0.0	0.358	0.138
9	12	1	9.327	2.986	2.986	0.0	6.342	3.032
11	12	1	6.309	5.505	5.505	0.0	0.805	0.223
10	11	1	8.850	7.610	-7.610	0.0	4.776	-0.948
8	11	1	8.930	4.154	4.154	0.0	4.776	2.303
6	11	1	8.507	7.198	-7.198	0.0	0.708	0.352
2	11	1	39.092	40.082	-40.082	0.0	-0.990	-1.260
0	11	1	6.477	6.697	6.697	0.0	-0.220	-0.102
-2	11	1	24.867	23.320	-23.320	0.0	1.547	1.807
-4	11	1	7.315	8.564	-8.564	0.0	-1.248	-0.536
-6	11	1	14.101	9.913	-9.913	0.0	4.188	3.062
-8	11	1	13.246	11.924	11.924	0.0	1.322	0.930
-12	11	1	8.216	1.382	-1.382	0.0	6.833	2.531
0	12	0	203.351	196.774	196.774	0.0	6.577	2.160
-11	10	1	9.760	14.564	14.564	0.0	-4.804	-1.845
-9	10	1	15.690	18.329	-18.329	0.0	-2.639	-1.709
-7	10	1	21.991	22.554	22.554	0.0	-0.563	-0.585
-5	10	1	33.189	32.225	-32.225	0.0	0.964	1.174
-3	10	1	55.021	51.858	51.858	0.0	3.163	3.446
-1	10	1	35.916	35.225	-35.225	0.0	0.691	0.943
1	10	1	12.248	14.061	-14.061	0.0	-1.812	-1.580
3	10	1	39.066	44.286	44.286	0.0	-5.220	-6.500
5	10	1	30.003	36.042	-36.042	0.0	-6.039	-6.644
7	10	1	15.187	19.793	19.793	0.0	-4.606	-3.203
9	10	1	15.513	12.663	-12.663	0.0	2.851	2.125
11	10	1	12.442	14.206	14.206	0.0	-1.763	-0.793
10	9	1	17.781	17.719	17.719	0.0	0.063	0.042
8	9	1	8.427	0.440	0.440	0.0	7.987	3.901
4	9	1	26.888	30.939	30.939	0.0	-4.051	-4.732
2	9	1	46.187	47.643	-47.643	0.0	-1.456	-1.813
0	9	1	95.340	95.864	95.864	0.0	-0.524	-0.360
-2	9	1	53.657	50.436	-50.436	0.0	3.261	3.695
-4	9	1	27.135	25.629	25.629	0.0	1.506	2.032

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	12	0	202.513	156.774	196.774	0.0	5.739	1.851 *
-6	9	1	17.587	18.373	18.373	0.0	-0.786	-0.660
-8	9	1	6.168	5.381	-5.381	0.0	0.787	0.303
-10	9	1	10.907	11.186	11.186	0.0	-0.279	-0.139
-12	9	1	23.782	22.323	-22.323	0.0	1.459	1.190
-13	8	1	2.894	4.264	4.264	0.0	-1.370	-0.271
-11	8	1	14.384	13.100	-13.100	0.0	1.284	0.836
-9	8	1	8.789	8.551	-8.551	0.0	0.238	0.105
-7	8	1	7.721	6.891	6.891	0.0	0.830	0.359
-5	8	1	15.610	15.629	-15.629	0.0	-0.019	-0.015
-3	8	1	6.698	1.457	-1.457	0.0	5.241	3.093
-1	8	1	13.440	13.043	-13.043	0.0	0.397	0.517
1	8	1	11.560	11.015	-11.015	0.0	0.545	0.594
3	8	1	3.715	9.844	-9.844	0.0	-6.129	-2.098
5	8	1	16.193	20.904	-20.904	0.0	-4.711	-3.759
7	8	1	13.007	11.821	11.821	0.0	1.187	0.856
11	8	1	10.942	9.473	-9.473	0.0	1.469	0.655
12	7	1	16.590	16.612	16.612	0.0	-0.022	-0.012
10	7	1	24.982	22.531	-22.531	0.0	2.451	2.187
8	7	1	3.044	2.814	2.814	0.0	0.231	0.057
0	12	0	202.407	156.774	196.774	0.0	5.633	1.856 *
6	7	1	52.216	57.031	57.031	0.0	-4.755	-5.036
4	7	1	40.142	45.438	-45.438	0.0	-5.295	-6.819
2	7	1	23.879	27.957	27.957	0.0	-4.078	-6.331
0	7	1	125.952	126.537	-126.537	0.0	-0.586	-0.309
-2	7	1	80.188	78.021	78.021	0.0	2.167	1.767
-4	7	1	5.286	2.925	2.925	0.0	2.361	1.057
-6	7	1	32.836	33.383	33.383	0.0	-0.547	-0.681
-8	7	1	15.946	15.590	-15.590	0.0	-0.045	-0.035
-10	7	1	19.476	17.747	-17.747	0.0	1.728	1.472
-12	7	1	43.355	41.875	41.875	0.0	1.479	1.363
