H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
2	6	6	8.986	10.025	-10.025	0.0	-1.039	-0.277	
-9	7	6	7.140	6.243	6.243	0.0	0.897	0.189	
-5	7	6	21.649	21.613	21.613	0.0	0.036	0.018	
-3	7	6	16.719	17.576	-17.576	0.0	-0.856	-0.338	
-1	7	6	28.360	27.053	27.053	0.0	1.308	0.929	
-8	8	6	8.459	15.425	15.425	0.0	-6.966	-1.524	
-6	8	6	25.079	23.890	-23.890	0.0	1.189	0.685	
-4	8	6	10.816	11.376	11.376	0.0	-0.559	-0.155	
-2	8	6	12.136	5.669	5.669	0.0	6.466	2.522	
0	8	6	41.996	40.206	-40.206	0.0	1.790	1.305	
0	12	0	208.316	210.970	210.970	0.0	-2.654	-0.839	*
2	8	6	37.907	38.945	38.945	0.0	-1.038	-0.570	
-7	9	6	7.832	4.822	-4.822	0.0	3.010	0.728	
-5	9	6	21.006	23.104	23.104	0.0	-2.097	-0.972	
-3	9	6	45.525	47.137	-47.137	0.0	-1.612	-0.996	
-1	9	6	19.341	20.672	20.672	0.0	-1.331	-0.547	
1	9	6	10.272	12.719	-12.719	0.0	-2.446	-0.653	
-8	10	6	9.613	9.114	9.114	0.0	0.499	0.136	
-6	10	6	11.311	12.347	12.347	0.0	-1.036	-0.323	
-4	10	6	22.424	21.875	21.875	0.0	0.549	0.347	
-2	10	6	17.544	20.789	20.789	0.0	-3.245	-1.163	
0	10	6	20.594	20.708	20.708	0.0	-0.114	-0.050	
2	10	6	4.963	2.305	2.305	0.0	2.658	0.536	
-7	11	6	38.253	38.514	38.514	0.0	-0.261	-0.155	
-5	11	6	13.999	13.744	-13.744	0.0	0.255	0.093	
-3	11	6	96.721	98.685	98.685	0.0	-1.963	-1.069	
1	11	6	23.991	26.074	26.074	0.0	-2.083	-0.954	
-6	12	6	35.384	35.811	35.811	0.0	-0.426	-0.277	
-4	12	6	26.876	27.060	27.060	0.0	-0.183	-0.107	
0	12	0	208.151	210.970	210.970	0.0	-2.819	-0.891	*
-2	12	6	8.376	6.379	-6.379	0.0	1.997	0.574	
0	12	6	44.799	44.290	44.290	0.0	0.509	0.338	
-5	13	6	29.003	29.758	-29.758	0.0	-0.755	-0.404	
-3	13	6	46.333	46.721	46.721	0.0	-0.389	-0.252	
-1	13	6	20.611	21.299	-21.299	0.0	-0.688	-0.290	
-2	14	6	11.575	7.421	7.421	0.0	4.154	1.326	
-7	0	7	7.238	5.623	5.623	0.0	1.615	0.363	
-5	0	7	7.074	2.404	2.404	0.0	4.670	1.261	
-3	0	7	4.023	4.192	-4.192	0.0	-0.169	-0.027	
-1	0	7	11.295	11.234	-11.234	0.0	0.060	0.017	
-7	2	7	24.123	20.529	20.529	0.0	3.594	2.028	
-5	2	7	33.768	32.893	-32.893	0.0	0.876	0.548	
-3	2	7	29.152	30.460	30.460	0.0	-1.308	-0.682	
-1	2	7	12.070	9.628	-9.628	0.0	2.442	0.783	
0	12	0	208.513	210.970	210.970	0.0	-2.456	-0.775	*
-4	3	7	10.256	8.092	-8.092	0.0	2.164	0.664	
-2	3	7	2.407	11.489	-11.489	0.0	-9.082	-1.080	

K-RICHTERITE 600C 1/24/73

RESULTS OF STRUCTURE FACTOR CALCULATIONS

ALL REFLECTIONS	NUMERATOR	DENOMINATOR	NUMBER	R
WEIGHTED R	2671.33	1192863.00	1319	0.047
UNWEIGHTED R	2939.57	54111.63	1319	0.054
RANGES OF F(OBS)				
	2189.88	14770.51	893	0.148
	273.32	11077.96	232	0.025
	99.82	6162.16	73	0.016
	58.94	3559.71	29	0.017
	35.23	1680.69	11	0.021
	148.02	6973.66	34	0.021
	132.05	9610.90	46	0.014
	2.36	276.66	1	0.009
RANGES OF (SIN(THETA)/LAMBDA)**2				
	218.16	5385.06	84	0.041
	460.92	20533.92	188	0.022
	294.93	5736.63	150	0.051
	259.00	5015.84	154	0.052
	339.20	4633.55	168	0.073
	410.44	4240.02	187	0.097
	441.41	4318.27	189	0.102
	515.59	4250.00	199	0.121
UNREJECTED REFLECTIONS				
WEIGHTED R	1758.37	780118.75	1133	0.047
UNWEIGHTED R	2358.45	35067.94	1133	0.067
RANGES OF F(OBS)				
	1932.96	13350.93	817	0.145
	226.21	9900.69	208	0.023
	83.79	5508.39	65	0.015
	45.56	2919.53	24	0.016
	35.23	1680.69	11	0.021
	15.12	777.50	4	0.019
	17.25	654.07	3	0.026
	2.36	276.66	1	0.009
RANGES OF (SIN(THETA)/LAMBDA)**2				
	161.56	4455.02	69	0.036
	182.99	4757.42	101	0.038
	264.86	5268.48	136	0.050
	241.67	4569.93	142	0.053
	306.11	4273.59	155	0.072
	355.48	3884.57	172	0.092
	372.74	3937.88	173	0.095
	473.11	3922.71	185	0.121

SUM FCAL 54008.74
STANDARD DEV OF UNIT WEIGHT OBS 1.31

K-RICHTERITE 6000 1/24/73

ATOM	PARAMETER	OLD	CHANGE	NEW	ERROR	SHIFT/ERROR
	EXTINCTION CORRECTION	0.0		0.0		
	SCALE FACTOR 1	0.6065	0.0000	0.6065	0.00178	0.01
ATOM 1 O(1)	EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.1104516	-0.0000061	0.1104454	0.0002823	-0.02
	Y	0.9147131	0.0000027	0.9147158	0.0001473	0.02
	Z	0.8914194	0.0000151	0.8914344	0.0005260	0.03
	BETA11	0.0033418	0.0000140	0.0033558	0.0003060	0.05
	BETA22	0.0011902	-0.0000012	0.0011890	0.0000875	-0.01
	BETA33	0.0117504	0.0000183	0.0117687	0.0011143	0.02
	BETA12	0.0001990	0.0000001	0.0001991	0.0001239	0.00
	BETA13	0.0008819	-0.0000320	0.0008499	0.0004622	-0.07
	BETA23	-0.0006424	-0.0000012	-0.0006437	0.0002271	-0.01
ATOM 2 O(2)	EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.1186472	0.0000025	0.1186497	0.0002801	0.01
	Y	0.8308489	-0.0000009	0.8308479	0.0001539	-0.01
	Z	0.3922855	-0.0000027	0.3922827	0.0005277	-0.01
	BETA11	0.0028470	-0.0000046	0.0028423	0.0002975	-0.02
	BETA22	0.0014607	0.0000004	0.0014611	0.0000903	0.00
	BETA33	0.0107164	-0.0000043	0.0107121	0.0010710	-0.00
	BETA12	0.0002126	-0.0000003	0.0002122	0.0001241	-0.00
	BETA13	0.0012015	0.0000286	0.0012300	0.0004411	0.06
	BETA23	-0.0006457	0.0000051	-0.0006407	0.0002317	0.02
ATOM 3 F(3)	EQUIPOINT FRACTION = 0.500					
	OCCUPANCY SPECIES 2	1.00000		1.00000		
	X	0.1025367	0.0000079	0.1025446	0.0003769	0.02
	Y	0.0		0.0		
	Z	0.3874061	-0.0000098	0.3873963	0.0006593	-0.01
	BETA11	0.0056564	-0.0000201	0.0056363	0.0004251	-0.05
	BETA22	0.0016507	0.0000021	0.0016527	0.0001141	0.02
	BETA33	0.0136620	0.0000018	0.0136638	0.0014075	0.00
	BETA12	0.0		0.0		
	BETA13	0.0013755	0.0000405	0.0014160	0.0006132	0.07
	BETA23	0.0		0.0		
ATOM 4 O(4)	EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.3614950	0.0000027	0.3614977	0.0003476	0.01
	Y	0.7531439	-0.0000007	0.7531432	0.0001641	-0.00
	Z	0.5593535	-0.0000037	0.5593497	0.0006586	-0.01
	BETA11	0.0067035	0.0000019	0.0067054	0.0003908	0.00
	BETA22	0.0012106	0.0000000	0.0012106	0.0000876	0.00
	BETA33	0.0193784	0.0000085	0.0193869	0.0013138	0.01
	BETA12	0.0011990	0.0000002	0.0011992	0.0001455	0.00
	BETA13	0.0028457	-0.0000031	0.0028426	0.0005691	-0.01
	BETA23	0.0004639	-0.0000022	0.0004617	0.0002615	-0.01
ATOM 5 O(5)	EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.3432378	-0.0000070	0.3432308	0.0003018	-0.02
	Y	0.8716636	0.0000032	0.8716667	0.0001604	0.02
	Z	0.2502073	0.0000118	0.2502190	0.0005642	0.02
	BETA11	0.0038519	-0.0000125	0.0038395	0.0003274	-0.04

BETA22	0.0017134	0.0000013	0.0017146	0.0000945	0.01
BETA33	0.0134349	0.0000108	0.0134458	0.0011212	0.01
BETA12	0.0002411	-0.0000015	0.0002396	0.0001352	-0.01
BETA13	0.0014925	0.0000023	0.0014948	0.0004740	0.00
BETA23	0.0017477	0.0000033	0.0017510	0.0002571	0.01
ATOM 6 U(6) EQUIPOINT FRACTION = 1.000					
OCCUPANCY SPECIES 1	1.00000		1.00000		
X	0.3395632	-0.0000052	0.3395580	0.0003074	-0.02
Y	0.8819065	0.0000028	0.8819093	0.0001617	0.02
Z	0.7517768	0.0000126	0.7517894	0.0005507	0.02
BETA11	0.0044371	-0.0000096	0.0044275	0.0003385	-0.03
BETA22	0.0017604	0.0000014	0.0017618	0.0000949	0.01
BETA33	0.0123918	0.0000070	0.0123988	0.0010921	0.01
BETA12	-0.0002242	-0.0000021	-0.0002263	0.0001378	-0.01
BETA13	0.0029583	0.0000239	0.0029822	0.0004729	0.05
BETA23	-0.0019737	0.0000009	-0.0019728	0.0002636	0.00
ATOM 7 U(7) EQUIPOINT FRACTION = 0.500					
OCCUPANCY SPECIES 1	1.00000		1.00000		
X	0.3330688	0.0000075	0.3330762	0.0004586	0.02
Y	0.0		0.0		
Z	0.0286837	0.0000067	0.0286904	0.0009064	0.01
BETA11	0.0049632	0.0000115	0.0049747	0.0004854	0.02
BETA22	0.0007326	-0.0000014	0.0007313	0.0001117	-0.01
BETA33	0.0245996	-0.0000041	0.0245955	0.0018687	-0.00
BETA12	0.0		0.0		
BETA13	0.0012709	-0.0000324	0.0012385	0.0007449	-0.04
BETA23	0.0		0.0		
ATOM 8 T(1) EQUIPOINT FRACTION = 1.000					
OCCUPANCY SPECIES 3	1.00000		1.00000		
X	0.2753478	0.0000027	0.2753505	0.0001153	0.02
Y	0.9155345	0.0000002	0.9155347	0.0000526	0.00
Z	0.9768988	-0.0000049	0.9768940	0.0002142	-0.02
BETA11	0.0025957	0.0000033	0.0025990	0.0001094	0.03
BETA22	0.0007477	-0.0000001	0.0007476	0.0000302	-0.00
BETA33	0.0086199	0.0000002	0.0086201	0.0003773	0.00
BETA12	0.0000142	0.0000001	0.0000142	0.0000464	0.00
BETA13	0.0008002	-0.0000073	0.0007928	0.0001569	-0.05
BETA23	-0.0000679	0.0000010	-0.0000670	0.0000846	0.01
ATOM 9 T(2) EQUIPOINT FRACTION = 1.000					
OCCUPANCY SPECIES 3	1.00000		1.00000		
X	0.2851254	-0.0000032	0.2851222	0.0001179	-0.03
Y	0.8291326	-0.0000007	0.8291318	0.0000541	-0.01
Z	0.4805529	0.0000036	0.4805564	0.0002158	0.02
BETA11	0.0028816	0.0000000	0.0028816	0.0001124	0.00
BETA22	0.0008536	0.0000001	0.0008537	0.0000301	0.00
BETA33	0.0086769	0.0000003	0.0086772	0.0003752	0.00
BETA12	0.0002710	0.0000010	0.0002720	0.0000466	0.02
BETA13	0.0012244	0.0000044	0.0012288	0.0001593	0.03
BETA23	0.0002159	-0.0000023	0.0002137	0.0000848	-0.03
ATOM 10 M(1) EQUIPOINT FRACTION = 0.500					
OCCUPANCY SPECIES 4	1.00000		1.00000		
X	0.0		0.0		
Y	0.9100387	0.0000000	0.9100387	0.0001050	0.00
Z	0.5000000		0.5000000		
BETA11	0.0036948	-0.0000098	0.0036850	0.0002131	-0.05
BETA22	0.0010932	0.0000012	0.0010944	0.0000581	0.02

Atom	Parameter	Old value	Shift	New value	Error	Shift/Error
	BETA33	0.0115938	-0.0000124	0.0115814	0.0007415	-0.02
	BETA12	0.0		0.0		
	BETA13	0.0016112	0.0000241	0.0016353	0.0003137	0.08
	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	0.8196930	-0.0000005	0.8196925	0.0001020	-0.00
	Z	0.0		0.0		
	BETA11	0.0038250	0.0000095	0.0038346	0.0002175	0.04
	BETA22	0.0010264	-0.0000004	0.0010260	0.0000585	-0.01
	BETA33	0.0123412	0.0000074	0.0123486	0.0007424	0.01
	BETA12	0.0		0.0		
	BETA13	0.0004652	-0.0000208	0.0004444	0.0003125	-0.07
	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	0.0038861	0.0000018	0.0038879	0.0003000	0.01
	BETA22	0.0009041	0.0000001	0.0009042	0.0000774	0.00
	BETA33	0.0102634	0.0000238	0.0102872	0.0010020	0.02
	BETA12	0.0		0.0		
	BETA13	0.0027743	-0.0000191	0.0027552	0.0004363	-0.04
	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	0.7217319	0.0000002	0.7217320	0.0000978	0.00
	Z	0.5000000		0.5000000		
	BETA11	0.0085775	-0.0000051	0.0085724	0.0002441	-0.02
	BETA22	0.0013912	0.0000003	0.0013915	0.0000536	0.01
	BETA33	0.0180245	0.0000052	0.0180296	0.0007033	0.01
	BETA12	0.0		0.0		
	BETA13	-0.0025636	0.0000066	-0.0025570	0.0003209	0.02
	BETA23	0.0		0.0		
ATOM 14 A	EQUIPOINT FRACTION = 0.500					
	OCCUPANCY SPECIES 7	0.50000		0.50000		
	X	0.4756192	0.0002923	0.4759115	0.0014954	0.19
	Y	0.0		0.0		
	Z	0.5272543	-0.0004057	0.5268487	0.0041311	-0.10
	BETA11	0.0152012	0.0004831	0.0156843	0.0020173	0.24
	BETA22	0.0033870	-0.0000086	0.0033784	0.0001248	-0.07
	BETA33	0.0454191	0.0006947	0.0461138	0.0058411	0.12
	BETA12	0.0		0.0		
	BETA13	-0.0109371	-0.0006001	-0.0115371	0.0023317	-0.26
	BETA23	0.0		0.0		

