H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-5	3	2	17.781	20.103	20.103	0.0	-2.322	-2.482	
-7	3	2	84.627	84.115	-84.115	0.0	0.512	0.384	
-9	3	2	57.315	57.005	57.005	0.0	0.310	0.308	
-11	3	2	7.571	9.688	-9.688	0.0	-2.117	-0.779	
-13	3	2	15.222	14.485	-14.485	0.0	0.738	0.410	
-12	4	2	38.836	37.932	37.932	0.0	0.904	0.891	
-10	4	2	39.207	38.114	-38.114	0.0	1.093	1.180	
-8	4	2	5.692	4.384	4.384	0.0	1.308	0.427	
-6	4	2	76.464	76.087	76.087	0.0	0.377	0.312	
-4	4	2	72.714	69.969	-69.969	0.0	2.745	2.411	
-2	4	2	10.175	10.370	10.370	0.0	-0.195	-0.198	
0	4	2	78.097	74.527	74.527	0.0	3.570	2.975	
2	4	2	68.619	73.589	73.589	0.0	-4.970	-4.617	
4	4	2	75.970	76.265	-76.265	0.0	-0.295	-0.246	
6	4	2	63.324	62.774	62.774	0.0	0.550	0.515	
8	4	2	16.458	12.525	12.525	0.0	3.933	2.991	
10	4	2	28.124	25.912	-25.912	0.0	2.211	2.054	
9	5	2	15.522	14.924	14.924	0.0	0.599	0.392	
7	5	2	37.310	35.957	-35.957	0.0	1.353	1.564	
0	12	0	202.874	196.774	196.774	0.0	6.101	2.010	*
5	5	2	9.010	5.229	-5.229	0.0	3.781	1.956	
3	5	2	27.523	27.547	27.547	0.0	-0.023	-0.031	
1	5	2	66.236	70.471	-70.471	0.0	-4.235	-4.067	
-1	5	2	44.405	42.759	-42.759	0.0	1.645	2.194	
-3	5	2	41.237	38.430	38.430	0.0	2.807	3.787	
-5	5	2	17.199	15.410	-15.410	0.0	1.789	1.748	
-7	5	2	39.392	40.057	-40.057	0.0	-0.665	-0.793	
-9	5	2	37.389	37.212	37.212	0.0	0.177	0.201	
-11	5	2	12.566	11.056	-11.056	0.0	1.510	0.896	
-13	5	2	10.969	3.531	3.531	0.0	7.438	3.649	
-12	6	2	3.768	0.194	-0.194	0.0	3.574	0.833	
-10	6	2	14.807	14.526	14.526	0.0	0.281	0.192	
-8	6	2	14.393	17.369	-17.369	0.0	-2.977	-1.906	
-6	6	2	16.069	14.459	14.459	0.0	1.610	1.352	
-4	6	2	8.824	10.659	-10.659	0.0	-1.834	-1.130	
2	6	2	5.780	3.187	3.187	0.0	2.593	1.272	
6	6	2	13.537	13.346	13.346	0.0	0.191	0.129	
0	12	0	202.689	196.774	196.774	0.0	5.915	1.949	*
8	6	2	19.264	19.008	-19.008	0.0	0.256	0.223	
10	6	2	11.834	8.426	8.426	0.0	3.408	1.875	
11	7	2	10.360	11.497	-11.497	0.0	-1.137	-0.428	
9	7	2	15.610	13.317	13.317	0.0	2.294	1.511	
5	7	2	18.152	19.953	19.953	0.0	-1.801	-1.408	
3	7	2	2.700	6.932	-6.932	0.0	-4.232	-1.087	
1	7	2	27.788	32.314	32.314	0.0	-4.525	-6.254	
-1	7	2	39.763	40.378	40.378	0.0	-0.615	-0.840	
-3	7	2	33.586	32.425	-32.425	0.0	1.161	1.586	
-5	7	2	34.662	35.708	35.708	0.0	-1.046	-1.261	
-9	7	2	17.419	17.423	17.423	0.0	-0.004	-0.003	
-11	7	2	16.943	17.495	-17.495	0.0	-0.552	-0.368	
-13	7	2	14.816	16.561	16.561	0.0	-1.745	-0.887	
-12	8	2	17.552	17.128	17.128	0.0	0.424	0.273	
-10	8	2	11.869	14.742	-14.742	0.0	-2.873	-1.508	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-8	8	2	4.121	3.997	3.997	0.0	0.124	0.036	
-6	8	2	20.570	20.478	-20.478	0.0	0.092	0.085	
-4	8	2	26.888	25.669	-25.669	0.0	1.219	1.470	
0	12	0	202.230	196.774	196.774	0.0	5.457	1.803	*
-2	8	2	55.506	52.286	52.286	0.0	3.220	3.509	
0	8	2	90.468	93.907	-93.907	0.0	-3.439	-2.482	
2	8	2	62.142	68.635	68.635	0.0	-6.493	-6.399	
4	8	2	32.492	35.911	-35.911	0.0	-3.419	-3.875	
6	8	2	6.830	3.693	3.693	0.0	3.137	1.284	
8	8	2	8.392	2.715	-2.715	0.0	5.678	2.513	
10	8	2	9.839	9.068	-9.068	0.0	0.771	0.314	
9	9	2	4.227	3.581	3.581	0.0	0.646	0.170	
7	9	2	28.574	29.092	-29.092	0.0	-0.518	-0.549	
5	9	2	26.482	28.403	28.403	0.0	-1.921	-2.155	
3	9	2	57.827	66.271	-66.271	0.0	-8.444	-8.543	
1	9	2	22.494	21.569	-21.569	0.0	0.925	1.027	
-1	9	2	15.752	15.719	15.719	0.0	0.033	0.030	
-3	9	2	76.164	74.441	-74.441	0.0	1.723	1.436	
-5	9	2	27.118	27.440	27.440	0.0	-0.322	-0.348	
-7	9	2	40.292	41.810	-41.810	0.0	-1.518	-1.703	
-9	9	2	18.434	18.111	18.111	0.0	0.323	0.258	
-11	9	2	4.086	5.603	-5.603	0.0	-1.517	-0.371	
-12	10	2	4.712	4.651	4.651	0.0	0.061	0.015	
0	12	0	203.227	196.774	196.774	0.0	6.454	2.120	*
-10	10	2	23.049	21.914	21.914	0.0	1.135	1.081	
-8	10	2	33.471	33.387	33.387	0.0	0.084	0.093	
-6	10	2	15.134	16.182	16.182	0.0	-1.048	-0.757	
-4	10	2	43.743	43.221	43.221	0.0	0.522	0.603	
-2	10	2	26.306	26.148	26.148	0.0	0.157	0.176	
0	10	2	47.908	48.302	48.302	0.0	-0.394	-0.456	
2	10	2	30.603	31.902	31.902	0.0	-1.299	-1.517	
4	10	2	45.111	51.888	51.888	0.0	-6.777	-7.529	
6	10	2	11.851	11.768	11.768	0.0	0.083	0.055	
8	10	2	8.895	11.597	11.597	0.0	-2.702	-1.074	
10	10	2	8.507	5.985	5.985	0.0	2.522	0.902	
7	11	2	41.166	45.821	45.821	0.0	-4.655	-4.976	
5	11	2	12.690	12.605	-12.605	0.0	0.085	0.060	
3	11	2	117.621	134.996	134.996	0.0	-17.375	-9.652	*
1	11	2	78.644	81.359	81.359	0.0	-2.715	-2.182	
-1	11	2	13.678	15.982	15.982	0.0	-2.304	-1.642	
-3	11	2	113.174	110.733	110.733	0.0	2.440	1.411	
-5	11	2	13.007	14.115	-14.115	0.0	-1.108	-0.675	
-7	11	2	122.651	123.298	123.298	0.0	-0.647	-0.344	
0	12	0	202.248	196.774	196.774	0.0	5.474	1.809	*
-11	11	2	31.609	30.367	30.367	0.0	1.242	1.126	
-12	12	2	24.311	23.777	-23.777	0.0	0.534	0.412	
-10	12	2	15.037	16.612	16.612	0.0	-1.575	-0.897	
-8	12	2	14.693	15.378	15.378	0.0	-0.686	-0.446	
-6	12	2	79.403	79.411	79.411	0.0	-0.008	-0.007	
-4	12	2	32.112	29.130	29.130	0.0	2.982	3.379	
-2	12	2	134.282	133.809	-133.809	0.0	0.473	0.232	
0	12	2	180.954	183.032	183.032	0.0	-2.077	-0.764	
2	12	2	12.407	11.365	-11.365	0.0	1.043	0.639	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
4	12	2	41.704	47.253	47.253	0.0	-5.549	-6.288	
6	12	2	19.246	21.854	-21.854	0.0	-2.608	-2.038	
8	12	2	18.205	17.736	17.736	0.0	0.469	0.340	
10	12	2	17.728	19.979	19.979	0.0	-2.251	-1.250	
9	13	2	15.055	14.405	-14.405	0.0	0.650	0.357	
5	13	2	32.121	37.490	-37.490	0.0	-5.369	-5.850	
3	13	2	43.205	48.560	48.560	0.0	-5.355	-6.130	
1	13	2	11.392	13.704	-13.704	0.0	-2.312	-1.224	
-1	13	2	48.799	49.595	-49.595	0.0	-0.795	-0.858	
0	12	0	203.307	196.774	196.774	0.0	6.533	2.146	*
-3	13	2	36.807	35.046	35.046	0.0	1.761	1.975	
-5	13	2	50.997	51.656	-51.656	0.0	-0.659	-0.698	
-7	13	2	41.475	39.899	39.899	0.0	1.576	1.734	
-9	13	2	11.675	10.687	-10.687	0.0	0.988	0.535	
-11	13	2	1.456	8.084	8.084	0.0	-6.628	-1.061	
-10	14	2	2.365	3.123	-3.123	0.0	-0.758	-0.143	
-8	14	2	3.309	6.427	6.427	0.0	-3.118	-0.718	
-6	14	2	8.842	2.544	-2.544	0.0	6.298	3.274	
-4	14	2	6.804	4.774	-4.774	0.0	2.029	0.839	
-2	14	2	9.522	10.545	10.545	0.0	-1.024	-0.511	
0	14	2	7.236	3.701	-3.701	0.0	3.535	1.462	
2	14	2	11.525	11.381	11.381	0.0	0.144	0.085	
4	14	2	1.624	2.122	2.122	0.0	-0.499	-0.099	
6	14	2	3.909	6.141	6.141	0.0	-2.232	-0.566	
7	15	2	15.187	15.611	-15.611	0.0	-0.425	-0.261	
5	15	2	24.205	30.298	30.298	0.0	-6.092	-5.270	
3	15	2	17.808	19.684	-19.684	0.0	-1.876	-1.563	
-1	15	2	27.674	27.692	27.692	0.0	-0.019	-0.021	
0	12	0	202.239	196.774	196.774	0.0	5.465	1.806	*
-3	15	2	29.156	27.994	-27.994	0.0	1.162	1.330	
-5	15	2	30.533	29.684	29.684	0.0	0.849	0.916	
-7	15	2	26.262	24.995	-24.995	0.0	1.267	1.293	
-9	15	2	20.340	21.205	21.205	0.0	-0.864	-0.649	
-11	15	2	6.857	6.763	-6.763	0.0	0.094	0.027	
-10	16	2	2.047	2.740	-2.740	0.0	-0.692	-0.123	
-6	16	2	8.021	5.081	-5.081	0.0	2.941	1.203	
-4	16	2	15.107	14.341	-14.341	0.0	0.766	0.533	
-2	16	2	18.390	15.950	15.950	0.0	2.440	2.266	
0	16	2	38.819	39.318	-39.318	0.0	-0.499	-0.566	
2	16	2	21.390	20.301	20.301	0.0	1.090	1.064	
4	16	2	18.408	21.580	-21.580	0.0	-3.172	-2.462	
6	16	2	5.612	1.303	1.303	0.0	4.309	1.353	
3	17	2	9.539	3.080	-3.080	0.0	6.460	3.453	
1	17	2	9.883	1.087	1.087	0.0	8.797	5.274	
-1	17	2	2.700	6.153	6.153	0.0	-3.452	-0.766	
0	12	0	202.319	196.774	196.774	0.0	5.545	1.832	*
-3	17	2	3.265	4.363	-4.363	0.0	-1.098	-0.260	
-9	17	2	8.948	3.773	3.773	0.0	5.175	2.102	
-8	18	2	7.210	5.919	-5.919	0.0	1.290	0.433	
-6	18	2	8.816	8.483	8.483	0.0	0.332	0.138	
-4	18	2	9.398	2.899	2.899	0.0	6.499	3.363	
-2	18	2	13.360	13.613	13.613	0.0	-0.253	-0.159	
0	18	2	3.636	1.405	1.405	0.0	2.230	0.584	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
2	18	2	13.784	11.862	11.862	0.0	1.922	1.245	
6	18	2	9.583	11.765	11.765	0.0	-2.182	-0.889	
5	19	2	4.156	4.358	4.358	0.0	-0.202	-0.049	
-7	19	2	24.806	23.648	-23.648	0.0	1.158	0.944	
-9	19	2	15.875	17.138	17.138	0.0	-1.263	-0.656	
0	12	0	200.757	196.774	196.774	0.0	3.983	1.324	*
-8	20	2	3.477	0.086	-0.086	0.0	3.391	0.716	
-6	20	2	8.657	12.612	12.612	0.0	-3.955	-1.575	
-4	20	2	32.889	30.215	-30.215	0.0	2.674	2.681	
0	20	2	25.741	23.245	-23.245	0.0	2.496	2.227	
2	20	2	20.296	21.293	21.293	0.0	-0.997	-0.748	
4	20	2	40.840	41.976	-41.976	0.0	-1.136	-1.139	
6	20	2	14.719	13.896	13.896	0.0	0.823	0.442	
5	21	2	29.483	28.484	28.484	0.0	0.999	0.884	
3	21	2	10.272	11.886	11.886	0.0	-1.614	-0.690	
-1	21	2	24.241	21.562	21.562	0.0	2.679	2.318	
-3	21	2	12.990	14.173	14.173	0.0	-1.183	-0.604	
-5	21	2	24.885	22.321	22.321	0.0	2.564	2.202	
-7	21	2	13.404	13.392	-13.392	0.0	0.012	0.006	
-6	22	2	17.252	15.434	15.434	0.0	1.818	1.164	
-4	22	2	28.662	25.437	25.437	0.0	3.225	2.877	
-2	22	2	10.625	8.042	8.042	0.0	2.583	1.134	
0	22	2	39.701	37.832	37.832	0.0	1.869	1.810	
2	22	2	12.548	13.436	13.436	0.0	-0.888	-0.417	
0	12	0	201.418	196.774	196.774	0.0	4.645	1.539	*
4	22	2	27.206	27.813	27.813	0.0	-0.607	-0.474	
1	23	2	20.058	18.156	18.156	0.0	1.902	1.382	
-1	23	2	13.422	8.769	-8.769	0.0	4.653	2.535	
-3	23	2	18.699	18.767	18.767	0.0	-0.068	-0.040	
-2	24	2	45.490	43.053	-43.053	0.0	2.437	2.227	
0	24	2	39.922	36.603	36.603	0.0	3.319	3.058	
-3	22	3	9.557	10.628	10.628	0.0	-1.072	-0.406	
-1	22	3	14.013	10.655	-10.655	0.0	3.358	1.874	
2	21	3	21.320	19.571	-19.571	0.0	1.748	1.348	
0	21	3	16.925	16.516	16.516	0.0	0.409	0.255	
-2	21	3	21.214	18.830	-18.830	0.0	2.384	1.972	
-4	21	3	6.054	8.728	8.728	0.0	-2.674	-0.761	
-7	20	3	7.218	7.096	7.096	0.0	0.122	0.038	
-3	20	3	8.551	10.539	10.539	0.0	-1.988	-0.729	
-1	20	3	7.024	0.893	0.893	0.0	6.131	2.118	
3	20	3	4.853	8.321	8.321	0.0	-3.468	-0.841	
0	12	0	201.065	196.774	196.774	0.0	4.292	1.426	*
4	19	3	27.947	29.796	-29.796	0.0	-1.849	-1.704	
2	19	3	20.261	20.270	20.270	0.0	-0.009	-0.006	
0	19	3	14.975	13.281	-13.281	0.0	1.694	1.073	
-2	19	3	21.064	19.055	19.055	0.0	2.009	1.626	
-4	19	3	12.645	10.709	-10.709	0.0	1.936	1.125	
-6	19	3	4.359	0.042	0.042	0.0	4.317	1.073	
-8	19	3	8.772	0.916	-0.916	0.0	7.855	3.049	
-9	18	3	54.165	52.890	52.890	0.0	1.275	1.175	
-7	18	3	51.941	50.837	-50.837	0.0	1.104	1.034	
-5	18	3	25.159	23.233	23.233	0.0	1.925	1.774	
-3	18	3	15.425	14.223	-14.223	0.0	1.202	0.792	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-1	18	3	57.403	55.609	55.609	0.0	1.795	1.709	
1	18	3	23.508	22.559	-22.559	0.0	0.949	0.867	
3	18	3	27.373	30.208	-30.208	0.0	-2.834	-2.471	
5	18	3	33.445	37.058	37.058	0.0	-3.613	-3.356	
6	17	3	37.839	43.138	43.138	0.0	-5.299	-4.728	
4	17	3	26.244	28.016	-28.016	0.0	-1.772	-1.545	
2	17	3	53.167	56.290	56.290	0.0	-3.122	-2.973	
0	17	3	11.101	8.808	-8.808	0.0	2.294	1.256	
-2	17	3	83.603	81.458	81.458	0.0	2.145	1.578	
0	12	0	201.110	196.774	196.774	0.0	4.336	1.441	*
-4	17	3	6.415	5.273	5.273	0.0	1.142	0.377	
-6	17	3	13.237	13.377	13.377	0.0	-0.140	-0.076	
-8	17	3	21.082	20.140	20.140	0.0	0.942	0.684	
-9	16	3	23.147	23.863	23.863	0.0	-0.717	-0.542	
-7	16	3	10.104	9.767	9.767	0.0	0.337	0.158	
-5	16	3	41.140	40.039	40.039	0.0	1.101	1.199	
-3	16	3	28.891	28.698	28.698	0.0	0.194	0.201	
-1	16	3	43.619	42.768	42.768	0.0	0.852	0.919	
1	16	3	32.774	34.114	34.114	0.0	-1.340	-1.406	
3	16	3	22.785	24.879	24.879	0.0	-2.094	-1.784	
5	16	3	17.984	19.963	19.963	0.0	-1.978	-1.367	
7	16	3	11.657	11.998	11.998	0.0	-0.341	-0.141	
6	15	3	10.686	8.495	-8.495	0.0	2.191	0.989	
4	15	3	16.387	18.567	18.567	0.0	-2.180	-1.471	
2	15	3	19.890	22.947	-22.947	0.0	-3.057	-2.405	
0	15	3	31.556	33.573	33.573	0.0	-2.017	-2.176	
-2	15	3	24.744	23.013	-23.013	0.0	1.731	1.736	
-4	15	3	14.146	14.326	14.326	0.0	-0.181	-0.114	
-6	15	3	10.757	13.830	13.830	0.0	-3.073	-1.457	
-8	15	3	6.839	9.255	-9.255	0.0	-2.416	-0.787	
0	12	0	201.736	196.774	196.774	0.0	4.962	1.644	*
-10	15	3	16.272	15.059	15.059	0.0	1.214	0.716	
-11	14	3	10.748	8.839	8.839	0.0	1.909	0.819	
-9	14	3	29.853	29.954	-29.954	0.0	-0.101	-0.088	
-7	14	3	24.779	23.105	23.105	0.0	1.674	1.568	
-5	14	3	51.270	50.141	-50.141	0.0	1.129	1.185	
-3	14	3	28.459	28.673	28.673	0.0	-0.214	-0.226	
-1	14	3	40.381	39.724	-39.724	0.0	0.657	0.730	
1	14	3	13.793	17.617	-17.617	0.0	-3.825	-2.449	
3	14	3	8.048	6.106	6.106	0.0	1.942	0.840	
5	14	3	26.976	30.926	-30.926	0.0	-3.949	-3.729	
7	14	3	9.345	10.401	10.401	0.0	-1.056	-0.424	
8	13	3	7.527	6.610	6.610	0.0	0.917	0.307	
6	13	3	8.127	8.118	-8.118	0.0	0.009	0.003	
4	13	3	18.805	19.426	19.426	0.0	-0.621	-0.513	
2	13	3	20.296	23.418	-23.418	0.0	-3.122	-2.564	
0	13	3	29.218	29.894	29.894	0.0	-0.676	-0.744	
-2	13	3	11.613	12.472	-12.472	0.0	-0.859	-0.521	
-4	13	3	17.817	15.160	15.160	0.0	2.656	2.315	
-6	13	3	8.992	6.765	-6.765	0.0	2.227	1.056	
-8	13	3	2.824	1.688	-1.688	0.0	1.136	0.242	
0	12	0	200.201	196.774	196.774	0.0	3.427	1.142	*
-10	13	3	4.474	3.453	3.453	0.0	1.021	0.246	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-11	12	3	9.363	8.152	8.152	0.0	1.211	0.485	
-9	12	3	6.124	4.054	-4.054	0.0	2.070	0.680	
-7	12	3	2.550	10.846	10.846	0.0	-8.296	-1.709	
-5	12	3	9.680	4.364	4.364	0.0	5.316	2.924	
-1	12	3	9.892	11.069	11.069	0.0	-1.177	-0.567	
1	12	3	15.646	15.830	15.830	0.0	-0.184	-0.151	
3	12	3	3.609	0.665	0.665	0.0	2.944	0.776	
7	12	3	6.786	3.177	3.177	0.0	3.609	1.243	
8	11	3	8.321	8.422	8.422	0.0	-0.100	-0.037	
6	11	3	11.692	15.320	-15.320	0.0	-3.627	-1.803	
4	11	3	8.471	10.875	-10.875	0.0	-2.403	-1.036	
2	11	3	10.836	9.472	-9.472	0.0	1.365	0.899	
0	11	3	10.748	7.681	7.681	0.0	3.068	1.738	
-2	11	3	32.527	32.492	-32.492	0.0	0.035	0.039	
-4	11	3	10.475	5.973	5.973	0.0	4.501	2.406	
-8	11	3	5.462	1.524	-1.524	0.0	3.938	1.290	
0	12	0	201.074	196.774	196.774	0.0	4.301	1.429	*
-10	11	3	7.730	5.162	-5.162	0.0	2.568	1.032	
-12	11	3	8.569	4.143	4.143	0.0	4.426	1.655	
-11	10	3	8.304	4.337	4.337	0.0	3.967	1.503	
-9	10	3	13.334	13.315	-13.315	0.0	0.019	0.012	
-7	10	3	30.497	29.952	29.952	0.0	0.545	0.618	
-5	10	3	53.467	51.631	-51.631	0.0	1.836	1.909	
-3	10	3	48.985	49.609	49.609	0.0	-0.624	-0.674	
-1	10	3	10.554	8.009	-8.009	0.0	2.545	1.400	
1	10	3	22.802	24.999	-24.999	0.0	-2.197	-2.092	
3	10	3	16.590	19.981	19.981	0.0	-3.391	-2.725	
5	10	3	4.068	5.662	-5.662	0.0	-1.593	-0.432	
7	10	3	11.181	5.658	5.658	0.0	5.522	3.113	
9	10	3	14.931	17.132	-17.132	0.0	-2.201	-1.080	
8	9	3	5.859	1.951	1.951	0.0	3.908	1.191	
6	9	3	11.445	10.775	-10.775	0.0	0.670	0.384	
4	9	3	25.291	26.209	26.209	0.0	-0.918	-1.010	
2	9	3	20.287	22.515	-22.515	0.0	-2.227	-1.842	
0	9	3	55.585	58.594	58.594	0.0	-3.009	-3.099	
-2	9	3	47.432	48.998	-48.998	0.0	-1.567	-1.740	
-4	9	3	37.707	39.063	39.063	0.0	-1.356	-1.552	
0	12	0	200.218	196.774	196.774	0.0	3.445	1.148	*
-6	9	3	15.752	17.894	17.894	0.0	-2.142	-1.527	
-8	9	3	31.124	30.134	-30.134	0.0	0.990	1.089	
-10	9	3	19.537	18.070	18.070	0.0	1.468	1.171	
-12	9	3	11.772	16.346	-16.346	0.0	-4.574	-1.892	
-13	8	3	10.907	10.748	10.748	0.0	0.159	0.067	
-11	8	3	4.218	3.555	-3.555	0.0	0.663	0.166	
-9	8	3	10.386	12.705	-12.705	0.0	-2.319	-1.090	
-5	8	3	12.663	11.287	-11.287	0.0	1.376	0.804	
-1	8	3	8.807	12.206	-12.206	0.0	-3.399	-1.689	
1	8	3	7.210	2.940	-2.940	0.0	4.270	1.633	
5	8	3	19.952	22.123	-22.123	0.0	-2.171	-1.822	
7	8	3	7.501	0.558	-0.558	0.0	6.943	2.770	
6	7	3	33.886	35.117	35.117	0.0	-1.231	-1.328	
4	7	3	61.798	64.129	-64.129	0.0	-2.331	-2.220	
2	7	3	23.958	26.157	26.157	0.0	-2.198	-2.224	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	12	0	200.642	196.774	196.774	0.0	3.868	1.285	*
0	7	3	36.577	36.982	-36.982	0.0	-0.405	-0.504	
-2	7	3	90.654	91.120	91.120	0.0	-0.466	-0.332	
-4	7	3	28.812	29.390	-29.390	0.0	-0.578	-0.675	
-6	7	3	11.410	11.597	-11.597	0.0	-0.187	-0.106	
-8	7	3	22.088	20.313	20.313	0.0	1.775	1.812	
-10	7	3	3.812	2.114	-2.114	0.0	1.698	0.444	
-12	7	3	34.795	36.014	36.014	0.0	-1.219	-1.132	
-13	6	3	16.661	12.846	12.846	0.0	3.815	2.484	
-11	6	3	13.819	12.155	12.155	0.0	1.664	1.009	
-9	6	3	116.659	118.792	118.792	0.0	-2.133	-1.185	
-7	6	3	77.691	80.293	-80.293	0.0	-2.602	-2.034	
-5	6	3	101.164	100.446	100.446	0.0	0.718	0.460	
-3	6	3	36.657	37.192	37.192	0.0	-0.536	-0.667	
-1	6	3	178.545	183.876	183.876	0.0	-5.330	-1.987	
1	6	3	25.044	27.230	27.230	0.0	-2.187	-2.478	
3	6	3	13.387	18.246	-18.246	0.0	-4.860	-3.059	
5	6	3	100.731	100.989	100.989	0.0	-0.257	-0.164	
9	6	3	65.901	60.166	60.166	0.0	5.735	4.744	
10	5	3	4.315	5.141	5.141	0.0	-0.826	-0.185	
0	12	0	200.801	196.774	196.774	0.0	4.027	1.338	*
8	5	3	31.053	28.792	28.792	0.0	2.261	2.228	
6	5	3	80.461	76.604	76.604	0.0	3.858	2.934	
4	5	3	30.365	29.002	-29.002	0.0	1.363	1.529	
2	5	3	91.766	95.291	95.291	0.0	-3.526	-2.466	
0	5	3	17.799	18.010	18.010	0.0	-0.211	-0.206	
-2	5	3	183.081	187.673	187.673	0.0	-4.592	-1.673	
-4	5	3	23.570	24.027	24.027	0.0	-0.457	-0.518	
-6	5	3	31.353	30.050	30.050	0.0	1.303	1.539	
-8	5	3	49.488	50.534	50.534	0.0	-1.047	-1.108	
-10	5	3	15.284	15.488	15.488	0.0	-0.204	-0.139	
-12	5	3	58.806	59.829	59.829	0.0	-1.023	-0.920	
-13	4	3	16.263	17.226	17.226	0.0	-0.962	-0.565	
-11	4	3	7.801	0.802	0.802	0.0	6.998	2.744	
-9	4	3	7.113	11.838	11.838	0.0	-4.726	-1.722	
-7	4	3	6.389	2.337	-2.337	0.0	4.052	1.422	
-5	4	3	8.948	10.539	10.539	0.0	-1.591	-0.842	
-3	4	3	7.483	7.885	7.885	0.0	-0.402	-0.206	
-1	4	3	11.119	11.263	11.263	0.0	-0.144	-0.098	
1	4	3	11.631	10.742	10.742	0.0	0.888	0.592	
0	12	0	200.395	196.774	196.774	0.0	3.621	1.207	*
5	4	3	5.904	7.215	-7.215	0.0	-1.311	-0.472	
7	4	3	7.642	4.051	4.051	0.0	3.591	1.524	
9	4	3	10.713	10.913	10.913	0.0	-0.200	-0.083	
10	3	3	8.860	7.971	7.971	0.0	0.889	0.324	
8	3	3	10.510	8.967	-8.967	0.0	1.543	0.763	
6	3	3	35.060	35.200	-35.200	0.0	-0.141	-0.150	
4	3	3	7.227	6.152	6.152	0.0	1.075	0.414	
2	3	3	58.674	58.065	-58.065	0.0	0.609	0.622	
0	3	3	33.092	32.874	32.874	0.0	0.218	0.287	
-2	3	3	94.307	93.579	-93.579	0.0	0.728	0.503	
-4	3	3	17.587	15.534	15.534	0.0	2.053	2.115	
-6	3	3	12.460	11.866	11.866	0.0	0.594	0.398	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-8	3	3	43.425	43.875	-43.875	0.0	-0.450	-0.505	
-10	3	3	12.958	13.099	13.099	0.0	-0.101	-0.062	
-12	3	3	19.184	20.181	-20.181	0.0	-0.997	-0.668	
-13	2	3	8.260	5.713	-5.713	0.0	2.547	0.946	
-11	2	3	9.839	9.326	9.326	0.0	0.514	0.238	
-9	2	3	27.938	28.219	-28.219	0.0	-0.281	-0.292	
-7	2	3	44.096	44.046	44.046	0.0	0.050	0.056	
-5	2	3	66.854	65.554	-65.554	0.0	1.301	1.198	
0	12	0	200.704	196.774	196.774	0.0	3.930	1.306	*
-3	2	3	86.259	85.224	85.224	0.0	1.035	0.777	
-1	2	3	6.477	6.138	-6.138	0.0	0.339	0.178	
1	2	3	10.828	9.962	-9.962	0.0	0.865	0.602	
3	2	3	44.493	44.387	44.387	0.0	0.106	0.121	
5	2	3	11.295	6.803	-6.803	0.0	4.492	3.012	
7	2	3	23.200	21.754	21.754	0.0	1.445	1.332	
9	2	3	22.485	22.078	-22.078	0.0	0.407	0.297	
10	1	3	8.127	6.947	-6.947	0.0	1.180	0.418	
8	1	3	15.310	11.928	11.928	0.0	3.383	2.356	
6	1	3	0.962	10.174	-10.174	0.0	-9.212	-1.570	
2	1	3	21.699	20.760	-20.760	0.0	0.939	1.023	
0	1	3	35.421	36.821	36.821	0.0	-1.400	-1.911	
-2	1	3	22.379	22.270	-22.270	0.0	0.109	0.137	
-4	1	3	26.076	24.722	24.722	0.0	1.354	1.724	
-12	1	3	7.889	4.346	-4.346	0.0	3.543	1.394	
-13	0	3	12.372	8.460	-8.460	0.0	3.912	2.015	
0	12	0	201.268	196.774	196.774	0.0	4.495	1.489	*
-11	0	3	7.757	10.767	10.767	0.0	-3.010	-1.111	
-9	0	3	11.869	12.164	-12.164	0.0	-0.295	-0.183	
-7	0	3	5.356	6.509	6.509	0.0	-1.153	-0.365	
-5	0	3	7.130	6.840	-6.840	0.0	0.290	0.124	
-3	0	3	23.438	24.836	-24.836	0.0	-1.399	-1.781	
1	0	3	7.413	0.601	0.601	0.0	6.811	3.590	
3	0	3	16.246	16.481	-16.481	0.0	-0.236	-0.188	
5	0	3	9.001	7.832	-7.832	0.0	1.169	0.589	
7	0	3	10.351	7.659	-7.659	0.0	2.692	1.387	