-13	6	1	38.016	34.855	34.855	0.0	3.161	2.866
-11	6	1	6.336	0.827	0.827	0.0	5.509	1.897
-9	6	1	92.772	92.969	92.969	0.0	-0.198	-0.135
-7	6	1	96.363	97.727	-97.727	0.0	-1.364	-0.909
-5	6	1	182.931	192.701	192.701	0.0	-9.770	-3.560
-3	6	1	158.929	152.406	152.406	0.0	6.523	2.738
-1	6	1	123.401	122.378	122.378	0.0	1.023	0.552
1	6	1	45.905	42.384	-42.384	0.0	3.521	4.640
3	6	1	42.712	47.943	47.943	0.0	-5.171	-6.894
5	6	1	201.092	224.488	224.488	0.0	-23.396	-7.752 *
0	12	0	202.707	156.774	196.774	0.0	5.933	1.954 *
7	6	1	40.019	38.945	-38.945	0.0	1.074	1.267
9	6	1	66.439	64.829	64.829	0.0	1.610	1.415
11	6	1	20.799	19.340	-19.340	0.0	1.459	1.034
12	5	1	36.957	35.868	35.868	0.0	1.089	0.935
10	5	1	10.113	10.767	-10.767	0.0	-0.654	-0.300
8	5	1	31.212	30.539	30.539	0.0	0.673	0.763
6	5	1	128.387	129.498	129.498	0.0	-1.111	-0.570
4	5	1	23.288	25.347	25.347	0.0	-2.059	-2.622
2	5	1	102.743	128.507	128.507	0.0	-25.763	-16.588 *
0	5	1	70.755	69.266	-69.266	0.0	1.488	1.371
-2	5	1	219.800	220.785	220.785	0.0	-0.985	-0.300

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-4	5	1	94.069	94.015	94.015	0.0	0.054	0.037
-6	5	1	89.860	91.025	91.025	0.0	-1.166	-0.836
-8	5	1	17.375	17.109	17.109	0.0	0.266	0.216
-10	5	1	7.677	3.229	3.229	0.0	4.448	1.931
-12	5	1	66.386	62.169	62.169	0.0	4.218	3.540
-13	4	1	16.996	16.832	16.832	0.0	0.164	0.100
-11	4	1	4.968	9.479	-9.479	0.0	-4.511	-1.214
-7	4	1	13.519	12.174	12.174	0.0	1.345	1.023
0	12	0	202.521	156.774	196.774	0.0	5.748	1.893
-5	4	1	19.996	19.771	19.771	0.0	0.225	0.300
-3	4	1	8.295	6.829	6.829	5.0	1.466	1.298
-1	4	1	6.804	8.707	8.707	0.0	-1.903	-1.307
1	4	1	7.977	3.821	3.821	0.0	4.156	3.596
5	4	1	6.045	2.520	2.520	0.0	3.525	1.548
7	4	1	15.160	13.200	13.200	0.0	1.960	1.452
9	4	1	17.658	16.816	16.816	0.0	0.842	0.696
11	4	1	8.604	11.043	-11.043	0.0	-2.439	-0.883
12	3	1	22.952	22.505	-22.505	0.0	0.447	0.303
10	3	1	14.516	11.395	11.395	0.0	3.121	2.170
8	3	1	10.748	10.342	-10.342	0.0	0.406	0.234
6	3	1	25.714	25.595	-25.595	0.0	0.120	0.134
4	3	1	21.902	21.157	-21.157	0.0	0.746	1.069
2	3	1	103.723	115.305	-115.305	0.0	-11.582	-7.415
-2	3	1	145.418	142.383	-142.383	0.0	3.036	1.393
-4	3	1	17.419	15.320	-15.320	0.0	2.100	3.173
-8	3	1	22.379	19.176	-19.176	0.0	3.202	3.128
-10	3	1	8.542	8.815	8.815	0.0	-0.273	-0.118
0	12	0	203.201	156.774	196.774	0.0	6.427	2.111
-12	3	1	33.842	32.607	-32.607	0.0	1.235	1.261
-13	2	1	18.355	15.339	-15.339	0.0	3.016	2.057
-11	2	1	20.173	17.043	-17.043	0.0	3.130	2.687
-9	2	1	27.815	27.496	-27.496	0.0	0.319	0.356
-7	2	1	45.914	44.789	-44.789	0.0	1.124	1.327
-5	2	1	53.750	52.558	-52.558	0.0	1.191	1.350
-3	2	1	124.346	123.623	-123.623	0.0	0.723	0.388
1	2	1	9.063	7.652	-7.652	0.0	1.411	1.311
3	2	1	100.352	101.775	101.775	0.0	-1.423	-0.938
5	2	1	31.194	31.791	-31.791	0.0	-0.597	-0.768
7	2	1	34.689	35.685	35.685	0.0	-0.996	-1.075
9	2	1	23.835	22.129	-22.129	0.0	1.706	1.806
11	2	1	26.579	23.304	-23.304	0.0	3.275	2.922
12	1	1	7.704	0.720	0.720	0.0	6.984	2.406