MAXIMUM SHIFT/ERROR = -0.26

AVERAGE SHIFT/ERROR = 0.03

K-RICHTERITE 800C, 3/6/73

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	12	0	199.934	202.599	202.599	0.0	-2.666	-0.886	*
4	0	0	11.987	41.305	41.305	0.0	-29.318	-63.204	*
6	0	0	39.492	86.579	86.579	0.0	-47.087	-66.221	*
8	0	0	44.337	102.030	102.030	0.0	-57.693	-71.700	*
10	0	0	75.340	51.346	51.346	0.0	23.994	15.030	*
12	0	0	7.381	5.059	-5.059	0.0	2.321	0.507	
13	1	0	27.308	27.863	-27.863	0.0	-0.555	-0.264	
11	1	0	50.941	50.915	50.915	0.0	0.025	0.019	
9	1	0	17.546	19.735	19.735	0.0	-2.189	-1.063	
7	1	0	71.748	72.999	72.999	0.0	-1.251	-1.021	
5	1	0	117.824	115.077	-115.077	0.0	2.746	1.528	
3	1	0	137.865	136.924	136.924	0.0	0.940	0.454	
-3	1	0	136.219	136.924	136.924	0.0	-0.705	-0.344	*
-5	1	0	116.271	115.077	-115.077	0.0	1.194	0.671	*
-7	1	0	71.168	72.999	72.999	0.0	-1.831	-1.497	*
-9	1	0	18.861	19.735	19.735	0.0	-0.874	-0.458	*
-11	1	0	49.098	50.915	50.915	0.0	-1.817	-1.185	*
-13	1	0	24.751	27.863	-27.863	0.0	-3.112	-0.961	*
-12	2	0	9.824	13.696	13.696	0.0	-3.872	-0.723	*
-10	2	0	3.882	3.988	-3.988	0.0	-0.106	-0.018	*
-8	2	0	11.201	11.096	-11.096	0.0	0.105	0.039	*
0	12	0	199.261	202.599	202.599	0.0	-3.339	-1.114	*
-6	2	0	29.668	30.966	-30.966	0.0	-1.297	-1.208	*
-4	2	0	4.948	2.452	2.452	0.0	2.496	1.056	*
4	2	0	8.457	2.452	2.452	0.0	6.006	4.726	
6	2	0	30.859	30.966	-30.966	0.0	-0.107	-0.113	
8	2	0	14.109	11.096	-11.096	0.0	3.014	1.720	
10	2	0	6.304	3.988	-3.988	0.0	2.316	0.603	
12	2	0	3.9[illegible]	13.696	13.696	0.0	-9.731	-1.314	
13	3	0	17.629	16.896	16.896	0.0	0.734	0.282	
11	3	0	20.258	18.068	-18.068	0.0	2.190	1.200	
9	3	0	17.049	16.010	16.010	0.0	1.039	0.577	
7	3	0	53.912	53.400	-53.400	0.0	0.512	0.488	
5	3	0	58.208	56.661	56.661	0.0	1.547	1.557	
3	3	0	85.485	87.398	-87.398	0.0	-1.914	-1.452	
-3	3	0	84.180	87.398	-87.398	0.0	-3.218	-2.473	*
-5	3	0	57.193	56.661	56.661	0.0	0.532	0.547	*
-7	3	0	52.659	53.400	-53.400	0.0	-0.740	-0.692	*
-9	3	0	20.051	16.010	16.010	0.0	4.041	2.500	*
-11	3	0	19.430	18.068	-18.068	0.0	1.362	0.549	*
-13	3	0	7.878	16.896	16.896	0.0	-9.018	-1.238	*
-12	4	0	8.375	8.319	8.319	0.0	0.056	0.010	*
0	12	0	198.484	202.599	202.599	0.0	-4.115	-1.377	*
-8	4	0	12.153	2.721	2.721	0.0	9.432	4.308	*
-6	4	0	11.045	13.319	13.319	0.0	-2.274	-0.853	*
-4	4	0	7.888	7.784	7.784	0.0	0.104	0.052	*
-2	4	0	136.715	143.150	143.150	0.0	-6.435	-3.134	*
2	4	0	138.506	143.150	143.150	0.0	-4.644	-2.233	
4	4	0	10.528	7.784	7.784	0.0	2.744	2.189	
6	4	0	14.213	13.319	13.319	0.0	0.894	0.492	
8	4	0	6.118	2.721	2.721	0.0	3.397	0.875	
12	4	0	11.542	8.319	8.319	0.0	3.223	0.991	
13	5	0	16.646	19.563	19.563	0.0	-2.917	-0.899	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
11	5	0	13.198	15.360	-15.360	0.0	-2.162	-0.663	
7	5	0	7.557	4.021	-4.021	0.0	3.536	1.167	
3	5	0	77.949	78.259	-78.259	0.0	-0.310	-0.254	
1	5	0	14.410	17.164	-17.164	0.0	-2.754	-2.732	
-1	5	0	14.037	17.164	-17.164	0.0	-3.127	-2.896	*
-3	5	0	77.793	78.259	-78.259	0.0	-0.465	-0.384	*
0	12	0	199.240	202.599	202.599	0.0	-3.359	-1.120	*
-5	5	0	6.801	13.788	-13.788	0.0	-6.987	-2.219	*
-7	5	0	8.758	4.021	-4.021	0.0	4.737	1.681	*
-11	5	0	17.660	15.360	-15.360	0.0	2.300	0.834	*
-13	5	0	6.646	19.563	19.563	0.0	-12.917	-1.559	*
-12	6	0	18.271	11.536	-11.536	0.0	6.735	2.419	*
-10	6	0	19.213	23.746	23.746	0.0	-4.533	-1.718	*
-8	6	0	23.240	25.960	-25.960	0.0	-2.721	-1.725	*
-6	6	0	17.784	15.846	15.846	0.0	1.938	1.256	*
-4	6	0	4.068	2.963	2.963	0.0	1.106	0.297	*
-2	6	0	18.053	19.940	19.940	0.0	-1.887	-1.959	*
0	6	0	14.523	14.220	14.220	0.0	0.303	0.293	
2	6	0	17.867	19.940	19.940	0.0	-2.073	-2.157	
4	6	0	2.764	2.963	2.963	0.0	-0.199	-0.044	
6	6	0	17.991	15.846	15.846	0.0	2.145	1.468	
8	6	0	23.975	25.960	-25.960	0.0	-1.986	-1.513	
10	6	0	23.416	23.746	23.746	0.0	-0.330	-0.212	
12	6	0	16.242	11.536	-11.536	0.0	4.706	1.966	
11	7	0	17.039	18.116	-18.116	0.0	-1.078	-0.442	
9	7	0	42.836	42.947	42.947	0.0	-0.111	-0.096	
0	12	0	201.580	202.599	202.599	0.0	-1.020	-0.336	*
7	7	0	30.320	29.281	-29.281	0.0	1.039	0.882	
5	7	0	11.656	4.212	4.212	0.0	7.444	4.069	
3	7	0	55.123	52.643	52.643	0.0	2.480	2.600	
1	7	0	14.907	15.598	-15.598	0.0	-0.692	-0.677	
-1	7	0	14.203	15.598	-15.598	0.0	-1.396	-1.253	*
-3	7	0	54.988	52.643	52.643	0.0	2.346	2.504	*
-5	7	0	9.265	4.212	4.212	0.0	5.053	1.923	*
-7	7	0	28.809	29.281	-29.281	0.0	-0.472	-0.360	*
-9	7	0	42.867	42.947	42.947	0.0	-0.080	-0.063	*
-11	7	0	21.356	18.116	-18.116	0.0	3.239	1.425	*
-12	8	0	30.734	29.070	29.070	0.0	1.664	0.752	*
-10	8	0	38.012	39.064	-39.064	0.0	-1.052	-0.686	*
-8	8	0	17.639	17.102	-17.102	0.0	0.538	0.273	*
-6	8	0	66.065	68.688	68.688	0.0	-2.624	-2.175	*
-4	8	0	96.820	97.690	-97.690	0.0	-0.870	-0.573	*
-2	8	0	26.821	31.125	31.125	0.0	-4.304	-4.920	*
0	8	0	44.916	41.875	41.875	0.0	3.041	3.844	
2	8	0	27.774	31.125	31.125	0.0	-3.351	-4.306	
4	8	0	99.221	97.690	-97.690	0.0	1.531	0.996	
6	8	0	68.953	68.688	68.688	0.0	0.265	0.223	
0	12	0	199.571	202.599	202.599	0.0	-3.028	-1.009	*
8	8	0	17.453	17.102	-17.102	0.0	0.351	0.206	
10	8	0	37.525	39.064	-39.064	0.0	-1.539	-1.097	
12	8	0	27.950	29.070	29.070	0.0	-1.121	-0.572	
11	9	0	10.859	13.395	-13.395	0.0	-2.536	-0.651	
9	9	0	33.861	33.745	33.745	0.0	0.116	0.104	

K-RICHTERITE 800C, 3/6/73 STRUCTURE FACTORS PAGE 3

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
7	9	0	83.746	84.639	-84.639	0.0	-0.893	-0.643	
1	9	0	78.280	77.560	-77.560	0.0	0.720	0.583	
-1	9	0	77.731	77.560	-77.560	0.0	0.171	0.139	*
-5	9	0	8.582	10.611	10.611	0.0	-2.030	-0.665	*
-7	9	0	82.276	84.639	-84.639	0.0	-2.363	-1.692	*
-9	9	0	33.426	33.745	33.745	0.0	-0.319	-0.237	*
-11	9	0	13.136	13.395	-13.395	0.0	-0.259	-0.064	*
-12	10	0	25.703	19.554	19.554	0.0	6.149	2.441	*
-10	10	0	17.650	20.377	20.377	0.0	-2.727	-0.874	*
-8	10	0	26.801	27.210	27.210	0.0	-0.410	-0.242	*
-6	10	0	16.397	14.537	14.537	0.0	1.860	0.970	*
-4	10	0	60.609	61.732	61.732	0.0	-1.123	-1.006	*
0	12	0	199.809	202.599	202.599	0.0	-2.790	-0.928	*
-2	10	0	46.107	48.151	48.151	0.0	-2.044	-2.202	*
0	10	0	104.087	104.368	104.368	0.0	-0.281	-0.175	
2	10	0	45.693	48.151	48.151	0.0	-2.459	-2.688	
4	10	0	60.723	61.732	61.732	0.0	-1.009	-0.930	
6	10	0	16.045	14.537	14.537	0.0	1.508	0.799	
8	10	0	27.929	27.210	27.210	0.0	0.719	0.486	
10	10	0	18.002	20.377	20.377	0.0	-2.375	-0.960	
12	10	0	22.971	19.554	19.554	0.0	3.417	1.677	
11	11	0	55.454	53.176	53.176	0.0	2.278	1.794	
7	11	0	118.010	119.070	119.070	0.0	-1.060	-0.571	
5	11	0	39.192	39.966	-39.966	0.0	-0.774	-0.699	
3	11	0	72.783	74.396	74.396	0.0	-1.613	-1.297	
1	11	0	119.273	118.397	118.397	0.0	0.876	0.479	
-1	11	0	117.968	118.397	118.397	0.0	-0.428	-0.236	*
-3	11	0	73.694	74.396	74.396	0.0	-0.702	-0.570	*
-5	11	0	36.904	39.966	-39.966	0.0	-3.062	-2.683	*
-7	11	0	117.047	119.070	119.070	0.0	-2.023	-1.093	*
-9	11	0	6.108	1.408	1.408	0.0	4.700	0.928	*
-11	11	0	52.887	53.176	53.176	0.0	-0.289	-0.173	*
0	12	0	199.209	202.599	202.599	0.0	-3.390	-1.131	*
-10	12	0	41.169	42.867	42.867	0.0	-1.698	-0.932	*
-8	12	0	45.982	47.988	47.988	0.0	-2.006	-1.571	*
-6	12	0	33.498	36.280	-36.280	0.0	-2.782	-2.274	*
-4	12	0	55.020	54.568	54.568	0.0	0.452	0.427	*
-2	12	0	44.626	43.698	-43.698	0.0	0.929	0.966	*
0	12	0	199.023	202.599	202.599	0.0	-3.577	-1.194	*
2	12	0	45.144	43.698	-43.698	0.0	1.446	1.512	
4	12	0	53.850	54.568	54.568	0.0	-0.718	-0.680	
6	12	0	34.181	36.280	-36.280	0.0	-2.099	-1.780	
8	12	0	45.693	47.988	47.988	0.0	-2.295	-1.875	
10	12	0	44.419	42.867	42.867	0.0	1.552	1.186	
11	13	0	19.606	20.249	20.249	0.0	-0.643	-0.233	
9	13	0	23.188	25.501	-25.501	0.0	-2.313	-1.146	
7	13	0	37.877	37.648	37.648	0.0	0.229	0.204	
5	13	0	59.036	58.762	-58.762	0.0	0.274	0.235	
3	13	0	14.865	15.683	-15.683	0.0	-0.818	-0.429	
1	13	0	6.853	3.973	3.973	0.0	2.880	0.936	
-1	13	0	6.811	3.973	3.973	0.0	2.839	0.919	*
-3	13	0	14.793	15.683	-15.683	0.0	-0.890	-0.473	*
-5	13	0	59.419	58.762	-58.762	0.0	0.657	0.560	*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	12	0	198.557	202.599	202.599	0.0	-4.043	-1.353	*
-7	13	0	35.600	37.648	37.648	0.0	-2.048	-1.568	*
-9	13	0	19.730	25.501	-25.501	0.0	-5.770	-1.995	*
-11	13	0	18.975	20.249	20.249	0.0	-1.274	-0.350	*
-8	14	0	7.847	0.869	-0.869	0.0	6.978	1.504	*
-6	14	0	4.048	2.812	-2.812	0.0	1.236	0.217	*
-4	14	0	12.898	11.990	11.990	0.0	0.909	0.423	*
-2	14	0	30.165	30.409	30.409	0.0	-0.244	-0.224	*
0	14	0	13.147	8.461	-8.461	0.0	4.685	2.631	
2	14	0	28.592	30.409	30.409	0.0	-1.818	-1.418	
4	14	0	8.861	11.990	11.990	0.0	-3.128	-1.005	
6	14	0	7.743	2.812	-2.812	0.0	4.931	1.472	
8	14	0	6.977	0.869	-0.869	0.0	6.108	1.478	
9	15	0	28.436	29.235	29.235	0.0	-0.799	-0.467	
7	15	0	45.672	43.889	-43.889	0.0	1.783	1.728	
5	15	0	23.240	26.601	26.601	0.0	-3.361	-1.745	
1	15	0	10.548	8.443	-8.443	0.0	2.105	0.863	
0	12	0	198.370	202.599	202.599	0.0	-4.229	-1.416	*
-5	15	0	27.008	26.601	26.601	0.0	0.407	0.271	*
-7	15	0	43.757	43.889	-43.889	0.0	-0.132	-0.099	*
-9	15	0	29.326	29.235	29.235	0.0	0.091	0.043	*
-10	16	0	15.300	16.978	-16.978	0.0	-1.678	-0.369	*
-8	16	0	5.466	11.883	-11.883	0.0	-6.417	-0.978	*
-6	16	0	30.227	31.044	31.044	0.0	-0.817	-0.555	*
-4	16	0	41.376	46.243	-46.243	0.0	-4.867	-3.546	*
-2	16	0	1.925	6.029	6.029	0.0	-4.103	-0.636	*
0	16	0	7.143	4.201	4.201	0.0	2.942	0.932	
4	16	0	44.916	46.243	-46.243	0.0	-1.326	-1.241	
6	16	0	26.780	31.044	31.044	0.0	-4.264	-2.325	
8	16	0	12.774	11.883	-11.883	0.0	0.891	0.323	
10	16	0	19.896	16.978	-16.978	0.0	2.918	1.076	
9	17	0	14.078	13.831	13.831	0.0	0.247	0.076	
7	17	0	11.356	10.055	-10.055	0.0	1.301	0.416	
5	17	0	10.134	6.498	-6.498	0.0	3.637	1.351	
3	17	0	21.573	26.078	26.078	0.0	-4.505	-2.316	
1	17	0	15.217	15.247	-15.247	0.0	-0.030	-0.015	
0	12	0	199.623	202.599	202.599	0.0	-2.976	-0.991	*
-1	17	0	16.335	15.247	-15.247	0.0	1.088	0.583	*
-3	17	0	24.917	26.078	26.078	0.0	-1.162	-0.800	*
-7	17	0	7.702	10.055	-10.055	0.0	-2.353	-0.428	*
-9	17	0	15.051	13.831	13.831	0.0	1.221	0.321	*
-8	18	0	19.989	11.329	-11.329	0.0	8.660	3.536	*
-6	18	0	24.720	20.595	20.595	0.0	4.125	2.304	*
-4	18	0	3.478	2.565	2.565	0.0	0.913	0.143	*
-2	18	0	17.163	17.229	17.229	0.0	-0.066	-0.029	*
0	18	0	18.343	16.010	16.010	0.0	2.333	1.355	
2	18	0	18.323	17.229	17.229	0.0	1.094	0.559	
4	18	0	2.847	2.565	2.565	0.0	0.282	0.046	
6	18	0	18.623	20.595	20.595	0.0	-1.972	-0.772	
8	18	0	15.609	11.329	-11.329	0.0	4.271	1.705	
7	19	0	19.523	18.464	-18.464	0.0	1.059	0.397	
3	19	0	27.049	25.960	-25.960	0.0	1.089	0.768	
-1	19	0	8.054	4.988	-4.988	0.0	3.065	0.847	*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-3	19	0	24.368	25.960	-25.960	0.0	-1.592	-0.814	*
0	12	0	199.209	202.599	202.599	0.0	-3.390	-1.131	*
-5	19	0	8.551	2.129	2.129	0.0	6.421	1.426	*
-7	19	0	17.670	18.464	-18.464	0.0	-0.794	-0.229	*
-8	20	0	9.917	5.073	-5.073	0.0	4.844	0.854	*
-6	20	0	10.631	5.380	5.380	0.0	5.252	1.176	*
-4	20	0	23.498	26.818	-26.818	0.0	-3.319	-1.286	*
-2	20	0	25.372	28.843	28.843	0.0	-3.470	-1.662	*
0	20	0	45.061	46.587	-46.587	0.0	-1.526	-1.210	
2	20	0	27.515	28.843	28.843	0.0	-1.328	-0.756	
4	20	0	27.877	26.818	-26.818	0.0	1.059	0.615	
6	20	0	11.977	5.380	5.380	0.0	6.597	1.950	
8	20	0	7.215	5.073	-5.073	0.0	2.142	0.354	
5	21	0	35.496	34.515	34.515	0.0	0.981	0.588	
1	21	0	23.923	23.189	23.189	0.0	0.734	0.403	
-1	21	0	19.544	23.189	23.189	0.0	-3.645	-1.374	*
-5	21	0	35.558	34.515	34.515	0.0	1.043	0.586	*
-7	21	0	6.211	5.624	-5.624	0.0	0.587	0.081	*
-6	22	0	2.754	3.645	3.645	0.0	-0.891	-0.095	*
0	12	0	199.281	202.599	202.599	0.0	-3.318	-1.107	*
-4	22	0	36.097	35.817	35.817	0.0	0.280	0.157	*
-2	22	0	14.441	14.721	14.721	0.0	-0.280	-0.079	*
0	22	0	50.817	50.102	50.102	0.0	0.714	0.487	
2	22	0	6.905	14.721	14.721	0.0	-7.816	-1.342	
4	22	0	37.297	35.817	35.817	0.0	1.480	0.904	
5	23	0	41.345	39.161	-39.161	0.0	2.184	1.422	
3	23	0	24.968	25.770	25.770	0.0	-0.801	-0.347	
1	23	0	8.778	8.321	8.321	0.0	0.458	0.094	
-3	23	0	30.600	25.770	25.770	0.0	4.830	2.925	*
-5	23	0	40.682	39.161	-39.161	0.0	1.521	0.805	*
-2	24	0	35.289	37.786	-37.786	0.0	-2.497	-1.219	*
0	24	0	73.487	71.267	71.267	0.0	2.220	1.458	
2	24	0	34.306	37.786	-37.786	0.0	-3.481	-1.577	
1	25	0	6.242	1.216	-1.216	0.0	5.026	0.720	
-1	25	0	5.269	1.216	-1.216	0.0	4.053	0.519	*
-3	24	1	12.091	1.347	1.347	0.0	10.744	2.794	*
1	24	1	13.675	1.249	1.249	0.0	12.426	4.208	*
0	12	0	199.437	202.599	202.599	0.0	-3.163	-1.054	*
4	23	1	6.594	0.445	0.445	0.0	6.150	1.058	
2	23	1	12.546	7.052	7.052	0.0	5.494	1.694	
0	23	1	11.511	14.718	14.718	0.0	-3.207	-0.743	
-2	23	1	9.451	4.917	-4.917	0.0	4.534	0.975	
-4	23	1	7.981	9.568	9.568	0.0	-1.587	-0.276	
-5	22	1	18.260	20.396	-20.396	0.0	-2.135	-0.650	
5	22	1	12.101	5.180	-5.180	0.0	6.921	2.118	
6	21	1	6.594	10.832	-10.832	0.0	-4.233	-0.738	
2	21	1	32.111	29.846	-29.846	0.0	2.265	1.578	
0	21	1	25.217	25.075	25.075	0.0	0.142	0.082	
-2	21	1	38.125	38.560	-38.560	0.0	-0.434	-0.292	
-4	21	1	11.366	9.867	9.867	0.0	1.499	0.422	
-7	20	1	14.410	17.305	17.305	0.0	-2.895	-0.761	
-5	20	1	4.627	7.066	-7.066	0.0	-2.439	-0.387	
0	12	0	200.741	202.599	202.599	0.0	-1.858	-0.615	*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-3	20	1	7.774	11.791	11.791	0.0	-4.017	-0.831
3	20	1	15.683	12.345	12.345	0.0	3.338	1.437
7	20	1	19.461	17.666	17.666	0.0	1.795	0.718
8	19	1	2.764	9.108	-9.108	0.0	-6.344	-0.787
6	19	1	24.016	24.544	24.544	0.0	-0.528	-0.260
4	19	1	17.795	17.377	-17.377	0.0	0.418	0.176
2	19	1	9.058	8.212	8.212	0.0	0.846	0.254
0	19	1	33.001	31.344	-31.344	0.0	1.657	1.202
-2	19	1	30.817	32.202	32.202	0.0	-1.385	-0.893
-4	19	1	18.064	15.466	-15.466	0.0	2.597	1.259
-6	19	1	1.687	10.082	10.082	0.0	-8.395	-0.973
-8	19	1	4.306	3.376	-3.376	0.0	0.931	0.122
-9	18	1	35.351	34.363	34.363	0.0	0.988	0.548
-7	18	1	69.077	70.212	-70.212	0.0	-1.135	-0.794
-5	18	1	67.866	67.704	67.704	0.0	0.162	0.116
-1	18	1	2.246	8.806	8.806	0.0	-6.560	-0.957
0	12	0	200.192	202.599	202.599	0.0	-2.407	-0.799 *
1	18	1	23.975	22.711	-22.711	0.0	1.263	0.916
3	18	1	12.888	12.553	-12.553	0.0	0.335	0.135
5	18	1	57.369	57.613	57.613	0.0	-0.245	-0.182
7	18	1	35.972	33.909	-33.909	0.0	2.063	1.464
8	17	1	8.323	3.075	-3.075	0.0	5.248	1.299
6	17	1	73.145	72.006	72.006	0.0	1.139	0.799
4	17	1	2.795	5.634	-5.634	0.0	-2.839	-0.453
2	17	1	61.034	61.125	61.125	0.0	-0.091	-0.077
0	17	1	54.243	54.481	-54.481	0.0	-0.238	-0.213
-2	17	1	103.228	103.282	103.282	0.0	-0.054	-0.032
-4	17	1	12.795	11.089	11.089	0.0	1.706	0.712
-6	17	1	43.850	42.627	42.627	0.0	1.223	1.024
-10	17	1	10.642	1.989	-1.989	0.0	8.652	1.737
-9	16	1	28.695	28.361	28.361	0.0	0.334	0.150
-7	16	1	24.461	19.536	19.536	0.0	4.925	3.122
-5	16	1	57.204	56.146	56.146	0.0	1.057	0.978
-3	16	1	48.632	48.527	48.527	0.0	0.106	0.093
-1	16	1	60.382	59.988	59.988	0.0	0.394	0.345
1	16	1	43.281	45.909	45.909	0.0	-2.628	-2.162
0	12	0	200.451	202.599	202.599	0.0	-2.148	-0.713 *
3	16	1	40.424	40.363	40.363	0.0	0.061	0.047
5	16	1	48.539	48.526	48.526	0.0	0.013	0.011
7	16	1	30.693	30.165	30.165	0.0	0.528	0.346
9	16	1	29.761	30.208	30.208	0.0	-0.446	-0.229
10	15	1	8.292	12.300	12.300	0.0	-4.009	-0.760
8	15	1	13.944	10.294	10.294	0.0	3.650	1.351
6	15	1	8.426	3.579	-3.579	0.0	4.848	1.608
2	15	1	26.418	25.568	-25.568	0.0	0.850	0.740
0	15	1	54.326	54.048	54.048	0.0	0.278	0.258
-2	15	1	48.850	47.994	-47.994	0.0	0.855	0.835
-4	15	1	18.706	18.399	18.399	0.0	0.307	0.178
-6	15	1	21.356	19.879	19.879	0.0	1.476	0.888
-8	15	1	11.718	7.433	-7.433	0.0	4.285	1.323
-10	15	1	15.973	14.357	14.357	0.0	1.616	0.465
-11	14	1	8.499	5.075	5.075	0.0	3.424	0.585
-9	14	1	30.662	27.731	-27.731	0.0	2.931	1.817