-12	0	4	6.971	2.290	-2.290	0.0	4.681	1.574	
-10	0	4	35.077	36.580	36.580	0.0	-1.503	-1.534	
-8	0	4	21.020	23.914	-23.914	0.0	-2.895	-2.504	
-6	0	4	132.376	136.922	136.922	0.0	-4.546	-2.260	
-4	0	4	129.640	128.738	128.738	0.0	0.902	0.458	
-2	0	4	81.123	81.372	-81.372	0.0	-0.249	-0.195	
0	0	4	155.602	153.201	153.201	0.0	2.401	1.023	
2	0	4	6.468	3.127	3.127	0.0	3.342	1.221	
4	0	4	118.274	112.363	112.363	0.0	5.911	3.236	
0	12	0	201.515	196.774	196.774	0.0	4.742	1.571	*
6	0	4	8.692	8.842	8.842	0.0	-0.150	-0.061	
8	0	4	27.294	23.839	23.839	0.0	3.455	2.837	
9	1	4	22.167	18.548	-18.548	0.0	3.620	2.486	
7	1	4	20.623	17.335	17.335	0.0	3.288	2.605	
5	1	4	6.768	5.239	5.239	0.0	1.529	0.570	
3	1	4	73.808	72.724	72.724	0.0	1.084	0.897	
1	1	4	8.895	2.673	-2.673	0.0	6.222	2.902	
-1	1	4	45.402	42.892	-42.892	0.0	2.510	2.903	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-3	1	4	122.378	124.432	124.432	0.0	-2.054	-1.103	
-5	1	4	12.654	13.762	-13.762	0.0	-1.108	-0.675	
-7	1	4	77.099	77.669	77.669	0.0	-0.569	-0.461	
-9	1	4	19.193	18.323	-18.323	0.0	0.871	0.759	
-11	1	4	21.585	25.944	25.944	0.0	-4.359	-3.207	
-13	1	4	8.833	7.328	7.328	0.0	1.505	0.572	
-10	2	4	4.280	4.987	-4.987	0.0	-0.707	-0.187	
-8	2	4	4.006	9.535	9.535	0.0	-5.529	-1.464	
-6	2	4	6.989	7.480	-7.480	0.0	-0.491	-0.184	
-4	2	4	7.942	7.164	-7.164	0.0	0.778	0.350	
-2	2	4	9.910	10.297	-10.297	0.0	-0.387	-0.205	
0	12	0	200.942	196.774	196.774	0.0	4.168	1.385	*
0	2	4	18.037	17.708	-17.708	0.0	0.329	0.261	
2	2	4	14.746	16.652	-16.652	0.0	-1.906	-1.301	
8	2	4	6.124	1.378	-1.378	0.0	4.746	1.442	
7	3	4	15.866	12.558	-12.558	0.0	3.309	2.118	
5	3	4	19.361	19.002	19.002	0.0	0.359	0.264	
3	3	4	36.913	38.011	-38.011	0.0	-1.098	-1.257	
1	3	4	14.622	7.267	7.267	0.0	7.355	5.448	
-1	3	4	40.275	41.881	41.881	0.0	-1.606	-1.802	
-3	3	4	69.457	70.993	-70.993	0.0	-1.536	-1.360	
-5	3	4	41.122	40.259	40.259	0.0	0.863	0.987	
-7	3	4	21.558	22.548	-22.548	0.0	-0.990	-0.943	
-9	3	4	17.278	17.668	17.668	0.0	-0.390	-0.285	
-11	3	4	14.234	15.010	-15.010	0.0	-0.776	-0.442	
-12	4	4	10.439	10.888	10.888	0.0	-0.449	-0.187	
-8	4	4	17.040	19.167	19.167	0.0	-2.127	-1.535	
-6	4	4	15.425	15.277	-15.277	0.0	0.148	0.113	
0	12	0	201.004	196.774	196.774	0.0	4.230	1.406	*
-4	4	4	9.680	4.336	4.336	0.0	5.345	2.753	
-2	4	4	44.828	44.308	44.308	0.0	0.520	0.601	
0	4	4	51.014	52.512	-52.512	0.0	-1.498	-1.571	
2	4	4	62.548	61.242	61.242	0.0	1.306	1.223	
4	4	4	13.448	11.966	-11.966	0.0	1.483	0.960	
6	4	4	11.092	7.627	7.627	0.0	3.466	1.785	
8	4	4	6.715	3.758	3.758	0.0	2.957	0.873	
5	5	4	6.318	3.341	-3.341	0.0	2.977	1.045	
3	5	4	21.885	20.917	-20.917	0.0	0.967	0.906	
-1	5	4	6.927	8.358	8.358	0.0	-1.431	-0.525	
-3	5	4	31.997	33.284	-33.284	0.0	-1.286	-1.401	
-5	5	4	14.878	14.105	14.105	0.0	0.773	0.534	
-11	5	4	9.142	9.329	-9.329	0.0	-0.187	-0.073	
-13	5	4	14.172	15.123	15.123	0.0	-0.951	-0.453	
-10	6	4	10.836	15.607	15.607	0.0	-4.771	-2.071	
0	12	0	201.136	196.774	196.774	0.0	4.362	1.450	*
-8	6	4	5.118	9.129	-9.129	0.0	-4.011	-1.128	
-6	6	4	6.557	3.564	3.564	0.0	2.993	1.233	
-4	6	4	7.757	3.596	-3.596	0.0	4.161	1.786	
-2	6	4	6.001	5.891	5.891	0.0	0.110	0.038	
0	6	4	12.195	8.798	-8.798	0.0	3.398	2.016	
2	6	4	8.789	8.076	-8.076	0.0	0.714	0.358	
4	6	4	6.654	1.188	-1.188	0.0	5.466	2.051	
6	6	4	9.989	10.764	10.764	0.0	-0.775	-0.343	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
8	6	4	12.831	11.774	-11.774	0.0	1.057	0.532	
7	7	4	14.349	13.909	-13.909	0.0	0.440	0.246	
5	7	4	15.752	14.338	14.338	0.0	1.414	0.943	
3	7	4	22.061	21.984	21.984	0.0	0.078	0.073	
1	7	4	17.772	15.450	-15.450	0.0	2.322	2.088	
-1	7	4	14.799	15.855	15.855	0.0	-1.057	-0.735	
-3	7	4	15.496	15.751	15.751	0.0	-0.255	-0.186	
-5	7	4	13.996	14.272	14.272	0.0	-0.276	-0.180	
-7	7	4	24.717	23.662	-23.662	0.0	1.055	1.107	
-9	7	4	30.647	33.127	33.127	0.0	-2.479	-2.381	
-11	7	4	15.363	14.783	-14.783	0.0	0.580	0.344	
-12	8	4	28.688	30.937	30.937	0.0	-2.249	-1.807	
0	12	0	201.092	196.774	196.774	0.0	4.318	1.435	*
-10	8	4	37.539	38.386	-38.386	0.0	-0.847	-0.842	
-8	8	4	7.395	2.884	2.884	0.0	4.511	1.787	
-6	8	4	25.609	25.527	25.527	0.0	0.081	0.082	
-4	8	4	36.913	37.748	-37.748	0.0	-0.835	-0.956	
-2	8	4	2.850	6.905	-6.905	0.0	-4.054	-0.955	
0	8	4	16.519	15.351	-15.351	0.0	1.168	0.988	
2	8	4	42.190	43.512	43.512	0.0	-1.322	-1.441	
4	8	4	57.350	58.565	-58.565	0.0	-1.215	-1.157	
6	8	4	21.788	21.524	21.524	0.0	0.263	0.197	
7	9	4	29.200	29.225	-29.225	0.0	-0.025	-0.021	
5	9	4	9.019	12.516	12.516	0.0	-3.497	-1.295	
3	9	4	17.578	16.063	-16.063	0.0	1.515	1.201	
1	9	4	32.968	35.434	-35.434	0.0	-2.465	-2.686	
-1	9	4	11.737	11.786	11.786	0.0	-0.049	-0.030	
-3	9	4	21.946	22.041	-22.041	0.0	-0.094	-0.091	
-5	9	4	9.760	9.807	9.807	0.0	-0.047	-0.023	
-7	9	4	41.140	40.558	-40.558	0.0	0.582	0.640	
-9	9	4	38.166	38.080	38.080	0.0	0.085	0.089	
-11	9	4	10.713	9.448	-9.448	0.0	1.264	0.537	
0	12	0	201.048	196.774	196.774	0.0	4.274	1.420	*
-10	10	4	12.831	11.054	11.054	0.0	1.777	0.973	
-8	10	4	21.540	22.785	22.785	0.0	-1.245	-0.993	
-6	10	4	23.500	23.096	23.096	0.0	0.404	0.372	
-4	10	4	31.962	32.179	32.179	0.0	-0.217	-0.243	
-2	10	4	14.966	14.878	14.878	0.0	0.088	0.065	
0	10	4	27.126	30.443	30.443	0.0	-3.317	-3.356	
2	10	4	10.016	9.165	9.165	0.0	0.851	0.421	
4	10	4	24.003	26.493	26.493	0.0	-2.490	-2.060	
6	10	4	13.025	13.341	13.341	0.0	-0.316	-0.161	
7	11	4	40.875	39.467	39.467	0.0	1.408	1.375	
5	11	4	15.416	12.953	12.953	0.0	2.463	1.604	
3	11	4	52.232	57.543	57.543	0.0	-5.311	-5.233	
1	11	4	45.358	47.496	47.496	0.0	-2.139	-2.203	
-1	11	4	4.465	3.660	-3.660	0.0	0.805	0.230	
-3	11	4	84.838	83.103	83.103	0.0	1.735	1.285	
-5	11	4	12.645	13.032	13.032	0.0	-0.386	-0.224	
-7	11	4	98.013	97.146	97.146	0.0	0.867	0.558	
-9	11	4	29.059	31.292	-31.292	0.0	-2.233	-1.977	
-11	11	4	28.044	28.073	28.073	0.0	-0.029	-0.024	
-10	12	4	36.886	37.138	37.138	0.0	-0.252	-0.230	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	12	0	201.163	196.774	196.774	0.0	4.389	1.458	*
-8	12	4	19.546	20.591	-20.591	0.0	-1.045	-0.745	
-6	12	4	34.839	32.294	32.294	0.0	2.545	2.856	
-4	12	4	81.573	80.692	80.692	0.0	0.881	0.666	
-2	12	4	47.476	48.767	-48.767	0.0	-1.291	-1.355	
0	12	4	39.269	39.881	39.881	0.0	-0.612	-0.654	
2	12	4	22.555	25.627	-25.627	0.0	-3.072	-2.578	
4	12	4	72.969	81.149	81.149	0.0	-8.180	-6.574	
6	12	4	24.841	25.447	-25.447	0.0	-0.606	-0.464	
5	13	4	14.181	9.563	-9.563	0.0	4.618	2.769	
3	13	4	4.527	4.684	4.684	0.0	-0.157	-0.040	
1	13	4	6.795	0.981	-0.981	0.0	5.813	2.211	
-1	13	4	32.633	33.530	-33.530	0.0	-0.897	-0.977	
-3	13	4	22.326	19.264	19.264	0.0	3.061	3.017	
-5	13	4	18.214	16.092	-16.092	0.0	2.122	1.636	
-7	13	4	40.663	40.551	40.551	0.0	0.112	0.112	
-9	13	4	37.795	36.299	-36.299	0.0	1.497	1.462	
-10	14	4	5.718	4.774	-4.774	0.0	0.944	0.261	
-8	14	4	7.898	9.370	9.370	0.0	-1.472	-0.515	
-6	14	4	7.218	5.413	-5.413	0.0	1.805	0.633	
-4	14	4	4.227	1.091	-1.091	0.0	3.136	0.840	
0	12	0	200.915	196.774	196.774	0.0	4.142	1.376	*
-2	14	4	12.019	11.400	11.400	0.0	0.619	0.349	
0	14	4	11.189	8.045	-8.045	0.0	3.145	1.722	
2	14	4	8.701	4.593	4.593	0.0	4.108	1.833	
4	14	4	7.015	0.210	0.210	0.0	6.806	2.337	
6	14	4	1.474	6.391	6.391	0.0	-4.917	-0.743	
5	15	4	15.381	16.368	16.368	0.0	-0.987	-0.533	
3	15	4	7.642	2.902	-2.902	0.0	4.740	1.796	
1	15	4	10.651	6.060	-6.060	0.0	4.591	2.323	
-1	15	4	21.699	20.408	20.408	0.0	1.291	1.109	
-3	15	4	17.322	15.953	-15.953	0.0	1.369	1.014	
-5	15	4	19.961	17.950	17.950	0.0	2.011	1.605	
-7	15	4	22.326	21.198	-21.198	0.0	1.128	0.887	
-9	15	4	24.497	25.384	25.384	0.0	-0.887	-0.703	
-8	16	4	8.004	0.652	-0.652	0.0	7.352	2.636	
-6	16	4	17.622	15.714	15.714	0.0	1.909	1.327	
-4	16	4	15.152	15.938	-15.938	0.0	-0.786	-0.457	
-2	16	4	7.307	7.673	-7.673	0.0	-0.366	-0.131	
0	16	4	7.413	6.675	-6.675	0.0	0.738	0.257	
2	16	4	17.967	17.575	17.575	0.0	0.392	0.269	
4	16	4	30.727	32.412	-32.412	0.0	-1.685	-1.469	
0	12	0	201.789	196.774	196.774	0.0	5.015	1.657	*
3	17	4	8.321	7.275	7.275	0.0	1.046	0.373	
1	17	4	12.063	14.149	-14.149	0.0	-2.086	-1.037	
-3	17	4	9.230	13.462	13.462	0.0	-4.232	-1.648	
-7	17	4	7.677	8.168	-8.168	0.0	-0.490	-0.157	
-6	18	4	6.001	7.961	7.961	0.0	-1.961	-0.534	
-4	18	4	7.518	0.787	-0.787	0.0	6.732	2.399	
-2	18	4	9.169	8.068	8.068	0.0	1.100	0.447	
1	19	4	9.407	5.592	-5.592	0.0	3.815	1.538	
-3	19	4	21.099	21.400	-21.400	0.0	-0.301	-0.220	
-5	19	4	12.090	12.012	12.012	0.0	0.077	0.036	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-4	20	4	12.407	10.228	-10.228	0.0	2.179	0.961	
-2	20	4	13.166	12.815	12.815	0.0	0.351	0.176	
0	20	4	31.521	31.487	-31.487	0.0	0.034	0.029	
-3	18	5	40.796	40.485	-40.485	0.0	0.311	0.289	
-1	18	5	32.924	33.583	33.583	0.0	-0.659	-0.549	
0	12	0	200.951	196.774	196.774	0.0	4.177	1.388	*
-2	17	5	45.314	43.436	43.436	0.0	1.878	1.851	
-4	17	5	10.483	8.245	-8.245	0.0	2.239	0.933	
-6	17	5	9.045	7.663	7.663	0.0	1.382	0.504	
-7	16	5	13.263	7.059	7.059	0.0	6.204	3.316	
-5	16	5	18.858	23.572	23.572	0.0	-4.714	-2.671	
-3	16	5	13.793	13.281	13.281	0.0	0.511	0.276	
-1	16	5	25.670	25.835	25.835	0.0	-0.165	-0.129	
1	16	5	18.381	19.510	19.510	0.0	-1.129	-0.703	
2	15	5	11.031	10.539	-10.539	0.0	0.492	0.206	
0	15	5	21.038	18.411	18.411	0.0	2.626	2.205	
-2	15	5	19.784	18.629	-18.629	0.0	1.156	0.813	
-4	15	5	17.834	14.617	14.617	0.0	3.217	2.322	
-6	15	5	13.837	14.434	14.434	0.0	-0.597	-0.300	
-8	15	5	20.517	18.870	-18.870	0.0	1.647	1.098	
-7	14	5	25.264	22.190	22.190	0.0	3.075	2.765	
-5	14	5	48.879	48.770	-48.770	0.0	0.109	0.105	
-3	14	5	28.318	27.171	27.171	0.0	1.147	1.121	
-1	14	5	15.937	16.852	-16.852	0.0	-0.915	-0.549	
1	14	5	13.263	15.389	-15.389	0.0	-2.125	-1.016	
0	12	0	200.527	196.774	196.774	0.0	3.753	1.251	*
3	14	5	3.468	3.116	-3.116	0.0	0.352	0.073	
4	13	5	8.357	8.064	8.064	0.0	0.293	0.101	
2	13	5	4.845	7.565	-7.565	0.0	-2.720	-0.664	
0	13	5	17.878	18.293	18.293	0.0	-0.415	-0.283	
-2	13	5	12.495	16.039	-16.039	0.0	-3.543	-1.701	
-4	13	5	9.989	11.269	11.269	0.0	-1.280	-0.551	
-6	13	5	7.783	0.336	-0.336	0.0	7.447	2.813	
-8	13	5	9.654	9.514	-9.514	0.0	0.140	0.054	
-9	12	5	9.319	9.978	-9.978	0.0	-0.660	-0.236	
-7	12	5	10.889	7.973	7.973	0.0	2.917	1.360	
-3	12	5	7.192	0.770	0.770	0.0	6.422	2.434	
-1	12	5	5.242	0.782	-0.782	0.0	4.460	1.283	
1	12	5	11.225	9.793	9.793	0.0	1.432	0.670	
4	11	5	3.989	1.431	1.431	0.0	2.558	0.582	
2	11	5	10.607	9.429	-9.429	0.0	1.178	0.536	
-2	11	5	9.001	8.638	-8.638	0.0	0.363	0.154	
0	12	0	200.448	196.774	196.774	0.0	3.674	1.225	*
-6	11	5	7.704	4.700	-4.700	0.0	3.003	1.101	
-9	10	5	17.649	15.952	-15.952	0.0	1.697	1.105	
-7	10	5	20.173	19.451	19.451	0.0	0.722	0.531	
-5	10	5	24.894	26.689	-26.689	0.0	-1.796	-1.565	
-3	10	5	24.832	25.144	25.144	0.0	-0.312	-0.297	
-1	10	5	10.113	12.603	-12.603	0.0	-2.490	-1.098	
1	10	5	6.257	0.134	-0.134	0.0	6.122	2.053	
3	10	5	2.656	1.212	1.212	0.0	1.444	0.283	
5	10	5	3.194	4.973	-4.973	0.0	-1.779	-0.354	
4	9	5	29.571	27.615	27.615	0.0	1.956	1.831	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
2	9	5	22.935	24.332	-24.332	0.0	-1.397	-1.190	
0	9	5	26.844	27.375	27.375	0.0	-0.531	-0.510	
-2	9	5	12.416	13.508	-13.508	0.0	-1.092	-0.592	
-4	9	5	14.172	16.993	16.993	0.0	-2.821	-1.700	
-8	9	5	19.934	22.487	-22.487	0.0	-2.552	-1.830	
-10	9	5	22.344	22.383	22.383	0.0	-0.040	-0.030	
0	12	0	200.545	196.774	196.774	0.0	3.771	1.257	*
-9	8	5	3.618	0.947	-0.947	0.0	2.671	0.594	
-5	8	5	8.207	9.203	-9.203	0.0	-0.996	-0.411	
-3	8	5	5.259	0.230	0.230	0.0	5.029	1.553	
-1	8	5	9.416	10.493	-10.493	0.0	-1.077	-0.462	
3	8	5	5.339	3.844	3.844	0.0	1.494	0.434	
5	8	5	14.040	9.356	-9.356	0.0	4.683	2.708	
6	7	5	3.971	7.644	7.644	0.0	-3.673	-0.760	
4	7	5	43.249	41.386	-41.386	0.0	1.863	1.820	
2	7	5	46.143	46.606	46.606	0.0	-0.463	-0.452	
0	7	5	10.157	13.888	-13.888	0.0	-3.731	-1.639	
-2	7	5	24.038	23.328	23.328	0.0	0.710	0.694	
-4	7	5	22.052	22.938	-22.938	0.0	-0.885	-0.803	
-6	7	5	3.247	5.980	5.980	0.0	-2.732	-0.621	
-8	7	5	32.739	32.618	32.618	0.0	0.121	0.124	
-10	7	5	12.231	10.064	-10.064	0.0	2.167	1.077	
-11	6	5	7.315	11.242	-11.242	0.0	-3.927	-1.144	
-9	6	5	91.086	94.050	94.050	0.0	-2.964	-2.011	
-7	6	5	15.990	15.802	-15.802	0.0	0.188	0.129	
0	12	0	199.998	196.774	196.774	0.0	3.224	1.075	*
-5	6	5	63.483	63.992	63.992	0.0	-0.509	-0.461	
-3	6	5	42.578	42.903	-42.903	0.0	-0.325	-0.361	
-1	6	5	110.191	109.582	109.582	0.0	0.609	0.358	
1	6	5	31.803	31.278	31.278	0.0	0.526	0.552	
3	6	5	9.045	4.449	4.449	0.0	4.597	1.996	
5	6	5	39.940	35.939	35.939	0.0	4.000	4.047	
6	5	5	33.974	31.551	31.551	0.0	2.423	2.129	
4	5	5	29.333	26.755	-26.755	0.0	2.577	2.434	
2	5	5	88.245	85.270	85.270	0.0	2.975	2.094	
0	5	5	19.387	16.105	16.105	0.0	3.283	3.049	
-2	5	5	69.687	70.217	70.217	0.0	-0.530	-0.458	
-6	5	5	25.335	26.262	26.262	0.0	-0.927	-0.921	
-8	5	5	59.115	60.540	60.540	0.0	-1.425	-1.324	
-12	5	5	34.177	36.514	36.514	0.0	-2.337	-1.906	
-9	4	5	13.749	13.177	13.177	0.0	0.571	0.334	
-5	4	5	4.139	8.268	8.268	0.0	-4.129	-1.112	
0	12	0	200.730	196.774	196.774	0.0	3.956	1.315	*
1	4	5	1.068	3.811	3.811	0.0	-2.743	-0.463	
3	4	5	10.616	9.446	9.446	0.0	1.169	0.564	
6	3	5	17.084	15.847	-15.847	0.0	1.237	0.697	
4	3	5	17.102	16.246	16.246	0.0	0.856	0.554	
2	3	5	41.722	40.413	-40.413	0.0	1.309	1.387	
0	3	5	15.778	16.953	16.953	0.0	-1.175	-0.832	
-2	3	5	34.998	34.841	-34.841	0.0	0.157	0.178	
-4	3	5	11.075	9.390	9.390	0.0	1.684	0.999	
-8	3	5	33.912	33.649	-33.649	0.0	0.264	0.272	
-10	3	5	23.826	25.168	25.168	0.0	-1.341	-1.056	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-12	3	5	13.078	17.352	-17.352	0.0	-4.274	-1.870	
-11	2	5	13.713	8.862	8.862	0.0	4.852	2.956	
-9	2	5	21.417	22.080	-22.080	0.0	-0.663	-0.537	
-7	2	5	30.921	31.000	31.000	0.0	-0.080	-0.082	
-5	2	5	45.014	47.206	-47.206	0.0	-2.193	-2.344	
-3	2	5	44.193	45.347	45.347	0.0	-1.154	-1.294	
0	12	0	201.163	196.774	196.774	0.0	4.389	1.454	*
-1	2	5	12.398	11.181	-11.181	0.0	1.217	0.758	
1	2	5	6.424	2.274	2.274	0.0	4.150	1.452	
3	2	5	3.812	9.305	9.305	0.0	-5.492	-1.240	
6	1	5	13.272	10.186	-10.186	0.0	3.086	1.649	
4	1	5	9.954	9.763	9.763	0.0	0.191	0.083	
2	1	5	12.001	6.790	-6.790	0.0	5.211	3.318	
0	1	5	16.881	16.132	16.132	0.0	0.750	0.555	
-2	1	5	13.678	11.353	-11.353	0.0	2.325	1.626	
-4	1	5	12.619	12.623	12.623	0.0	-0.004	-0.003	
-8	1	5	3.503	1.458	-1.458	0.0	2.045	0.509	
-12	1	5	5.586	2.489	-2.489	0.0	3.097	0.824	
-11	0	5	12.787	11.154	11.154	0.0	1.633	0.830	
-9	0	5	9.213	10.027	-10.027	0.0	-0.814	-0.344	
-7	0	5	5.904	4.600	4.600	0.0	1.304	0.440	
-5	0	5	7.289	3.182	3.182	0.0	4.107	1.797	
-3	0	5	13.501	12.366	-12.366	0.0	1.135	0.780	
-1	0	5	11.437	13.007	-13.007	0.0	-1.571	-0.873	
0	12	0	201.048	196.774	196.774	0.0	4.274	1.420	*
1	0	5	7.933	1.780	1.780	0.0	6.153	2.651	
3	0	5	8.339	8.190	-8.190	0.0	0.149	0.062	
7	0	5	7.545	8.460	-8.460	0.0	-0.915	-0.276	
-10	0	6	69.096	71.585	71.585	0.0	-2.489	-1.972	
-8	0	6	25.335	25.294	-25.294	0.0	0.041	0.037	
-6	0	6	14.110	15.581	15.581	0.0	-1.471	-0.882	
-4	0	6	83.471	81.740	81.740	0.0	1.731	1.274	
-2	0	6	21.020	20.367	20.367	0.0	0.653	0.529	
0	0	6	48.137	45.268	45.268	0.0	2.869	2.878	
2	0	6	30.727	29.715	-29.715	0.0	1.012	0.875	
4	0	6	82.906	73.638	73.638	0.0	9.268	6.564	
1	1	6	20.605	17.141	17.141	0.0	3.464	2.865	
-1	1	6	4.853	4.790	-4.790	0.0	0.064	0.017	
-3	1	6	59.503	58.879	58.879	0.0	0.625	0.580	
-5	1	6	15.319	12.272	-12.272	0.0	3.047	2.171	
-7	1	6	44.572	46.121	46.121	0.0	-1.549	-1.513	
-9	1	6	27.021	26.598	-26.598	0.0	0.422	0.344	
-10	2	6	1.950	3.579	-3.579	0.0	-1.628	-0.277	
0	12	0	201.383	196.774	196.774	0.0	4.609	1.527	*
-8	2	6	11.295	5.024	5.024	0.0	6.272	3.260	
-6	2	6	8.101	4.471	-4.471	0.0	3.630	1.496	
-4	2	6	8.321	1.651	-1.651	0.0	6.671	2.842	
-2	2	6	8.154	0.727	-0.727	0.0	7.426	2.815	
0	2	6	9.680	5.514	-5.514	0.0	4.166	1.896	
2	2	6	5.709	8.582	-8.582	0.0	-2.872	-0.743	
4	2	6	8.666	7.694	-7.694	0.0	0.971	0.327	
1	3	6	14.207	11.833	-11.833	0.0	2.374	1.325	
-1	3	6	18.390	16.115	16.115	0.0	2.275	1.663	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-3	3	6	22.441	22.600	-22.600	0.0	-0.159	-0.135	
-5	3	6	20.420	21.178	21.178	0.0	-0.758	-0.609	
-7	3	6	25.944	24.900	-24.900	0.0	1.044	0.970	
-9	3	6	16.934	19.990	19.990	0.0	-3.056	-1.698	
-10	4	6	27.100	27.172	-27.172	0.0	-0.072	-0.056	
-8	4	6	4.465	4.841	4.841	0.0	-0.376	-0.089	
-6	4	6	17.022	19.487	19.487	0.0	-2.465	-1.561	
-2	4	6	4.492	3.241	-3.241	0.0	1.250	0.326	
0	12	0	200.368	196.774	196.774	0.0	3.595	1.198	*
2	4	6	36.348	33.590	33.590	0.0	2.758	2.541	
4	4	6	27.541	24.458	-24.458	0.0	3.083	2.569	
3	5	6	6.971	3.604	3.604	0.0	3.368	1.046	
1	5	6	17.622	18.192	-18.192	0.0	-0.569	-0.347	
-7	5	6	13.210	12.268	-12.268	0.0	0.943	0.483	
-9	5	6	20.349	22.931	22.931	0.0	-2.581	-1.701	
-10	6	6	7.616	7.766	7.766	0.0	-0.151	-0.047	
-8	6	6	2.136	1.450	-1.450	0.0	0.686	0.121	
-6	6	6	2.418	4.741	4.741	0.0	-2.323	-0.447	
-4	6	6	9.875	7.746	-7.746	0.0	2.128	0.980	
-2	6	6	6.583	2.606	2.606	0.0	3.977	1.314	
2	6	6	3.680	6.677	-6.677	0.0	-2.997	-0.632	
1	7	6	3.865	5.273	5.273	0.0	-1.408	-0.313	
-1	7	6	15.760	16.105	16.105	0.0	-0.344	-0.212	
-3	7	6	14.631	17.683	-17.683	0.0	-3.052	-1.729	
0	12	0	200.907	196.774	196.774	0.0	4.133	1.373	*
-5	7	6	16.987	19.676	19.676	0.0	-2.689	-1.587	
-7	7	6	4.359	4.906	-4.906	0.0	-0.547	-0.126	
-8	8	6	15.037	15.213	15.213	0.0	-0.176	-0.093	
-6	8	6	16.758	18.373	-18.373	0.0	-1.615	-0.934	
-2	8	6	16.740	16.266	16.266	0.0	0.474	0.293	
0	8	6	39.463	39.098	-39.098	0.0	0.365	0.360	
2	8	6	28.265	26.573	26.573	0.0	1.692	1.410	
-1	9	6	12.593	12.672	12.672	0.0	-0.080	-0.039	
-3	9	6	41.343	41.195	-41.195	0.0	0.148	0.146	
-5	9	6	26.156	27.268	27.268	0.0	-1.112	-0.863	
-7	9	6	6.380	9.870	-9.870	0.0	-3.490	-0.942	
-8	10	6	9.354	11.951	11.951	0.0	-2.597	-0.881	
-6	10	6	6.495	8.742	8.742	0.0	-2.248	-0.656	
-4	10	6	18.302	18.922	18.922	0.0	-0.621	-0.393	
-2	10	6	17.217	13.475	13.475	0.0	3.741	2.465	
0	10	6	14.754	15.614	15.614	0.0	-0.859	-0.470	
0	12	0	201.039	196.774	196.774	0.0	4.265	1.417	*
1	11	6	11.551	11.253	11.253	0.0	0.298	0.121	
-3	11	6	77.514	77.810	77.810	0.0	-0.296	-0.225	
-5	11	6	13.096	14.642	-14.642	0.0	-1.547	-0.718	
-7	11	6	39.101	39.024	39.024	0.0	0.077	0.073	
-6	12	6	28.044	25.346	25.346	0.0	2.698	2.389	
-4	12	6	37.539	38.114	38.114	0.0	-0.574	-0.525	
-2	12	6	19.352	17.649	-17.649	0.0	1.703	1.163	
0	12	6	40.072	39.555	39.555	0.0	0.517	0.500	
-1	13	6	12.487	13.339	-13.339	0.0	-0.852	-0.394	
-3	13	6	35.933	39.001	39.001	0.0	-3.067	-2.431	
-5	13	6	28.997	28.522	-28.522	0.0	0.475	0.399	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-4	14	6	4.827	2.C76	-2.076	0.0	2.751	0.682	
-2	14	5	9.778	3.859	3.859	0.0	5.919	2.258	
-5	6	7	64.048	64.107	64.107	0.0	-0.059	-0.049	
-3	6	7	38.386	38.861	-38.861	0.0	-0.474	-0.413	
-2	5	7	25.397	24.148	24.148	0.0	1.249	0.996	
-4	5	7	9.213	8.622	8.622	0.0	0.590	0.217	
0	12	0	200.686	196.774	196.774	0.0	3.912	1.300	*
-6	5	7	20.049	18.982	18.982	0.0	1.067	0.738	
-5	4	7	9.689	7.482	7.482	0.0	2.207	0.881	
-3	4	7	7.527	1.442	1.442	0.0	6.085	2.022	
-2	3	7	16.731	13.128	-13.128	0.0	3.603	2.281	
-4	3	7	3.856	0.800	-0.800	0.0	3.056	0.663	
-6	3	7	7.280	2.226	2.226	0.0	5.054	1.613	
-7	2	7	20.270	19.959	19.959	0.0	0.311	0.2C6	
-5	2	7	30.744	31.358	-31.358	0.0	-0.614	-0.543	
-3	2	7	22.458	22.852	22.852	0.0	-0.394	-0.270	
0	1	7	7.342	5.711	5.711	0.0	1.631	0.490	
-2	1	7	4.659	4.747	-4.747	0.0	-0.088	-0.021	
-6	1	7	1.774	0.745	-0.745	0.0	1.029	0.173	
-1	0	7	12.4C7	7.670	-7.670	0.0	4.737	2.324	