8	1	1	11.472	13.533	13.533	0.0	-2.062	-1.263
6	1	1	9.213	5.148	-5.148	0.0	4.065	2.303
4	1	1	13.369	13.674	13.674	0.0	-0.304	-0.332
2	1	1	48.561	50.301	-50.301	0.0	-1.740	-2.215
-4	1	1	24.691	25.780	-25.780	0.0	-1.090	-1.764
0	12	0	202.424	156.774	196.774	0.0	5.651	1.861
-6	1	1	2.762	5.572	5.572	0.0	-2.810	-0.856
-8	1	1	9.248	7.812	7.812	0.0	1.436	0.733
-10	1	1	5.339	3.790	-3.790	0.0	1.549	0.513
-12	1	1	3.989	0.627	0.627	0.0	3.361	0.862
-13	0	1	12.310	12.516	-12.516	0.0	-0.606	-0.285

H	K	L	F(0BS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-11	0	1	9.760	7.777	7.777	0.0	1.983	1.003
-7	0	1	3.865	3.861	-3.861	0.0	0.004	0.001
-5	0	1	12.098	10.020	-10.020	0.0	2.078	2.265
-3	0	1	21.470	20.109	-20.109	0.0	1.361	2.268
3	0	1	30.153	30.355	-30.355	0.0	-0.202	-0.332
5	0	1	4.827	3.081	-3.081	0.0	1.746	0.730
9	0	1	3.177	6.776	-6.776	0.0	-3.599	-0.862
-12	0	2	47.956	45.196	-45.196	0.0	2.800	2.859
-10	0	2	74.126	72.388	-72.388	0.0	1.738	1.427
-8	0	2	62.645	64.684	64.684	0.0	-2.039	-1.909
-6	0	2	98.640	98.622	98.622	0.0	0.017	0.012
-4	0	2	156.440	156.976	156.976	0.0	-0.536	-0.228
0	12	0	202.327	156.774	196.774	0.0	5.554	1.835
-2	0	2	113.712	107.542	-107.542	0.0	5.770	3.370
0	0	2	253.853	265.477	265.477	0.0	-11.623	-3.070
2	0	2	124.601	120.132	120.132	0.0	4.470	2.378
4	0	2	188.323	189.491	189.491	0.0	-1.168	-0.414
6	0	2	44.899	43.673	-43.673	0.0	1.226	1.349
8	0	2	44.899	41.725	41.725	0.0	3.174	3.330
10	0	2	70.737	65.728	65.728	0.0	5.009	3.888
11	1	2	45.931	41.178	41.178	0.0	4.753	4.379
9	1	2	26.147	23.578	-23.578	0.0	2.569	2.426
7	1	2	57.641	56.028	56.028	0.0	1.613	1.576
5	1	2	41.201	40.786	-40.786	0.0	0.416	0.491
3	1	2	76.896	76.578	76.578	0.0	0.318	0.265
1	1	2	118.115	114.183	114.183	0.0	3.933	2.206
-1	1	2	4.853	4.155	-4.155	0.0	0.699	0.390
-3	1	2	4.448	3.862	3.862	0.0	0.585	0.328
-5	1	2	21.188	20.307	-20.307	0.0	0.881	1.160
-7	1	2	162.555	163.757	163.757	0.0	-1.202	-0.492
-9	1	2	30.886	30.104	-30.104	0.0	0.782	0.904
-11	1	2	25.962	26.672	26.672	0.0	-0.711	-0.694
-13	1	2	5.683	3.507	3.507	0.0	2.176	0.626
0	12	0	203.192	196.774	196.774	0.0	6.418	2.108
-10	2	2	9.928	1.507	1.507	0.0	8.420	4.632
-8	2	2	8.119	7.870	7.870	0.0	0.249	0.110
-6	2	2	26.076	26.040	-26.040	0.0	0.036	0.045
-4	2	2	20.843	19.338	-19.338	0.0	1.506	2.216
-2	2	2	20.552	20.466	-20.466	0.0	0.086	0.138
0	2	2	30.347	28.958	-28.958	0.0	1.389	2.282
2	2	2	13.016	11.974	-11.974	0.0	1.042	1.192
4	2	2	8.992	5.699	5.699	0.0	3.293	1.838
6	2	2	6.512	10.415	-10.415	0.0	-3.902	-1.340
8	2	2	13.810	10.803	-10.803	0.0	3.007	2.028
10	2	2	11.763	11.736	-11.736	0.0	0.027	0.014
11	3	2	17.852	14.719	-14.719	0.0	3.132	2.028
9	3	2	29.191	26.121	26.121	0.0	3.071	3.163
7	3	2	59.080	57.803	-57.803	0.0	1.276	1.226
5	3	2	44.056	44.903	44.903	0.0	-0.808	-0.906
1	3	2	66.113	65.761	-65.761	0.0	0.352	0.341
-1	3	2	5.039	7.795	7.795	0.0	-2.756	-1.569
-3	3	2	24.629	21.328	21.328	0.0	3.301	5.269
0	12	0	202.592	196.774	196.774	0.0	5.818	1.917

*