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-7	14	1	30.569	30.721	30.721	0.0	-0.152	-0.113	
-5	14	1	70.485	72.631	-72.631	0.0	-2.146	-1.711	
-3	14	1	35.931	37.490	37.490	0.0	-1.559	-1.458	
0	12	0	199.116	202.599	202.599	0.0	-3.484	-1.163	*
-1	14	1	32.153	33.150	-33.150	0.0	-0.997	-0.887	
1	14	1	42.442	43.656	-43.656	0.0	-1.213	-1.093	
3	14	1	20.672	23.820	23.820	0.0	-3.148	-2.058	
5	14	1	39.896	41.098	-41.098	0.0	-1.202	-1.090	
7	14	1	11.014	9.769	9.769	0.0	1.245	0.426	
9	14	1	28.592	28.586	-28.586	0.0	0.006	0.003	
10	13	1	10.507	9.194	-9.194	0.0	1.313	0.343	
8	13	1	10.859	10.782	10.782	0.0	.077	0.024	
6	13	1	15.269	12.022	-12.022	0.0	3.247	1.827	
4	13	1	17.629	17.514	17.514	0.0	0.115	0.070	
2	13	1	34.233	35.123	-35.123	0.0	-0.890	-0.797	
0	13	1	31.335	33.322	33.322	0.0	-1.987	-1.679	
-2	13	1	41.883	41.563	-41.563	0.0	0.320	0.320	
-4	13	1	30.237	30.903	30.903	0.0	-0.666	-0.568	
-6	13	1	12.857	8.555	-8.555	0.0	4.302	2.085	
-8	13	1	8.323	1.904	-1.904	0.0	6.419	1.829	
-11	12	1	2.609	9.414	9.414	0.0	-6.806	-0.756	
-9	12	1	9.958	2.000	-2.000	0.0	7.959	2.440	
-7	12	1	17.225	13.225	13.225	0.0	4.000	2.251	
0	12	0	199.820	202.599	202.599	0.0	-2.780	-0.925	*
-5	12	1	15.507	16.676	16.676	0.0	-1.169	-0.556	
-3	12	1	17.184	15.555	15.555	0.0	1.629	1.038	
-1	12	1	26.511	26.142	26.142	0.0	0.369	0.336	
1	12	1	30.268	30.855	30.855	0.0	-0.587	-0.537	
3	12	1	12.091	12.515	12.515	0.0	-0.424	-0.192	
5	12	1	19.078	17.906	17.906	0.0	1.172	0.850	
7	12	1	9.410	10.587	10.587	0.0	-1.177	-0.362	
9	12	1	5.952	7.804	7.804	0.0	-1.852	-0.363	
11	12	1	9.627	3.941	3.941	0.0	5.686	1.395	
10	11	1	15.838	13.060	-13.060	0.0	2.778	1.264	
6	11	1	9.058	16.003	-16.003	0.0	-6.945	-1.954	
2	11	1	49.399	51.531	-51.531	0.0	-2.132	-2.065	
0	11	1	10.310	4.375	-4.375	0.0	5.935	3.017	
-2	11	1	30.600	29.846	-29.846	0.0	0.754	0.751	
-4	11	1	9.379	11.041	-11.041	0.0	-1.662	-0.589	
-6	11	1	13.478	15.734	-15.734	0.0	-2.256	-1.002	
-8	11	1	13.085	13.137	13.137	0.0	-0.052	-0.020	
-10	11	1	12.919	13.120	-13.120	0.0	-0.201	-0.063	
0	12	0	199.613	202.599	202.599	0.0	-2.987	-0.995	*
-11	10	1	18.343	16.044	16.044	0.0	2.300	0.902	
-9	10	1	13.581	19.955	-19.955	0.0	-6.373	-2.072	
-7	10	1	19.461	21.179	21.179	0.0	-1.717	-1.033	
-5	10	1	30.517	30.837	-30.837	0.0	-0.320	-0.300	
-3	10	1	53.694	55.376	55.376	0.0	-1.681	-1.608	
-1	10	1	33.674	33.265	-33.265	0.0	0.409	0.449	
3	10	1	44.688	45.330	45.330	0.0	-0.642	-0.634	
5	10	1	33.612	32.858	-32.858	0.0	0.754	0.668	
7	10	1	18.219	21.838	21.838	0.0	-3.619	-1.743	
9	10	1	12.225	14.185	-14.185	0.0	-1.959	-0.662	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
10	9	1	15.766	18.422	18.422	0.0	-2.656	-0.963	
8	9	1	9.358	2.711	2.711	0.0	6.647	2.547	
6	9	1	12.577	12.483	-12.483	0.0	0.095	0.042	
4	9	1	35.175	33.566	33.566	0.0	1.609	1.715	
2	9	1	62.897	64.216	-64.216	0.0	-1.319	-1.233	
0	9	1	90.143	88.352	88.352	0.0	1.791	1.273	
-2	9	1	59.709	60.060	-60.060	0.0	-0.351	-0.345	
0	12	0	199.437	202.599	202.599	0.0	-3.163	-1.054	*
-4	9	1	25.248	22.009	22.009	0.0	3.239	3.300	
-6	9	1	12.919	13.844	13.844	0.0	-0.925	-0.417	
-8	9	1	3.002	2.334	-2.334	0.0	0.668	0.116	
-10	9	1	15.341	11.548	11.548	0.0	3.793	1.549	
-12	9	1	20.320	23.065	-23.065	0.0	-2.745	-0.849	
-13	8	1	10.497	4.541	4.541	0.0	5.956	1.121	
-11	8	1	13.219	14.457	-14.457	0.0	-1.238	-0.345	
-9	8	1	11.863	11.020	-11.020	0.0	0.843	0.304	
-7	8	1	11.770	15.070	15.070	0.0	-3.300	-1.248	
-5	8	1	12.588	16.162	-16.162	0.0	-3.574	-1.571	
-3	8	1	13.302	8.067	8.067	0.0	5.235	3.826	
-1	8	1	3.499	0.323	0.323	0.0	3.176	0.964	
3	8	1	4.472	1.412	1.412	0.0	3.060	0.906	
5	8	1	22.701	23.328	-23.328	0.0	-0.627	-0.489	
7	8	1	22.360	23.060	23.060	0.0	-0.700	-0.529	
11	8	1	10.994	10.827	-10.827	0.0	0.167	0.047	
12	7	1	8.105	10.461	10.461	0.0	-2.355	-0.467	
10	7	1	18.416	16.395	-16.395	0.0	2.020	0.945	
0	12	0	199.281	202.599	202.599	0.0	-3.318	-1.107	*
8	7	1	9.813	12.038	-12.038	0.0	-2.224	-0.741	
6	7	1	63.798	64.387	64.387	0.0	-0.589	-0.511	
4	7	1	63.518	63.546	-63.546	0.0	-0.028	-0.025	
2	7	1	13.716	12.529	12.529	0.0	1.187	0.936	
0	7	1	132.368	133.502	-133.502	0.0	-1.135	-0.568	
-2	7	1	62.483	61.789	61.789	0.0	0.694	0.690	
-4	7	1	11.025	7.556	-7.556	0.0	3.469	1.980	
-6	7	1	31.521	33.434	33.434	0.0	-1.913	-1.742	
-8	7	1	28.602	27.100	-27.100	0.0	1.502	1.434	
-10	7	1	15.424	11.203	-11.203	0.0	4.221	1.793	
-12	7	1	36.604	35.913	35.913	0.0	0.691	0.369	
-13	6	1	48.695	46.947	46.947	0.0	1.748	1.046	
-9	6	1	94.770	95.737	95.737	0.0	-0.967	-0.621	
-7	6	1	90.464	91.763	-91.763	0.0	-1.299	-0.898	
-5	6	1	186.694	192.828	192.828	0.0	-6.134	-2.183	
-3	6	1	162.895	159.304	159.304	0.0	3.591	1.466	
-1	6	1	130.349	135.132	135.132	0.0	-4.783	-2.435	
1	6	1	53.694	41.546	-41.546	0.0	12.149	13.582	*
3	6	1	69.812	70.166	70.166	0.0	-0.354	-0.311	
0	12	0	199.168	202.599	202.599	0.0	-3.432	-1.145	*
5	6	1	218.184	222.340	222.340	0.0	-4.157	-1.268	
7	6	1	30.879	30.017	-30.017	0.0	0.862	0.690	
9	6	1	75.392	76.034	76.034	0.0	-0.643	-0.466	
11	6	1	29.875	30.253	-30.253	0.0	-0.378	-0.223	
12	5	1	32.908	32.655	32.655	0.0	0.253	0.149	
10	5	1	3.903	0.414	0.414	0.0	3.489	0.611	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
8	5	1	19.834	18.455	18.455	0.0	1.379	1.029	
6	5	1	146.042	149.338	149.338	0.0	-3.295	-1.480	
4	5	1	12.122	13.707	13.707	0.0	-1.586	-0.772	
2	5	1	118.207	118.123	118.123	0.0	0.084	0.047	
0	5	1	80.744	81.951	-81.951	0.0	-1.208	-0.969	
-2	5	1	208.784	213.180	213.180	0.0	-4.396	-1.408	
-4	5	1	91.737	90.550	90.550	0.0	1.187	0.637	
-6	5	1	95.919	97.970	97.970	0.0	-2.051	-1.357	
-8	5	1	8.261	5.719	5.719	0.0	2.541	0.830	
-10	5	1	15.258	13.106	13.106	0.0	2.152	1.052	
-12	5	1	61.945	61.321	61.321	0.0	0.624	0.418	
-13	4	1	18.540	20.439	20.439	0.0	-1.899	-0.539	
-11	4	1	14.379	14.413	-14.413	0.0	-0.035	-0.012	
0	12	0	199.095	202.599	202.599	0.0	-3.504	-1.170	*
-7	4	1	16.366	16.939	16.939	0.0	-0.573	-0.348	
-5	4	1	25.527	23.618	23.618	0.0	1.910	2.171	
-3	4	1	18.084	19.124	19.124	0.0	-1.039	-1.193	
-1	4	1	23.633	25.248	25.248	0.0	-1.615	-2.166	
1	4	1	18.095	17.134	17.134	0.0	0.961	1.036	
3	4	1	7.060	11.085	11.085	0.0	-4.025	-1.873	
5	4	1	8.892	4.092	4.092	0.0	4.800	1.972	
7	4	1	24.430	26.027	26.027	0.0	-1.596	-1.083	
9	4	1	18.260	17.237	17.237	0.0	1.024	0.540	
11	4	1	13.861	15.915	-15.915	0.0	-2.054	-0.713	
12	3	1	26.024	25.385	-25.385	0.0	0.639	0.340	
10	3	1	10.559	9.573	9.573	0.0	0.986	0.345	
8	3	1	7.753	10.449	-10.449	0.0	-2.696	-0.764	
6	3	1	39.026	38.009	-38.009	0.0	1.017	1.078	
4	3	1	22.660	23.219	-23.219	0.0	-0.559	-0.514	
2	3	1	131.115	136.040	-136.040	0.0	-4.925	-2.488	
-2	3	1	148.641	153.805	-153.805	0.0	-5.164	-2.318	
-4	3	1	23.830	22.239	-22.239	0.0	1.591	1.937	
-8	3	1	21.604	21.134	-21.134	0.0	0.470	0.319	
0	12	0	199.551	202.599	202.599	0.0	-3.049	-1.015	*
-10	3	1	12.753	7.646	7.646	0.0	5.107	2.103	
-12	3	1	33.239	34.442	-34.442	0.0	-1.203	-0.667	
-13	2	1	16.221	19.590	-19.590	0.0	-3.369	-0.886	
-11	2	1	17.960	19.517	19.517	0.0	-1.557	-0.603	
-9	2	1	27.929	26.957	-26.957	0.0	0.972	0.840	
-7	2	1	50.548	50.800	50.800	0.0	-0.252	-0.253	
-5	2	1	46.179	47.246	-47.246	0.0	-1.067	-1.238	
-3	2	1	130.784	132.495	132.495	0.0	-1.711	-0.870	
3	2	1	109.490	109.801	109.801	0.0	-0.310	-0.187	
5	2	1	25.734	25.818	-25.818	0.0	-0.084	-0.080	
7	2	1	42.256	41.358	41.358	0.0	0.898	0.832	
11	2	1	29.223	28.893	28.893	0.0	0.330	0.205	
12	1	1	11.646	9.416	9.416	0.0	2.229	0.652	
10	1	1	13.064	10.167	-10.167	0.0	2.897	1.261	
8	1	1	9.969	14.861	14.861	0.0	-4.892	-1.720	
6	1	1	11.232	13.222	-13.222	0.0	-1.990	-0.850	
4	1	1	14.368	13.625	13.625	0.0	0.743	0.627	
2	1	1	64.150	66.783	-66.783	0.0	-2.633	-2.579	
-4	1	1	20.848	21.793	21.793	0.0	-0.945	-1.109	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	12	0	200.172	202.599	202.599	0.0	-2.428	-0.806	*
-8	1	1	8.571	11.393	11.393	0.0	-2.821	-0.925	
-10	1	1	8.406	7.209	-7.209	0.0	1.196	0.365	
-12	1	1	1.884	5.829	5.829	0.0	-3.945	-0.462	
-13	0	1	10.352	15.468	-15.468	0.0	-5.116	-0.951	
-11	0	1	12.049	6.424	6.424	0.0	5.625	2.161	
-9	0	1	5.631	6.115	-6.115	0.0	-0.484	-0.124	
-5	0	1	8.809	5.021	-5.021	0.0	3.788	2.433	
-3	0	1	13.706	12.005	-12.005	0.0	1.701	1.374	
3	0	1	25.879	24.804	-24.804	0.0	1.076	1.450	
5	0	1	7.422	3.442	3.442	0.0	3.980	1.706	
-12	0	2	44.927	44.170	-44.170	0.0	0.757	0.554	
-10	0	2	69.605	68.611	68.611	0.0	0.994	0.796	
-8	0	2	72.069	74.122	74.122	0.0	-2.053	-1.648	
-6	0	2	95.847	94.655	94.655	0.0	1.192	0.793	
-4	0	2	158.620	161.361	161.361	0.0	-2.741	-1.148	
0	12	0	200.399	202.599	202.599	0.0	-2.200	-0.730	*
-2	0	2	101.882	96.365	-96.365	0.0	5.516	3.556	
0	0	2	271.702	275.327	275.327	0.0	-3.625	-0.894	
2	0	2	136.301	134.348	134.348	0.0	1.953	0.948	
4	0	2	209.002	214.423	214.423	0.0	-5.422	-1.726	
6	0	2	57.183	58.402	-58.402	0.0	-1.219	-1.094	
8	0	2	70.878	70.070	70.070	0.0	0.809	0.639	
10	0	2	61.251	59.321	59.321	0.0	1.930	1.511	
11	1	2	53.146	51.417	51.417	0.0	1.729	1.372	
9	1	2	31.873	30.528	-30.528	0.0	1.345	1.062	
7	1	2	45.620	47.543	47.543	0.0	-1.922	-1.755	
5	1	2	30.196	31.904	-31.904	0.0	-1.708	-1.370	
3	1	2	62.307	61.031	61.031	0.0	1.276	1.197	
1	1	2	117.151	110.949	110.949	0.0	6.202	3.489	
-1	1	2	21.159	21.485	-21.485	0.0	-0.326	-0.375	
-3	1	2	4.399	1.105	-1.105	0.0	3.295	1.113	
-5	1	2	26.128	25.257	-25.257	0.0	0.871	0.839	
-7	1	2	157.315	160.437	160.437	0.0	-3.121	-1.306	
-9	1	2	31.169	32.889	-32.889	0.0	-1.720	-1.539	
-11	1	2	31.418	31.058	31.058	0.0	0.359	0.266	
0	12	0	199.965	202.599	202.599	0.0	-2.635	-0.876	*
-12	2	2	11.097	2.266	2.266	0.0	8.832	2.655	
-10	2	2	4.741	1.045	-1.045	0.0	3.696	0.790	
-8	2	2	8.209	6.591	6.591	0.0	1.617	0.541	
-6	2	2	25.248	26.801	-26.801	0.0	-1.553	-1.283	
-4	2	2	10.921	11.294	-11.294	0.0	-0.373	-0.255	
-2	2	2	14.006	12.247	-12.247	0.0	1.758	1.654	
0	2	2	25.693	22.902	-22.902	0.0	2.791	3.693	
2	2	2	6.677	5.153	-5.153	0.0	1.524	0.645	
4	2	2	17.494	17.830	17.830	0.0	-0.336	-0.215	
6	2	2	9.534	6.916	-6.916	0.0	2.618	1.028	
8	2	2	3.644	14.757	-14.757	0.0	-11.113	-1.606	*
10	2	2	17.225	14.970	-14.970	0.0	2.255	1.228	
11	3	2	27.825	26.821	-26.821	0.0	1.005	0.599	
9	3	2	33.788	34.703	34.703	0.0	-0.915	-0.692	
7	3	2	60.785	60.912	-60.912	0.0	-0.127	-0.107	
5	3	2	28.778	28.738	28.738	0.0	0.040	0.033	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
3	3	2	10.755	7.215	7.215	0.0	3.541	2.038	
1	3	2	77.141	75.031	-75.031	0.0	2.110	1.740	
-3	3	2	18.074	14.147	14.147	0.0	3.927	4.202	
0	12	0	199.882	202.599	202.599	0.0	-2.718	-0.903	*
-5	3	2	11.729	17.714	17.714	0.0	-5.985	-2.753	
-7	3	2	82.348	83.430	-83.430	0.0	-1.081	-0.800	
-9	3	2	58.322	59.766	59.766	0.0	-1.444	-1.270	
-11	3	2	6.822	13.632	-13.632	0.0	-6.810	-1.347	
-13	3	2	11.998	10.761	-10.761	0.0	1.237	0.295	
-12	4	2	40.724	38.296	38.296	0.0	2.427	1.818	
-10	4	2	35.092	32.600	-32.600	0.0	2.492	2.244	
-8	4	2	8.302	2.435	-2.435	0.0	5.867	1.952	
-6	4	2	79.274	80.072	80.072	0.0	-0.799	-0.610	
-4	4	2	67.255	66.346	-66.346	0.0	0.910	0.821	
-2	4	2	20.217	21.996	21.996	0.0	-1.779	-2.092	
0	4	2	94.232	90.560	90.560	0.0	3.672	2.530	
2	4	2	66.489	69.207	69.207	0.0	-2.718	-2.498	
4	4	2	72.887	71.416	-71.416	0.0	1.470	1.214	
6	4	2	85.599	86.996	86.996	0.0	-1.397	-0.979	
8	4	2	11.221	0.850	-0.850	0.0	10.371	4.748	*
10	4	2	21.335	18.332	-18.332	0.0	3.003	1.893	
11	5	2	16.056	11.990	-11.990	0.0	4.065	1.906	
9	5	2	13.302	14.269	14.269	0.0	-0.967	-0.360	
7	5	2	33.467	33.688	-33.688	0.0	-0.221	-0.182	
0	12	0	199.530	202.599	202.599	0.0	-3.070	-1.023	*
5	5	2	29.606	30.929	-30.929	0.0	-1.323	-1.251	
3	5	2	33.302	29.753	29.753	0.0	3.549	4.043	
1	5	2	79.118	78.005	-78.005	0.0	1.113	0.881	
-1	5	2	60.392	59.701	-59.701	0.0	0.691	0.701	
-3	5	2	31.511	29.303	29.303	0.0	2.208	2.575	
-5	5	2	24.741	23.092	-23.092	0.0	1.648	1.621	
-7	5	2	38.322	39.074	-39.074	0.0	-0.752	-0.740	
-9	5	2	37.691	36.556	36.556	0.0	1.135	1.207	
-11	5	2	17.029	17.070	-17.070	0.0	-0.041	-0.018	
-13	5	2	12.526	6.999	6.999	0.0	5.527	1.439	
-12	6	2	8.312	5.306	-5.306	0.0	3.006	0.632	
-10	6	2	17.670	18.818	18.818	0.0	-1.147	-0.568	
-8	6	2	23.053	23.480	-23.480	0.0	-0.426	-0.336	
-6	6	2	19.410	20.086	20.086	0.0	-0.676	-0.441	
-4	6	2	5.849	6.263	-6.263	0.0	-0.415	-0.149	
0	6	2	10.269	9.604	9.604	0.0	0.665	0.397	
2	6	2	9.244	9.642	9.642	0.0	-0.398	-0.194	
4	6	2	6.946	9.498	9.498	0.0	-2.552	-0.788	
6	6	2	21.956	21.557	21.557	0.0	0.399	0.247	
0	12	0	199.851	202.599	202.599	0.0	-2.749	-0.914	*
8	6	2	25.786	25.711	-25.711	0.0	0.075	0.062	
10	6	2	16.563	18.146	18.146	0.0	-1.584	-0.636	
11	7	2	12.805	12.096	-12.096	0.0	0.709	0.211	
9	7	2	10.238	11.618	11.618	0.0	-1.380	-0.406	
5	7	2	12.536	11.515	11.515	0.0	1.021	0.429	
3	7	2	10.497	7.971	-7.971	0.0	2.526	1.230	
1	7	2	15.548	18.970	18.970	0.0	-3.422	-2.120	