NA RICHTERITE 900 C, JUNE, 1973

RESULTS OF STRUCTURE FACTOR CALCULATIONS

ALL REFLECTIONS	NUMERATOR	DENOMINATOR	NUMBER	R
WEIGHTED R	5452.46	1487452.00	1345	0.061
UNWEIGHTED R	3119.63	49604.55	1345	0.063
RANGES OF F(OBS)				
	1901.08	13311.34	933	0.143
	417.41	9716.75	223	0.043
	170.22	5176.40	66	0.033
	164.49	3466.00	31	0.047
	17.90	1278.50	9	0.014
	30.66	1235.32	7	0.025
	406.28	15167.17	75	0.027
	11.62	253.85	1	0.046
RANGES OF (SIN(THETA)/LAMBDA)**2				
	287.01	5050.06	87	0.057
	633.87	19671.79	190	0.032
	301.63	5179.81	147	0.058
	271.02	4597.29	155	0.059
	404.34	4259.43	184	0.095
	396.05	3470.29	181	0.114
	403.05	3745.69	199	0.108
	422.74	3632.12	202	0.116
UNREJECTED REFLECTIONS				
WEIGHTED R	4044.03	1005407.44	1158	0.063
UNWEIGHTED R	2376.02	30541.52	1158	0.078
RANGES OF F(OBS)				
	1762.01	12334.38	864	0.143
	374.12	8558.09	197	0.044
	144.00	4696.89	60	0.031
	47.44	2368.66	21	0.020
	16.84	1128.93	8	0.015
	30.66	1235.32	7	0.025
	0.99	219.80	1	0.004
	0.0	0.0	0	0.0
RANGES OF (SIN(THETA)/LAMBDA)**2				
	163.52	3714.16	68	0.044
	187.48	4027.79	102	0.047
	267.58	4771.32	134	0.056
	240.82	4017.69	140	0.060
	379.21	3978.86	172	0.095
	369.83	3182.25	166	0.116
	373.56	3472.53	185	0.108
	394.11	3378.74	191	0.117

SUM FCAL 48821.26

STANDARD DEV OF UNIT WEIGHT OBS 1.96

NA RICHTERITE 900 C, JUNE, 1973

ATOM		PARAMETER	OLD	CHANGE	NEW	ERROR	SHIFT/ERROR
		EXTINCTION CORRECTION	0.0		0.0		
		SCALE FACTOR 1	1.1332	0.0002	1.1334	0.00463	0.04
ATOM 1	O(1)	EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 1	1.00000		1.00000		
		X	0.1128876	-0.0000002	0.1128873	C.0003426	-0.00
		Y	0.9151734	-0.0000046	C.9151688	0.0001749	-0.03
		Z	0.8954085	0.0000137	C.8954221	C.0006527	0.02
		BETA11	0.0047224	-0.0000091	0.0047133	0.0003827	-0.02
		BETA22	0.0014432	0.0000034	0.0014466	0.C0C1C97	0.03
		BETA33	0.0160488	0.0000080	0.0160568	C.0013635	0.01
		BETA12	-0.0000391	0.0000022	-0.0000368	0.0001516	0.01
		BETA13	0.0041245	-0.0000055	0.0041190	C.0005908	-0.01
		BETA23	-0.0000708	-0.0000071	-C.C000779	0.0002778	-0.03
ATOM 2	O(2)	EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 1	1.C0000		1.00000		
		X	0.1195616	0.0000073	0.1195689	C.0003414	0.02
		Y	0.8320302	-0.0000002	0.8320301	0.C0C1940	-0.00
		Z	0.3918976	0.0000101	0.3919078	0.0006623	0.02
		BETA11	0.0044328	-0.0000056	C.0044272	0.0003742	-0.01
		BETA22	0.0018664	-0.0000033	0.0018632	C.0001174	-0.03
		BETA33	0.0163617	0.0000312	0.0163929	C.0013581	0.02
		BETA12	0.0001763	-0.0000017	0.0001746	0.0001635	-0.01
		BETA13	0.0022534	0.0000036	0.0022570	0.0005720	0.01
		BETA23	-0.0002650	-0.0000160	-0.0002811	0.0003034	-0.05
ATOM 3	F(3)	EQUIPOINT FRACTION = 0.500					
		OCCUPANCY SPECIES 2	1.C0000		1.00000		
		X	0.1029251	-0.0000242	0.1029009	C.0004885	-0.05
		Y	0.0		0.0		
		Z	0.3923900	-0.0000524	0.3923375	0.0009033	-0.06
		BETA11	0.0079301	0.0000018	0.0079319	0.0005655	0.00
		BETA22	0.0017917	0.0000114	C.0018030	0.0001419	0.08
		BETA33	0.0267304	-0.0000788	0.0266516	0.0020515	-0.04
		BETA12	0.0		0.0		
		BETA13	0.0039351	-0.0000003	0.0039349	0.0008648	-0.00
		BETA23	0.0		0.0		
ATOM 4	O(4)	EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 1	1.00000		1.00000		
		X	0.3625290	-0.0000201	0.3625089	0.0004292	-0.05
		Y	0.7533392	-0.0000099	0.7533293	C.0002017	-0.05
		Z	0.5650454	-0.0000236	0.5650218	C.0008159	-0.03
		BETA11	0.0088424	0.0000057	0.0088481	0.0005229	0.01
		BETA22	0.0014656	-0.0000011	0.0014645	0.0001094	-0.01
		BETA33	0.0264482	0.0000063	0.0264545	0.0018202	0.00
		BETA12	0.0012780	-0.0000030	0.0012750	0.0001828	-0.02
		BETA13	0.0062936	-0.0000048	0.0062888	0.0007959	-0.01
		BETA23	0.0000981	-0.0000055	0.0000927	C.0003183	-0.02
ATOM 5	O(5)	EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 1	1.C0000		1.00000		
		X	0.3461736	0.0000065	C.3461800	0.0003812	0.02
		Y	0.8724539	0.0000104	C.8724643	0.0002041	0.05
		Z	0.2623353	0.0000020	0.2623373	C.0007054	0.00
		BETA11	0.0057307	0.0000111	0.0057418	C.0004117	0.03

	BETA22	0.0023225	-0.0000080	0.0023145	0.0001222	-0.07
	BETA33	0.0182529	0.0000211	0.0182740	0.0014676	0.01
	BETA12	0.0001421	0.0000004	0.0001424	0.0001764	0.00
	BETA13	0.0034519	0.0000071	0.0034589	0.0006249	0.01
	BETA23	0.0025184	-0.0000020	0.0025164	0.0003329	-0.01
ATOM 6 O(6)	EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.3421390	0.0000138	0.3421528	0.0003934	0.04
	Y	0.8813721	-0.0000059	0.8813662	0.0002026	-0.03
	Z	0.7602293	0.0000122	0.7602414	0.0007056	0.02
	BETA11	0.0067164	-0.0000013	0.0067151	0.0004330	-0.00
	BETA22	0.0022424	-0.0000035	0.0022389	0.0001211	-0.03
	BETA33	0.0179389	0.0000165	0.0179555	0.0014765	0.01
	BETA12	0.0001262	-0.0000050	0.0001212	0.0001811	-0.03
	BETA13	0.0044693	-0.0000018	0.0044675	0.0006425	-0.00
	BETA23	-0.0022095	0.0000065	-0.0022030	0.0003374	0.02
ATOM 7 O(7)	EQUIPOINT FRACTION = 0.500					
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.3402463	0.0000054	0.3402517	0.0005616	0.01
	Y	0.0		0.0		
	Z	0.0417705	0.0000223	0.0417929	0.0011376	0.02
	BETA11	0.0066812	0.0000245	0.0067057	0.0006134	0.04
	BETA22	0.0009924	-0.0000106	0.0009818	0.0001403	-0.08
	BETA33	0.0345275	0.0000389	0.0345664	0.0026657	0.01
	BETA12	0.0		0.0		
	BETA13	0.0027050	0.0000118	0.0027168	0.0010219	0.01
	BETA23	0.0		0.0		
ATOM 8 T(1)	EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 3	1.00000		1.00000		
	X	0.2793974	-0.0000021	0.2793953	0.0001460	-0.01
	Y	0.9161841	0.0000020	0.9161860	0.0000621	0.03
	Z	0.9857123	0.0000060	0.9857183	0.0002737	0.02
	BETA11	0.0037970	0.0000011	0.0037981	0.0001380	0.01
	BETA22	0.0010822	0.0000023	0.0010845	0.0000373	0.06
	BETA33	0.0130745	0.0000051	0.0130795	0.0004921	0.01
	BETA12	0.0001054	0.0000018	0.0001072	0.0000589	0.03
	BETA13	0.0030022	0.0000013	0.0030035	0.0002101	0.01
	BETA23	-0.0001636	0.0000044	-0.0001592	0.0001051	0.04
ATOM 9 T(2)	EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 3	1.00000		1.00000		
	X	0.2870086	-0.0000039	0.2870046	0.0001453	-0.03
	Y	0.8298824	-0.0000022	0.8298802	0.0000655	-0.03
	Z	0.4874550	-0.0000126	0.4874424	0.0002710	-0.05
	BETA11	0.0041917	0.0000032	0.0041949	0.0001386	0.02
	BETA22	0.0012026	-0.0000001	0.0012025	0.0000372	-0.00
	BETA33	0.0126782	0.0000005	0.0126787	0.0004717	0.00
	BETA12	0.0002568	0.0000022	0.0002590	0.0000605	0.04
	BETA13	0.0031592	0.0000021	0.0031613	0.0002043	0.01
	BETA23	0.0000086	0.0000036	0.0000121	0.0001071	0.03
ATOM 10 M(1)	EQUIPOINT FRACTION = 0.500					
	OCCUPANCY SPECIES 4	1.00000		1.00000		
	X	0.0		0.0		
	Y	0.9104138	0.0000043	0.9104180	0.0001279	0.03
	Z	0.5000000		0.5000000		
	BETA11	0.0054529	0.0000004	0.0054532	0.0002780	0.00
	BETA22	0.0014555	0.0000039	0.0014594	0.0000736	0.05

		BETA33	0.0153300	-0.0000176	0.0153124	0.0009565	-0.02
		BETA12	0.0		0.0		
		BETA13	0.0035333	-0.0000044	0.0035289	0.0004178	-0.01
		BETA23	0.0		0.0		
ATOM 11	M(2)	EQUIPOINT FRACTION = 0.500					
		OCCUPANCY SPECIES 4	1.00000		1.00000		
		X	0.0		0.0		
		Y	0.8193905	0.0000047	0.8193952	0.0001305	0.04
		Z	0.0		0.0		
		BETA11	0.0055395	-0.0000016	0.0055379	0.0002775	-0.01
		BETA22	0.0015152	0.0000034	0.0015186	0.0000747	0.05
		BETA33	0.0175277	0.0000395	0.0175672	0.0009739	0.04
		BETA12	0.0		0.0		
		BETA13	0.0032839	0.0000064	0.0032903	0.0004142	0.02
		BETA23	0.0		0.0		
ATOM 12	M(3)	EQUIPOINT FRACTION = 0.250					
		OCCUPANCY SPECIES 4	1.00000		1.00000		
		X	0.0		0.0		
		Y	0.0		0.0		
		Z	0.0		0.0		
		BETA11	0.0055648	0.0000068	0.0055716	0.0003812	0.02
		BETA22	0.0013086	0.0000025	0.0013111	0.0000982	0.03
		BETA33	0.0178108	-0.0000193	0.0177915	0.0013644	-0.01
		BETA12	0.0		0.0		
		BETA13	0.0058588	0.0000058	0.0058646	0.0005888	0.01
		BETA23	0.0		0.0		
ATOM 13	M(4)	EQUIPOINT FRACTION = 0.500					
		OCCUPANCY SPECIES 5	0.50000		0.50000		
		OCCUPANCY SPECIES 6	0.50000		0.50000		
		TOTAL OCCUPANCY (FIXED) =	1.00000				
		X	0.0		0.0		
		Y	0.7234599	0.0000006	0.7234604	0.0001315	0.00
		Z	0.5000000		0.5000000		
		BETA11	0.0130135	-0.0000098	0.0130036	0.0003579	-0.03
		BETA22	0.0019238	-0.0000029	0.0019209	0.0000727	-0.04
		BETA33	0.0252596	0.0000189	0.0252784	0.0010114	0.02
		BETA12	0.0		0.0		
		BETA13	-0.0016909	-0.0000080	-0.0016989	0.0004669	-0.02
		BETA23	0.0		0.0		
ATOM 14	A	EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 6	0.25000		0.25000		
		X	0.4675266	-0.0004222	0.4671044	0.0028664	-0.15
		Y	0.9846402	0.0040829	0.9887230	0.0021748	1.88
		Z	0.5536271	-0.0010806	0.5525465	0.0047755	-0.23
		BETA11	0.0267081	-0.0013651	0.0253430	0.0051942	-0.26
		BETA22	0.0064071	0.0025469	0.0089540	0.0019378	1.31
		BETA33	0.0611226	0.0021842	0.0633068	0.0139337	0.16
		BETA12	-0.0014076	-0.0013687	-0.0027763	0.0017319	-0.79
		BETA13	-0.0130833	0.0000745	-0.0130088	0.0048035	0.02
		BETA23	-0.0002241	-0.0004797	-0.0007038	0.0025830	-0.19

MAXIMUM SHIFT/ERROR = 1.88

AVERAGE SHIFT/ERROR = 0.07

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
6	0	0	106.192	105.729	105.729	0.0	0.463	0.287	
8	0	0	105.158	110.846	110.846	0.0	-5.688	-3.533	
10	0	0	70.303	69.843	69.843	0.0	0.460	0.404	
12	0	0	21.168	20.518	-20.518	0.0	0.650	0.615	
13	1	0	29.487	28.984	-28.984	0.0	0.502	0.469	
11	1	0	60.179	60.429	60.429	0.0	-0.250	-0.242	
9	1	0	22.905	23.838	23.838	0.0	-0.933	-1.122	
7	1	0	76.608	78.354	78.354	0.0	-1.746	-1.467	
5	1	0	106.386	106.228	-106.228	0.0	0.158	0.099	
3	1	0	144.432	152.183	152.183	0.0	-7.751	-3.594	
-3	1	0	142.665	152.183	152.183	0.0	-9.518	-4.460	*
-5	1	0	105.608	106.228	-106.228	0.0	-0.620	-0.389	*
-7	1	0	75.649	78.354	78.354	0.0	-2.705	-2.286	*
-9	1	0	22.478	23.838	23.838	0.0	-1.360	-1.697	*
-11	1	0	59.872	60.429	60.429	0.0	-0.557	-0.539	*
-13	1	0	30.213	28.984	-28.984	0.0	1.229	1.216	*
-12	2	0	9.435	10.109	10.109	0.0	-0.675	-0.360	*
-8	2	0	14.174	12.897	-12.897	0.0	1.278	1.264	*
0	12	0	208.452	217.361	217.361	0.0	-8.908	-2.860	*
-6	2	0	32.856	34.660	-34.660	0.0	-1.804	-2.707	*
-4	2	0	11.726	12.149	-12.149	0.0	-0.423	-0.673	*
4	2	0	11.554	12.149	-12.149	0.0	-0.595	-0.903	
6	2	0	34.272	34.660	-34.660	0.0	-0.389	-0.590	
8	2	0	12.205	12.897	-12.897	0.0	-0.692	-0.563	
12	2	0	6.320	10.109	10.109	0.0	-3.790	-1.318	
13	3	0	17.177	14.191	14.191	0.0	2.986	2.203	
11	3	0	19.453	16.930	-16.930	0.0	2.523	2.675	
9	3	0	18.555	19.309	19.309	0.0	-0.754	-0.812	
7	3	0	51.995	52.788	-52.788	0.0	-0.793	-0.913	
5	3	0	61.497	61.570	61.570	0.0	-0.073	-0.076	
3	3	0	79.955	82.228	-82.228	0.0	-2.274	-1.874	
-3	3	0	79.356	82.228	-82.228	0.0	-2.873	-2.398	*
-5	3	0	59.827	61.570	61.570	0.0	-1.743	-1.862	*
-7	3	0	51.965	52.788	-52.788	0.0	-0.823	-0.947	*
-9	3	0	19.640	19.309	19.309	0.0	0.332	0.395	*
-11	3	0	17.649	16.930	-16.930	0.0	0.719	0.722	*
-13	3	0	16.496	14.191	14.191	0.0	2.305	1.729	*
-12	4	0	22.089	21.051	21.051	0.0	1.038	0.998	*
0	12	0	208.198	217.361	217.361	0.0	-9.163	-2.942	*
-10	4	0	4.890	3.948	-3.948	0.0	0.942	0.367	*
-8	4	0	10.513	8.784	8.784	0.0	1.728	1.261	*
-6	4	0	5.893	8.296	8.296	0.0	-2.403	-1.332	*
-4	4	0	11.614	10.236	10.236	0.0	1.377	2.043	*
-2	4	0	124.073	129.585	129.585	0.0	-5.513	-2.969	*
2	4	0	125.870	129.585	129.585	0.0	-3.716	-1.977	
4	4	0	11.808	10.236	10.236	0.0	1.572	2.307	
6	4	0	6.896	8.296	8.296	0.0	-1.400	-0.882	
8	4	0	6.844	8.784	8.784	0.0	-1.941	-0.960	
10	4	0	5.062	3.948	-3.948	0.0	1.114	0.422	
12	4	0	19.431	21.051	21.051	0.0	-1.620	-1.258	
11	5	0	18.734	18.241	-18.241	0.0	0.493	0.454	
7	5	0	7.480	7.280	-7.280	0.0	0.200	0.114	
5	5	0	4.291	8.637	-8.637	0.0	-4.346	-2.088	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
3	5	0	72.317	72.888	-72.888	0.0	-0.571	-0.519	
-3	5	0	71.830	72.888	-72.888	0.0	-1.058	-0.968	*
-5	5	0	8.888	8.637	-8.637	0.0	0.251	0.233	*
0	12	0	208.475	217.361	217.361	0.0	-8.886	-2.853	*
-7	5	0	9.135	7.280	-7.280	0.0	1.855	1.264	*
-9	5	0	1.116	1.218	1.218	0.0	-0.102	-0.024	*
-11	5	0	16.511	18.241	-18.241	0.0	-1.731	-1.409	*
-10	6	0	16.241	16.689	16.689	0.0	-0.448	-0.413	*
-8	6	0	20.801	22.443	-22.443	0.0	-1.642	-1.994	*
-6	6	0	5.631	4.469	4.469	0.0	1.162	0.613	*
-4	6	0	6.769	6.140	-6.140	0.0	0.629	0.532	*
-2	6	0	11.419	9.750	9.750	0.0	1.669	2.592	*
0	6	0	4.822	0.575	0.575	0.0	4.247	3.241	
2	6	0	10.528	9.750	9.750	0.0	0.778	1.094	
4	6	0	6.380	6.140	-6.140	0.0	0.240	0.188	
6	6	0	7.832	4.469	4.469	0.0	3.363	2.315	
8	6	0	20.719	22.443	-22.443	0.0	-1.725	-2.003	
10	6	0	14.841	16.689	16.689	0.0	-1.848	-1.514	
12	6	0	6.559	3.429	-3.429	0.0	3.130	1.118	
11	7	0	6.118	7.480	-7.480	0.0	-1.362	-0.487	
9	7	0	49.831	50.598	50.598	0.0	-0.766	-0.867	
7	7	0	39.431	40.033	-40.033	0.0	-0.602	-0.788	
5	7	0	22.823	23.591	23.591	0.0	-0.768	-1.127	
0	12	0	205.278	217.361	217.361	0.0	-12.083	-3.936	*
3	7	0	60.674	59.144	59.144	0.0	1.529	1.621	
1	7	0	8.079	7.085	-7.085	0.0	0.994	1.135	
-1	7	C	8.701	7.085	-7.085	0.0	1.616	2.016	*
-3	7	0	59.648	59.144	59.144	0.0	0.503	0.542	*
-5	7	0	22.688	23.591	23.591	0.0	-0.903	-1.370	*
-7	7	0	39.640	40.033	-40.033	0.0	-0.392	-0.509	*
-9	7	0	49.210	50.598	50.598	0.0	-1.388	-1.571	*
-11	7	0	6.702	7.480	-7.480	0.0	-0.778	-0.321	*
-12	8	0	35.956	36.193	36.193	0.0	-0.237	-0.247	*
-10	8	0	57.881	57.868	-57.868	0.0	0.013	0.013	*
-8	8	0	3.287	2.219	2.219	0.0	1.068	0.353	*
-6	8	0	60.614	60.945	60.945	0.0	-0.332	-0.338	*
-4	8	0	108.221	111.165	-111.165	0.0	-2.944	-1.803	*
-2	8	0	29.981	32.208	32.208	0.0	-2.227	-3.966	*
0	8	0	42.628	37.857	37.857	0.0	4.771	6.926	
2	8	0	30.333	32.208	32.208	0.0	-1.875	-3.339	
4	8	0	109.876	111.165	-111.165	0.0	-1.289	-0.775	
6	8	0	60.853	60.945	60.945	0.0	-0.092	-0.094	
8	8	0	3.609	2.219	2.219	0.0	1.390	0.475	
10	8	0	57.768	57.868	-57.868	0.0	-0.100	-0.099	
0	12	0	205.158	217.361	217.361	0.0	-12.203	-3.975	*
12	8	0	35.732	36.193	36.193	0.0	-0.461	-0.485	
11	9	0	9.038	7.768	-7.768	0.0	1.270	0.608	
9	9	0	31.681	30.774	30.774	0.0	0.906	1.175	
7	9	0	94.908	97.324	-97.324	0.0	-2.417	-1.655	
5	9	0	19.064	20.621	20.621	0.0	-1.558	-1.857	
1	9	0	76.068	75.602	-75.602	0.0	0.466	0.402	
-1	9	0	75.672	75.602	-75.602	0.0	0.070	0.060	*
-3	9	0	4.777	3.239	-3.239	0.0	1.539	0.934	*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-5	9	0	18.809	20.621	20.621	0.0	-1.812	-2.180	*
-7	9	0	94.758	97.324	-97.324	0.0	-2.566	-1.758	*
-9	9	0	30.573	30.774	30.774	0.0	-0.202	-0.254	*
-11	9	0	6.200	7.768	-7.768	0.0	-1.568	-0.569	*
-12	10	0	18.562	18.740	18.740	0.0	-0.178	-0.141	*
-10	10	0	24.770	25.134	25.134	0.0	-0.365	-0.381	*
-8	10	0	24.193	23.108	23.108	0.0	1.085	1.393	*
-6	10	0	16.990	14.351	14.351	0.0	2.638	3.118	*
-4	10	0	51.007	52.229	52.229	0.0	-1.223	-1.432	*
-2	10	0	35.844	37.319	37.319	0.0	-1.475	-2.264	*
0	10	0	85.832	85.599	85.599	0.0	0.233	0.179	
0	12	0	207.846	217.361	217.361	0.0	-9.515	-3.062	*
2	10	0	35.297	37.319	37.319	0.0	-2.021	-3.067	
4	10	0	50.894	52.229	52.229	0.0	-1.335	-1.578	
6	10	0	14.399	14.351	14.351	0.0	0.048	0.044	
8	10	0	23.631	23.108	23.108	0.0	0.523	0.641	
10	10	0	24.687	25.134	25.134	0.0	-0.447	-0.470	
12	10	0	18.944	18.740	18.740	0.0	0.204	0.152	
11	11	0	59.932	59.759	59.759	0.0	0.173	0.159	
9	11	0	8.888	10.282	10.282	0.0	-1.394	-0.760	
7	11	0	138.052	140.852	140.852	0.0	-2.800	-1.340	
5	11	0	37.431	38.088	-38.088	0.0	-0.656	-0.885	
3	11	0	91.800	95.266	95.266	0.0	-3.465	-2.475	
1	11	0	126.079	128.551	128.551	0.0	-2.472	-1.300	
-1	11	0	125.375	128.551	128.551	0.0	-3.176	-1.683	*
-3	11	0	92.519	95.266	95.266	0.0	-2.747	-1.941	*
-5	11	0	37.267	38.088	-38.088	0.0	-0.821	-1.107	*
-7	11	0	136.690	140.852	140.852	0.0	-4.162	-2.014	*
-9	11	0	10.153	10.282	10.282	0.0	-0.129	-0.083	*
-11	11	0	61.422	59.759	59.759	0.0	1.663	1.553	*
-10	12	0	66.229	66.117	66.117	0.0	0.113	0.100	*
-8	12	0	43.669	43.838	43.838	0.0	-0.169	-0.204	*
0	12	0	209.433	217.361	217.361	0.0	-7.928	-2.533	*
-6	12	0	22.134	23.169	-23.169	0.0	-1.035	-1.304	*
-4	12	0	50.722	50.238	50.238	0.0	0.485	0.563	*
-2	12	0	44.650	43.572	-43.572	0.0	1.078	1.384	*
0	12	0	209.793	217.361	217.361	0.0	-7.568	-2.412	*
2	12	0	44.784	43.572	-43.572	0.0	1.212	1.572	
4	12	0	51.261	50.238	50.238	0.0	1.024	1.169	
6	12	0	23.429	23.169	-23.169	0.0	0.260	0.351	
8	12	0	43.100	43.838	43.838	0.0	-0.738	-0.881	
10	12	0	66.769	66.117	66.117	0.0	0.652	0.569	
11	13	0	19.521	18.892	18.892	0.0	0.628	0.499	
9	13	0	20.651	22.060	-22.060	0.0	-1.408	-1.262	
7	13	0	49.105	49.012	49.012	0.0	0.093	0.105	
5	13	0	70.190	71.690	-71.690	0.0	-1.499	-1.344	
3	13	0	12.123	12.007	-12.007	0.0	0.116	0.094	
1	13	0	15.747	15.289	15.289	0.0	0.458	0.510	
-1	13	0	16.728	15.289	15.289	0.0	1.439	1.685	*
-3	13	0	9.944	12.007	-12.007	0.0	-2.063	-1.420	*
-5	13	0	69.494	71.690	-71.690	0.0	-2.195	-1.981	*
-7	13	0	48.109	49.012	49.012	0.0	-0.903	-1.040	*
-9	13	0	22.284	22.060	-22.060	0.0	0.224	0.241	*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	12	0	209.800	217.361	217.361	0.0	-7.561	-2.410	*
-11	13	0	18.944	18.892	18.892	0.0	0.052	0.044	*
-2	14	0	25.466	26.092	26.092	0.0	-0.626	-0.828	*
0	14	0	8.521	10.187	-10.187	0.0	-1.666	-0.980	
2	14	0	25.975	26.092	26.092	0.0	-0.117	-0.156	
4	14	0	2.726	3.419	3.419	0.0	-0.693	-0.206	
6	14	0	5.197	7.185	-7.185	0.0	-1.989	-0.765	
10	14	0	4.702	0.592	-0.592	0.0	4.111	1.242	
9	15	0	35.350	34.678	34.678	0.0	0.671	0.766	
7	15	0	52.033	50.639	-50.639	0.0	1.393	1.525	
5	15	0	41.220	41.164	41.164	0.0	0.056	0.069	
3	15	0	5.751	5.584	5.584	0.0	0.167	0.083	
-1	15	0	5.054	1.690	-1.690	0.0	3.364	1.459	*
-3	15	0	5.653	5.584	5.584	0.0	0.069	0.034	*
-5	15	0	40.367	41.164	41.164	0.0	-0.797	-1.004	*
0	12	0	208.722	217.361	217.361	0.0	-8.639	-2.767	*
-7	15	0	49.487	50.639	-50.639	0.0	-1.153	-1.241	*
-9	15	0	33.755	34.678	34.678	0.0	-0.923	-0.995	*
-10	16	0	32.504	32.118	-32.118	0.0	0.387	0.400	*
-6	16	0	26.035	26.932	26.932	0.0	-0.897	-1.130	*
-4	16	0	55.177	56.379	-56.379	0.0	-1.202	-1.284	*
-2	16	0	2.171	3.900	3.900	0.0	-1.728	-0.471	*
0	16	0	0.389	1.142	1.142	0.0	-0.752	-0.155	
2	16	0	6.147	3.900	3.900	0.0	2.248	1.210	
4	16	0	56.271	56.379	-56.379	0.0	-0.108	-0.114	
6	16	0	26.230	26.932	26.932	0.0	-0.702	-0.876	
8	16	0	3.033	3.930	-3.930	0.0	-0.898	-0.223	
10	16	0	33.351	32.118	-32.118	0.0	1.233	1.238	
9	17	0	15.545	17.031	17.031	0.0	-1.486	-1.018	
7	17	0	17.222	18.160	-18.160	0.0	-0.938	-0.778	
3	17	0	23.017	26.360	26.360	0.0	-3.343	-3.783	
1	17	0	13.942	14.426	-14.426	0.0	-0.483	-0.471	
-1	17	0	13.306	14.426	-14.426	0.0	-1.120	-0.977	*
-3	17	0	25.556	26.360	26.360	0.0	-0.804	-1.064	*
0	12	0	208.797	217.361	217.361	0.0	-8.564	-2.743	*
-7	17	0	18.233	18.160	-18.160	0.0	0.073	0.069	*
-9	17	0	17.065	17.031	17.031	0.0	0.034	0.027	*
-8	18	0	4.605	6.333	-6.333	0.0	-1.728	-0.504	*
-6	18	0	19.356	19.847	19.847	0.0	-0.491	-0.490	*
-2	18	0	19.947	19.824	19.824	0.0	0.123	0.142	*
0	18	0	15.163	15.462	15.462	0.0	-0.299	-0.287	
2	18	0	19.783	19.824	19.824	0.0	-0.041	-0.045	
4	18	0	2.688	3.280	3.280	0.0	-0.592	-0.160	
6	18	0	20.097	19.847	19.847	0.0	0.250	0.251	
8	18	0	5.009	6.333	-6.333	0.0	-1.324	-0.394	
7	19	0	25.414	23.899	-23.899	0.0	1.514	1.476	
5	19	0	8.431	9.213	9.213	0.0	-0.781	-0.386	
3	19	0	25.361	26.346	-26.346	0.0	-0.985	-1.154	
1	19	0	5.264	1.577	1.577	0.0	3.687	1.534	
-3	19	0	25.518	26.346	-26.346	0.0	-0.828	-1.014	*
-5	19	0	9.584	9.213	9.213	0.0	0.372	0.212	*
-7	19	0	23.751	23.899	-23.899	0.0	-0.148	-0.136	*
0	12	0	209.396	217.361	217.361	0.0	-7.965	-2.545	*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-6	20	0	4.837	3.727	-3.727	0.0	1.110	0.350	*
-4	20	0	37.544	37.983	-37.983	0.0	-0.439	-0.506	*
-2	20	0	23.834	24.622	24.622	0.0	-0.789	-0.885	*
0	20	0	60.352	60.866	-60.866	0.0	-0.515	-0.502	
2	20	0	25.136	24.622	24.622	0.0	0.514	0.602	
4	20	0	38.038	37.983	-37.983	0.0	0.055	0.064	
6	20	0	6.896	3.727	-3.727	0.0	3.169	1.283	
7	21	0	3.018	7.197	-7.197	0.0	-4.180	-0.887	
5	21	0	39.992	39.488	39.488	0.0	0.504	0.547	
3	21	0	8.574	3.780	3.780	0.0	4.793	2.581	
1	21	0	24.058	24.904	24.904	0.0	-0.846	-0.876	
-1	21	0	24.365	24.904	24.904	0.0	-0.539	-0.571	*
-3	21	0	1.707	3.780	3.780	0.0	-2.073	-0.445	*
-5	21	0	40.060	39.488	39.488	0.0	0.572	0.626	*
-7	21	0	8.574	7.197	-7.197	0.0	1.376	0.574	*
-6	22	0	13.036	13.008	13.008	0.0	0.028	0.017	*
-4	22	0	45.653	44.820	44.820	0.0	0.833	0.904	*
-2	22	0	20.786	21.068	21.068	0.0	-0.282	-0.269	*
0	22	0	58.360	59.394	59.394	0.0	-1.035	-1.001	
2	22	0	22.598	21.068	21.068	0.0	1.531	1.622	
0	12	0	207.412	217.361	217.361	0.0	-9.949	-3.209	*
4	22	0	45.578	44.820	44.820	0.0	0.758	0.803	
6	22	0	7.495	13.008	13.008	0.0	-5.513	-1.809	
5	23	0	43.512	43.441	-43.441	0.0	0.070	0.070	
3	23	0	40.464	41.447	41.447	0.0	-0.983	-1.050	
1	23	0	14.594	14.293	14.293	0.0	0.301	0.209	
-1	23	0	14.309	14.293	14.293	0.0	0.016	0.011	*
-3	23	0	40.726	41.447	41.447	0.0	-0.721	-0.776	*
-5	23	0	44.919	43.441	-43.441	0.0	1.478	1.518	*
-2	24	0	45.578	45.623	-45.623	0.0	-0.044	-0.048	*
0	24	0	89.614	89.718	89.718	0.0	-0.104	-0.072	
2	24	0	45.189	45.623	-45.623	0.0	-0.434	-0.446	
-3	24	1	5.474	5.370	5.370	0.0	0.103	0.034	
-1	24	1	4.837	4.681	4.681	0.0	0.156	0.046	
4	23	1	4.568	0.617	0.617	0.0	3.951	1.132	
2	23	1	12.010	13.596	13.596	0.0	-1.586	-0.864	
0	23	1	18.809	18.221	18.221	0.0	0.588	0.531	
-4	23	1	14.010	14.141	14.141	0.0	-0.132	-0.088	
-5	22	1	30.033	30.470	-30.470	0.0	-0.437	-0.452	
0	12	0	209.463	217.361	217.361	0.0	-7.898	-2.523	*
-3	22	1	18.323	17.353	17.353	0.0	0.970	0.869	
-1	22	1	8.544	5.597	-5.597	0.0	2.947	1.452	
1	22	1	24.807	24.342	-24.342	0.0	0.465	0.496	
3	22	1	10.633	9.649	9.649	0.0	0.983	0.523	
5	22	1	8.588	6.928	-6.928	0.0	1.660	0.722	
6	21	1	7.503	7.956	-7.956	0.0	-0.453	-0.166	
4	21	1	6.732	3.183	3.183	0.0	3.549	1.378	
2	21	1	25.593	25.670	-25.670	0.0	-0.076	-0.080	
0	21	1	31.898	33.625	33.625	0.0	-1.727	-1.971	
-2	21	1	43.092	42.130	-42.130	0.0	0.963	1.108	
-4	21	1	11.584	12.698	12.698	0.0	-1.115	-0.668	
-6	21	1	2.628	4.744	4.744	0.0	-2.116	-0.479	
-7	20	1	20.292	18.068	18.068	0.0	2.224	1.967	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-5	20	1	6.612	3.842	-3.842	0.0	2.770	1.174	
-3	20	1	16.421	16.014	16.014	0.0	0.407	0.372	
-1	20	1	5.489	1.407	1.407	0.0	4.082	1.736	
1	20	1	8.544	6.992	6.992	0.0	1.552	0.890	
3	20	1	12.954	13.822	13.822	0.0	-0.868	-0.604	
5	20	1	9.697	10.241	-10.241	0.0	-0.544	-0.271	
7	20	1	19.221	19.950	19.950	0.0	-0.729	-0.507	
0	12	0	207.194	217.361	217.361	0.0	-10.166	-3.280	*
6	19	1	31.217	31.835	31.835	0.0	-0.619	-0.672	
4	19	1	11.164	12.794	-12.794	0.0	-1.629	-1.017	
2	19	1	7.076	5.294	5.294	0.0	1.782	0.868	
0	19	1	41.452	40.667	-40.667	0.0	0.785	0.953	
-2	19	1	43.332	43.337	43.337	0.0	-0.005	-0.006	
-4	19	1	11.247	11.259	-11.259	0.0	-0.013	-0.009	
-6	19	1	8.574	6.690	6.690	0.0	1.884	1.023	
-8	19	1	4.500	2.354	-2.354	0.0	2.146	0.638	
-9	18	1	37.229	36.781	36.781	0.0	0.449	0.504	
-7	18	1	88.468	88.497	-88.497	0.0	-0.029	-0.020	
-5	18	1	85.758	85.537	85.537	0.0	0.221	0.163	
-3	18	1	6.065	4.333	4.333	0.0	1.732	0.820	
-1	18	1	5.249	4.552	4.552	0.0	0.697	0.299	
1	18	1	24.260	24.728	-24.728	0.0	-0.468	-0.578	
3	18	1	19.835	19.617	-19.617	0.0	0.218	0.231	
5	18	1	78.098	77.452	77.452	0.0	0.646	0.513	
7	18	1	46.896	46.400	-46.400	0.0	0.496	0.514	
8	17	1	15.515	15.961	15.961	0.0	-0.446	-0.314	
6	17	1	81.662	82.189	82.189	0.0	-0.527	-0.405	
4	17	1	7.390	8.102	8.102	0.0	-0.712	-0.367	
0	12	0	206.798	217.361	217.361	0.0	-10.563	-3.416	*
2	17	1	78.322	78.118	78.118	0.0	0.204	0.164	
0	17	1	45.653	45.959	-45.959	0.0	-0.306	-0.364	
-2	17	1	123.533	126.178	126.178	0.0	-2.645	-1.407	
-4	17	1	21.924	21.731	21.731	0.0	0.193	0.224	
-6	17	1	49.232	49.730	49.730	0.0	-0.498	-0.545	
-8	17	1	18.323	19.696	19.696	0.0	-1.373	-1.215	
-10	17	1	5.840	6.997	-6.997	0.0	-1.157	-0.372	
-9	16	1	38.165	36.938	36.938	0.0	1.227	1.344	
-7	16	1	22.411	21.919	21.919	0.0	0.492	0.557	
-5	16	1	61.991	61.793	61.793	0.0	0.198	0.193	
-3	16	1	45.204	45.988	45.988	0.0	-0.784	-0.952	
-1	16	1	60.981	61.120	61.120	0.0	-0.140	-0.140	
1	16	1	48.888	49.137	49.137	0.0	-0.249	-0.287	
3	16	1	36.046	36.673	36.673	0.0	-0.627	-0.797	
5	16	1	55.732	55.655	55.655	0.0	0.077	0.080	
7	16	1	29.270	28.573	28.573	0.0	0.697	0.782	
9	16	1	39.483	38.088	38.088	0.0	1.395	1.422	
8	15	1	9.435	10.251	10.251	0.0	-0.817	-0.423	
6	15	1	6.971	7.733	-7.733	0.0	-0.762	-0.348	
0	12	0	207.292	217.361	217.361	0.0	-10.069	-3.248	*
2	15	1	24.006	24.194	-24.194	0.0	-0.188	-0.251	