-1	7	2	40.993	38.887	38.887	0.0	2.106	2.556	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-3	7	2	37.401	37.228	-37.228	0.0	0.173	0.181	
-5	7	2	33.912	33.276	33.276	0.0	0.636	0.641	
-9	7	2	12.101	17.035	17.035	0.0	-4.934	-1.549	
-11	7	2	20.062	17.633	-17.633	0.0	2.429	1.227	
-13	7	2	22.587	22.075	22.075	0.0	0.513	0.185	
-12	8	2	9.813	14.063	14.063	0.0	-4.249	-0.852	
-10	8	2	13.861	10.916	-10.916	0.0	2.945	1.200	
-8	8	2	6.656	1.372	1.372	0.0	5.284	1.590	
-6	8	2	21.635	21.945	-21.945	0.0	-0.310	-0.252	
-4	8	2	23.022	19.770	-19.770	0.0	3.252	2.799	
0	12	0	200.265	202.599	202.599	0.0	-2.335	-0.775	*
-2	8	2	55.082	54.302	54.302	0.0	0.780	0.817	
0	8	2	88.352	85.810	-85.810	0.0	2.542	1.843	
2	8	2	81.054	81.037	81.037	0.0	0.017	0.013	
4	8	2	41.811	41.495	-41.495	0.0	0.316	0.288	
6	8	2	15.300	15.075	15.075	0.0	0.225	0.116	
8	8	2	11.936	5.747	-5.747	0.0	6.188	2.856	
9	9	2	4.337	1.223	1.223	0.0	3.114	0.543	
7	9	2	37.618	36.427	-36.427	0.0	1.192	1.099	
5	9	2	23.457	24.583	24.583	0.0	-1.126	-0.851	
3	9	2	68.435	69.522	-69.522	0.0	-1.087	-0.899	
1	9	2	37.598	37.040	-37.040	0.0	0.558	0.548	
-1	9	2	12.878	12.923	12.923	0.0	-0.045	-0.023	
-3	9	2	79.522	79.677	-79.677	0.0	-0.155	-0.119	
-5	9	2	22.029	22.871	22.871	0.0	-0.842	-0.573	
-7	9	2	41.272	41.105	-41.105	0.0	0.168	0.161	
-9	9	2	17.660	16.651	16.651	0.0	1.009	0.557	
-13	9	2	8.892	2.087	2.087	0.0	6.805	1.199	
0	12	0	199.406	202.599	202.599	0.0	-3.194	-1.064	*
-10	10	2	18.002	22.408	22.408	0.0	-4.406	-1.709	
-8	10	2	36.966	37.376	37.376	0.0	-0.410	-0.346	
-6	10	2	20.496	18.618	18.618	0.0	1.879	1.330	
-4	10	2	50.931	50.705	50.705	0.0	0.226	0.217	
-2	10	2	28.271	30.891	30.891	0.0	-2.620	-2.040	
0	10	2	62.514	62.547	62.547	0.0	-0.033	-0.030	
2	10	2	42.918	43.091	43.091	0.0	-0.173	-0.161	
4	10	2	71.065	71.686	71.686	0.0	-0.621	-0.508	
6	10	2	17.474	14.484	14.484	0.0	2.990	1.782	
8	10	2	19.720	15.875	15.875	0.0	3.845	2.208	
10	10	2	7.215	6.711	6.711	0.0	0.504	0.112	
7	11	2	43.840	44.427	44.427	0.0	-0.587	-0.485	
5	11	2	19.648	15.253	-15.253	0.0	4.395	3.997	
3	11	2	126.757	129.608	129.608	0.0	-2.851	-1.453	
1	11	2	90.598	90.484	90.485	0.0	0.114	0.078	
-1	11	2	5.062	3.334	-3.334	0.0	1.728	0.445	
-3	11	2	108.569	109.773	109.773	0.0	-1.204	-0.713	
-5	11	2	18.354	17.994	-17.994	0.0	0.360	0.246	
-7	11	2	125.701	127.065	127.065	0.0	-1.363	-0.695	
0	12	0	199.095	202.599	202.599	0.0	-3.504	-1.170	*
-11	11	2	33.923	32.919	32.919	0.0	1.004	0.564	
-12	12	2	22.722	20.848	-20.848	0.0	1.875	0.704	
-10	12	2	9.617	12.072	12.072	0.0	-2.455	-0.570	
-8	12	2	16.480	16.121	16.121	0.0	0.359	0.173	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-6	12	2	75.299	75.515	75.515	0.0	-0.216	-0.166	
-4	12	2	27.059	26.457	26.457	0.0	0.603	0.456	
-2	12	2	125.515	127.061	-127.061	0.0	-1.546	-0.800	
0	12	2	188.143	189.263	189.263	0.0	-1.120	-0.394	
2	12	2	20.269	19.635	-19.635	0.0	0.634	0.408	
4	12	2	65.433	66.000	66.000	0.0	-0.567	-0.462	
6	12	2	30.041	28.767	-28.767	0.0	1.274	1.005	
8	12	2	24.865	25.521	25.521	0.0	-0.656	-0.362	
10	12	2	9.027	11.110	11.110	0.0	-2.083	-0.462	
9	13	2	15.196	14.391	-14.391	0.0	0.805	0.286	
7	13	2	9.099	7.038	-7.038	0.0	2.061	0.577	
5	13	2	40.165	40.022	-40.022	0.0	0.143	0.125	
3	13	2	38.778	40.264	40.264	0.0	-1.487	-1.365	
1	13	2	11.749	13.691	-13.691	0.0	-1.942	-0.772	
-1	13	2	60.268	60.885	-60.885	0.0	-0.617	-0.546	
0	12	0	200.813	202.599	202.599	0.0	-1.786	-0.591	*
-3	13	2	33.788	35.145	35.145	0.0	-1.357	-1.193	
-5	13	2	52.432	51.437	-51.437	0.0	0.994	0.937	
-7	13	2	36.252	35.748	35.748	0.0	0.504	0.427	
-9	13	2	15.020	10.408	-10.408	0.0	4.612	1.968	
-10	14	2	6.149	3.619	-3.619	0.0	2.530	0.430	
-6	14	2	6.108	2.263	-2.263	0.0	3.845	0.949	
-4	14	2	2.412	0.632	0.632	0.0	1.780	0.327	
-2	14	2	19.244	19.946	19.946	0.0	-0.702	-0.449	
2	14	2	14.140	18.619	18.619	0.0	-4.478	-1.859	
4	14	2	11.791	8.702	8.702	0.0	3.089	1.356	
6	14	2	18.623	15.719	15.719	0.0	2.903	1.764	
9	15	2	18.084	14.492	14.492	0.0	3.593	1.662	
7	15	2	18.768	19.032	-19.032	0.0	-0.264	-0.116	
5	15	2	23.902	24.760	24.760	0.0	-0.858	-0.564	
3	15	2	23.064	23.491	-23.491	0.0	-0.428	-0.294	
0	12	0	199.633	202.599	202.599	0.0	-2.966	-0.987	*
-1	15	2	24.637	25.353	25.353	0.0	-0.716	-0.554	
-3	15	2	33.281	34.907	-34.907	0.0	-1.626	-1.266	
-5	15	2	28.053	28.615	28.615	0.0	-0.562	-0.407	
-7	15	2	24.440	27.438	-27.438	0.0	-2.998	-1.601	
-9	15	2	19.399	21.386	21.386	0.0	-1.987	-0.741	
-8	16	2	8.716	3.295	-3.295	0.0	5.421	1.406	
-4	16	2	13.281	14.682	-14.682	0.0	-1.401	-0.597	
-2	16	2	17.795	15.217	15.217	0.0	2.577	1.516	
0	16	2	35.465	37.091	-37.091	0.0	-1.626	-1.414	
2	16	2	23.219	25.469	25.469	0.0	-2.250	-1.315	
4	16	2	21.873	24.651	-24.651	0.0	-2.778	-1.346	
8	16	2	9.047	6.003	-6.003	0.0	3.044	0.794	
5	17	2	5.248	1.057	-1.057	0.0	4.192	0.861	
3	17	2	9.306	1.509	-1.509	0.0	7.797	2.737	
0	12	0	199.768	202.599	202.599	0.0	-2.831	-0.942	*
-1	17	2	6.667	6.010	6.010	0.0	0.657	0.162	
-3	17	2	11.687	5.150	-5.150	0.0	6.537	3.607	
-5	17	2	8.478	4.330	4.330	0.0	4.148	1.366	
-7	17	2	1.863	3.407	3.407	0.0	-1.543	-0.195	
-8	18	2	11.832	7.974	-7.974	0.0	3.858	1.078	
-6	18	2	11.925	11.664	11.664	0.0	0.262	0.083	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-4	18	2	6.170	3.978	3.978	0.0	2.192	0.508	
-2	18	2	17.267	16.152	16.152	0.0	1.115	0.560	
2	18	2	18.157	16.289	16.289	0.0	1.868	0.982	
4	18	2	13.923	8.790	8.790	0.0	5.133	2.217	
6	18	2	16.314	16.209	16.209	0.0	0.105	0.037	
3	19	2	4.306	2.448	-2.448	0.0	1.858	0.329	
1	19	2	18.457	19.414	-19.414	0.0	-0.957	-0.396	
-1	19	2	3.602	4.915	-4.915	0.0	-1.313	-0.232	
-3	19	2	15.859	16.834	-16.834	0.0	-0.975	-0.365	
-7	19	2	23.571	25.963	-25.963	0.0	-2.392	-1.007	
0	12	0	200.575	202.599	202.599	0.0	-2.024	-0.670	*
-9	19	2	17.784	17.459	17.459	0.0	0.326	0.092	
-6	20	2	9.037	12.921	12.921	0.0	-3.884	-0.829	
-4	20	2	27.049	29.241	-29.241	0.0	-2.191	-1.059	
-2	20	2	11.905	10.019	10.019	0.0	1.886	0.634	
2	20	2	20.579	22.859	22.859	0.0	-2.279	-1.052	
4	20	2	43.871	44.333	-44.333	0.0	-0.462	-0.356	
6	20	2	22.349	24.498	24.498	0.0	-2.149	-0.854	
5	21	2	29.834	28.715	28.715	0.0	1.119	0.573	
3	21	2	14.078	17.768	17.768	0.0	-3.690	-1.171	
1	21	2	8.923	3.398	3.398	0.0	5.525	1.590	
-1	21	2	24.565	22.746	22.746	0.0	1.819	1.096	
-3	21	2	16.583	17.562	17.562	0.0	-0.979	-0.376	
-5	21	2	22.080	22.840	22.840	0.0	-0.760	-0.317	
-6	22	2	14.503	15.684	15.684	0.0	-1.181	-0.311	
-4	22	2	26.759	27.290	27.290	0.0	-0.531	-0.247	
0	22	2	44.171	43.533	43.533	0.0	0.638	0.423	
0	12	0	199.996	202.599	202.599	0.0	-2.604	-0.865	*
2	22	2	8.903	12.548	12.548	0.0	-3.646	-0.755	
4	22	2	39.388	36.982	36.982	0.0	2.406	1.589	
1	23	2	23.136	22.102	22.102	0.0	1.034	0.502	
-1	23	2	19.337	16.454	-16.454	0.0	2.883	1.273	
-3	23	2	18.851	18.951	18.951	0.0	-0.100	-0.035	
-2	24	2	40.486	41.936	-41.936	0.0	-1.451	-0.768	
0	24	2	39.554	39.225	39.225	0.0	0.329	0.182	
-3	22	3	16.408	12.259	12.259	0.0	4.148	1.751	
-1	22	3	13.540	12.321	-12.321	0.0	1.219	0.410	
2	21	3	30.351	27.621	-27.621	0.0	2.730	1.852	
0	21	3	12.132	14.982	14.982	0.0	-2.850	-0.841	
-2	21	3	20.672	21.811	-21.811	0.0	-1.138	-0.518	
-7	20	3	8.706	11.049	11.049	0.0	-2.344	-0.475	
-5	20	3	9.679	7.962	-7.962	0.0	1.716	0.461	
-3	20	3	10.497	12.401	12.401	0.0	-1.904	-0.462	
1	20	3	12.101	8.366	8.366	0.0	3.735	1.300	
0	12	0	198.174	202.599	202.599	0.0	-4.426	-1.484	*
4	19	3	32.908	34.253	-34.253	0.0	-1.344	-0.749	
2	19	3	16.759	20.027	20.027	0.0	-3.268	-1.217	
0	19	3	5.942	8.338	-8.338	0.0	-2.396	-0.466	
-2	19	3	15.186	14.073	14.073	0.0	1.113	0.489	
-4	19	3	11.501	9.178	-9.178	0.0	2.323	0.794	
-6	19	3	6.791	2.839	2.839	0.0	3.952	0.854	
-9	18	3	50.372	51.639	51.639	0.0	-1.267	-0.814	
-7	18	3	50.113	50.674	-50.674	0.0	-0.561	-0.392	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-5	18	3	25.921	23.001	23.001	0.0	2.920	2.082	
-3	18	3	16.273	17.475	-17.475	0.0	-1.202	-0.516	
-1	18	3	62.990	61.825	61.825	0.0	1.165	0.945	
1	18	3	27.505	30.811	-30.811	0.0	-3.307	-1.909	
3	18	3	13.054	17.419	-17.419	0.0	-4.365	-1.286	
5	18	3	29.078	30.851	30.851	0.0	-1.773	-0.983	
6	17	3	55.309	55.841	55.841	0.0	-0.532	-0.410	
4	17	3	39.730	41.932	-41.932	0.0	-2.202	-1.534	
2	17	3	54.761	55.359	55.359	0.0	-0.599	-0.487	
0	17	3	6.967	10.877	-10.877	0.0	-3.910	-0.882	
0	12	0	198.039	202.599	202.599	0.0	-4.560	-1.529	*
-2	17	3	77.152	79.108	79.108	0.0	-1.956	-1.404	
-6	17	3	7.246	10.234	10.234	0.0	-2.988	-0.634	
-8	17	3	14.306	17.866	17.866	0.0	-3.560	-1.008	
-9	16	3	22.298	26.618	26.618	0.0	-4.320	-1.682	
-7	16	3	11.884	7.948	7.948	0.0	3.936	1.379	
-5	16	3	44.347	43.482	43.482	0.0	0.864	0.790	
-3	16	3	29.295	29.268	29.268	0.0	0.027	0.020	
-1	16	3	53.715	53.421	53.421	0.0	0.294	0.249	
1	16	3	40.103	39.083	39.083	0.0	1.019	0.887	
3	16	3	32.411	32.865	32.865	0.0	-0.454	-0.291	
5	16	3	20.859	20.307	20.307	0.0	0.552	0.266	
7	16	3	21.873	21.943	21.943	0.0	-0.070	-0.030	
6	15	3	15.103	14.520	-14.520	0.0	0.583	0.251	
4	15	3	23.209	21.325	21.325	0.0	1.883	1.357	
2	15	3	26.242	25.722	-25.722	0.0	0.519	0.360	
0	15	3	32.598	32.703	32.703	0.0	-0.105	-0.094	
-2	15	3	16.946	18.311	-18.311	0.0	-1.365	-0.650	
-4	15	3	8.054	12.931	12.931	0.0	-4.877	-1.286	
-6	15	3	13.716	16.862	16.862	0.0	-3.145	-1.185	
0	12	0	198.195	202.599	202.599	0.0	-4.405	-1.477	*
-8	15	3	12.795	9.641	-9.641	0.0	3.154	1.084	
-10	15	3	18.664	15.326	15.326	0.0	3.338	1.382	
-7	14	3	21.997	22.084	22.084	0.0	-0.087	-0.050	
-5	14	3	48.529	49.461	-49.461	0.0	-0.932	-0.777	
-3	14	3	32.194	32.483	32.483	0.0	-0.290	-0.236	
-1	14	3	46.117	46.227	-46.227	0.0	-0.110	-0.104	
1	14	3	6.853	7.867	-7.867	0.0	-1.014	-0.271	
3	14	3	12.484	4.071	4.071	0.0	8.413	5.393	
5	14	3	24.544	27.635	-27.635	0.0	-3.091	-1.575	
7	14	3	10.807	10.808	10.808	0.0	-0.001	-0.000	
8	13	3	9.317	8.105	8.105	0.0	1.211	0.319	
6	13	3	10.869	14.111	-14.111	0.0	-3.242	-0.889	
4	13	3	20.683	20.586	20.586	0.0	0.097	0.063	
2	13	3	30.175	32.403	-32.403	0.0	-2.228	-1.445	
0	13	3	25.269	25.741	25.741	0.0	-0.472	-0.370	
-2	13	3	12.784	14.240	-14.240	0.0	-1.456	-0.607	
-4	13	3	10.507	12.418	12.418	0.0	-1.911	-0.684	
0	12	0	200.172	202.599	202.599	0.0	-2.428	-0.806	*
-11	12	3	16.759	9.575	9.575	0.0	7.184	2.991	
-9	12	3	1.170	3.551	-3.551	0.0	-2.381	-0.298	
-7	12	3	12.464	11.809	11.809	0.0	0.655	0.269	
-5	12	3	6.304	4.740	4.740	0.0	1.565	0.412	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-3	12	3	8.913	10.204	10.204	0.0	-1.292	-0.418	
-1	12	3	14.813	15.677	15.677	0.0	-0.863	-0.406	
1	12	3	25.279	25.434	25.434	0.0	-0.155	-0.114	
3	12	3	7.929	4.745	4.745	0.0	3.185	0.964	
5	12	3	13.478	14.442	14.442	0.0	-0.964	-0.349	
7	12	3	6.470	3.591	3.591	0.0	2.879	0.670	
8	11	3	11.263	8.589	8.589	0.0	2.674	0.859	
6	11	3	17.432	18.533	-18.533	0.0	-1.101	-0.483	
4	11	3	16.035	17.932	-17.932	0.0	-1.897	-0.894	
2	11	3	14.710	17.956	-17.956	0.0	-3.246	-1.508	
0	11	3	6.066	4.668	4.668	0.0	1.398	0.350	
-2	11	3	34.130	34.103	-34.103	0.0	0.027	0.023	
-6	11	3	5.983	2.100	-2.100	0.0	3.884	1.006	
0	12	0	200.110	202.599	202.599	0.0	-2.490	-0.827	*
-12	11	3	15.186	5.629	5.629	0.0	9.557	3.342	
-11	10	3	2.526	3.826	3.826	0.0	-1.301	-0.172	
-9	10	3	18.343	15.764	-15.764	0.0	2.580	1.753	
-7	10	3	28.592	28.177	28.177	0.0	0.414	0.315	
-5	10	3	51.531	52.624	-52.624	0.0	-1.093	-0.971	
-3	10	3	53.042	53.643	53.643	0.0	-0.601	-0.554	
-1	10	3	10.486	13.912	-13.912	0.0	-3.425	-1.235	
1	10	3	17.960	17.254	-17.254	0.0	0.706	0.447	
3	10	3	21.428	20.937	20.937	0.0	0.491	0.337	
5	10	3	5.776	0.315	0.315	0.0	5.461	1.309	
7	10	3	8.406	2.762	2.762	0.0	5.644	1.593	
9	10	3	18.975	15.373	-15.373	0.0	3.602	1.718	
6	9	3	19.327	19.952	-19.952	0.0	-0.626	-0.369	
4	9	3	28.902	29.747	29.747	0.0	-0.845	-0.664	
2	9	3	35.786	35.148	-35.148	0.0	0.638	0.624	
0	9	3	55.630	57.030	57.030	0.0	-1.400	-1.312	
-2	9	3	50.672	50.152	-50.152	0.0	0.520	0.491	
0	12	0	198.785	202.599	202.599	0.0	-3.815	-1.275	*
-4	9	3	33.488	33.444	33.444	0.0	0.044	0.045	
-6	9	3	18.416	20.196	20.196	0.0	-1.780	-1.119	
-8	9	3	29.140	29.606	-29.606	0.0	-0.466	-0.336	
-10	9	3	22.277	19.515	19.515	0.0	2.762	1.864	
-12	9	3	14.938	16.920	-16.920	0.0	-1.983	-0.581	
-13	8	3	14.327	11.780	11.780	0.0	2.547	0.702	
-11	8	3	9.886	6.971	-6.971	0.0	2.915	0.844	
-9	8	3	14.058	13.222	-13.222	0.0	0.835	0.385	
-5	8	3	13.675	12.662	-12.662	0.0	1.012	0.526	
-3	8	3	8.126	1.610	1.610	0.0	6.516	2.450	
-1	8	3	9.037	8.320	-8.320	0.0	0.717	0.273	
1	8	3	12.888	11.080	11.080	0.0	1.808	0.891	
3	8	3	12.246	10.359	10.359	0.0	1.887	0.842	
5	8	3	25.155	26.393	-26.393	0.0	-1.238	-0.841	
9	8	3	6.615	4.458	4.458	0.0	2.157	0.495	
10	7	3	11.076	2.543	2.543	0.0	8.533	2.830	
8	7	3	3.665	8.813	-8.813	0.0	-5.148	-0.825	
6	7	3	37.660	38.958	38.958	0.0	-1.298	-1.008	
0	12	0	198.981	202.599	202.599	0.0	-3.618	-1.208	*
4	7	3	76.551	78.946	-78.946	0.0	-2.395	-1.830	
2	7	3	20.300	19.017	19.017	0.0	1.283	0.918	

K-RICHTERITE 800C, 3/6/73 STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	7	3	38.312	38.176	-38.178	0.0	0.133	0.137	
-2	7	3	76.696	77.244	77.244	0.0	-0.548	-0.430	
-4	7	3	31.873	30.895	-30.895	0.0	0.979	0.963	
-6	7	3	9.989	12.447	-12.447	0.0	-[illegible].457	-0.827	
-8	7	3	17.846	15.320	15.320	0.0	2.526	1.600	
-10	7	3	8.157	0.003	0.003	0.0	8.154	2.309	
-12	7	3	31.459	31.473	31.473	0.0	-0.014	-0.007	
-13	6	3	17.029	17.867	17.867	0.0	-0.838	-0.275	
-11	6	3	13.540	8.432	8.432	0.0	5.108	1.901	
-9	6	3	113.217	115.020	115.020	0.0	-1.803	-1.003	
-7	6	3	78.176	78.486	-78.486	0.0	-0.310	-0.234	
-5	6	3	100.950	101.102	101.102	0.0	-0.152	-0.095	
-3	6	3	33.509	34.180	34.180	0.0	-0.671	-0.615	
-1	6	3	197.201	198.480	198.480	0.0	-1.279	-0.431	
1	6	3	20.051	18.612	18.612	0.0	1.439	1.132	
3	6	3	8.054	7.462	7.463	0.0	0.591	0.184	
5	6	3	92.607	93.519	93.519	0.0	-0.912	-0.605	
7	6	3	14.813	8.912	8.912	0.0	5.902	3.086	
0	12	0	198.660	202.599	202.599	0.0	-3.939	-1.317	*
9	6	3	71.955	72.607	72.607	0.0	-0.652	-0.455	
10	5	3	18.757	19.570	19.570	0.0	-0.813	-0.353	
8	5	3	18.219	18.658	18.658	0.0	-0.439	-0.203	
6	5	3	94.284	94.223	94.223	0.0	0.061	0.039	
4	5	3	45.237	44.531	-44.531	0.0	0.706	0.693	
2	5	3	93.021	93.573	93.573	0.0	-0.552	-0.370	
0	5	3	21.045	21.540	21.540	0.0	-0.495	-0.336	
-2	5	3	176.932	179.413	179.413	0.0	-2.481	-0.931	
-4	5	3	21.915	24.819	24.819	0.0	-2.904	-2.161	
-6	5	3	27.360	28.660	28.660	0.0	-1.300	-1.067	
-8	5	3	48.560	48.368	48.368	0.0	0.192	0.161	
-10	5	3	20.258	18.872	18.872	0.0	1.387	0.830	
-12	5	3	55.102	57.535	57.535	0.0	-2.432	-1.567	
-13	4	3	17.557	18.287	18.287	0.0	-0.730	-0.236	
-11	4	3	11.656	0.964	-0.964	0.0	10.692	4.171	*
-9	4	3	10.807	11.539	11.539	0.0	-0.732	-0.268	
-5	4	3	9.606	10.843	10.843	0.0	-1.236	-0.472	
-3	4	3	13.592	11.954	11.954	0.0	1.638	0.903	
-1	4	3	23.488	22.290	22.290	0.0	1.198	1.036	
0	12	0	199.592	202.599	202.599	0.0	-3.007	-1.002	*
1	4	3	20.548	19.827	19.827	0.0	0.721	0.516	
3	4	3	12.163	12.602	12.602	0.0	-0.438	-0.186	
5	4	3	13.043	12.531	-12.531	0.0	0.512	0.259	
7	4	3	13.757	12.954	12.954	0.0	0.803	0.365	
9	4	3	19.430	15.868	15.868	0.0	3.562	2.023	
8	3	3	3.406	8.185	-8.185	0.0	-4.779	-0.767	
6	3	3	45.092	47.970	-47.970	0.0	-2.878	-2.294	
2	3	3	71.655	72.318	-72.318	0.0	-0.663	-0.542	
0	3	3	29.699	29.078	29.078	0.0	0.622	0.629	
-2	3	3	95.899	94.947	-94.947	0.0	0.952	0.637	
-4	3	3	12.702	5.474	5.474	0.0	7.227	4.177	
-6	3	3	14.306	12.937	12.937	0.0	1.369	0.803	
-8	3	3	42.256	44.232	-44.232	0.0	-1.976	-1.674	
-10	3	3	10.497	12.533	12.533	0.0	-2.037	-0.636	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-12	3	3	21.035	21.111	-21.111	0.0	-0.076	-0.034	
-11	2	3	11.501	9.367	9.367	0.0	2.134	0.693	
-9	2	3	26.946	28.426	-28.426	0.0	-1.480	-1.052	
0	12	0	200.182	202.599	202.599	0.0	-2.417	-0.803	*
-7	2	3	44.036	44.901	44.901	0.0	-0.864	-0.865	
-5	2	3	59.823	60.831	-60.831	0.0	-1.009	-0.898	
-3	2	3	94.863	95.195	95.195	0.0	-0.332	-0.224	
-1	2	3	10.279	10.920	-10.920	0.0	-0.640	-0.331	
1	2	3	12.909	6.512	6.512	0.0	6.396	3.666	
3	2	3	46.500	48.116	48.116	0.0	-1.616	-1.548	
7	2	3	24.792	23.313	23.313	0.0	1.479	1.121	
9	2	3	22.784	20.016	-20.016	0.0	2.768	1.894	
10	1	3	16.977	14.501	-14.501	0.0	2.476	1.224	
8	1	3	14.348	13.308	13.308	0.0	1.040	0.449	
6	1	3	14.182	15.575	-15.575	0.0	-1.393	-0.589	
2	1	3	32.028	32.227	-32.227	0.0	-0.199	-0.194	
0	1	3	29.958	30.058	30.058	0.0	-0.100	-0.105	
-2	1	3	23.581	24.579	-24.579	0.0	-0.997	-0.800	
-4	1	3	20.372	20.907	20.907	0.0	-0.534	-0.435	
-6	1	3	4.834	2.456	-2.456	0.0	2.378	0.591	
0	12	0	199.219	202.599	202.599	0.0	-3.380	-1.128	*
-13	0	3	12.691	11.619	-11.619	0.0	1.072	0.286	
-11	0	3	6.635	8.887	8.887	0.0	-2.251	-0.475	
-9	0	3	13.261	13.330	-13.330	0.0	-0.069	-0.032	
-5	0	3	8.199	9.157	-9.157	0.0	-0.958	-0.324	
-3	0	3	18.405	19.862	-19.862	0.0	-1.456	-1.149	
1	0	3	12.101	12.251	12.251	0.0	-0.150	-0.071	
3	0	3	15.610	17.412	-17.412	0.0	-1.801	-0.962	
7	0	3	7.018	9.839	-9.839	0.0	-2.820	-0.717	
9	0	3	3.644	10.972	10.972	0.0	-7.329	-1.124	
-10	0	4	32.784	33.289	33.289	0.0	-0.505	-0.376	
-8	0	4	20.227	22.523	-22.523	0.0	-2.296	-1.245	
-6	0	4	137.471	139.329	139.329	0.0	-1.858	-0.880	
-4	0	4	109.584	110.254	110.254	0.0	-0.670	-0.391	
-2	0	4	57.463	58.009	-58.009	0.0	-0.546	-0.504	
0	0	4	158.340	159.574	159.574	0.0	-1.234	-0.512	
0	12	0	197.967	202.599	202.599	0.0	-4.633	-1.554	*
4	0	4	136.891	139.528	139.528	0.0	-2.636	-1.231	
6	0	4	7.381	9.987	9.987	0.0	-2.606	-0.596	
8	0	4	41.293	40.632	40.632	0.0	0.661	0.484	
9	1	4	20.538	17.768	-17.768	0.0	2.770	1.499	
7	1	4	8.758	12.601	12.601	0.0	-3.843	-0.942	
3	1	4	61.282	61.523	61.523	0.0	-0.241	-0.203	
1	1	4	10.662	8.268	8.268	0.0	2.394	0.987	
-1	1	4	64.709	64.325	-64.325	0.0	0.383	0.332	
-3	1	4	126.022	128.542	128.542	0.0	-2.520	-1.292	
-5	1	4	15.869	13.458	-13.458	0.0	2.411	1.445	
-7	1	4	71.396	71.138	71.138	0.0	0.258	0.207	
-9	1	4	10.310	16.310	-16.310	0.0	-6.000	-1.704	
-11	1	4	23.074	24.497	24.497	0.0	-1.423	-0.754	
-12	2	4	7.971	0.597	-0.597	0.0	7.374	1.819	
-10	2	4	8.488	6.122	-6.122	0.0	2.367	0.702	
-6	2	4	7.484	9.700	-9.700	0.0	-2.216	-0.617	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	12	0	200.047	202.599	202.599	0.0	-2.552	-0.848	*
-4	2	4	4.689	4.207	-4.207	0.0	0.483	0.108	
-2	2	4	8.913	4.989	-4.989	0.0	3.924	1.454	
0	2	4	12.960	15.729	-15.729	0.0	-2.769	-1.213	
2	2	4	16.376	16.697	-16.697	0.0	-0.321	-0.182	
4	2	4	7.505	0.844	0.844	0.0	6.661	2.057	
6	2	4	4.224	8.463	8.463	0.0	-4.240	-0.710	
9	3	4	16.180	15.020	15.020	0.0	1.160	0.490	
7	3	4	18.323	16.082	-16.082	0.0	2.241	1.157	
5	3	4	18.043	16.049	16.049	0.0	1.994	1.224	
3	3	4	35.610	35.130	-35.130	0.0	0.480	0.419	
1	3	4	14.472	11.093	-11.093	0.0	3.379	1.741	
-1	3	4	45.910	49.285	49.285	0.0	-3.375	-3.192	
-3	3	4	71.903	72.001	-72.001	0.0	-0.098	-0.081	
-5	3	4	37.949	36.722	36.722	0.0	1.228	1.199	
-7	3	4	18.074	19.172	-19.172	0.0	-1.098	-0.589	
-9	3	4	14.503	16.615	16.615	0.0	-2.112	-0.889	
-11	3	4	17.598	13.355	-13.355	0.0	4.243	2.244	
-13	3	4	13.809	3.769	-3.769	0.0	10.040	3.629	*
-12	4	4	11.842	7.554	7.554	0.0	4.288	1.383	
0	12	0	198.257	202.599	202.599	0.0	-4.343	-1.455	*
-10	4	4	6.315	3.657	-3.657	0.0	2.657	0.588	
-8	4	4	15.300	17.610	17.610	0.0	-2.310	-1.022	
-6	4	4	11.283	16.351	-16.351	0.0	-5.067	-1.795	
-2	4	4	32.701	34.592	34.592	0.0	-1.891	-1.568	
0	4	4	44.057	44.032	-44.032	0.0	0.025	0.024	
2	4	4	73.880	75.343	75.343	0.0	-1.463	-1.123	
4	4	4	17.142	17.433	-17.433	0.0	-0.291	-0.149	
6	4	4	19.410	17.424	17.424	0.0	1.986	1.267	
8	4	4	6.811	4.600	4.600	0.0	2.211	0.516	
7	5	4	8.147	1.185	-1.185	0.0	6.962	1.968	
5	5	4	14.658	12.155	-12.155	0.0	2.504	1.317	
3	5	4	21.687	20.977	-20.977	0.0	0.710	0.437	
1	5	4	21.097	20.020	-20.020	0.0	1.077	0.739	
-1	5	4	2.226	8.078	8.078	0.0	-5.852	-0.921	
-3	5	4	35.258	36.906	-35.906	0.0	-1.648	-1.419	
-5	5	4	7.422	10.014	10.014	0.0	-2.592	-0.683	
-11	5	4	10.176	11.924	-11.924	0.0	-1.748	-0.468	
0	12	0	199.105	202.599	202.599	0.0	-3.494	-1.166	*
-13	5	4	16.408	17.815	17.815	0.0	-1.407	-0.441	
-12	6	4	12.608	3.310	-3.310	0.0	9.299	3.473	
-10	6	4	13.830	15.884	15.884	0.0	-2.054	-0.766	
-8	6	4	13.271	13.351	-13.351	0.0	-0.081	-0.034	
-6	6	4	8.416	5.842	5.842	0.0	2.574	0.943	
-4	6	4	11.832	2.091	-2.091	0.0	9.741	5.293	
0	6	4	7.577	3.078	-3.078	0.0	4.499	1.407	
2	6	4	11.211	6.602	-6.602	0.0	4.609	2.316	
4	6	4	3.571	7.175	7.175	0.0	-3.604	-0.655	
6	6	4	15.145	16.462	16.462	0.0	-1.317	-0.472	
8	6	4	9.348	15.695	-15.695	0.0	-6.347	-1.545	
7	7	4	15.041	10.751	-10.751	0.0	4.290	2.055	
3	7	4	30.900	32.067	32.067	0.0	-1.167	-0.895	
1	7	4	19.575	20.600	-20.600	0.0	-1.025	-0.600	