0	15	1	53.755	53.409	53.409	0.0	0.345	0.384	
-2	15	1	58.390	58.965	-58.965	0.0	-0.576	-0.601	
-4	15	1	18.165	17.100	17.100	0.0	1.066	1.248	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-6	15	1	19.408	20.561	20.561	0.0	-1.152	-1.175	
-8	15	1	12.565	13.972	-13.972	0.0	-1.407	-0.940	
-10	15	1	10.580	11.932	11.932	0.0	-1.351	-0.716	
-9	14	1	30.288	30.952	-30.952	0.0	-0.663	-0.764	
-7	14	1	27.922	27.509	27.509	0.0	0.413	0.515	
-5	14	1	85.091	86.846	-86.846	0.0	-1.755	-1.317	
-3	14	1	38.442	39.266	39.266	0.0	-0.823	-1.078	
-1	14	1	35.155	35.783	-35.783	0.0	-0.628	-0.847	
1	14	1	61.003	62.348	-62.348	0.0	-1.345	-1.351	
3	14	1	17.873	21.619	21.619	0.0	-3.746	-3.939	
5	14	1	45.121	45.790	-45.790	0.0	-0.668	-0.790	
7	14	1	3.841	8.249	8.249	0.0	-4.408	-1.294	
9	14	1	40.838	40.448	-40.448	0.0	0.391	0.408	
10	13	1	2.546	2.538	-2.538	0.0	0.008	0.002	
8	13	1	14.841	16.182	16.182	0.0	-1.342	-1.054	
0	12	0	207.067	217.361	217.361	0.0	-10.294	-3.321	*
6	13	1	4.006	2.431	-2.431	0.0	1.575	0.558	
4	13	1	18.884	18.909	18.909	0.0	-0.025	-0.030	
2	13	1	22.763	23.033	-23.033	0.0	-0.270	-0.354	
0	13	1	45.473	46.344	46.344	0.0	-0.871	-1.087	
-2	13	1	37.372	37.221	-37.221	0.0	0.151	0.205	
-4	13	1	38.255	39.011	39.011	0.0	-0.755	-0.980	
-10	13	1	3.175	6.878	6.878	0.0	-3.704	-0.937	
-11	12	1	13.852	10.668	10.668	0.0	3.184	2.562	
-9	12	1	7.211	5.228	-5.228	0.0	1.983	1.015	
-7	12	1	12.325	14.895	14.895	0.0	-2.570	-1.917	
-5	12	1	17.177	14.453	14.453	0.0	2.724	3.083	
-3	12	1	12.362	12.629	12.629	0.0	-0.267	-0.239	
-1	12	1	19.566	19.448	19.448	0.0	0.117	0.163	
1	12	1	19.708	20.369	20.369	0.0	-0.661	-0.866	
3	12	1	9.607	9.388	9.388	0.0	0.219	0.153	
5	12	1	9.180	11.175	11.175	0.0	-1.995	-1.313	
7	12	1	12.512	13.408	13.408	0.0	-0.896	-0.704	
9	12	1	9.143	5.885	5.885	0.0	3.258	1.813	
0	12	0	207.464	217.361	217.361	0.0	-9.897	-3.193	*
10	11	1	13.351	11.724	-11.724	0.0	1.627	1.065	
8	11	1	7.937	1.393	1.393	0.0	6.544	3.833	
6	11	1	10.071	9.038	-9.038	0.0	1.033	0.802	
4	11	1	8.686	7.826	-7.826	0.0	0.860	0.557	
2	11	1	48.888	49.165	-49.165	0.0	-0.278	-0.337	
0	11	1	1.542	0.226	0.226	0.0	1.317	0.370	
-2	11	1	24.560	24.244	-24.244	0.0	0.316	0.474	
-4	11	1	12.025	12.665	-12.665	0.0	-0.639	-0.554	
-6	11	1	13.523	13.445	-13.445	0.0	0.078	0.071	
-8	11	1	11.793	9.617	9.617	0.0	2.176	1.783	
-10	11	1	13.298	12.612	-12.612	0.0	0.686	0.530	
-11	10	1	17.297	18.828	18.828	0.0	-1.532	-1.210	
-9	10	1	22.396	22.393	-22.393	0.0	0.003	0.003	
-7	10	1	19.977	20.185	20.185	0.0	-0.207	-0.247	
-5	10	1	31.673	31.876	-31.876	0.0	-0.203	-0.286	
-3	10	1	57.139	56.349	56.349	0.0	0.790	0.865	
-1	10	1	38.817	38.749	-38.749	0.0	0.068	0.099	
1	10	1	10.520	10.756	-10.756	0.0	-0.236	-0.233	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
3	10	1	52.033	51.504	51.504	0.0	0.528	0.613	
0	12	0	207.981	217.361	217.361	0.0	-9.380	-3.019	*
5	10	1	41.145	40.441	-40.441	0.0	0.705	0.905	
7	10	1	21.093	21.699	21.699	0.0	-0.606	-0.658	
9	10	1	14.332	14.679	-14.679	0.0	-0.347	-0.258	
11	10	1	18.532	18.747	18.747	0.0	-0.215	-0.167	
10	9	1	25.354	25.191	25.191	0.0	0.163	0.166	
8	9	1	6.499	2.510	2.510	0.0	3.989	1.966	
4	9	1	34.309	33.470	33.470	0.0	0.839	1.192	
2	9	1	56.361	55.231	-55.231	0.0	1.129	1.257	
0	9	1	100.756	100.810	100.810	0.0	-0.054	-0.036	
-2	9	1	52.781	51.822	-51.822	0.0	0.959	1.134	
-4	9	1	24.081	24.064	24.064	0.0	0.017	0.025	
-6	9	1	22.104	22.514	22.514	0.0	-0.411	-0.512	
-10	9	1	15.882	15.303	15.303	0.0	0.579	0.505	
-12	9	1	26.866	27.485	-27.485	0.0	-0.618	-0.635	
-11	8	1	15.597	16.121	-16.121	0.0	-0.524	-0.438	
-9	8	1	16.585	14.100	-14.100	0.0	2.485	2.699	
-7	8	1	7.009	6.839	6.839	0.0	0.170	0.087	
-5	8	1	17.641	17.159	-17.159	0.0	0.482	0.613	
0	12	0	210.152	217.361	217.361	0.0	-7.209	-2.292	*
-3	8	1	7.121	2.838	2.838	0.0	4.283	3.667	
-1	8	1	11.561	11.198	-11.198	0.0	0.363	0.495	
1	8	1	11.599	10.840	-10.840	0.0	0.759	1.034	
3	8	1	10.191	8.967	-8.967	0.0	1.224	1.229	
5	8	1	21.640	21.271	-21.271	0.0	0.369	0.483	
7	8	1	16.735	17.215	17.215	0.0	-0.480	-0.525	
11	8	1	13.635	14.993	-14.993	0.0	-1.358	-0.836	
12	7	1	22.306	21.844	21.844	0.0	0.462	0.384	
10	7	1	34.661	33.256	-33.256	0.0	1.405	1.661	
6	7	1	60.995	62.073	62.073	0.0	-1.077	-1.090	
4	7	1	47.263	47.546	-47.546	0.0	-0.283	-0.357	
2	7	1	29.030	28.247	28.247	0.0	0.783	1.394	
0	7	1	130.235	132.236	-132.236	0.0	-2.001	-1.024	
-2	7	1	75.934	75.998	75.998	0.0	-0.065	-0.056	
-4	7	1	9.495	8.274	8.274	0.0	1.221	1.156	
-6	7	1	33.253	32.128	32.128	0.0	1.125	1.651	
-8	7	1	19.932	21.711	-21.711	0.0	-1.778	-1.996	
-10	7	1	24.620	23.948	-23.948	0.0	0.672	0.761	
0	12	0	210.092	217.361	217.361	0.0	-7.269	-2.317	*
-12	7	1	54.758	54.556	54.556	0.0	0.202	0.199	
-13	6	1	48.229	46.268	46.268	0.0	1.961	2.046	
-11	6	1	12.145	8.420	8.420	0.0	3.725	3.109	
-9	6	1	107.622	109.454	109.454	0.0	-1.832	-1.112	
-7	6	1	99.924	102.480	-102.480	0.0	-2.556	-1.673	
-5	6	1	192.893	205.207	205.207	0.0	-12.315	-4.272	*
-3	6	1	163.406	163.163	163.163	0.0	0.243	0.099	
-1	6	1	131.710	134.623	134.623	0.0	-2.913	-1.479	
1	6	1	54.047	43.785	-43.785	0.0	10.262	12.128	*
3	6	1	54.975	53.456	53.456	0.0	1.520	1.750	
5	6	1	244.626	256.302	256.302	0.0	-11.677	-3.196	*
7	6	1	42.912	41.713	-41.713	0.0	1.200	1.541	
9	6	1	79.603	79.735	79.735	0.0	-0.133	-0.104	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
11	6	1	18.502	17.847	-17.847	0.0	0.655	0.524	
12	5	1	54.900	53.067	53.067	0.0	1.834	1.762	
10	5	1	15.852	14.127	-14.127	0.0	1.724	1.515	
8	5	1	44.837	44.227	44.227	0.0	0.610	0.734	
6	5	1	139.370	142.930	142.930	0.0	-3.560	-1.698	
4	5	1	24.245	24.659	24.659	0.0	-0.414	-0.666	
2	5	1	130.407	135.845	135.845	0.0	-5.438	-2.783	
0	12	0	207.404	217.361	217.361	0.0	-9.957	-3.212	*
0	5	1	75.117	72.983	-72.983	0.0	2.134	1.875	
-2	5	1	208.333	220.030	220.030	0.0	-11.697	-3.764	*
-4	5	1	98.974	98.492	98.492	0.0	0.482	0.322	
-6	5	1	95.087	97.945	97.945	0.0	-2.858	-1.967	
-8	5	1	24.081	23.696	23.696	0.0	0.385	0.499	
-10	5	1	7.907	4.830	4.830	0.0	3.077	1.851	
-12	5	1	86.686	85.709	85.709	0.0	0.977	0.705	
-13	4	1	22.366	20.423	20.423	0.0	1.943	1.880	
-11	4	1	15.590	15.831	-15.831	0.0	-0.241	-0.201	
-9	4	1	5.137	0.031	-0.031	0.0	5.106	2.304	
-7	4	1	7.555	9.331	9.331	0.0	-1.775	-1.049	
-5	4	1	20.239	19.871	19.871	0.0	0.369	0.640	
-3	4	1	4.919	3.653	3.653	0.0	1.267	0.989	
-1	4	1	9.532	10.046	10.046	0.0	-0.514	-0.630	
1	4	1	9.277	4.187	4.187	0.0	5.091	7.009	
3	4	1	0.809	1.272	-1.272	0.0	-0.463	-0.146	
5	4	1	5.406	4.867	4.868	0.0	0.539	0.281	
7	4	1	13.014	14.317	14.317	0.0	-1.303	-1.130	
9	4	1	17.050	17.522	17.522	0.0	-0.472	-0.457	
11	4	1	19.109	17.410	-17.410	0.0	1.699	1.543	
0	12	0	207.307	217.361	217.361	0.0	-10.054	-3.243	*
12	3	1	32.467	32.787	-32.787	0.0	-0.320	-0.328	
10	3	1	11.299	11.224	11.224	0.0	0.075	0.051	
8	3	1	13.171	13.810	-13.810	0.0	-0.639	-0.558	
6	3	1	29.382	30.084	-30.084	0.0	-0.702	-1.030	
4	3	1	26.102	24.622	-24.622	0.0	1.481	2.637	
2	3	1	114.413	119.215	-119.215	0.0	-4.801	-2.800	
-2	3	1	141.040	144.488	-144.488	0.0	-3.448	-1.639	
-4	3	1	21.857	20.757	-20.757	0.0	1.100	2.128	
-8	3	1	27.218	25.290	-25.290	0.0	1.928	2.575	
-10	3	1	9.802	6.692	6.692	0.0	3.109	2.108	
-12	3	1	41.640	41.580	-41.580	0.0	0.060	0.065	
-13	2	1	19.491	18.003	-18.003	0.0	1.488	1.334	
-11	2	1	23.661	22.713	22.713	0.0	0.948	1.073	
-9	2	1	25.279	25.497	-25.497	0.0	-0.218	-0.283	
-7	2	1	49.030	49.623	49.623	0.0	-0.592	-0.719	
-5	2	1	49.629	49.708	-49.708	0.0	-0.079	-0.099	
-3	2	1	126.723	131.563	131.563	0.0	-4.839	-2.555	
1	2	1	9.285	7.264	-7.264	0.0	2.020	2.594	
3	2	1	109.494	109.780	109.780	0.0	-0.286	-0.174	
0	12	0	208.048	217.361	217.361	0.0	-9.313	-2.997	*
5	2	1	29.951	29.377	-29.377	0.0	0.574	0.902	
7	2	1	43.938	42.560	42.560	0.0	1.378	1.737	
9	2	1	23.025	22.521	-22.521	0.0	0.504	0.601	
11	2	1	35.470	34.120	34.120	0.0	1.350	1.541	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
10	1	1	6.814	3.540	-3.540	0.0	3.274	1.567	
8	1	1	15.006	15.187	15.187	0.0	-0.182	-0.197	
4	1	1	9.000	10.912	10.912	0.0	-1.911	-1.863	
2	1	1	50.093	50.802	-50.802	0.0	-0.709	-0.911	
-4	1	1	21.460	23.470	23.470	0.0	-2.010	-3.890	
-6	1	1	8.072	7.657	7.657	0.0	0.415	0.336	
-8	1	1	5.511	6.860	6.860	0.0	-1.349	-0.583	
-12	1	1	6.058	1.019	1.019	0.0	5.039	2.103	
-13	0	1	15.260	16.088	-16.088	0.0	-0.827	-0.576	
-9	0	1	10.797	12.784	-12.784	0.0	-1.986	-1.442	
-7	0	1	6.649	8.052	-8.052	0.0	-1.403	-0.774	
-5	0	1	10.835	9.609	-9.609	0.0	1.226	1.621	
0	12	0	209.141	217.361	217.361	0.0	-8.220	-2.626	*
-3	0	1	20.322	18.679	-18.679	0.0	1.643	3.274	
3	0	1	31.988	32.132	-32.132	0.0	-0.144	-0.253	
9	0	1	8.866	8.180	-8.180	0.0	0.685	0.412	
11	0	1	1.902	1.563	-1.563	0.0	0.339	0.074	
-12	0	2	50.393	49.821	-49.821	0.0	0.572	0.596	
-10	0	2	91.261	90.124	90.124	0.0	1.137	0.800	
-8	0	2	67.375	69.691	69.691	0.0	-2.316	-2.148	
-6	0	2	112.833	115.793	115.793	0.0	-2.959	-1.733	
-4	0	2	161.294	168.672	168.672	0.0	-7.378	-3.060	
-2	0	2	114.046	109.354	-109.354	0.0	4.693	2.737	
0	0	2	251.335	273.828	273.828	0.0	-22.493	-5.996	*
2	0	2	134.278	131.933	131.933	0.0	2.346	1.165	
4	0	2	199.527	207.641	207.641	0.0	-8.114	-2.716	
6	0	2	44.807	45.121	-45.121	0.0	-0.314	-0.389	
8	0	2	54.646	54.955	54.955	0.0	-0.309	-0.327	
10	0	2	97.042	96.109	96.109	0.0	0.932	0.610	
11	1	2	58.704	57.931	57.931	0.0	0.774	0.728	
9	1	2	29.959	29.048	-29.048	0.0	0.911	1.086	
0	12	0	206.723	217.361	217.361	0.0	-10.638	-3.440	*
7	1	2	65.735	65.416	65.416	0.0	0.320	0.301	
5	1	2	46.552	46.063	-46.063	0.0	0.489	0.610	
3	1	2	82.216	82.408	82.408	0.0	-0.192	-0.153	
1	1	2	118.966	116.945	116.945	0.0	2.021	1.134	
-1	1	2	4.949	4.067	-4.067	0.0	0.883	0.637	
-3	1	2	5.256	1.206	1.206	0.0	4.050	3.005	
-5	1	2	26.417	25.787	-25.787	0.0	0.630	1.051	
-7	1	2	170.370	176.238	176.238	0.0	-5.868	-2.298	
-9	1	2	28.656	29.504	-29.504	0.0	-0.848	-1.133	
-11	1	2	24.994	25.768	25.768	0.0	-0.773	-0.883	
-13	1	2	9.809	7.853	7.853	0.0	1.956	1.062	
-12	2	2	6.941	3.082	-3.082	0.0	3.859	1.777	
-8	2	2	6.372	4.372	4.372	0.0	2.000	0.957	
-6	2	2	29.367	29.556	-29.556	0.0	-0.189	-0.281	
-4	2	2	20.584	21.459	-21.459	0.0	-0.875	-1.479	
-2	2	2	20.502	21.411	-21.411	0.0	-0.909	-1.686	
0	2	2	30.588	30.211	-30.211	0.0	0.376	0.679	
2	2	2	6.769	8.001	-8.001	0.0	-1.232	-0.956	
4	2	2	8.192	7.733	7.733	0.0	0.459	0.331	
0	12	0	207.232	217.361	217.361	0.0	-10.129	-3.267	*
6	2	2	12.490	12.815	-12.815	0.0	-0.325	-0.265	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
8	2	2	15.627	17.149	-17.149	0.0	-1.522	-1.320	
10	2	2	16.541	15.516	-15.516	0.0	1.024	0.855	
11	3	2	17.836	16.292	-16.292	0.0	1.544	1.297	
9	3	2	33.029	33.821	33.821	0.0	-0.792	-0.945	
7	3	2	71.718	71.333	-71.333	0.0	0.385	0.336	
5	3	2	51.089	52.374	52.374	0.0	-1.285	-1.479	
1	3	2	75.387	71.628	-71.628	0.0	3.759	3.281	
-1	3	2	6.971	5.345	5.345	0.0	1.626	1.562	
-3	3	2	24.680	20.908	20.908	0.0	3.772	6.996	
-5	3	2	21.752	23.178	23.178	0.0	-1.426	-2.215	
-7	3	2	89.262	90.948	-90.948	0.0	-1.686	-1.230	
-9	3	2	64.552	64.530	64.530	0.0	0.022	0.021	
-11	3	2	7.563	7.844	-7.844	0.0	-0.282	-0.139	
-13	3	2	19.903	21.294	-21.294	0.0	-1.391	-1.113	
-12	4	2	48.820	48.697	48.697	0.0	0.124	0.132	
-10	4	2	46.334	46.651	-46.651	0.0	-0.317	-0.368	
-8	4	2	13.201	11.338	11.338	0.0	1.863	1.605	
-6	4	2	84.193	84.658	84.658	0.0	-0.466	-0.360	
0	12	0	209.957	217.361	217.361	0.0	-7.403	-2.360	*
-4	4	2	71.913	69.762	-69.762	0.0	2.151	1.941	
-2	4	2	11.629	12.422	12.422	0.0	-0.794	-1.165	
0	4	2	87.330	80.336	80.336	0.0	6.994	5.277	
2	4	2	80.816	82.319	82.319	0.0	-1.503	-1.217	
4	4	2	83.309	83.921	-83.921	0.0	-0.612	-0.478	
6	4	2	72.160	74.037	74.037	0.0	-1.878	-1.639	
8	4	2	24.066	23.876	23.876	0.0	0.189	0.220	
10	4	2	35.080	35.490	-35.490	0.0	-0.410	-0.453	
11	5	2	11.044	7.411	-7.411	0.0	3.633	2.047	
9	5	2	17.162	15.286	15.286	0.0	1.876	1.898	
7	5	2	46.874	46.590	-46.590	0.0	0.283	0.332	
5	5	2	8.978	5.602	-5.602	0.0	3.376	2.312	
3	5	2	28.910	26.551	26.551	0.0	2.360	3.752	
1	5	2	75.934	74.722	-74.722	0.0	1.212	1.044	
-1	5	2	49.270	47.517	-47.517	0.0	1.753	2.229	
-3	5	2	36.743	32.573	32.573	0.0	4.170	6.400	
-5	5	2	20.659	19.322	-19.322	0.0	1.337	1.941	
-7	5	2	44.784	45.772	-45.772	0.0	-0.987	-1.210	
-9	5	2	38.929	39.786	39.786	0.0	-0.857	-1.091	
-11	5	2	13.822	14.128	-14.128	0.0	-0.305	-0.240	
0	12	0	209.044	217.361	217.361	0.0	-8.317	-2.664	*
-13	5	2	6.776	2.179	-2.179	0.0	4.598	1.827	
-10	6	2	12.767	13.610	13.610	0.0	-0.844	-0.629	
-8	6	2	17.761	17.881	-17.881	0.0	-0.120	-0.133	
-6	6	2	9.285	12.936	12.936	0.0	-3.652	-2.379	
-4	6	2	10.693	11.856	-11.856	0.0	-1.164	-1.110	
2	6	2	3.467	6.119	6.119	0.0	-2.652	-1.135	
6	6	2	13.987	14.441	14.441	0.0	-0.454	-0.433	
8	6	2	23.519	23.959	-23.959	0.0	-0.440	-0.520	
10	6	2	7.278	8.050	8.050	0.0	-0.772	-0.320	
11	7	2	10.213	12.911	-12.911	0.0	-2.698	-1.178	
9	7	2	19.079	18.530	18.530	0.0	0.548	0.535	
7	7	2	4.875	1.764	-1.764	0.0	3.110	1.286	
5	7	2	28.184	26.980	26.980	0.0	1.204	1.692	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
3	7	2	10.206	9.505	-9.505	0.0	0.701	0.588	
1	7	2	33.118	33.058	33.058	0.0	0.061	0.097	
-1	7	2	44.979	44.313	44.313	0.0	0.666	0.899	
0	12	0	208.041	217.361	217.361	0.0	-9.320	-2.999	*
-3	7	2	35.552	34.061	-34.061	0.0	1.491	2.262	
-5	7	2	38.472	39.555	39.555	0.0	-1.083	-1.475	
-7	7	2	9.599	6.692	6.692	0.0	2.908	2.012	
-9	7	2	24.006	24.525	24.525	0.0	-0.519	-0.630	
-11	7	2	16.585	18.973	-18.973	0.0	-2.388	-1.909	
-13	7	2	21.827	21.367	21.367	0.0	0.460	0.418	
-12	8	2	22.007	22.239	22.239	0.0	-0.233	-0.211	
-10	8	2	17.304	17.046	-17.046	0.0	0.258	0.258	
-8	8	2	3.452	3.090	3.090	0.0	0.362	0.122	
-6	8	2	22.411	21.870	-21.870	0.0	0.541	0.695	
-4	8	2	22.658	21.070	-21.070	0.0	1.588	2.356	
-2	8	2	54.975	53.578	53.578	0.0	1.397	1.582	
0	8	2	98.929	97.240	-97.240	0.0	1.689	1.128	
2	8	2	80.157	79.794	79.794	0.0	0.363	0.294	
4	8	2	37.454	37.314	-37.314	0.0	0.139	0.181	
6	8	2	6.447	4.227	4.227	0.0	2.220	1.154	
8	8	2	6.267	0.254	0.254	0.0	6.013	2.769	
10	8	2	12.258	12.414	-12.414	0.0	-0.156	-0.094	
9	9	2	1.737	0.098	0.098	0.0	1.639	0.349	
7	9	2	36.817	38.437	-38.437	0.0	-1.620	-1.949	
0	12	0	207.449	217.361	217.361	0.0	-9.912	-3.197	*
5	9	2	29.217	28.153	28.153	0.0	1.064	1.528	
3	9	2	75.821	78.054	-78.054	0.0	-2.232	-1.887	
1	9	2	29.405	28.089	-28.089	0.0	1.315	1.930	
-1	9	2	14.489	13.224	13.224	0.0	1.264	1.443	
-3	9	2	84.417	84.502	-84.502	0.0	-0.084	-0.065	
-5	9	2	17.020	19.228	19.228	0.0	-2.209	-2.218	
-7	9	2	46.716	47.186	-47.186	0.0	-0.470	-0.565	
-9	9	2	13.680	15.915	15.915	0.0	-2.235	-1.705	
-11	9	2	14.204	11.603	-11.603	0.0	2.601	2.131	
-12	10	2	7.450	3.655	3.655	0.0	3.795	1.630	
-10	10	2	29.644	29.227	29.227	0.0	0.417	0.485	
-8	10	2	35.148	35.321	35.321	0.0	-0.174	-0.227	
-6	10	2	17.529	17.260	17.260	0.0	0.269	0.283	
-4	10	2	45.586	45.065	45.065	0.0	0.521	0.656	
-2	10	2	24.747	25.492	25.492	0.0	-0.745	-1.047	
0	10	2	54.077	54.152	54.152	0.0	-0.075	-0.085	
2	10	2	33.643	33.755	33.755	0.0	-0.112	-0.159	
4	10	2	61.587	61.992	61.992	0.0	-0.405	-0.403	
6	10	2	13.987	14.349	14.349	0.0	-0.362	-0.314	
8	10	2	11.726	13.050	13.050	0.0	-1.324	-0.830	
0	12	0	207.456	217.361	217.361	0.0	-9.904	-3.195	*
10	10	2	12.018	10.441	10.441	0.0	1.577	0.892	
9	11	2	3.355	4.350	4.350	0.0	-0.995	-0.256	
7	11	2	59.550	59.387	59.387	0.0	0.163	0.160	
5	11	2	10.356	11.870	-11.870	0.0	-1.515	-1.082	
3	11	2	152.571	156.092	156.092	0.0	-3.521	-1.532	
1	11	2	88.101	87.289	87.289	0.0	0.812	0.599	
-1	11	2	15.605	15.828	15.828	0.0	-0.223	-0.242	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	16	2	46.462	45.854	-45.854	0.0	0.608	0.725	
0	12	0	207.614	217.361	217.361	0.0	-9.747	-3.137	*
2	16	2	23.983	24.412	24.412	0.0	-0.429	-0.511	
4	16	2	27.046	26.777	-26.777	0.0	0.269	0.324	
6	16	2	2.591	1.243	-1.243	0.0	1.348	0.335	
8	16	2	5.885	3.682	-3.682	0.0	2.204	0.730	
7	17	2	1.018	4.271	4.271	0.0	-3.253	-0.566	
5	17	2	2.538	3.939	3.939	0.0	-1.401	-0.354	
3	17	2	7.024	5.159	-5.159	0.0	1.865	0.919	
1	17	2	3.197	2.055	2.055	0.0	1.142	0.347	
-1	17	2	7.840	7.015	7.015	0.0	0.825	0.465	
-3	17	2	10.498	8.219	-8.219	0.0	2.278	1.690	
-5	17	2	4.291	4.441	4.441	0.0	-0.150	-0.052	
-9	17	2	8.319	5.113	5.113	0.0	3.206	1.557	
-8	18	2	3.542	1.860	-1.860	0.0	1.682	0.456	
-6	18	2	12.482	13.626	13.626	0.0	-1.144	-0.772	
-4	18	2	3.145	5.859	5.859	0.0	-2.714	-0.757	
-2	18	2	20.254	18.723	18.723	0.0	1.532	1.843	
0	18	2	7.503	4.273	4.273	0.0	3.230	1.843	
2	18	2	19.146	19.583	19.583	0.0	-0.437	-0.446	
4	18	2	8.259	10.465	10.465	0.0	-2.206	-1.041	
0	12	0	207.187	217.361	217.361	0.0	-10.174	-3.282	*
6	18	2	17.746	17.465	17.465	0.0	0.281	0.232	
5	19	2	7.518	10.120	10.120	0.0	-2.602	-1.004	
3	19	2	3.092	2.846	-2.846	0.0	0.247	0.067	
1	19	2	19.596	16.671	-16.671	0.0	2.925	3.228	
-1	19	2	6.043	2.702	-2.702	0.0	3.340	1.544	
-3	19	2	14.886	15.139	-15.139	0.0	-0.254	-0.212	
-5	19	2	9.644	9.545	9.545	0.0	0.099	0.058	
-7	19	2	32.190	32.271	-32.271	0.0	-0.081	-0.089	
-8	20	2	7.360	2.058	-2.058	0.0	5.303	2.146	
-6	20	2	11.778	11.124	11.124	0.0	0.654	0.414	
-4	20	2	42.942	42.800	-42.800	0.0	0.142	0.167	
-2	20	2	2.074	2.984	2.984	0.0	-0.910	-0.206	
0	20	2	31.089	30.958	-30.958	0.0	0.131	0.145	
2	20	2	25.541	24.900	24.900	0.0	0.640	0.701	
4	20	2	59.565	59.344	-59.344	0.0	0.222	0.208	
5	21	2	40.127	38.622	38.622	0.0	1.505	1.570	
3	21	2	14.833	15.002	15.002	0.0	-0.169	-0.115	
-1	21	2	27.360	26.033	26.033	0.0	1.327	1.528	
-3	21	2	19.116	18.624	18.624	0.0	0.492	0.463	
0	12	0	209.179	217.361	217.361	0.0	-8.182	-2.614	*
-5	21	2	25.024	25.047	25.047	0.0	-0.023	-0.022	
-7	21	2	15.515	15.390	-15.390	0.0	0.125	0.091	
-6	22	2	24.508	24.073	24.073	0.0	0.435	0.430	
-4	22	2	36.892	37.388	37.388	0.0	-0.495	-0.533	
-2	22	2	11.471	12.355	12.355	0.0	-0.884	-0.498	
0	22	2	54.496	54.062	54.062	0.0	0.434	0.436	
2	22	2	20.157	18.597	18.597	0.0	1.560	1.418	
1	23	2	26.065	26.808	26.808	0.0	-0.743	-0.714	
-1	23	2	12.392	10.331	-10.331	0.0	2.061	1.280	
-3	23	2	27.226	27.604	27.604	0.0	-0.378	-0.371	
-3	22	3	10.603	12.433	12.433	0.0	-1.830	-0.951	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-1	22	3	17.566	17.260	-17.260	0.0	0.306	0.242	
1	22	3	7.540	5.831	-5.831	0.0	1.709	0.671	
2	21	3	27.832	27.992	-27.992	0.0	-0.160	-0.155	
0	21	3	20.988	22.155	22.155	0.0	-1.167	-1.005	
-2	21	3	24.852	24.398	-24.398	0.0	0.454	0.463	
-4	21	3	8.701	7.433	7.433	0.0	1.267	0.613	
-7	20	3	14.002	12.528	12.528	0.0	1.474	0.994	
-5	20	3	9.345	8.717	-8.717	0.0	0.628	0.315	
0	12	0	210.205	217.361	217.361	0.0	-7.156	-2.276	*
-3	20	3	16.076	15.991	15.991	0.0	0.085	0.069	
-1	20	3	7.623	3.080	3.080	0.0	4.542	2.121	
1	20	3	9.135	8.488	8.488	0.0	0.647	0.325	
3	20	3	9.120	11.150	11.150	0.0	-2.030	-0.901	
4	19	3	38.877	40.109	-40.109	0.0	-1.233	-1.317	
2	19	3	22.950	24.638	24.638	0.0	-1.688	-1.610	
0	19	3	14.496	14.433	-14.433	0.0	0.063	0.046	
-2	19	3	23.721	23.255	23.255	0.0	0.466	0.494	
-4	19	3	9.727	8.873	-8.873	0.0	0.853	0.507	
-6	19	3	2.231	2.352	-2.352	0.0	-0.121	-0.027	
-8	19	3	11.059	4.323	-4.323	0.0	6.736	4.410	
-7	18	3	62.516	62.525	-62.525	0.0	-0.009	-0.009	
-5	18	3	21.243	21.537	21.537	0.0	-0.295	-0.283	
-3	18	3	15.814	15.213	-15.213	0.0	0.601	0.508	
-1	18	3	75.522	75.273	75.273	0.0	0.249	0.204	
1	18	3	29.981	30.104	-30.104	0.0	-0.123	-0.137	
3	18	3	42.710	42.236	-42.236	0.0	0.474	0.519	
5	18	3	56.495	56.223	56.223	0.0	0.272	0.259	
6	17	3	60.651	61.109	61.109	0.0	-0.458	-0.413	
4	17	3	37.109	36.700	-36.700	0.0	0.410	0.464	
0	12	0	207.382	217.361	217.361	0.0	-9.979	-3.219	*
2	17	3	77.701	77.132	77.132	0.0	0.569	0.455	
0	17	3	10.760	8.526	-8.526	0.0	2.234	1.456	
-2	17	3	100.509	99.413	99.413	0.0	1.095	0.703	
-4	17	3	13.403	12.777	12.777	0.0	0.626	0.489	
-6	17	3	18.907	18.456	18.456	0.0	0.451	0.430	
-8	17	3	28.521	28.897	28.897	0.0	-0.376	-0.401	
-9	16	3	32.475	32.399	32.399	0.0	0.075	0.081	
-7	16	3	13.441	12.224	12.224	0.0	1.217	0.979	
-5	16	3	52.392	52.775	52.775	0.0	-0.383	-0.406	
-3	16	3	32.287	32.108	32.108	0.0	0.179	0.224	
-1	16	3	54.174	54.396	54.396	0.0	-0.222	-0.235	
1	16	3	43.774	44.117	44.117	0.0	-0.343	-0.402	
3	16	3	31.786	32.052	32.052	0.0	-0.266	-0.320	
5	16	3	29.120	29.845	29.845	0.0	-0.725	-0.774	
6	15	3	13.598	12.730	-12.730	0.0	0.868	0.604	
4	15	3	19.011	19.727	19.727	0.0	-0.715	-0.677	
2	15	3	32.272	31.402	-31.402	0.0	0.870	1.151	
0	15	3	34.227	33.307	33.307	0.0	0.919	1.181	
-2	15	3	26.731	27.030	-27.030	0.0	-0.298	-0.369	
-4	15	3	12.183	12.101	12.101	0.0	0.082	0.063	
0	12	0	209.508	217.361	217.361	0.0	-7.853	-2.509	*
-6	15	3	12.385	12.329	12.329	0.0	0.055	0.042	
-8	15	3	14.631	14.124	-14.124	0.0	0.507	0.391	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-10	15	3	13.448	13.881	13.881	0.0	-0.433	-0.267	
-11	14	3	6.110	8.123	8.123	0.0	-2.013	-0.689	
-9	14	3	38.285	38.591	-38.591	0.0	-0.306	-0.340	
-7	14	3	22.156	19.911	19.911	0.0	2.245	2.751	
-5	14	3	58.876	59.814	-59.814	0.0	-0.938	-0.935	
-3	14	3	31.673	31.406	31.406	0.0	0.268	0.347	
-1	14	3	48.730	48.779	-48.779	0.0	-0.048	-0.056	
1	14	3	20.322	21.240	-21.240	0.0	-0.918	-1.030	
3	14	3	6.874	8.971	8.971	0.0	-2.097	-0.997	
5	14	3	42.418	41.430	-41.430	0.0	0.989	1.138	
7	14	3	12.594	13.148	13.148	0.0	-0.553	-0.344	
8	13	3	7.128	9.788	9.788	0.0	-2.660	-0.963	
6	13	3	7.667	7.523	-7.523	0.0	0.144	0.066	
4	13	3	24.725	24.064	24.064	0.0	0.661	0.795	
2	13	3	28.686	27.772	-27.772	0.0	0.914	1.299	
0	13	3	39.303	39.375	39.375	0.0	-0.072	-0.093	
-2	13	3	12.355	11.497	-11.497	0.0	0.858	0.749	
-4	13	3	18.779	17.684	17.684	0.0	1.095	1.240	
0	12	0	210.017	217.361	217.361	0.0	-7.343	-2.341	*
-8	13	3	6.215	0.087	0.087	0.0	6.128	2.756	
-10	13	3	12.857	7.759	7.759	0.0	5.097	3.868	
-11	12	3	16.331	12.257	12.257	0.0	4.074	3.804	
-9	12	3	7.143	3.029	-3.029	0.0	4.114	1.998	
-7	12	3	13.792	12.658	12.658	0.0	1.135	1.017	
-5	12	3	3.512	3.849	3.849	0.0	-0.337	-0.111	
-3	12	3	7.623	7.930	7.930	0.0	-0.307	-0.178	
-1	12	3	14.976	16.726	16.726	0.0	-1.750	-1.569	
1	12	3	19.708	20.820	20.820	0.0	-1.112	-1.314	
3	12	3	7.870	4.258	4.258	0.0	3.612	2.254	
5	12	3	2.785	6.795	6.795	0.0	-4.010	-1.088	
7	12	3	7.855	6.841	6.841	0.0	1.013	0.454	
8	11	3	8.334	10.298	10.298	0.0	-1.964	-0.841	
6	11	3	21.393	22.811	-22.811	0.0	-1.419	-1.446	
4	11	3	18.046	17.427	-17.427	0.0	0.619	0.661	
2	11	3	8.177	10.440	-10.440	0.0	-2.263	-1.362	
0	11	3	6.447	3.492	3.492	0.0	2.955	1.500	
-2	11	3	36.278	37.991	-37.991	0.0	-1.713	-2.178	
0	12	0	209.808	217.361	217.361	0.0	-7.553	-2.407	*
-6	11	3	3.901	2.766	-2.766	0.0	1.135	0.398	
-8	11	3	7.847	9.154	-9.154	0.0	-1.307	-0.651	
-10	11	3	4.717	5.786	-5.786	0.0	-1.069	-0.349	
-12	11	3	6.222	5.282	5.282	0.0	0.941	0.348	
-11	10	3	7.405	1.626	1.626	0.0	5.779	2.634	
-9	10	3	14.114	13.268	-13.268	0.0	0.846	0.739	
-7	10	3	31.351	32.096	32.096	0.0	-0.744	-0.975	
-5	10	3	61.183	61.680	-61.680	0.0	-0.498	-0.500	
-3	10	3	53.058	53.583	53.583	0.0	-0.525	-0.584	
1	10	3	29.172	29.196	-29.196	0.0	-0.023	-0.031	
3	10	3	19.917	21.482	21.482	0.0	-1.564	-1.916	
7	10	3	8.970	6.999	6.999	0.0	1.971	1.097	
9	10	3	26.162	27.008	-27.008	0.0	-0.846	-0.784	
8	9	3	10.902	8.055	8.055	0.0	2.847	1.769	
6	9	3	13.673	15.394	-15.394	0.0	-1.721	-1.368	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
4	9	3	27.705	29.600	29.600	0.0	-1.895	-2.388	
2	9	3	23.265	23.287	-23.287	0.0	-0.022	-0.029	
0	9	3	61.999	64.091	64.091	0.0	-2.092	-2.085	
0	12	0	205.577	217.361	217.361	0.0	-11.784	-3.829	*
-2	9	3	54.391	54.125	-54.125	0.0	0.266	0.294	
-4	9	3	44.088	44.233	44.233	0.0	-0.145	-0.179	
-6	9	3	24.448	24.519	24.519	0.0	-0.071	-0.094	
-8	9	3	33.059	33.865	-33.865	0.0	-0.806	-1.016	
-10	9	3	24.021	24.435	24.435	0.0	-0.414	-0.436	
-12	9	3	15.949	16.792	-16.792	0.0	-0.843	-0.612	
-9	8	3	16.061	16.249	-16.249	0.0	-0.187	-0.171	
-5	8	3	18.150	16.649	-16.649	0.0	1.501	1.643	
-3	8	3	7.480	1.285	-1.285	0.0	6.195	3.830	
-1	8	3	11.606	10.382	-10.382	0.0	1.224	1.021	
3	8	3	4.635	0.952	0.952	0.0	3.683	1.552	
5	8	3	25.885	26.584	-26.584	0.0	-0.698	-0.864	
7	8	3	6.335	3.397	3.397	0.0	2.938	1.358	
9	8	3	8.027	5.622	5.622	0.0	2.405	1.078	
8	7	3	12.415	9.871	9.871	0.0	2.543	1.836	
6	7	3	41.295	41.642	41.642	0.0	-0.347	-0.429	
4	7	3	73.792	74.849	-74.849	0.0	-1.057	-0.905	
0	12	0	205.420	217.361	217.361	0.0	-11.941	-3.890	*
2	7	3	23.714	25.087	25.087	0.0	-1.373	-1.667	
0	7	3	39.206	38.580	-38.580	0.0	0.626	0.862	
-2	7	3	96.398	96.734	96.734	0.0	-0.336	-0.229	
-4	7	3	32.310	31.738	-31.738	0.0	0.572	0.796	
-6	7	3	18.210	18.571	-18.571	0.0	-0.361	-0.389	
-8	7	3	20.464	20.027	20.027	0.0	0.437	0.482	
-12	7	3	43.347	43.241	43.241	0.0	0.106	0.113	
-13	6	3	11.127	14.355	14.355	0.0	-3.229	-1.585	
-11	6	3	23.302	22.856	22.856	0.0	0.446	0.492	
-9	6	3	132.781	136.411	136.411	0.0	-3.630	-1.802	
-7	6	3	82.680	83.535	-83.535	0.0	-0.855	-0.664	
-5	6	3	107.315	108.488	108.488	0.0	-1.173	-0.719	
-3	6	3	45.488	45.083	45.083	0.0	0.405	0.510	
-1	6	3	200.425	202.642	202.642	0.0	-2.217	-0.740	
1	6	3	31.606	32.470	32.470	0.0	-0.864	-1.240	
3	6	3	14.751	17.651	-17.651	0.0	-2.900	-2.599	
5	6	3	124.020	126.901	126.901	0.0	-2.881	-1.527	
9	6	3	87.001	85.873	85.873	0.0	1.127	0.805	
0	12	0	206.109	217.361	217.361	0.0	-11.252	-3.647	*
10	5	3	10.453	8.367	8.367	0.0	2.086	1.067	
8	5	3	43.774	43.399	43.399	0.0	0.375	0.424	
6	5	3	94.226	94.647	94.647	0.0	-0.421	-0.288	
4	5	3	34.953	34.892	-34.892	0.0	0.061	0.083	
2	5	3	103.878	105.013	105.013	0.0	-1.135	-0.718	
0	5	3	19.588	19.459	19.459	0.0	0.129	0.182	
-2	5	3	195.102	196.549	196.549	0.0	-1.448	-0.496	
-4	5	3	26.335	27.041	27.041	0.0	-0.707	-1.015	
-6	5	3	32.669	32.831	32.831	0.0	-0.162	-0.216	
-8	5	3	61.445	62.258	62.258	0.0	-0.814	-0.805	
-10	5	3	18.607	19.148	19.148	0.0	-0.541	-0.528	
-12	5	3	77.311	77.156	77.156	0.0	0.155	0.123	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-13	4	3	19.835	18.950	18.950	0.0	0.886	0.773	
-11	4	3	3.160	0.436	-0.436	0.0	2.724	0.803	
-9	4	3	9.360	8.300	8.300	0.0	1.059	0.690	
-7	4	3	0.404	8.994	-8.994	0.0	-8.590	-1.557	
-5	4	3	7.952	8.850	8.850	0.0	-0.898	-0.538	
-3	4	3	8.259	4.836	4.836	0.0	3.423	2.540	
-1	4	3	13.882	13.015	13.015	0.0	0.868	0.974	
1	4	3	10.333	13.134	13.134	0.0	-2.801	-2.067	
0	12	0	206.438	217.361	217.361	0.0	-10.923	-3.541	*
3	4	3	2.823	1.292	1.292	0.0	1.531	0.454	
5	4	3	7.667	9.147	-9.147	0.0	-1.480	-0.813	
7	4	3	4.186	5.613	5.613	0.0	-1.428	-0.498	
9	4	3	19.708	16.978	16.978	0.0	2.729	2.804	
10	3	3	9.292	10.104	10.104	0.0	-0.812	-0.368	
8	3	3	12.976	11.293	-11.293	0.0	1.683	1.371	
6	3	3	44.627	44.789	-44.789	0.0	-0.162	-0.195	
4	3	3	8.753	3.810	3.810	0.0	4.943	3.252	
2	3	3	63.144	63.273	-63.273	0.0	-0.128	-0.127	
0	3	3	31.269	31.317	31.317	0.0	-0.049	-0.074	
-2	3	3	103.953	101.103	-101.103	0.0	2.849	1.812	
-4	3	3	15.372	12.510	12.510	0.0	2.863	3.324	
-6	3	3	8.252	9.838	9.838	0.0	-1.586	-0.905	
-8	3	3	51.621	52.696	-52.696	0.0	-1.076	-1.207	
-10	3	3	6.013	11.151	11.151	0.0	-5.138	-1.972	
-12	3	3	23.766	24.106	-24.106	0.0	-0.340	-0.329	
-13	2	3	9.876	4.598	-4.598	0.0	5.278	2.937	
-11	2	3	12.392	10.496	10.496	0.0	1.897	1.456	
-9	2	3	24.013	24.539	-24.539	0.0	-0.526	-0.639	
-7	2	3	49.442	49.802	49.802	0.0	-0.360	-0.415	
0	12	0	209.718	217.361	217.361	0.0	-7.643	-2.436	*
-5	2	3	68.940	68.216	-68.216	0.0	0.724	0.671	
-3	2	3	96.525	94.082	94.082	0.0	2.443	1.664	
1	2	3	7.233	9.819	-9.819	0.0	-2.585	-1.548	
3	2	3	49.547	50.517	50.517	0.0	-0.970	-1.147	
7	2	3	29.382	30.291	30.291	0.0	-0.909	-1.104	
9	2	3	29.397	28.918	-28.918	0.0	0.479	0.520	
10	1	3	9.914	6.743	-6.743	0.0	3.171	1.641	
8	1	3	15.080	15.574	15.574	0.0	-0.494	-0.407	
6	1	3	12.527	13.304	-13.304	0.0	-0.777	-0.656	
2	1	3	20.539	20.561	-20.561	0.0	-0.022	-0.028	
0	1	3	36.952	37.052	37.052	0.0	-0.100	-0.148	
-2	1	3	26.574	24.919	-24.919	0.0	1.655	2.632	
-4	1	3	26.072	26.111	26.111	0.0	-0.039	-0.057	
-6	1	3	2.321	0.750	-0.750	0.0	1.571	0.435	
-8	1	3	6.544	1.671	-1.671	0.0	4.873	2.646	
-10	1	3	9.757	8.171	8.171	0.0	1.585	1.038	
0	12	0	208.932	217.361	217.361	0.0	-8.429	-2.700	*
-13	0	3	9.135	9.199	-9.199	0.0	-0.064	-0.031	
-11	0	3	10.595	8.645	8.645	0.0	1.950	1.329	
-9	0	3	17.491	17.187	-17.187	0.0	0.305	0.320	
-7	0	3	3.856	1.295	1.295	0.0	2.561	0.879	
-5	0	3	13.538	13.726	-13.726	0.0	-0.189	-0.189	
-3	0	3	25.998	26.257	-26.257	0.0	-0.259	-0.422	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
1	0	3	6.911	2.492	2.492	0.0	4.419	2.981	
3	0	3	17.641	17.753	-17.753	0.0	-0.112	-0.127	
5	0	3	12.617	11.517	-11.517	0.0	1.100	1.006	
7	0	3	10.573	9.765	-9.765	0.0	0.808	0.553	
-12	0	4	9.816	4.248	4.248	0.0	5.569	3.508	
-10	0	4	42.793	42.556	42.556	0.0	0.236	0.279	
-8	0	4	22.516	23.612	-23.612	0.0	-1.096	-1.296	
-6	0	4	151.201	157.941	157.941	0.0	-6.741	-2.961	
-4	0	4	137.955	140.720	140.720	0.0	-2.765	-1.328	
-2	0	4	81.153	82.726	-82.727	0.0	-1.574	-1.244	
0	0	4	167.352	170.952	170.952	0.0	-3.600	-1.431	
2	0	4	11.688	11.114	11.114	0.0	0.575	0.436	
0	12	0	205.420	217.361	217.361	0.0	-11.941	-3.890	*
4	0	4	137.034	138.631	138.631	0.0	-1.597	-0.770	
6	0	4	16.174	14.989	14.989	0.0	1.185	1.076	
8	0	4	38.742	38.530	38.530	0.0	0.212	0.227	
7	1	4	22.785	22.285	22.285	0.0	0.501	0.527	
5	1	4	11.658	9.127	9.127	0.0	2.531	1.965	
3	1	4	84.253	86.227	86.227	0.0	-1.975	-1.498	
-1	1	4	49.973	49.284	-49.284	0.0	0.689	0.801	
-3	1	4	131.193	133.060	133.060	0.0	-1.866	-0.941	
-5	1	4	11.629	12.564	-12.564	0.0	-0.935	-0.661	
-7	1	4	80.591	81.579	81.579	0.0	-0.988	-0.781	
-9	1	4	18.023	18.426	-18.426	0.0	-0.403	-0.390	
-11	1	4	27.076	27.843	27.843	0.0	-0.767	-0.840	
-13	1	4	14.549	10.634	10.634	0.0	3.915	3.022	
-12	2	4	10.468	5.872	-5.872	0.0	4.596	2.842	
-10	2	4	12.684	9.128	-9.128	0.0	3.556	2.844	
-8	2	4	5.803	5.223	5.223	0.0	0.580	0.252	
-6	2	4	12.063	12.104	-12.104	0.0	-0.041	-0.031	
-4	2	4	9.584	8.541	-8.541	0.0	1.044	0.677	
-2	2	4	13.770	11.716	-11.716	0.0	2.054	1.804	
0	12	0	206.161	217.361	217.361	0.0	-11.200	-3.630	*
0	2	4	22.344	21.572	-21.572	0.0	0.772	0.954	
2	2	4	18.704	18.544	-18.544	0.0	0.160	0.193	
6	2	4	0.831	3.277	3.277	0.0	-2.446	-0.493	
7	3	4	16.009	15.941	-15.941	0.0	0.068	0.057	
5	3	4	25.743	25.618	25.618	0.0	0.125	0.153	
3	3	4	44.043	45.177	-45.177	0.0	-1.133	-1.389	
1	3	4	10.505	4.630	4.630	0.0	5.875	4.311	
-1	3	4	47.188	48.287	48.287	0.0	-1.099	-1.299	
-3	3	4	76.390	76.467	-76.467	0.0	-0.077	-0.064	
-5	3	4	41.632	41.345	41.345	0.0	0.287	0.359	
-7	3	4	19.925	19.466	-19.466	0.0	0.459	0.528	
-9	3	4	19.970	19.114	19.114	0.0	0.855	0.872	
-11	3	4	17.125	19.249	-19.249	0.0	-2.124	-1.669	
-13	3	4	5.174	5.759	-5.759	0.0	-0.585	-0.177	
-12	4	4	14.534	14.831	14.831	0.0	-0.297	-0.202	
-8	4	4	17.806	18.952	18.952	0.0	-1.146	-1.196	
-6	4	4	11.778	14.151	-14.151	0.0	-2.372	-1.770	
0	12	0	208.976	217.361	217.361	0.0	-8.384	-2.685	*
-4	4	4	17.050	15.125	15.125	0.0	1.925	1.933	
-2	4	4	45.653	46.174	46.174	0.0	-0.521	-0.627	