K-RICHTERITE 800C, 3/6/73

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-1	7	4	14.658	11.501	11.501	0.0	3.157	1.796	
-3	7	4	11.377	13.949	13.949	0.0	-2.572	-1.045	
-5	7	4	16.035	17.596	17.596	0.0	-1.561	-0.744	
-7	7	4	23.737	23.528	-23.528	0.0	0.208	0.148	
0	12	0	198.495	202.599	202.599	0.0	-4.105	-1.374	*
-9	7	4	31.293	33.955	33.955	0.0	-2.662	-1.781	
-11	7	4	10.569	14.908	-14.908	0.0	-4.339	-1.054	
-12	8	4	27.877	29.384	29.384	0.0	-1.506	-0.776	
-10	8	4	38.001	36.906	-36.906	0.0	1.096	0.841	
-6	8	4	22.432	21.563	21.563	0.0	0.869	0.598	
-4	8	4	38.384	38.133	-38.133	0.0	0.252	0.247	
-2	8	4	6.615	6.572	-6.572	0.0	0.043	0.012	
0	8	4	8.654	4.209	-4.209	0.0	4.445	1.648	
2	8	4	40.786	40.610	40.610	0.0	0.176	0.159	
4	8	4	60.651	62.022	-62.022	0.0	-1.371	-1.119	
6	8	4	38.912	39.016	39.016	0.0	-0.104	-0.081	
7	9	4	35.092	33.317	-33.317	0.0	1.775	1.313	
3	9	4	7.360	10.807	-10.807	0.0	-3.447	-0.829	
1	9	4	45.196	44.123	-44.123	0.0	1.072	0.981	
-1	9	4	5.435	7.420	7.420	0.0	-1.985	-0.496	
-3	9	4	24.575	22.005	-22.005	0.0	2.570	2.237	
-5	9	4	14.027	10.186	10.186	0.0	3.841	1.944	
0	12	0	198.578	202.599	202.599	0.0	-4.022	-1.346	*
-7	9	4	37.235	38.460	-38.460	0.0	-1.225	-0.886	
-9	9	4	35.827	35.627	35.627	0.0	0.201	0.160	
-11	9	4	9.430	9.546	-9.546	0.0	-0.116	-0.029	
-10	10	4	12.878	10.720	10.720	0.0	2.157	0.783	
-8	10	4	22.236	20.854	20.854	0.0	1.381	0.899	
-6	10	4	26.614	25.743	25.743	0.0	0.871	0.682	
-4	10	4	35.030	35.415	35.415	0.0	-0.385	-0.336	
-2	10	4	20.838	19.499	19.499	0.0	1.339	0.904	
0	10	4	37.856	35.753	35.753	0.0	2.104	2.254	
2	10	4	13.499	10.899	10.899	0.0	2.600	1.193	
4	10	4	38.974	40.467	40.467	0.0	-1.493	-1.094	
6	10	4	23.043	21.564	21.564	0.0	1.479	0.844	
7	11	4	35.538	37.678	37.678	0.0	-2.140	-1.337	
5	11	4	22.815	25.506	25.506	0.0	-2.691	-1.227	
3	11	4	45.548	46.632	46.632	0.0	-1.084	-0.934	
1	11	4	55.692	55.951	55.951	0.0	-0.258	-0.227	
-1	11	4	14.223	15.232	-15.232	0.0	-1.008	-0.407	
-3	11	4	88.590	90.011	90.011	0.0	-1.420	-0.957	
-5	11	4	11.521	9.470	9.470	0.0	2.052	0.816	
-7	11	4	96.665	96.970	96.970	0.0	-0.305	-0.190	
0	12	0	199.261	202.599	202.599	0.0	-3.339	-1.114	*
-9	11	4	27.836	30.763	-30.763	0.0	-2.928	-1.682	
-11	11	4	27.349	27.299	27.299	0.0	0.050	0.029	
-10	12	4	33.488	35.321	35.321	0.0	-1.833	-1.190	
-8	12	4	25.507	23.189	-23.189	0.0	2.318	1.615	
-6	12	4	31.966	33.275	33.275	0.0	-1.309	-0.883	
-4	12	4	72.069	72.714	72.714	0.0	-0.645	-0.487	
-2	12	4	42.960	44.105	-44.105	0.0	-1.145	-1.027	
0	12	4	38.954	37.614	37.614	0.0	1.340	1.070	
2	12	4	24.130	24.290	-24.290	0.0	-0.160	-0.108	