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	4	4	54.983	57.903	-57.903	0.0	-2.920	-3.145	
2	4	4	76.121	77.002	77.002	0.0	-0.881	-0.735	
4	4	4	7.907	10.872	-10.872	0.0	-2.965	-1.559	
6	4	4	10.558	9.430	9.430	0.0	1.128	0.742	
8	4	4	8.222	9.870	9.870	0.0	-1.648	-0.705	
7	5	4	6.110	1.147	-1.147	0.0	4.963	1.910	
5	5	4	8.970	4.177	-4.177	0.0	4.794	3.093	
3	5	4	27.929	28.953	-28.953	0.0	-1.023	-1.327	
1	5	4	5.152	7.983	-7.983	0.0	-2.831	-1.099	
-1	5	4	9.098	7.492	7.492	0.0	1.606	1.036	
-3	5	4	39.678	40.635	-40.635	0.0	-0.957	-1.217	
-5	5	4	14.010	12.322	12.322	0.0	1.688	1.610	
-7	5	4	4.395	0.566	0.566	0.0	3.830	1.413	
-11	5	4	17.619	16.895	-16.895	0.0	0.724	0.616	
-10	6	4	9.517	12.069	12.069	0.0	-2.552	-1.358	
-8	6	4	12.048	11.740	-11.740	0.0	0.308	0.219	
0	12	0	209.104	217.361	217.361	0.0	-8.257	-2.638	*
-4	6	4	4.365	3.670	-3.670	0.0	0.695	0.255	
-2	6	4	4.560	6.330	6.330	0.0	-1.770	-0.637	
0	6	4	9.959	11.301	-11.301	0.0	-1.343	-0.875	
2	6	4	10.857	9.134	-9.134	0.0	1.723	1.412	
4	6	4	5.339	1.173	1.173	0.0	4.166	1.766	
6	6	4	15.889	15.408	15.408	0.0	0.481	0.449	
8	6	4	15.395	14.120	-14.120	0.0	1.275	0.946	
7	7	4	17.918	18.424	-18.424	0.0	-0.506	-0.407	
5	7	4	23.834	23.127	23.127	0.0	0.707	0.807	
3	7	4	24.088	25.532	25.532	0.0	-1.444	-1.692	
1	7	4	16.900	18.065	-18.065	0.0	-1.165	-1.179	
-1	7	4	18.233	18.674	18.674	0.0	-0.441	-0.471	
-3	7	4	19.640	20.926	20.926	0.0	-1.285	-1.467	
-5	7	4	23.137	22.348	22.348	0.0	0.789	1.023	
-7	7	4	24.620	24.282	-24.282	0.0	0.338	0.422	
-9	7	4	39.820	39.520	39.520	0.0	0.300	0.357	
-11	7	4	16.541	13.865	-13.865	0.0	2.675	2.335	
-12	8	4	38.727	37.817	37.817	0.0	0.910	1.021	
-10	8	4	48.394	49.090	-49.090	0.0	-0.696	-0.732	
0	12	0	209.029	217.361	217.361	0.0	-8.332	-2.668	*
-8	8	4	5.736	4.560	4.560	0.0	1.176	0.491	
-6	8	4	28.394	29.264	29.264	0.0	-0.870	-1.076	
-4	8	4	39.768	39.857	-39.857	0.0	-0.089	-0.113	
-2	8	4	3.721	8.098	-8.098	0.0	-4.377	-1.443	
0	8	4	15.530	16.044	-16.044	0.0	-0.515	-0.467	
2	8	4	56.143	56.112	56.112	0.0	0.032	0.033	
4	8	4	71.306	71.435	-71.435	0.0	-0.129	-0.110	
6	8	4	28.985	28.489	28.489	0.0	0.496	0.581	
8	8	4	12.460	11.479	11.479	0.0	0.980	0.592	
7	9	4	43.294	43.453	-43.453	0.0	-0.159	-0.171	
5	9	4	15.904	14.383	14.383	0.0	1.521	1.391	
3	9	4	23.534	22.402	-22.402	0.0	1.132	1.399	
1	9	4	45.443	44.818	-44.818	0.0	0.625	0.752	
-1	9	4	9.906	8.637	8.637	0.0	1.269	0.897	
-3	9	4	30.191	28.673	-28.673	0.0	1.518	2.007	
-5	9	4	7.608	4.729	4.729	0.0	2.879	1.532	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-7	9	4	49.067	48.138	-48.138	0.0	0.929	1.043	
-9	9	4	38.090	38.552	38.552	0.0	-0.461	-0.531	
-11	9	4	11.329	15.141	-15.141	0.0	-3.812	-1.981	
-10	10	4	15.964	15.803	15.803	0.0	0.161	0.136	
0	12	0	209.149	217.361	217.361	0.0	-8.212	-2.624	*
-8	10	4	22.621	23.386	23.386	0.0	-0.765	-0.786	
-6	10	4	26.821	26.346	26.346	0.0	0.475	0.572	
-4	10	4	35.649	35.555	35.555	0.0	0.094	0.123	
-2	10	4	15.215	15.606	15.606	0.0	-0.390	-0.370	
0	10	4	35.290	35.633	35.633	0.0	-0.343	-0.445	
2	10	4	7.166	8.994	8.994	0.0	-1.828	-0.875	
4	10	4	35.567	37.521	37.521	0.0	-1.954	-2.211	
6	10	4	20.464	20.629	20.629	0.0	-0.165	-0.153	
7	11	4	60.187	60.072	60.072	0.0	0.115	0.105	
5	11	4	19.199	20.153	20.153	0.0	-0.954	-0.822	
3	11	4	73.380	73.489	73.489	0.0	-0.109	-0.091	
1	11	4	58.173	57.885	57.885	0.0	0.288	0.294	
-3	11	4	101.048	99.901	99.901	0.0	1.147	0.736	
-5	11	4	17.574	16.987	16.987	0.0	0.587	0.589	
-7	11	4	117.319	118.404	118.404	0.0	-1.086	-0.604	
-9	11	4	31.164	30.826	-30.826	0.0	0.338	0.392	
-11	11	4	31.359	32.960	32.960	0.0	-1.601	-1.645	
-10	12	4	46.447	46.554	46.554	0.0	-0.108	-0.112	
-8	12	4	28.154	29.250	-29.250	0.0	-1.096	-1.144	
0	12	0	208.700	217.361	217.361	0.0	-8.661	-2.774	*
-6	12	4	43.002	41.489	41.489	0.0	1.513	1.804	
-4	12	4	97.918	96.615	96.615	0.0	1.303	0.861	
-2	12	4	56.323	56.186	-56.186	0.0	0.137	0.141	
0	12	4	45.398	45.259	45.259	0.0	0.140	0.164	
2	12	4	23.205	23.902	-23.902	0.0	-0.698	-0.757	
4	12	4	108.416	109.393	109.393	0.0	-0.977	-0.582	
6	12	4	33.590	33.940	-33.940	0.0	-0.350	-0.368	
5	13	4	11.202	10.911	-10.911	0.0	0.291	0.171	
3	13	4	4.298	5.854	5.854	0.0	-1.556	-0.496	
1	13	4	4.178	3.334	-3.334	0.0	0.844	0.285	
-1	13	4	38.330	39.255	-39.255	0.0	-0.925	-1.133	
-3	13	4	19.483	18.597	18.597	0.0	0.886	0.995	
-5	13	4	18.090	16.506	-16.506	0.0	1.584	1.603	
-7	13	4	47.158	46.742	46.742	0.0	0.416	0.459	
-9	13	4	46.102	45.765	-45.765	0.0	0.337	0.366	
-10	14	4	6.522	6.395	-6.395	0.0	0.127	0.046	
-8	14	4	13.104	12.688	12.688	0.0	0.416	0.283	
-6	14	4	9.697	6.012	-6.012	0.0	3.684	2.321	
-2	14	4	15.477	15.504	15.504	0.0	-0.027	-0.025	
0	12	0	207.307	217.361	217.361	0.0	-10.054	-3.243	*
0	14	4	11.329	11.524	-11.524	0.0	-0.195	-0.133	
2	14	4	8.034	8.693	8.693	0.0	-0.659	-0.321	
4	14	4	9.405	2.565	2.565	0.0	6.840	3.887	
6	14	4	13.980	13.868	13.868	0.0	0.112	0.073	
5	15	4	25.571	25.368	25.368	0.0	0.203	0.201	
3	15	4	4.410	2.405	-2.405	0.0	2.005	0.632	
1	15	4	7.960	10.693	-10.693	0.0	-2.734	-1.281	
-1	15	4	27.248	26.617	26.617	0.0	0.631	0.787	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-3	15	4	16.705	16.132	-16.132	0.0	0.573	0.535	
-5	15	4	23.684	22.867	22.867	0.0	0.817	0.880	
-7	15	4	26.297	26.217	-26.217	0.0	0.080	0.086	
-9	15	4	31.419	32.467	32.467	0.0	-1.048	-1.102	
-8	16	4	3.819	3.323	-3.323	0.0	0.496	0.137	
-6	16	4	15.844	17.625	17.625	0.0	-1.781	-1.336	
-4	16	4	21.610	21.189	-21.189	0.0	0.420	0.428	
-2	16	4	11.913	14.166	-14.166	0.0	-2.253	-1.475	
0	16	4	10.790	8.865	-8.865	0.0	1.925	1.218	
2	16	4	24.388	23.315	23.315	0.0	1.073	1.184	
4	16	4	44.126	45.433	-45.433	0.0	-1.308	-1.344	
3	17	4	11.861	8.875	8.875	0.0	2.986	1.936	
0	12	0	207.075	217.361	217.361	0.0	-10.286	-3.318	*
1	17	4	16.952	18.149	-18.149	0.0	-1.197	-0.993	
-1	17	4	11.044	3.328	3.328	0.0	7.717	5.855	
-3	17	4	16.076	15.392	15.392	0.0	0.684	0.582	
-5	17	4	8.791	6.454	-6.454	0.0	2.337	1.253	
-7	17	4	5.241	9.168	-9.168	0.0	-3.926	-1.197	
-6	18	4	12.849	13.216	13.216	0.0	-0.367	-0.222	
-2	18	4	13.927	13.718	13.718	0.0	0.209	0.150	
0	18	4	6.657	6.524	6.524	0.0	0.133	0.053	
2	18	4	10.131	9.024	9.024	0.0	1.107	0.596	
1	19	4	10.723	7.871	-7.871	0.0	2.851	1.567	
-1	19	4	11.621	7.269	7.269	0.0	4.352	2.980	
-3	19	4	27.630	27.641	-27.641	0.0	-0.011	-0.011	
-5	19	4	14.489	15.826	15.826	0.0	-1.337	-0.911	
-4	20	4	15.357	14.913	-14.913	0.0	0.444	0.322	
-2	20	4	11.217	11.430	11.430	0.0	-0.214	-0.117	
0	20	4	45.331	45.980	-45.980	0.0	-0.649	-0.667	
-3	18	5	55.747	53.593	-53.593	0.0	2.153	2.115	
0	17	5	1.513	2.122	2.122	0.0	-0.610	-0.117	
-2	17	5	60.052	58.740	58.740	0.0	1.312	1.234	
0	12	0	207.172	217.361	217.361	0.0	-10.189	-3.287	*
-4	17	5	9.689	7.833	-7.833	0.0	1.856	0.946	
-6	17	5	10.663	10.864	10.864	0.0	-0.202	-0.106	
-7	16	5	11.119	9.798	9.798	0.0	1.322	0.732	
-5	16	5	34.242	34.147	34.147	0.0	0.094	0.104	
-3	16	5	18.278	15.987	15.987	0.0	2.291	2.026	
-1	16	5	37.327	37.401	37.401	0.0	-0.074	-0.081	
1	16	5	28.978	28.525	28.525	0.0	0.453	0.488	
2	15	5	13.770	13.075	-13.075	0.0	0.695	0.489	
0	15	5	19.004	18.252	18.252	0.0	0.752	0.640	
-2	15	5	24.186	24.980	-24.980	0.0	-0.795	-0.753	
-4	15	5	17.686	17.504	17.504	0.0	0.182	0.155	
-6	15	5	11.157	12.387	12.387	0.0	-1.230	-0.665	
-8	15	5	26.529	27.388	-27.388	0.0	-0.859	-0.819	
-7	14	5	24.103	25.247	25.247	0.0	-1.144	-1.047	
-5	14	5	66.372	65.207	-65.207	0.0	1.165	1.037	
-3	14	5	29.322	29.086	29.086	0.0	0.236	0.263	
-1	14	5	18.974	18.333	-18.333	0.0	0.641	0.564	
1	14	5	23.676	22.264	-22.264	0.0	1.413	1.486	
3	14	5	7.667	7.675	-7.675	0.0	-0.008	-0.003	
0	12	0	206.857	217.361	217.361	0.0	-10.503	-3.396	*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	13	5	26.102	25.625	25.625	0.0	0.477	0.510	
-2	13	5	20.651	19.750	-19.750	0.0	0.901	0.962	
-4	13	5	17.754	16.963	16.963	0.0	0.790	0.694	
-6	13	5	4.380	3.355	3.355	0.0	1.025	0.315	
-8	13	5	9.674	11.580	-11.580	0.0	-1.906	-0.860	
-9	12	5	8.019	8.827	-8.827	0.0	-0.808	-0.331	
-7	12	5	11.591	13.239	13.239	0.0	-1.648	-0.987	
-5	12	5	7.053	7.096	7.096	0.0	-0.043	-0.019	
-1	12	5	6.881	1.182	1.182	0.0	5.699	2.840	
1	12	5	16.795	15.251	15.251	0.0	1.544	1.442	
3	12	5	5.024	9.510	9.510	0.0	-4.486	-1.349	
2	11	5	12.774	13.573	-13.573	0.0	-0.799	-0.531	
0	11	5	9.487	2.711	-2.711	0.0	6.776	4.480	
-2	11	5	10.371	11.485	-11.485	0.0	-1.115	-0.680	
-4	11	5	4.523	0.867	-0.867	0.0	3.656	1.236	
-6	11	5	12.220	9.867	-9.867	0.0	2.353	1.595	
-8	11	5	8.656	2.778	2.778	0.0	5.878	3.008	
0	12	0	209.658	217.361	217.361	0.0	-7.703	-2.455	*
-9	10	5	16.593	16.922	-16.922	0.0	-0.329	-0.240	
-7	10	5	20.554	20.863	20.863	0.0	-0.309	-0.279	
-5	10	5	33.560	32.954	-32.954	0.0	0.607	0.723	
-3	10	5	27.271	28.354	28.354	0.0	-1.084	-1.292	
-1	10	5	14.534	13.915	-13.915	0.0	0.619	0.523	
1	10	5	4.455	1.127	1.127	0.0	3.328	1.117	
5	10	5	7.405	4.717	-4.717	0.0	2.688	1.068	
4	9	5	37.334	37.625	37.625	0.0	-0.291	-0.326	
2	9	5	27.817	28.689	-28.689	0.0	-0.872	-0.979	
0	9	5	34.841	35.599	35.599	0.0	-0.758	-0.920	
-2	9	5	15.327	14.100	-14.100	0.0	1.227	1.085	
-4	9	5	19.341	19.179	19.179	0.0	0.162	0.159	
-6	9	5	7.772	7.804	7.804	0.0	-0.032	-0.015	
-8	9	5	24.201	24.166	-24.166	0.0	0.035	0.037	
-10	9	5	26.784	27.666	27.666	0.0	-0.883	-0.807	
-11	8	5	5.309	1.001	-1.001	0.0	4.308	1.393	
-9	8	5	6.694	2.384	-2.384	0.0	4.310	1.766	
-7	8	5	5.833	2.377	-2.377	0.0	3.456	1.416	
-5	8	5	13.396	12.486	-12.486	0.0	0.910	0.686	
0	12	0	208.392	217.361	217.361	0.0	-8.968	-2.879	*
-1	8	5	12.819	14.135	-14.135	0.0	-1.316	-0.971	
1	8	5	8.701	1.418	1.418	0.0	7.283	4.462	
3	8	5	3.991	6.834	6.834	0.0	-2.843	-0.867	
5	8	5	12.377	14.432	-14.432	0.0	-2.054	-1.158	
6	7	5	8.596	6.324	6.324	0.0	2.272	1.084	
4	7	5	55.956	55.261	-55.261	0.0	0.695	0.693	
2	7	5	59.513	59.151	59.151	0.0	0.362	0.356	
0	7	5	16.885	15.633	-15.633	0.0	1.252	1.169	
-2	7	5	24.590	23.663	23.663	0.0	0.927	1.115	
-4	7	5	26.364	26.709	-26.709	0.0	-0.345	-0.404	
-6	7	5	2.508	2.879	2.879	0.0	-0.371	-0.094	
-8	7	5	36.802	35.974	35.974	0.0	0.829	0.988	
-10	7	5	13.238	11.388	-11.388	0.0	1.850	1.287	
-11	6	5	11.741	10.355	-10.355	0.0	1.386	0.823	
-9	6	5	111.119	111.195	111.195	0.0	-0.076	-0.044	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-7	6	5	9.899	8.899	-8.899	0.0	1.000	0.588	
-5	6	5	71.201	70.035	70.035	0.0	1.167	1.012	
-3	6	5	48.963	48.229	-48.229	0.0	0.734	0.824	
-1	6	5	136.510	136.818	136.818	0.0	-0.308	-0.149	
0	12	0	206.483	217.361	217.361	0.0	-10.878	-3.526	*
1	6	5	42.284	41.734	41.734	0.0	0.549	0.661	
3	6	5	8.791	5.407	5.407	0.0	3.384	1.899	
5	6	5	53.725	54.598	54.598	0.0	-0.873	-0.883	
6	5	5	43.107	42.582	42.582	0.0	0.525	0.548	
4	5	5	34.878	34.792	-34.792	0.0	0.087	0.106	
2	5	5	108.086	109.550	109.550	0.0	-1.464	-0.876	
0	5	5	20.397	19.710	19.710	0.0	0.687	0.771	
-2	5	5	79.558	79.955	79.955	0.0	-0.398	-0.314	
-6	5	5	30.183	29.764	29.764	0.0	0.419	0.509	
-8	5	5	72.774	72.914	72.914	0.0	-0.140	-0.118	
-10	5	5	6.290	6.778	6.778	0.0	-0.488	-0.183	
-11	4	5	2.007	2.690	2.690	0.0	-0.683	-0.141	
-9	4	5	13.815	11.673	11.673	0.0	2.142	1.663	
-5	4	5	8.184	6.482	6.482	0.0	1.703	0.910	
-3	4	5	5.309	5.175	-5.175	0.0	0.134	0.055	
1	4	5	6.005	6.788	6.788	0.0	-0.783	-0.324	
3	4	5	12.130	11.796	11.796	0.0	0.334	0.246	
0	12	0	207.022	217.361	217.361	0.0	-10.339	-3.343	*
5	4	5	12.385	7.552	-7.552	0.0	4.833	3.566	
6	3	5	25.391	25.265	-25.265	0.0	0.126	0.127	
4	3	5	19.775	19.635	19.635	0.0	0.140	0.142	
2	3	5	48.311	48.471	-48.471	0.0	-0.160	-0.176	
0	3	5	16.728	16.885	16.885	0.0	-0.157	-0.152	
-2	3	5	41.130	40.718	-40.718	0.0	0.412	0.514	
-4	3	5	5.444	7.564	7.564	0.0	-2.120	-0.840	
-6	3	5	2.508	4.387	-4.387	0.0	-1.878	-0.482	
-8	3	5	41.056	41.771	-41.771	0.0	-0.715	-0.853	
-10	3	5	27.211	27.486	27.486	0.0	-0.275	-0.285	
-12	3	5	21.340	20.590	-20.590	0.0	0.751	0.630	
-11	2	5	11.629	9.122	9.122	0.0	2.506	1.455	
-9	2	5	17.963	19.235	-19.235	0.0	-1.271	-1.103	
-7	2	5	38.892	37.795	37.795	0.0	1.097	1.331	
-5	2	5	52.639	51.868	-51.868	0.0	0.771	0.837	
-3	2	5	52.699	52.533	52.533	0.0	0.166	0.182	
-1	2	5	3.721	6.561	-6.561	0.0	-2.839	-0.901	
3	2	5	12.018	12.735	12.735	0.0	-0.717	-0.483	
5	2	5	6.043	3.238	3.238	0.0	2.805	1.118	
0	12	0	207.599	217.361	217.361	0.0	-9.762	-3.141	*
6	1	5	15.043	13.680	-13.680	0.0	1.363	0.963	
4	1	5	10.393	12.336	12.336	0.0	-1.943	-1.201	
2	1	5	10.026	7.005	-7.005	0.0	3.021	2.112	
0	1	5	18.997	19.876	19.876	0.0	-0.879	-0.939	
-2	1	5	14.317	13.985	-13.985	0.0	0.331	0.297	
-4	1	5	10.505	12.585	12.585	0.0	-2.080	-1.286	
-10	1	5	6.672	7.554	7.554	0.0	-0.882	-0.341	
-12	1	5	8.319	4.549	-4.549	0.0	3.770	1.736	
-11	0	5	11.381	10.753	10.753	0.0	0.629	0.356	
-9	0	5	10.483	12.186	-12.186	0.0	-1.703	-0.968	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-3	0	5	17.402	16.902	-16.902	0.0	0.500	0.498	
-1	0	5	15.844	15.768	-15.768	0.0	0.076	0.076	
3	0	5	6.866	6.146	-6.146	0.0	0.720	0.342	
5	0	5	9.008	6.711	-6.711	0.0	2.297	1.198	
-10	0	6	92.527	92.503	92.503	0.0	0.023	0.016	
0	12	0	208.722	217.361	217.361	0.0	-8.639	-2.767	*
-8	0	6	30.910	31.855	-31.855	0.0	-0.945	-1.002	
-6	0	6	19.895	21.659	21.659	0.0	-1.764	-1.540	
-4	0	6	102.395	104.096	104.096	0.0	-1.701	-1.066	
-2	0	6	30.131	29.847	29.847	0.0	0.284	0.336	
0	0	6	54.519	54.433	54.433	0.0	0.086	0.087	
2	0	6	32.826	33.217	-33.217	0.0	-0.390	-0.435	
4	0	6	108.565	109.053	109.053	0.0	-0.488	-0.287	
1	1	6	22.636	20.913	20.913	0.0	1.723	1.983	
-1	1	6	8.244	3.179	-3.179	0.0	5.065	2.750	
-3	1	6	69.913	69.539	69.539	0.0	0.374	0.327	
-5	1	6	14.684	14.308	-14.308	0.0	0.376	0.290	
-7	1	6	53.598	53.775	53.775	0.0	-0.178	-0.181	
-9	1	6	31.359	30.729	-30.729	0.0	0.630	0.657	
-10	2	6	6.994	6.780	-6.780	0.0	0.214	0.077	
-8	2	6	1.535	2.115	2.115	0.0	-0.580	-0.114	
-6	2	6	7.772	9.430	-9.430	0.0	-1.658	-0.705	
0	2	6	3.332	7.142	-7.142	0.0	-3.810	-0.998	
0	12	0	207.359	217.361	217.361	0.0	-10.002	-3.226	*
2	2	6	13.313	13.938	-13.938	0.0	-0.625	-0.403	
4	2	6	13.276	11.894	-11.894	0.0	1.382	0.942	
3	3	6	5.189	2.691	2.691	0.0	2.498	0.826	
1	3	6	16.705	16.744	-16.744	0.0	-0.038	-0.030	
-1	3	6	21.512	21.929	21.929	0.0	-0.416	-0.412	
-3	3	6	24.844	24.139	-24.139	0.0	0.705	0.766	
-5	3	6	24.964	24.924	24.924	0.0	0.040	0.041	
-7	3	6	29.015	28.250	-28.250	0.0	0.765	0.818	
-9	3	6	22.059	22.418	22.418	0.0	-0.359	-0.313	
-10	4	6	32.752	33.206	-33.206	0.0	-0.455	-0.471	
-8	4	6	5.840	6.197	6.197	0.0	-0.356	-0.121	
-6	4	6	22.778	24.021	24.021	0.0	-1.244	-1.186	
-4	4	6	3.684	2.605	-2.605	0.0	1.079	0.310	
-2	4	6	3.167	2.141	-2.141	0.0	1.026	0.279	
2	4	6	46.574	47.460	47.460	0.0	-0.886	-0.931	
3	5	6	2.935	2.611	2.611	0.0	0.324	0.079	
1	5	6	25.286	24.611	-24.611	0.0	0.675	0.710	
-1	5	6	6.559	2.738	2.738	0.0	3.821	1.690	
-3	5	6	5.496	4.927	4.927	0.0	0.569	0.212	
0	12	0	206.985	217.361	217.361	0.0	-10.376	-3.355	*
-5	5	6	5.548	5.375	-5.375	0.0	0.174	0.064	
-7	5	6	21.355	19.453	-19.453	0.0	1.902	1.924	
-9	5	6	21.662	23.064	23.064	0.0	-1.402	-1.185	
-10	6	6	6.252	6.651	6.651	0.0	-0.398	-0.136	
-8	6	6	7.593	4.876	-4.876	0.0	2.717	1.130	
-6	6	6	2.067	2.408	2.408	0.0	-0.342	-0.075	
-4	6	6	10.865	9.201	-9.201	0.0	1.664	1.063	
0	6	6	1.760	2.786	2.786	0.0	-1.026	-0.221	
2	6	6	7.563	9.851	-9.851	0.0	-2.289	-0.876	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
1	7	6	10.595	8.824	8.824	0.0	1.771	1.085	
-1	7	6	24.537	25.248	25.248	0.0	-0.710	-0.708	
-3	7	6	20.097	18.665	-18.665	0.0	1.433	1.428	
-5	7	6	26.222	25.959	25.959	0.0	0.263	0.288	
-7	7	6	7.039	2.695	-2.695	0.0	4.344	1.732	
-9	7	6	5.346	6.866	6.866	0.0	-1.520	-0.459	
-8	8	6	14.474	14.280	14.280	0.0	0.194	0.120	
-6	8	6	23.422	24.253	-24.253	0.0	-0.831	-0.787	
0	12	0	207.247	217.361	217.361	0.0	-10.114	-3.263	*
-2	8	6	20.449	19.705	19.705	0.0	0.744	0.715	
0	8	6	52.924	52.357	-52.357	0.0	0.567	0.582	
2	8	6	39.176	39.401	39.401	0.0	-0.225	-0.244	
-1	9	6	16.526	14.373	14.373	0.0	2.153	1.797	
-3	9	6	54.474	54.008	-54.008	0.0	0.465	0.471	
-5	9	6	28.102	27.202	27.202	0.0	0.900	0.977	
-7	9	6	10.520	10.850	-10.850	0.0	-0.329	-0.171	
-9	9	6	6.155	4.660	-4.660	0.0	1.495	0.513	
-8	10	6	10.850	12.550	12.550	0.0	-1.700	-0.808	
-6	10	6	10.213	11.806	11.806	0.0	-1.593	-0.785	
-4	10	6	22.134	22.556	22.556	0.0	-0.422	-0.386	
-2	10	6	18.869	17.356	17.356	0.0	1.514	1.366	
0	10	6	22.269	21.875	21.875	0.0	0.394	0.373	
2	10	6	7.001	0.088	0.088	0.0	6.914	2.806	
1	11	6	17.394	16.873	16.873	0.0	0.522	0.383	
-3	11	6	104.492	104.112	104.112	0.0	0.380	0.232	
-5	11	6	12.362	14.090	-14.090	0.0	-1.728	-0.970	
-7	11	6	48.918	48.870	48.870	0.0	0.048	0.048	
0	12	0	209.718	217.361	217.361	0.0	-7.643	-2.436	*
-6	12	6	32.879	33.126	33.126	0.0	-0.247	-0.254	
-4	12	6	48.244	49.073	49.073	0.0	-0.829	-0.846	
-2	12	6	18.929	19.372	-19.372	0.0	-0.443	-0.374	
0	12	6	51.269	50.975	50.975	0.0	0.294	0.293	
-1	13	6	17.042	16.616	-16.616	0.0	0.426	0.318	
-3	13	6	48.431	49.026	49.026	0.0	-0.595	-0.612	
-5	13	6	35.223	34.641	-34.641	0.0	0.582	0.653	
-4	14	6	4.373	0.079	0.079	0.0	4.294	1.207	
-5	6	7	82.403	81.690	81.690	0.0	0.713	0.526	
-3	6	7	50.423	49.553	-49.553	0.0	0.869	0.873	
-2	5	7	30.962	31.371	31.371	0.0	-0.409	-0.417	
-4	5	7	13.306	14.418	14.418	0.0	-1.113	-0.624	
-6	5	7	27.248	25.946	25.946	0.0	1.302	1.269	
-5	4	7	3.033	8.770	8.770	0.0	-5.738	-1.258	
-3	4	7	9.128	0.554	-0.554	0.0	8.574	4.075	
-1	4	7	2.508	3.582	-3.582	0.0	-1.074	-0.236	
-2	3	7	17.694	17.710	-17.710	0.0	-0.016	-0.012	
-4	3	7	2.875	2.957	-2.957	0.0	-0.082	-0.018	
-6	3	7	1.969	0.948	0.948	0.0	1.022	0.198	
-7	2	7	28.985	28.748	28.748	0.0	0.237	0.221	
0	12	0	207.067	217.361	217.361	0.0	-10.294	-3.321	*
-5	2	7	35.672	36.461	-36.461	0.0	-0.789	-0.829	
-3	2	7	27.682	28.059	28.059	0.0	-0.376	-0.361	
-1	2	7	6.275	3.478	-3.478	0.0	2.797	0.980	
-2	1	7	6.709	7.124	-7.124	0.0	-0.415	-0.144	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-4	1	7	13.231	9.776	9.776	0.0	3.455	2.319
-6	1	7	8.671	0.973	0.973	0.0	7.698	3.521
-7	0	7	0.532	2.037	2.037	0.0	-1.505	-0.244
-5	0	7	3.160	1.479	1.479	0.0	1.681	0.401
-3	0	7	2.883	4.228	-4.228	0.0	-1.345	-0.305
-1	0	7	11.082	12.749	-12.749	0.0	-1.667	-0.831