K-RICHTERITE 800C, 3/6/73 STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
4	12	4	91.799	92.873	92.873	0.0	-1.074	-0.665	
6	12	4	36.407	36.721	-36.721	0.0	-0.314	-0.223	
1	13	4	4.462	0.030	0.030	0.0	4.432	0.880	
-1	13	4	36.635	35.288	-35.288	0.0	1.347	1.112	
-3	13	4	19.554	21.431	21.431	0.0	-1.876	-1.040	
-5	13	4	21.894	18.344	-18.344	0.0	3.550	2.556	
-7	13	4	38.364	37.506	37.506	0.0	0.857	0.646	
-9	13	4	34.782	34.420	-34.420	0.0	0.361	0.243	
0	12	0	198.857	202.599	202.599	0.0	-3.742	-1.250	*
-8	14	4	7.598	10.248	10.248	0.0	-2.650	-0.600	
-6	14	4	9.989	8.002	-8.002	0.0	1.988	0.636	
-2	14	4	10.724	16.126	16.126	0.0	-5.402	-1.615	
2	14	4	11.729	9.030	9.030	0.0	2.698	0.968	
6	14	4	10.196	15.516	15.516	0.0	-5.319	-1.252	
1	15	4	14.172	15.016	-15.016	0.0	-0.844	-0.328	
-1	15	4	19.585	20.106	20.106	0.0	-0.521	-0.276	
-3	15	4	18.519	18.946	-18.945	0.0	-0.427	-0.205	
-5	15	4	21.180	18.393	18.393	0.0	2.786	1.722	
-7	15	4	20.269	23.423	-23.423	0.0	-3.154	-1.305	
-9	15	4	25.062	25.309	25.309	0.0	-0.247	-0.129	
-6	16	4	12.029	14.845	14.845	0.0	-2.816	-0.893	
-4	16	4	12.805	18.743	-18.743	0.0	-5.938	-1.812	
-2	16	4	11.397	9.877	-9.877	0.0	1.521	0.533	
0	12	0	200.534	202.599	202.599	0.0	-2.065	-0.685	*
0	16	4	3.985	2.037	-2.037	0.0	1.949	0.354	
2	16	4	15.641	14.443	14.443	0.0	1.198	0.479	
4	16	4	36.935	35.561	-35.561	0.0	1.374	1.026	
3	17	4	12.919	14.098	14.098	0.0	-1.179	-0.395	
1	17	4	15.621	15.888	-15.888	0.0	-0.267	-0.102	
-1	17	4	8.809	0.641	0.641	0.0	8.168	2.499	
-3	17	4	14.668	15.340	15.340	0.0	-0.672	-0.281	
-5	18	4	11.066	9.709	9.709	0.0	1.357	0.405	
-2	18	4	6.667	8.466	8.466	0.0	-1.800	-0.374	
0	18	4	6.377	7.690	7.690	0.0	-1.314	-0.255	
1	19	4	13.757	12.156	-12.156	0.0	1.601	0.574	
-1	19	4	8.240	6.383	6.383	0.0	1.857	0.457	
-3	19	4	26.097	25.286	-25.286	0.0	0.810	0.485	
-5	19	4	5.321	11.622	11 522	0.0	-6.301	-1.030	
-4	20	4	11.190	6.767	-6.767	0.0	4.423	1.376	
-2	20	4	15.310	10.532	10.532	0.0	4.778	2.414	
0	12	0	199.054	202.599	202.599	0.0	-3.546	-1.184	*
0	20	4	28.374	29.055	-29.055	0.0	-0.680	-0.380	
-3	18	5	45.703	44.596	-44.596	0.0	1.107	0.832	
-1	18	5	44.295	40.213	40.213	0.0	4.082	3.833	
-2	17	5	39.337	37.368	37.368	0.0	1.969	1.581	
-6	17	5	10.942	2.936	2.936	0.0	8.006	2.504	
-7	16	5	11.490	6.289	6.289	0.0	5.201	1.622	
-5	16	5	29.161	25.405	25.405	0.0	3.755	3.039	
-3	16	5	9.130	11.202	11.202	0.0	-2.072	-0.501	
-1	16	5	33.188	32.087	32.087	0.0	1.100	0.844	
1	16	5	13.395	21.037	21.037	0.0	-7.642	-1.986	
2	15	5	12.929	11.283	-11.283	0.0	1.646	0.535	
0	15	5	20.548	21.054	21.054	0.0	-0.505	-0.238	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-2	15	5	20.029	14.941	-14.941	0.0	5.080	2.908	
-4	15	5	13.074	11.101	11.101	0.0	1.973	0.763	
-6	15	5	18.457	18.038	18.038	0.0	0.419	0.182	
-8	15	5	20.258	18.817	-18.817	0.0	1.441	0.649	
-7	14	5	20.879	18.373	18.373	0.0	2.507	1.414	
-5	14	5	49.047	48.708	-48.708	0.0	0.339	0.261	
0	12	0	199.126	202.599	202.599	0.0	-3.473	-1.159	*
-3	14	5	32.266	32.875	32.875	0.0	-0.609	-0.452	
-1	14	5	24.047	24.686	-24.686	0.0	-0.639	-0.372	
1	14	5	10.533	10.624	-10.624	0.0	-0.066	-0.026	
4	13	5	2.660	7.295	7.295	0.0	-4.635	-0.626	
2	13	5	15.797	11.902	-11.902	0.0	3.895	1.728	
0	13	5	21.066	18.241	18.241	0.0	2.825	1.950	
-2	13	5	13.147	13.291	-13.291	0.0	-0.144	-0.051	
-6	13	5	2.898	2.670	2.670	0.0	0.229	0.035	
-8	13	5	16.842	10.852	-10.852	0.0	5.990	3.629	
-7	12	5	11.967	10.228	10.228	0.0	1.739	0.599	
1	12	5	15.352	16.918	16.918	0.0	-1.566	-0.595	
3	12	5	10.010	4.504	4.504	0.0	5.507	1.763	
4	11	5	7.681	2.515	-2.515	0.0	5.166	1.289	
2	11	5	15.983	10.507	-10.507	0.0	5.476	2.626	
0	12	0	198.453	202.599	202.599	0.0	-4.146	-1.388	*
-2	11	5	12.143	7.922	-7.922	0.0	4.220	1.822	
-4	11	5	8.199	0.553	0.553	0.0	7.645	2.253	
-6	11	5	5.869	6.175	-6.175	0.0	-0.306	-0.064	
-8	11	5	6.563	4.084	4.084	0.0	2.479	0.555	
-10	11	5	2.857	1.644	-1.644	0.0	1.213	0.173	
-9	10	5	16.035	15.370	-15.370	0.0	0.665	0.266	
-7	10	5	15.579	16.206	16.206	0.0	-0.627	-0.265	
-5	10	5	26.231	28.735	-28.735	0.0	-2.503	-1.453	
-3	10	5	27.494	27.074	27.074	0.0	0.421	0.347	
-1	10	5	16.625	17.411	-17.411	0.0	-0.786	-0.344	
1	10	5	11.873	5.908	5.908	0.0	5.965	2.335	
3	10	5	7.433	4.702	-4.702	0.0	2.731	0.694	
5	10	5	8.695	2.022	2.022	0.0	6.673	1.820	
4	9	5	31.200	32.065	32.065	0.0	-0.865	-0.583	
2	9	5	27.763	28.391	-28.391	0.0	-0.628	-0.383	
0	9	5	27.463	26.589	26.589	0.0	0.875	0.775	
-2	9	5	11.459	11.052	-11.052	0.0	0.407	0.150	
-4	9	5	15.082	11.853	11.853	0.0	3.229	1.757	
0	12	0	198.153	202.599	202.599	0.0	-4.446	-1.492	*
-8	9	5	19.989	23.387	-23.387	0.0	-3.398	-1.536	
-10	9	5	19.368	21.045	21.045	0.0	-1.677	-0.707	
-11	8	5	8.168	2.155	-2.155	0.0	6.012	1.493	
-9	8	5	4.410	1.573	-1.573	0.0	2.837	0.511	
-7	8	5	4.607	0.380	-0.380	0.0	4.227	0.774	
-5	8	5	10.093	8.935	-8.935	0.0	1.158	0.400	
-1	8	5	14.399	12.968	-12.968	0.0	1.431	0.772	
3	8	5	10.269	11.732	11.732	0.0	-1.463	-0.416	
5	8	5	11.066	10.975	-10.975	0.0	0.091	0.029	
6	7	5	11.635	11.964	11.964	0.0	-0.329	-0.101	
4	7	5	49.864	51.109	-51.109	0.0	-1.244	-0.900	
2	7	5	43.569	44.210	44.210	0.0	-0.650	-0.536	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	7	5	11.801	9.025	-9.025	0.0	2.776	1.100	
-2	7	5	12.712	11.142	11.142	0.0	1.570	0.633	
-4	7	5	14.741	17.307	-17.307	0.0	-2.566	-1.029	
-6	7	5	9.596	3.336	3.336	0.0	6.260	2.290	
-8	7	5	33.198	30.316	30.316	0.0	2.882	2.246	
-10	7	5	2.950	10.527	-10.527	0.0	-7.577	-1.022	
0	12	0	198.319	202.599	202.599	0.0	-4.281	-1.435	*
-9	6	5	87.607	85.042	85.042	0.0	2.565	1.729	
-7	6	5	15.217	14.267	-14.267	0.0	0.950	0.411	
-5	6	5	62.897	62.902	62.902	0.0	-0.004	-0.004	
-3	6	5	44.647	45.405	-45.405	0.0	-0.758	-0.639	
-1	6	5	121.716	121.113	121.113	0.0	0.603	0.316	
1	6	5	19.378	16.805	16.805	0.0	2.574	1.596	
3	6	5	32.318	31.515	31.515	0.0	0.803	0.577	
5	6	5	24.647	27.419	27.419	0.0	-2.772	-1.442	
6	5	5	43.674	43.336	43.336	0.0	0.338	0.239	
4	5	5	34.740	34.653	-34.653	0.0	0.088	0.064	
2	5	5	87.193	88.192	88.192	0.0	-0.999	-0.688	
0	5	5	23.105	24.280	24.280	0.0	-1.175	-0.766	
-2	5	5	58.591	60.530	60.530	0.0	-1.939	-1.662	
-4	5	5	5.083	8.707	8.707	0.0	-3.625	-0.760	
-6	5	5	19.202	21.195	21.195	0.0	-1.992	-0.957	
-8	5	5	59.119	60.344	60.344	0.0	-1.225	-0.888	
-10	5	5	6.573	2.766	2.766	0.0	3.807	0.833	
-12	5	5	33.736	33.878	33.878	0.0	-0.141	-0.082	
-11	4	5	7.298	0.685	0.685	0.0	6.613	1.555	
0	12	0	197.853	202.599	202.599	0.0	-4.747	-1.595	*
-9	4	5	11.625	13.163	13.163	0.0	-1.538	-0.494	
-5	4	5	12.381	8.667	8.667	0.0	3.713	1.699	
-3	4	5	4.617	2.434	-2.434	0.0	2.183	0.468	
-1	4	5	8.861	5.271	5.271	0.0	3.590	1.183	
1	4	5	7.091	9.450	9.450	0.0	-2.359	-0.608	
3	4	5	17.619	19.120	19.120	0.0	-1.501	-0.689	
5	4	5	15.621	9.943	-9.943	0.0	5.678	3.018	
6	3	5	27.577	27.395	-27.395	0.0	0.182	0.112	
4	3	5	13.033	18.523	18.523	0.0	-5.490	-1.635	
2	3	5	46.397	46.335	-46.335	0.0	0.062	0.056	
0	3	5	7.940	13.233	13.233	0.0	-5.293	-1.321	
-2	3	5	32.473	31.452	-31.452	0.0	1.021	0.841	
-4	3	5	5.228	2.042	2.042	0.0	3.186	0.745	
-6	3	5	9.234	3.932	3.932	0.0	5.301	1.945	
-8	3	5	34.254	34.926	-34.926	0.0	-0.672	-0.562	
-10	3	5	19.793	24.333	24.333	0.0	-4.541	-1.898	
-12	3	5	16.273	15.854	-15.854	0.0	0.419	0.145	
-9	2	5	20.331	19.169	-19.169	0.0	1.162	0.672	
0	12	0	198.246	202.599	202.599	0.0	-4.353	-1.459	*
-7	2	5	27.039	27.413	27.413	0.0	-0.374	-0.257	
-5	2	5	43.746	45.713	-45.713	0.0	-1.966	-1.564	
-3	2	5	50.516	52.359	52.359	0.0	-1.843	-1.603	
-1	2	5	14.958	16.334	-16.334	0.0	-1.376	-0.622	
1	2	5	15.859	13.718	13.718	0.0	2.141	1.062	
3	2	5	6.625	6.277	6.277	0.0	0.348	0.085	
5	2	5	10.745	10.589	10.589	0.0	0.156	0.047	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
7	2	5	15.227	17.718	17.718	0.0	-2.491	-0.829	
6	1	5	12.826	13.054	-13.054	0.0	-0.228	-0.075	
4	1	5	6.635	5.210	5.210	0.0	1.425	0.321	
2	1	5	7.577	9.610	-9.610	0.0	-2.033	-0.523	
0	1	5	17.774	14.917	14.917	0.0	2.857	1.996	
-2	1	5	9.700	10.215	-10.215	0.0	-0.515	-0.176	
-4	1	5	6.977	8.039	8.039	0.0	-1.062	-0.286	
-8	1	5	1.925	1.412	-1.412	0.0	0.514	0.078	
-10	1	5	6.863	3.063	3.063	0.0	3.800	0.854	
-11	0	5	11.532	10.576	10.576	0.0	0.956	0.293	
-9	0	5	9.254	11.047	-11.047	0.0	-1.793	-0.511	
0	12	0	197.956	202.599	202.599	0.0	-4.643	-1.559	*
-7	0	5	7.691	4.381	4.381	0.0	3.310	1.030	
-3	0	5	14.513	11.045	-11.045	0.0	3.468	2.092	
-1	0	5	13.095	12.557	-12.557	0.0	0.538	0.230	
1	0	5	9.493	6.315	6.315	0.0	3.178	1.121	
5	0	5	7.702	0.658	0.658	0.0	7.044	1.854	
7	0	5	11.635	14.551	-14.551	0.0	-2.916	-0.795	
-10	0	6	69.191	68.405	68.405	0.0	0.786	0.530	
-8	0	6	31.697	30.033	-30.033	0.0	1.664	1.202	
-6	0	6	22.525	25.358	25.358	0.0	-2.832	-1.346	
-4	0	6	71.468	70.478	70.478	0.0	0.990	0.739	
-2	0	6	29.585	28.767	28.767	0.0	0.818	0.528	
0	0	6	42.173	41.893	41.893	0.0	0.280	0.226	
2	0	6	17.877	20.387	-20.387	0.0	-2.510	-1.004	
4	0	6	85.433	83.166	83.166	0.0	2.267	1.450	
3	1	6	16.314	13.660	-13.660	0.0	2.654	1.087	
1	1	6	25.941	24.264	24.264	0.0	1.678	1.173	
-1	1	6	12.598	7.665	-7.665	0.0	4.933	1.945	
-3	1	6	62.452	62.370	62.370	0.0	0.082	0.066	
0	12	0	197.884	202.599	202.599	0.0	-4.715	-1.584	*
-5	1	6	17.608	16.058	-16.058	0.0	1.551	0.836	
-7	1	6	44.471	43.392	43.392	0.0	1.079	0.918	
-9	1	6	22.308	21.660	-21.660	0.0	0.648	0.346	
-10	2	6	2.339	2.841	-2.841	0.0	-0.501	-0.067	
-8	2	6	1.273	3.906	3.906	0.0	-2.632	-0.331	
-2	2	6	5.662	1.433	1.433	0.0	4.229	0.892	
2	2	6	5.631	9.246	-9.246	0.0	-3.614	-0.664	
4	2	6	12.888	9.981	-9.981	0.0	2.907	1.106	
3	3	6	16.076	10.503	10.503	0.0	5.573	3.019	
1	3	6	16.811	19.026	-19.026	0.0	-2.215	-0.872	
-1	3	6	15.931	18.445	18.445	0.0	-2.514	-0.962	
-3	3	6	23.757	21.868	-21.868	0.0	1.889	1.245	
-5	3	6	25.186	21.957	21.957	0.0	3.229	2.258	
-7	3	6	17.049	22.713	-22.713	0.0	-5.663	-1.919	
-9	3	6	17.381	17.451	17.451	0.0	-0.070	-0.030	
-10	4	6	25.869	27.495	-27.495	0.0	-1.626	-0.779	
-8	4	6	7.391	8.288	8.288	0.0	-0.897	-0.201	
0	12	0	198.402	202.599	202.599	0.0	-4.198	-1.405	*
-6	4	6	17.225	16.067	16.067	0.0	1.158	0.560	
0	4	6	7.257	3.435	3.435	0.0	3.822	0.933	
2	4	6	29.037	30.182	30.182	0.0	-1.145	-0.615	
4	4	6	21.045	25.052	-25.052	0.0	-4.007	-1.485	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
1	5	6	26.304	23.454	-23.454	0.0	2.850	1.947	
-3	5	6	6.118	4.893	4.893	0.0	1.224	0.288	
-5	5	6	0.694	1.691	-1.691	0.0	-0.997	-0.123	
-7	5	6	17.639	15.842	-15.842	0.0	1.797	0.790	
-9	5	6	22.867	20.607	20.607	0.0	2.260	1.236	
-10	6	6	14.472	6.792	6.792	0.0	7.679	3.346	
-8	6	6	3.696	4.222	-4.222	0.0	-0.527	-0.087	
-6	6	6	5.735	3.857	3.857	0.0	1.878	0.402	
-2	6	6	5.362	2.219	2.219	0.0	3.143	0.652	
0	6	6	7.971	5.426	5.426	0.0	2.545	0.661	
2	6	6	8.074	10.679	-10.679	0.0	-2.604	-0.633	
0	12	0	198.008	202.599	202.599	0.0	-4.591	-1.540	*
1	7	6	2.805	2.663	-2.663	0.0	0.142	0.022	
-1	7	6	22.701	22.084	22.084	0.0	0.617	0.350	
-3	7	6	18.788	17.585	-17.585	0.0	1.204	0.645	
-5	7	6	19.679	18.479	18.479	0.0	1.200	0.611	
-9	7	6	10.673	5.691	5.691	0.0	4.981	1.661	
-8	8	6	11.998	15.039	15.039	0.0	-3.042	-0.924	
-6	8	6	22.577	21.156	-21.156	0.0	1.421	0.798	
-4	8	6	8.457	8.161	8.161	0.0	0.296	0.076	
-2	8	6	2.391	5.046	5.046	0.0	-2.655	-0.374	
0	8	6	33.571	35.891	-35.891	0.0	-2.320	-1.433	
2	8	6	33.333	33.846	33.846	0.0	-0.514	-0.330	
1	9	6	15.051	10.389	-10.389	0.0	4.662	2.010	
-1	9	6	19.855	20.249	20.249	0.0	-0.395	-0.186	
-3	9	6	41.138	40.730	-40.730	0.0	0.408	0.304	
-5	9	6	22.846	22.405	22.405	0.0	0.442	0.242	
-7	9	6	8.375	4.696	-4.696	0.0	3.679	0.983	
-8	10	6	9.089	8.686	8.686	0.0	0.403	0.103	
0	12	0	197.884	202.599	202.599	0.0	-4.715	-1.583	*
-6	10	6	12.277	10.127	10.127	0.0	2.150	0.767	
-4	10	6	12.360	19.196	19.196	0.0	-6.836	-1.836	
-2	10	6	17.515	17.695	17.695	0.0	-0.180	-0.076	
0	10	6	18.799	18.312	18.312	0.0	0.487	0.242	
2	10	6	5.807	2.022	2.022	0.0	3.786	0.731	
1	11	6	22.815	23.249	23.249	0.0	-0.434	-0.227	
-1	11	6	1.718	9.623	-9.623	0.0	-7.905	-0.994	
-3	11	6	84.750	85.186	85.186	0.0	-0.437	-0.289	
-5	11	6	12.888	14.005	-14.005	0.0	-1.117	-0.379	
-7	11	6	34.709	34.459	34.459	0.0	0.250	0.171	
-6	12	6	30.300	31.393	31.393	0.0	-1.094	-0.630	
-4	12	6	24.772	22.486	22.486	0.0	2.285	1.592	
-2	12	6	4.327	7.648	-7.648	0.0	-3.321	-0.551	
0	12	6	36.241	39.120	39.120	0.0	-2.879	-1.599	
-1	13	6	22.391	18.916	-18.916	0.0	3.475	2.036	
-3	13	6	40.444	40.779	40.779	0.0	-0.335	-0.226	
-5	13	6	28.250	26.945	-26.945	0.0	1.305	1.001	
-2	14	6	5.352	5.477	5.477	0.0	-0.125	-0.022	
-4	7	7	6.004	5.889	5.889	0.0	0.115	0.021	
0	12	0	197.653	202.599	202.599	0.0	-4.747	-1.594	*
-5	6	7	60.827	59.529	59.529	0.0	1.298	0.979	
-3	6	7	39.150	39.963	-39.963	0.0	-0.813	-0.516	
-4	5	7	17.308	18.906	18.906	0.0	-1.598	-0.624	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-6	5	7	11.418	13.117	13.117	0.0	-1.699	-0.467	
-2	3	7	8.473	9.783	-9.783	0.0	-1.3[illegible]	-0.312	
-4	3	7	6.387	5.901	-5.901	0.0	0.486	0.099	
-7	2	7	13.664	16.304	16.304	0.0	-2.639	-2.804	
-5	2	7	29.979	30.070	-30.070	0.0	-0.091	-0.057	
-3	2	7	25.341	26.257	26.257	0.0	-0.915	-0.497	
-1	2	7	6.822	9.936	-9.936	0.0	-3.114	-0.605	
0	1	7	7.443	4.317	4.317	0.0	3.126	0.717	
-4	1	7	11.863	2.859	2.859	0.0	9.004	3.519	
-6	1	7	2.878	1.897	1.897	0.0	0.981	0.137	
0	12	0	197.108	202.599	202.599	0.0	-5.492	-1.850	*
-3	0	7	12.080	3.066	-3.066	0.0	9.014	3.820	
-1	0	7	10.880	10.049	-10.049	0.0	0.831	0.243	

K-RICHTERITE 800C, 3/6/73

RESULTS OF STRUCTURE FACTOR CALCULATIONS

ALL REFLECTIONS	NUMERATOR	DENOMINATOR	NUMBER	R
WEIGHTED R	16098.64	1261750.00	1338	0.113
UNWEIGHTED R	3148.08	51675.84	1338	0.061
RANGES OF F(OBS)				
	2344.74	15066.90	941	0.156
	338.71	9784.26	208	0.035
	106.92	5794.82	71	0.018
	40.37	2740.25	23	0.015
	38.32	1891.82	13	0.020
	261.46	15490.76	78	0.017
	13.97	635.97	3	0.022
	3.62	271.70	1	0.013
RANGES OF (SIN(THETA)/LAMBDA)**2				
	228.97	5468.17	91	0.042
	511.16	20016.92	193	0.026
	279.14	5449.54	144	0.051
	280.71	4844.52	160	0.058
	399.53	4343.86	173	0.092
	430.07	3856.43	184	0.112
	441.28	3662.01	187	0.121
	577.31	4036.19	206	0.143
UNREJECTED REFLECTIONS				
WEIGHTED R	1750.22	828645.25	1141	0.046
UNWEIGHTED R	2386.47	33148.22	1141	0.072
RANGES OF F(OBS)				
	2028.73	13753.59	857	0.148
	187.95	8574.82	182	0.022
	73.30	5155.83	63	0.014
	36.73	2388.96	20	0.015
	31.18	1618.89	11	0.019
	11.01	748.97	4	0.015
	13.97	635.97	3	0.022
	3.62	271.70	1	0.013
RANGES OF (SIN(THETA)/LAMBDA)**2				
	158.02	4571.41	74	0.035
	183.30	4634.82	104	0.040
	193.55	4977.13	130	0.039
	253.80	4412.38	146	0.058
	333.68	3939.57	157	0.085
	370.80	3544.60	169	0.105
	405.56	3349.17	173	0.121
	487.85	3720.86	188	0.131

SUM FCAL 51612.68
STANDARD DEV OF UNIT WEIGHT OBS 1.30

K-RICHTERITE 800C, 3/6/73

ATOM	PARAMETER	OLD	CHANGE	NEW	ERROR	SHIFT/ERROR
	EXTINCTION CORRECTION	0.0		0.0		
	SCALE FACTOR 1	0.9660	-0.0000	0.9660	0.00274	-0.00
ATOM 1 O(1)	EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.1108150	0.0000080	0.1108230	0.0002740	0.03
	Y	0.9145764	0.0000051	0.9145815	0.0001480	0.03
	Z	0.8909881	-0.0000095	0.8909785	0.0005265	-0.02
	BETA11	0.0038408	-0.0000311	0.0038097	0.0003091	-0.10
	BETA22	0.0014436	0.0000026	0.0014461	0.0000896	0.03
	BETA33	0.0164350	0.0000297	0.0164647	0.0011446	0.03
	BETA12	0.0001089	0.0000052	0.0001141	0.0001268	0.04
	BETA13	0.0020877	0.0000351	0.0021227	0.0004748	0.07
	BETA23	-0.0004255	-0.0000054	-0.0004308	0.0002361	-0.02
ATOM 2 O(2)	EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.1192549	0.0000006	0.1192555	0.0002762	0.00
	Y	0.8306174	0.0000059	0.8306232	0.0001541	0.04
	Z	0.3926241	0.0000012	0.3926253	0.0005370	0.00
	BETA11	0.0036893	-0.0000190	0.0036703	0.0003077	-0.06
	BETA22	0.0016624	0.0000002	0.0016627	0.0000925	0.00
	BETA33	0.0160847	0.0000278	0.0161125	0.0011389	0.02
	BETA12	0.0004902	-0.0000010	0.0004892	0.0001312	-0.01
	BETA13	0.0010818	0.0000175	0.0010993	0.0004539	0.04
	BETA23	-0.0004768	-0.0000032	-0.0004800	0.0002440	-0.01
ATOM 3 F(3)	EQUIPOINT FRACTION = 0.500					
	OCCUPANCY SPECIES 2	1.00000		1.00000		
	X	0.1013607	0.0000226	0.1013833	0.0003820	0.06
	Y	0.0		0.0		
	Z	0.3884387	-0.0000165	0.3884222	0.0006859	-0.02
	BETA11	0.0070173	-0.0000158	0.0070015	0.0004450	-0.04
	BETA22	0.0018149	-0.0000001	0.0018148	0.0001186	-0.00
	BETA33	0.0212255	-0.0000039	0.0212216	0.0015553	-0.00
	BETA12	0.0		0.0		
	BETA13	0.0004872	0.0000277	0.0005149	0.0006596	0.04
	BETA23	0.0		0.0		
ATOM 4 O(4)	EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.3613507	-0.0000051	0.3613455	0.0003386	-0.02
	Y	0.7537410	-0.0000053	0.7537357	0.0001618	-0.03
	Z	0.5591253	-0.0000053	0.5591199	0.0006439	-0.01
	BETA11	0.0081809	0.0000157	0.0081967	0.0004172	0.04
	BETA22	0.0013721	-0.0000015	0.0013706	0.0000907	-0.02
	BETA33	0.0232372	0.0000044	0.0232416	0.0013926	0.00
	BETA12	0.0014224	-0.0000029	0.0014195	0.0001530	-0.02
	BETA13	0.0029527	-0.0000114	0.0029413	0.0006052	-0.02
	BETA23	0.0006498	0.0000030	0.0006528	0.0002614	0.01
ATOM 5 O(5)	EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.3420107	0.0000303	0.3420410	0.0003100	0.10
	Y	0.8722124	0.0000029	0.8722153	0.0001593	0.02
	Z	0.2511258	-0.0000222	0.2511036	0.0005514	-0.04
	BETA11	0.0053092	0.0000210	0.0053301	0.0003509	0.06