NA RICHTERITE 400C, 3/13/73

RESULTS OF STRUCTURE FACTOR CALCULATIONS

	NUMERATOR	DENOMINATOR	NUMBER	R
ALL REFLECTIONS				
WEIGHTED R	3083.70	1953309.00	1384	0.040
UNWEIGHTED R	2462.30	55237.83	1384	0.045
RANGES OF F(OBS)				
	1288.50	12972.76	897	0.099
	190.72	12352.72	272	0.015
	73.04	5394.82	69	0.014
	74.37	4258.72	40	0.017
	80.30	3134.29	23	0.026
	17.09	662.42	4	0.026
	704.17	15966.90	77	0.044
	34.17	495.96	2	0.069
RANGES OF (SIN(THETA)/LAMBDA)**2				
	213.50	5156.62	86	0.041
	834.76	20084.05	184	0.042
	201.35	5801.30	146	0.035
	170.09	5114.88	156	0.033
	186.44	4808.66	170	0.039
	256.86	4760.90	202	0.054
	272.25	4723.78	210	0.058
	327.17	4789.40	230	0.068
UNREJECTED REFLECTIONS				
WEIGHTED R	2008.96	1449113.00	1201	0.037
UNWEIGHTED R	1600.09	35842.37	1201	0.045
RANGES OF F(OBS)				
	1223.67	12010.40	833	0.102
	156.30	10952.80	242	0.014
	61.28	4864.08	62	0.013
	59.56	3700.69	35	0.016
	66.62	2854.93	21	0.023
	17.09	662.42	4	0.026
	15.62	797.71	4	0.020
	0.0	0.0	0	0.0
RANGES OF (SIN(THETA)/LAMBDA)**2				
	139.21	3844.05	69	0.036
	122.29	4304.81	97	0.028
	182.24	5394.19	133	0.034
	149.90	4582.30	141	0.033
	179.46	4520.29	160	0.040
	249.27	4369.41	188	0.057
	262.12	4428.30	197	0.059
	315.71	4400.83	216	0.072

SUM FCAL 55733.33

STANDARD DEV OF UNIT WEIGHT OBS 1.35

NA RICHTERITE 400C, 3/13/73

ATOM		PARAMETER	OLD	CHANGE	NEW	ERROR	SHIFT/ERROR
		EXTINCTION CORRECTION	0.0		0.0		
		SCALE FACTOR 1	1.3355	-0.0000	1.3355	0.00325	-0.01
ATOM 1	O(1)	EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 1	1.00000		1.00000		
		X	0.1131963	0.0000002	0.1131964	0.0001677	0.00
		Y	0.9156628	0.0000005	0.9156633	0.0000856	0.01
		Z	0.8952785	0.0000010	0.8952795	0.0003266	0.00
		BETA11	0.0023978	-0.0000006	0.0023972	0.0001717	-0.00
		BETA22	0.0008340	0.0000002	0.0008343	0.0000484	0.00
		BETA33	0.0089840	-0.0000013	0.0089827	0.0006073	-0.00
		BETA12	0.0000893	0.0000000	0.0000893	0.0000678	0.00
		BETA13	0.0008248	0.0000009	0.0008258	0.0002644	0.00
		BETA23	-0.0002546	0.0000006	-0.0002540	0.0001258	0.01
ATOM 2	O(2)	EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 1	1.00000		1.00000		
		X	0.1191695	-0.0000012	0.1191683	0.0001663	-0.01
		Y	0.8324125	-0.0000001	0.8324124	0.0000936	-0.00
		Z	0.3923233	-0.0000020	0.3923212	0.0003267	-0.01
		BETA11	0.0024694	0.0000008	0.0024702	0.0001704	0.00
		BETA22	0.0011146	0.0000006	0.0011151	0.0000508	0.01
		BETA33	0.0098966	-0.0000034	0.0098932	0.0006156	-0.01
		BETA12	0.0001475	0.0000001	0.0001476	0.0000722	0.00
		BETA13	0.0011813	0.0000001	0.0011813	0.0002583	0.00
		BETA23	-0.0004540	0.0000009	-0.0004531	0.0001376	0.01
ATOM 3	F(3)	EQUIPOINT FRACTION = 0.500					
		OCCUPANCY SPECIES 2	1.00000		1.00000		
		X	0.1029299	0.0000021	0.1029321	0.0002239	0.01
		Y	0.0		0.0		
		Z	0.3906509	0.0000048	0.3906557	0.0004148	0.01
		BETA11	0.0045674	0.0000010	0.0045683	0.0002311	0.00
		BETA22	0.0010123	-0.0000018	0.0010104	0.0000596	-0.03
		BETA33	0.0134404	0.0000019	0.0134423	0.0008244	0.00
		BETA12	0.0		0.0		
		BETA13	0.0018481	-0.0000009	0.0018472	0.0003541	-0.00
		BETA23	0.0		0.0		
ATOM 4	O(4)	EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 1	1.00000		1.00000		
		X	0.3613861	0.0000005	0.3613866	0.0001973	0.00
		Y	0.7520770	0.0000003	0.7520773	0.0000978	0.00
		Z	0.5650235	0.0000003	0.5650237	0.0003821	0.00
		BETA11	0.0051101	0.0000001	0.0051101	0.0002087	0.00
		BETA22	0.0009604	0.0000006	0.0009610	0.0000509	0.01
		BETA33	0.0133682	-0.0000039	0.0133643	0.0007484	-0.01
		BETA12	0.0008913	0.0000004	0.0008917	0.0000809	0.00
		BETA13	0.0020737	-0.0000015	0.0020722	0.0003158	-0.00
		BETA23	0.0005332	-0.0000000	0.0005332	0.0001406	-0.00
ATOM 5	O(5)	EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 1	1.00000		1.00000		
		X	0.3476000	-0.0000005	0.3475996	0.0001798	-0.00
		Y	0.8709472	-0.0000003	0.8709469	0.0001021	-0.00
		Z	0.2601048	0.0000003	0.2601051	0.0003415	0.00
		BETA11	0.0034538	-0.0000003	0.0034534	0.0001826	-0.00

		BETA22	0.0013976	0.0000005	0.0013981	0.0000543	0.01
		BETA33	0.0114330	-0.0000010	0.0114320	0.0006739	-0.00
		BETA12	0.0001154	0.0000001	0.0001155	0.0000789	0.00
		BETA13	0.0014381	0.0000006	0.0014387	0.0002783	0.00
		BETA23	0.0018798	0.0000007	0.0018806	0.0001463	0.01
ATOM 6	O(6)	EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 1	1.00000		1.00000		
		X	0.3438634	-0.0000007	0.3438627	0.0001835	-0.00
		Y	0.8821423	0.0000004	0.8821427	0.0001003	0.00
		Z	0.7596895	-0.0000016	0.7596878	0.0003361	-0.00
		BETA11	0.0038270	-0.0000007	0.0038263	0.0001860	-0.00
		BETA22	0.0013899	-0.0000000	0.0013899	0.0000545	-0.00
		BETA33	0.0100329	-0.0000017	0.0100313	0.0006570	-0.00
		BETA12	-0.0001200	0.0000006	-0.0001194	0.0000777	0.01
		BETA13	0.0023632	-0.0000013	0.0023619	0.0002800	-0.00
		BETA23	-0.0016017	-0.0000003	-0.0016020	0.0001454	-0.00
ATOM 7	O(7)	EQUIPOINT FRACTION = 0.500					
		OCCUPANCY SPECIES 1	1.00000		1.00000		
		X	0.3419102	-0.0000000	0.3419102	0.0002612	-0.00
		Y	0.0		0.0		
		Z	0.0487048	-0.0000020	0.0487028	0.0005370	-0.00
		BETA11	0.0037657	-0.0000009	0.0037647	0.0002650	-0.00
		BETA22	0.0005296	0.0000007	0.0005303	0.0000653	0.01
		BETA33	0.0222700	-0.0000068	0.0222631	0.0011576	-0.01
		BETA12	0.0		0.0		
		BETA13	0.0014733	0.0000014	0.0014747	0.0004420	0.00
		BETA23	0.0		0.0		
ATOM 8	T(1)	EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 3	1.00000		1.00000		
		X	0.2803982	0.0000005	0.2803987	0.0000689	0.01
		Y	0.9158736	-0.0000001	0.9158735	0.0000311	-0.00
		Z	0.9857837	-0.0000005	0.9857832	0.0001302	-0.00
		BETA11	0.0022119	-0.0000000	0.0022119	0.0000661	-0.00
		BETA22	0.0005956	-0.0000002	0.0005955	0.0000178	-0.01
		BETA33	0.0070017	-0.0000009	0.0070009	0.0002293	-0.00
		BETA12	0.0000889	-0.0000001	0.0000888	0.0000269	-0.00
		BETA13	0.0011412	-0.0000001	0.0011411	0.0000965	-0.00
		BETA23	-0.0000024	-0.0000003	-0.0000028	0.0000471	-0.01
ATOM 9	T(2)	EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 3	1.00000		1.00000		
		X	0.2872177	0.0000003	0.2872179	0.0000682	0.00
		Y	0.8293691	-0.0000000	0.8293691	0.0000328	-0.00
		Z	0.4867428	0.0000009	0.4867436	0.0001301	0.01
		BETA11	0.0024052	-0.0000008	0.0024044	0.0000663	-0.01
		BETA22	0.0007121	-0.0000000	0.0007121	0.0000176	-0.00
		BETA33	0.0069977	-0.0000003	0.0069975	0.0002216	-0.00
		BETA12	0.0001964	0.0000001	0.0001964	0.0000273	0.00
		BETA13	0.0010355	-0.0000003	0.0010353	0.0000932	-0.00
		BETA23	0.0000379	-0.0000000	0.0000379	0.0000484	-0.00
ATOM 10	M(1)	EQUIPOINT FRACTION = 0.500					
		OCCUPANCY SPECIES 4	1.00000		1.00000		
		X	0.0		0.0		
		Y	0.9108672	-0.0000003	0.9108669	0.0000616	-0.00
		Z	0.5000000		0.5000000		
		BETA11	0.0030742	0.0000005	0.0030748	0.0001216	0.00
		BETA22	0.0008158	-0.0000002	0.0008157	0.0000326	-0.01

		BETA33	0.0085627	-0.0000014	0.0085613	0.0004322	-0.00
		BETA12	0.0		0.0		
		BETA13	0.0014790	-0.0000011	0.0014778	0.0001835	-0.01
		BETA23	0.0		0.0		
ATOM 11	M(2)	EQUIPOINT FRACTION = 0.500					
		OCCUPANCY SPECIES 4	1.00000		1.00000		
		X	0.0		0.0		
		Y	0.8205556	0.0000008	0.8205563	0.0000612	0.01
		Z	0.0		0.0		
		BETA11	0.0030517	-0.0000000	0.0030517	0.0001228	-0.00
		BETA22	0.0008432	-0.0000004	0.0008428	0.0000339	-0.01
		BETA33	0.0105584	-0.0000017	0.0105567	0.0004413	-0.00
		BETA12	0.0		0.0		
		BETA13	0.0014389	0.0000001	0.0014390	0.0001831	0.00
		BETA23	0.0		0.0		
ATOM 12	M(3)	EQUIPOINT FRACTION = 0.250					
		OCCUPANCY SPECIES 4	1.00000		1.00000		
		X	0.0		0.0		
		Y	0.0		0.0		
		Z	0.0		0.0		
		BETA11	0.0030760	0.0000001	0.0030761	0.0001658	0.00
		BETA22	0.0006463	-0.0000002	0.0006461	0.0000437	-0.01
		BETA33	0.0084178	-0.0000011	0.0084167	0.0005940	-0.00
		BETA12	0.0		0.0		
		BETA13	0.0018572	-0.0000001	0.0018572	0.0002533	-0.00
		BETA23	0.0		0.0		
ATOM 13	M(4)	EQUIPOINT FRACTION = 0.500					
		OCCUPANCY SPECIES 5	0.50000		0.50000		
		OCCUPANCY SPECIES 6	0.50000		0.50000		
		TOTAL OCCUPANCY (FIXED) =	1.00000				
		X	0.0		0.0		
		Y	0.7239429	-0.0000002	0.7239426	0.0000581	-0.00
		Z	0.5000000		0.5000000		
		BETA11	0.0072852	-0.0000011	0.0072841	0.0001321	-0.01
		BETA22	0.0011041	0.0000001	0.0011042	0.0000300	0.00
		BETA33	0.0141938	0.0000006	0.0141944	0.0004078	0.00
		BETA12	0.0		0.0		
		BETA13	-0.0016560	0.0000014	-0.0016546	0.0001785	0.01
		BETA23	0.0		0.0		
ATOM 14	A	EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 6	0.25000		0.25000		
		X	0.4716316	-0.0001199	0.4715117	0.0012070	-0.10
		Y	0.9887244	-0.0002624	0.9884620	0.0011939	-0.22
		Z	0.5399881	0.0000019	0.5399900	0.0026564	0.00
		BETA11	0.0176811	-0.0001475	0.0175336	0.0018934	-0.08
		BETA22	0.0040983	-0.0001819	0.0039164	0.0007764	-0.23
		BETA33	0.0486258	0.0000126	0.0486384	0.0056943	0.00
		BETA12	-0.0040281	0.0002754	-0.0037527	0.0011632	0.24
		BETA13	-0.0143386	0.0000573	-0.0142814	0.0022274	0.03
		BETA23	-0.0000530	0.0000426	-0.0000105	0.0013136	0.03

MAXIMUM SHIFT/ERROR = 0.24

AVERAGE SHIFT/ERROR = 0.01

NA RICHTERITE 600 C, JUNE, 1973 STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	12	0	206.015	211.538	211.538	0.0	-5.522	-1.791	*
4	0	0	4.473	12.218	12.218	0.0	-7.745	-5.119	
6	0	0	101.486	99.455	99.455	0.0	2.032	1.314	
8	0	0	99.676	103.900	103.900	0.0	-4.225	-2.747	
10	0	0	64.874	64.080	64.080	0.0	0.794	0.727	
12	0	0	20.043	20.460	-20.460	0.0	-0.418	-0.348	
13	1	0	28.294	26.807	-26.807	0.0	1.488	1.304	
11	1	0	56.051	56.064	56.064	0.0	-0.012	-0.012	
9	1	0	19.968	21.907	21.907	0.0	-1.939	-1.938	
7	1	0	76.747	77.151	77.151	0.0	-0.404	-0.337	
5	1	0	106.563	104.829	-104.829	0.0	1.734	1.076	
3	1	0	146.450	151.467	151.467	0.0	-5.017	-2.290	
-3	1	0	145.259	151.467	151.467	0.0	-6.207	-2.854	*
-5	1	0	106.836	104.829	-104.829	0.0	2.007	1.245	*
-7	1	0	77.128	77.151	77.151	0.0	-0.024	-0.020	*
-9	1	0	20.729	21.907	21.907	0.0	-1.179	-1.261	*
-11	1	0	56.986	56.064	56.064	0.0	0.922	0.929	*
-13	1	0	28.055	26.807	-26.807	0.0	1.248	1.170	*
-12	2	0	8.111	10.756	10.756	0.0	-2.645	-1.107	*
-10	2	0	3.861	3.562	-3.562	0.0	0.299	0.095	*
-8	2	0	14.867	10.436	-10.436	0.0	4.430	4.321	*
0	12	0	206.652	211.538	211.538	0.0	-4.886	-1.580	*
-6	2	0	31.817	32.277	-32.277	0.0	-0.460	-0.654	*
-4	2	0	10.402	11.823	-11.823	0.0	-1.421	-1.772	*
4	2	0	10.137	11.823	-11.823	0.0	-1.686	-1.999	
6	2	0	32.627	32.277	-32.277	0.0	0.351	0.511	
8	2	0	9.575	10.436	-10.436	0.0	-0.862	-0.472	
10	2	0	3.216	3.562	-3.562	0.0	-0.346	-0.098	
12	2	0	9.732	10.756	10.756	0.0	-1.024	-0.506	
13	3	0	15.189	12.406	12.406	0.0	2.783	1.781	
11	3	0	18.025	16.942	-16.942	0.0	1.083	1.056	
9	3	0	18.356	18.883	18.883	0.0	-0.527	-0.550	
7	3	0	51.074	51.600	-51.600	0.0	-0.526	-0.589	
5	3	0	61.715	61.340	61.340	0.0	0.376	0.385	
3	3	0	79.955	81.434	-81.434	0.0	-1.478	-1.216	
-3	3	0	78.839	81.434	-81.434	0.0	-2.595	-2.164	*
-5	3	0	60.922	61.340	61.340	0.0	-0.418	-0.436	*
-7	3	0	51.049	51.600	-51.600	0.0	-0.551	-0.628	*
-9	3	0	19.067	18.883	18.883	0.0	0.184	0.197	*
-11	3	0	16.644	16.942	-16.942	0.0	-0.298	-0.245	*
-13	3	0	13.866	12.406	12.406	0.0	1.460	0.901	*
-12	4	0	18.794	18.042	18.042	0.0	0.752	0.627	*
0	12	0	207.462	211.538	211.538	0.0	-4.075	-1.314	*
-10	4	0	1.083	4.411	-4.411	0.0	-3.328	-0.662	*
-8	4	0	11.047	7.236	7.236	0.0	3.811	2.743	*
-4	4	0	10.807	8.178	8.178	0.0	2.629	3.572	*
-2	4	0	124.993	129.333	129.333	0.0	-4.340	-2.322	*
2	4	0	126.548	129.333	129.333	0.0	-2.785	-1.471	
4	4	0	9.079	8.178	8.178	0.0	0.901	0.964	
6	4	0	4.366	6.738	6.738	0.0	-2.373	-0.935	
8	4	0	11.204	7.236	7.236	0.0	3.968	2.926	
10	4	0	8.723	4.411	-4.411	0.0	4.312	2.426	
12	4	0	20.555	18.042	18.042	0.0	2.513	2.156	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
11	5	0	17.413	16.340	-16.340	0.0	1.074	0.914	
9	5	0	6.152	1.089	1.089	0.0	5.062	2.310	
7	5	0	7.227	5.348	-5.348	0.0	1.878	0.912	
5	5	0	5.019	6.559	-6.559	0.0	-1.540	-0.810	
3	5	0	72.754	71.648	-71.648	0.0	1.106	0.991	
1	5	0	1.753	0.586	-0.586	0.0	1.167	0.436	
-3	5	0	72.183	71.648	-71.648	0.0	0.535	0.483	*
0	12	0	206.933	211.538	211.538	0.0	-4.604	-1.485	*
-7	5	0	9.914	5.348	-5.348	0.0	4.566	3.210	*
-11	5	0	16.735	16.340	-16.340	0.0	0.396	0.311	*
-12	6	0	4.242	4.201	-4.201	0.0	0.041	0.012	*
-10	6	0	16.239	17.228	17.228	0.0	-0.989	-0.848	*
-8	6	0	21.738	22.448	-22.448	0.0	-0.710	-0.818	*
-6	6	0	5.002	5.917	5.917	0.0	-0.915	-0.381	*
-4	6	0	5.226	5.154	-5.154	0.0	0.072	0.040	*
-2	6	0	10.294	9.530	9.530	0.0	0.764	0.906	*
0	6	0	4.085	0.775	-0.775	0.0	3.309	1.888	
2	6	0	9.244	9.530	9.530	0.0	-0.286	-0.314	
4	6	0	4.085	5.154	-5.154	0.0	-1.069	-0.509	
6	6	0	2.001	5.917	5.917	0.0	-3.916	-0.997	
8	6	0	21.878	22.448	-22.448	0.0	-0.570	-0.703	
10	6	0	14.503	17.228	17.228	0.0	-2.725	-2.047	
12	6	0	11.088	4.201	-4.201	0.0	6.887	3.967	
11	7	0	12.403	9.634	-9.634	0.0	2.768	1.830	
9	7	0	46.105	46.120	46.120	0.0	-0.016	-0.018	
7	7	0	38.845	37.817	-37.817	0.0	1.028	1.309	
5	7	0	19.389	20.273	20.273	0.0	-0.884	-1.090	
0	12	0	207.371	211.538	211.538	0.0	-4.166	-1.344	*
3	7	0	60.376	57.503	57.503	0.0	2.873	3.022	
1	7	0	8.508	6.098	-6.098	0.0	2.410	2.603	
-1	7	0	7.508	6.098	-6.098	0.0	1.410	1.353	*
-3	7	0	59.408	57.503	57.503	0.0	1.906	2.040	*
-5	7	0	20.448	20.273	20.273	0.0	0.175	0.230	*
-7	7	0	37.621	37.817	-37.817	0.0	-0.195	-0.244	*
-9	7	0	47.651	46.120	46.120	0.0	1.530	1.714	*
-11	7	0	13.263	9.634	-9.634	0.0	3.628	2.692	*
-12	8	0	34.769	33.022	33.022	0.0	1.746	1.869	*
-10	8	0	52.686	52.540	-52.540	0.0	0.146	0.151	*
-6	8	0	58.722	58.841	58.841	0.0	-0.119	-0.122	*
-4	8	0	107.861	109.274	-109.274	0.0	-1.413	-0.863	*
-2	8	0	28.551	30.537	30.537	0.0	-1.986	-3.431	*
0	8	0	41.524	36.214	36.214	0.0	5.310	7.737	
2	8	0	28.270	30.537	30.537	0.0	-2.267	-3.862	
4	8	0	107.919	109.274	-109.274	0.0	-1.355	-0.828	
6	8	0	59.499	58.841	58.841	0.0	0.658	0.669	
8	8	0	2.332	0.046	-0.046	0.0	2.285	0.578	
10	8	0	52.389	52.540	-52.540	0.0	-0.152	-0.156	
0	12	0	207.983	211.538	211.538	0.0	-3.554	-1.143	*
12	8	0	35.215	33.022	33.022	0.0	2.193	2.326	
11	9	0	8.607	6.849	-6.849	0.0	1.759	0.782	
9	9	0	31.908	31.669	31.669	0.0	0.238	0.291	
7	9	0	91.969	92.366	-92.366	0.0	-0.396	-0.277	
5	9	0	20.985	22.490	22.490	0.0	-1.505	-1.717	