	BETA22	0.0020352	-0.0000006	0.0020346	0.0000979	-0.01
	BETA33	0.0161914	-0.0000116	0.0161798	0.0011394	-0.01
	BETA12	0.0001403	-0.0000078	0.0001325	0.0001424	-0.05
	BETA13	0.0021380	-0.0000239	0.0021141	0.0004941	-0.05
	BETA23	0.0021466	0.0000009	0.0021475	0.0002657	0.00
ATOM 6 O(6)	EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.3386558	-0.0000040	0.3386518	0.0003038	-0.01
	Y	0.8814414	-0.0000057	0.8814356	0.0001566	-0.04
	Z	0.7513913	0.0000151	0.7514064	0.0005474	0.03
	BETA11	0.0050735	-0.0000355	0.0050380	0.0003461	-0.10
	BETA22	0.0019819	0.0000026	0.0019845	0.0000966	0.03
	BETA33	0.0176388	0.0000267	0.0176655	0.0011550	0.02
	BETA12	-0.0001242	0.0000107	-0.0001134	0.0001415	0.08
	BETA13	0.0032182	0.0000229	0.0032411	0.0004952	0.05
	BETA23	-0.0021183	-0.0000079	-0.0021262	0.0002737	-0.03
ATOM 7 O(7)	EQUIPOINT FRACTION = 0.500					
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.3314922	-0.0000322	0.3314600	0.0004518	-0.07
	Y	0.0		0.0		
	Z	0.0263935	0.0000312	0.0264247	0.0008857	0.04
	BETA11	0.0064085	-0.0000033	0.0064053	0.0005059	-0.01
	BETA22	0.0009475	-0.0000006	0.0009469	0.0001174	-0.01
	BETA33	0.0280098	-0.0000013	0.0280086	0.0019309	-0.00
	BETA12	0.0		0.0		
	BETA13	0.0021089	0.0000078	0.0021166	0.0007683	0.01
	BETA23	0.0		0.0		
ATOM 8 T(1)	EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 3	1.00000		1.00000		
	X	0.2748698	-0.0000143	0.2748554	0.0001165	-0.12
	Y	0.9157217	-0.0000008	0.9157208	0.0000526	-0.02
	Z	0.9768265	0.0000112	0.9768377	0.0002192	0.05
	BETA11	0.0033552	0.0000076	0.0033627	0.0001143	0.07
	BETA22	0.0009577	-0.0000001	0.0009576	0.0000310	-0.00
	BETA33	0.0115963	-0.0000076	0.0115888	0.0003881	-0.02
	BETA12	0.0001676	-0.0000029	0.0001647	0.0000489	-0.06
	BETA13	0.0014571	-0.0000076	0.0014495	0.0001660	-0.05
	BETA23	-0.0000678	0.0000025	-0.0000653	0.0000880	0.03
ATOM 9 T(2)	EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 3	1.00000		1.00000		
	X	0.2847525	-0.0000002	0.2847524	0.0001165	-0.00
	Y	0.8293477	-0.0000027	0.8293450	0.0000538	-0.05
	Z	0.4805126	-0.0000039	0.4805087	0.0002171	-0.02
	BETA11	0.0034390	0.0000036	0.0034426	0.0001103	0.03
	BETA22	0.0010322	-0.0000006	0.0010317	0.0000308	-0.02
	BETA33	0.0110665	-0.0000031	0.0110634	0.0003767	-0.01
	BETA12	0.0002314	-0.0000034	0.0002280	0.0000489	-0.07
	BETA13	0.0013204	-0.0000020	0.0013184	0.0001605	-0.01
	BETA23	0.0000681	0.0000016	0.0000696	0.0000886	0.02
ATOM 10 M(1)	EQUIPOINT FRACTION = 0.500					
	OCCUPANCY SPECIES 4	1.00000		1.00000		
	X	0.0		0.0		
	Y	0.9098220	0.0000027	0.9098247	0.0001049	0.03
	Z	0.5000000		0.5000000		
	BETA11	0.0049964	-0.0000180	0.0049784	0.0002274	-0.08
	BETA22	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

		BETA33	0.0133838	0.0000200	0.0134038	0.0007458	0.03
		BETA12	0.0		0.0		
		BETA13	0.0020237	0.0000225	0.0020463	0.0003256	0.07
		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	0.8191273	0.0000032	0.8191304	0.0001058	0.03
		Z	0.0		0.0		
		BETA11	0.0049834	-0.0000003	0.0049831	0.0002296	-0.00
		BETA22	0.0014460	-0.0000006	0.0014454	0.0000652	-0.01
		BETA33	0.0171309	0.0000097	0.0171406	0.0007997	0.01
		BETA12	0.0		0.0		
		BETA13	0.0016403	-0.0000060	0.0016343	0.0003339	-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	0.0053396	-0.0000226	0.0053170	0.0003235	-0.07
		BETA22	0.0012041	0.0000017	0.0012058	0.0000844	0.02
		BETA33	0.0151850	0.0000154	0.0152003	0.0010802	0.01
		BETA12	0.0		0.0		
		BETA13	0.0036033	0.0000276	0.0036309	0.0004690	0.06
		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	0.7216036	-0.0000015	0.7216021	0.0001017	-0.01
		Z	0.5000000		0.5000000		
		BETA11	0.0107333	0.0000183	0.0107516	0.0002666	0.07
		BETA22	0.0017201	-0.0000016	0.0017185	0.0000588	-0.03
		BETA33	0.0226398	0.0000042	0.0226440	0.0007625	0.01
		BETA12	0.0		0.0		
		BETA13	-0.0030167	-0.0000226	-0.0030394	0.0003523	-0.06
		BETA23	0.0		0.0		
ATOM 14	A	EQUIPOINT FRACTION = 0.500					
		OCCUPANCY SPECIES 7	0.50000		0.50000		
		X	0.4747868	-0.0000510	0.4747359	0.0016543	-0.03
		Y	0.0		0.0		
		Z	0.5336866	-0.0002387	0.5334479	0.0035738	-0.07
		BETA11	0.0188159	-0.0000701	0.0187458	0.0022656	-0.03
		BETA22	0.0042318	-0.0000013	0.0042305	0.0001453	-0.01
		BETA33	0.0488123	0.0004028	0.0492151	0.0063068	0.06
		BETA12	0.0		0.0		
		BETA13	-0.0109103	-0.0001078	-0.0110181	0.0021206	-0.05
		BETA23	0.0		0.0		

MAXIMUM SHIFT/ERROR = -0.12

AVERAGE SHIFT/ERROR = 0.03

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	12	0	203.217	204.739	204.739	0.0	-1.523	-0.501	*
6	0	0	96.256	93.930	93.930	0.0	2.326	1.583	
8	0	0	94.069	97.285	97.285	0.0	-3.216	-2.202	
10	0	0	60.374	58.573	58.573	0.0	1.801	1.720	
12	0	0	18.954	19.149	-19.149	0.0	-0.195	-0.145	
13	1	0	27.540	24.485	-24.485	0.0	3.056	2.721	
11	1	0	52.674	51.116	51.116	0.0	1.558	1.564	
9	1	0	19.359	19.666	19.666	0.0	-0.307	-0.306	
7	1	0	77.107	76.867	76.867	0.0	0.241	0.158	
5	1	0	107.138	103.674	-103.674	0.0	3.465	2.137	
3	1	0	147.950	150.480	150.480	0.0	-2.529	-1.143	
-3	1	0	145.688	150.480	150.480	0.0	-4.792	-2.200	*
-5	1	0	106.708	103.674	-103.674	0.0	3.034	1.881	*
-7	1	0	75.529	76.867	76.867	0.0	-1.338	-1.124	*
-9	1	0	19.418	19.666	19.666	0.0	-0.248	-0.249	*
-11	1	0	52.353	51.116	51.116	0.0	1.238	1.275	*
-13	1	0	26.696	24.485	-24.485	0.0	2.211	1.912	*
-12	2	0	11.212	9.902	9.902	0.0	1.310	0.666	*
-10	2	0	7.573	2.729	-2.729	0.0	4.844	2.342	*
-8	2	0	9.321	9.050	-9.050	0.0	0.270	0.146	*
0	12	0	203.402	204.739	204.739	0.0	-1.337	-0.439	*
-6	2	0	31.348	31.152	-31.152	0.0	0.196	0.280	*
-4	2	0	9.388	11.090	-11.090	0.0	-1.702	-1.768	*
4	2	0	8.823	11.090	-11.090	0.0	-2.267	-2.219	
6	2	0	31.187	31.152	-31.152	0.0	0.036	0.050	
8	2	0	2.955	9.050	-9.050	0.0	-6.096	-1.483	
10	2	0	4.635	2.729	-2.729	0.0	1.906	0.620	
12	2	0	12.782	9.902	9.902	0.0	2.881	1.706	
13	3	0	11.997	11.051	11.051	0.0	0.946	0.433	
11	3	0	19.047	15.723	-15.723	0.0	3.324	3.175	
9	3	0	17.240	16.748	16.748	0.0	0.492	0.452	
7	3	0	51.762	50.991	-50.991	0.0	0.771	0.861	
5	3	0	61.868	60.826	60.826	0.0	1.042	1.064	
3	3	0	79.860	79.823	-79.823	0.0	0.037	0.030	
-3	3	0	79.066	79.823	-79.823	0.0	-0.757	-0.631	*
-5	3	0	61.539	60.826	60.826	0.0	0.713	0.734	*
-7	3	0	50.851	50.991	-50.991	0.0	-0.141	-0.157	*
-9	3	0	19.739	16.748	16.748	0.0	2.991	3.343	*
-11	3	0	18.388	15.723	-15.723	0.0	2.665	2.304	*
-13	3	0	12.799	11.051	11.051	0.0	1.748	0.937	*
-12	4	0	16.472	15.731	15.731	0.0	0.741	0.513	*
0	12	0	203.504	204.739	204.739	0.0	-1.236	-0.405	*
-10	4	0	3.411	5.605	-5.605	0.0	-2.194	-0.588	*
-8	4	0	7.961	4.916	4.916	0.0	3.045	1.515	*
-6	4	0	1.553	5.359	5.359	0.0	-3.806	-0.898	*
-4	4	0	6.543	6.555	6.555	0.0	-0.012	-0.009	*
-2	4	0	125.560	129.138	129.138	0.0	-3.578	-1.900	*
2	4	0	127.840	129.138	129.138	0.0	-1.298	-0.677	
4	4	0	8.341	6.555	6.555	0.0	1.786	1.706	
6	4	0	2.904	5.359	5.359	0.0	-2.455	-0.729	
8	4	0	7.953	4.916	4.916	0.0	3.037	1.462	
10	4	0	8.350	5.605	-5.605	0.0	2.745	1.414	
12	4	0	15.560	15.731	15.731	0.0	-0.171	-0.104	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
13	5	0	13.373	17.540	17.540	0.0	-4.167	-1.920	
11	5	0	17.350	15.319	-15.319	0.0	2.031	1.718	
7	5	0	8.772	5.361	-5.361	0.0	3.411	1.942	
3	5	0	70.725	69.457	-69.457	0.0	1.268	1.164	
-3	5	0	70.193	69.457	-69.457	0.0	0.736	0.681	*
0	12	0	202.659	204.739	204.739	0.0	-2.080	-0.686	*
-5	5	0	1.663	3.548	-3.548	0.0	-1.884	-0.533	*
-7	5	0	6.847	5.361	-5.361	0.0	1.486	0.669	*
-11	5	0	15.425	15.319	-15.319	0.0	0.106	0.078	*
-13	5	0	16.869	17.540	17.540	0.0	-0.672	-0.425	*
-12	6	0	9.650	4.240	-4.240	0.0	5.410	2.727	*
-10	6	0	17.966	15.603	15.603	0.0	2.363	2.089	*
-8	6	0	20.879	22.865	-22.865	0.0	-1.986	-2.158	*
-6	6	0	7.556	6.898	6.898	0.0	0.658	0.354	*
-4	6	0	4.931	5.437	-5.437	0.0	-0.507	-0.254	*
-2	6	0	12.647	8.358	8.358	0.0	4.289	6.513	*
0	6	0	8.823	2.146	-2.146	0.0	6.677	7.061	
2	6	0	10.190	8.358	8.358	0.0	1.832	2.087	
4	6	0	4.880	5.437	-5.437	0.0	-0.558	-0.282	
6	6	0	7.742	6.898	6.898	0.0	0.844	0.450	
8	6	0	21.656	22.865	-22.865	0.0	-1.209	-1.377	
10	6	0	15.805	15.603	15.603	0.0	0.202	0.158	
12	6	0	7.497	4.240	-4.240	0.0	3.257	1.165	
11	7	0	11.997	13.155	-13.155	0.0	-1.158	-0.650	
9	7	0	44.071	42.457	42.457	0.0	1.614	1.820	
0	12	0	201.790	204.739	204.739	0.0	-2.949	-0.976	*
7	7	0	35.164	35.530	-35.530	0.0	-0.366	-0.434	
5	7	0	16.809	16.656	16.656	0.0	0.153	0.159	
3	7	0	58.407	56.338	56.338	0.0	2.069	2.249	
1	7	0	6.459	4.512	-4.512	0.0	1.947	1.478	
-1	7	0	7.691	4.512	-4.512	0.0	3.179	2.919	*
-3	7	0	57.909	56.338	56.338	0.0	1.571	1.723	*
-5	7	0	18.422	16.656	16.656	0.0	1.766	2.071	*
-7	7	0	34.852	35.530	-35.530	0.0	-0.679	-0.812	*
-9	7	0	43.472	42.457	42.457	0.0	1.014	1.155	*
-11	7	0	12.934	13.155	-13.155	0.0	-0.221	-0.142	*
-12	8	0	29.938	29.624	29.624	0.0	0.314	0.293	*
-10	8	0	46.528	46.719	-46.719	0.0	-0.191	-0.208	*
-8	8	0	8.375	4.381	-4.381	0.0	3.994	2.366	*
-6	8	0	57.461	57.677	57.677	0.0	-0.216	-0.224	*
-4	8	0	104.893	106.711	-106.711	0.0	-1.818	-1.139	*
-2	8	0	27.135	28.504	28.504	0.0	-1.369	-2.385	*
0	8	0	39.512	34.683	34.683	0.0	4.829	7.240	
2	8	0	26.611	28.504	28.504	0.0	-1.893	-3.203	
4	8	0	106.961	106.711	-106.711	0.0	0.250	0.154	
6	8	0	57.757	57.677	57.677	0.0	0.080	0.082	
0	12	0	202.161	204.739	204.739	0.0	-2.578	-0.853	*
8	8	0	3.318	4.381	-4.381	0.0	-1.063	-0.303	
10	8	0	48.774	46.719	-46.719	0.0	2.055	2.213	
12	8	0	30.563	29.624	29.624	0.0	0.939	0.843	
11	9	0	10.047	6.097	-6.097	0.0	3.950	1.982	
9	9	0	30.048	30.917	30.917	0.0	-0.870	-0.936	
7	9	0	86.749	86.615	-86.615	0.0	0.134	0.098	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
5	9	0	23.884	24.200	24.200	0.0	-0.315	-0.381	
1	9	0	74.752	71.379	-71.379	0.0	3.373	2.937	
-1	9	0	73.764	71.379	-71.379	0.0	2.385	2.092	*
-3	9	0	2.381	1.951	1.951	0.0	0.430	0.137	*
-5	9	0	23.344	24.200	24.200	0.0	-0.856	-1.014	*
-7	9	0	86.065	86.615	-86.615	0.0	-0.550	-0.407	*
-9	9	0	30.833	30.917	30.917	0.0	-0.084	-0.098	*
-11	9	0	4.264	6.097	-6.097	0.0	-1.834	-0.488	*
-12	10	0	17.468	15.595	15.595	0.0	1.873	1.344	*
-10	10	0	18.760	18.698	18.698	0.0	0.062	0.051	*
-8	10	0	22.795	24.452	24.452	0.0	-1.656	-1.691	*
-6	10	0	17.029	13.321	13.321	0.0	3.708	3.459	*
-4	10	0	48.706	48.645	48.645	0.0	0.062	0.072	*
0	12	0	202.541	204.739	204.739	0.0	-2.198	-0.725	*
-2	10	0	38.111	38.280	38.280	0.0	-0.169	-0.241	*
0	10	0	85.736	84.853	84.853	0.0	0.883	0.671	
2	10	0	37.528	38.280	38.280	0.0	-0.752	-1.035	
4	10	0	48.124	48.645	48.645	0.0	-0.521	-0.611	
6	10	0	15.062	13.321	13.321	0.0	1.741	1.442	
8	10	0	25.531	24.452	24.452	0.0	1.079	1.318	
10	10	0	20.170	18.698	18.698	0.0	1.472	1.321	
12	10	0	17.181	15.595	15.595	0.0	1.586	1.021	
11	11	0	48.858	48.928	48.928	0.0	-0.070	-0.068	
7	11	0	123.450	123.621	123.621	0.0	-0.172	-0.091	
5	11	0	36.236	36.585	-36.585	0.0	-0.349	-0.440	
3	11	0	86.960	87.805	87.805	0.0	-0.844	-0.629	
1	11	0	124.488	124.250	124.250	0.0	0.238	0.127	
-1	11	0	124.176	124.250	124.250	0.0	-0.074	-0.040	*
-3	11	0	86.454	87.805	87.805	0.0	-1.351	-1.013	*
-5	11	0	35.907	36.585	-36.585	0.0	-0.678	-0.837	*
-7	11	0	121.964	123.621	123.621	0.0	-1.658	-0.888	*
-9	11	0	4.804	4.764	4.764	0.0	0.040	0.013	*
-11	11	0	48.723	48.928	48.928	0.0	-0.205	-0.204	*
0	12	0	201.503	204.739	204.739	0.0	-3.236	-1.074	*
-10	12	0	53.839	53.104	53.104	0.0	0.735	0.719	*
-8	12	0	38.338	39.204	39.204	0.0	-0.866	-0.955	*
-6	12	0	23.825	24.061	-24.061	0.0	-0.235	-0.263	*
-4	12	0	47.465	46.892	46.892	0.0	0.573	0.653	*
-2	12	0	47.837	47.082	-47.082	0.0	0.754	0.893	*
0	12	0	201.857	204.739	204.739	0.0	-2.882	-0.953	*
2	12	0	48.613	47.082	-47.082	0.0	1.531	1.795	
4	12	0	47.254	46.892	46.892	0.0	0.362	0.413	
6	12	0	23.994	24.061	-24.061	0.0	-0.066	-0.077	
8	12	0	38.735	39.204	39.204	0.0	-0.469	-0.529	
10	12	0	55.317	53.104	53.104	0.0	2.212	2.131	
11	13	0	18.557	17.128	17.128	0.0	1.429	1.045	
9	13	0	21.081	21.651	-21.651	0.0	-0.569	-0.489	
7	13	0	45.498	45.862	45.862	0.0	-0.365	-0.404	
5	13	0	64.367	64.447	-64.447	0.0	-0.080	-0.076	
3	13	0	8.958	7.685	-7.685	0.0	1.273	0.698	
1	13	0	9.599	11.053	11.053	0.0	-1.453	-0.848	
-1	13	0	11.719	11.053	11.053	0.0	0.666	0.487	*
-3	13	0	9.388	7.685	-7.685	0.0	1.703	1.009	*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-5	13	0	64.291	64.447	-64.447	0.0	-0.156	-0.146	*
0	12	0	202.339	204.739	204.739	0.0	-2.401	-0.792	*
-7	13	0	46.190	45.862	45.862	0.0	0.328	0.363	*
-9	13	0	19.967	21.651	-21.651	0.0	-1.684	-1.404	*
-11	13	0	14.361	17.128	17.128	0.0	-2.767	-1.438	*
-10	14	0	3.377	1.002	-1.002	0.0	2.375	0.558	*
-6	14	0	8.384	6.728	-6.728	0.0	1.655	0.875	*
-2	14	0	22.677	21.580	21.580	0.0	1.097	1.249	*
0	14	0	10.663	10.624	-10.624	0.0	0.040	0.025	
2	14	0	21.681	21.580	21.580	0.0	0.101	0.106	
4	14	0	7.168	5.181	5.181	0.0	1.987	0.968	
6	14	0	7.067	6.728	-6.728	0.0	0.338	0.152	
10	14	0	5.099	1.002	-1.002	0.0	4.097	1.153	
9	15	0	27.650	28.549	28.549	0.0	-0.899	-0.851	
7	15	0	43.919	43.070	-43.070	0.0	0.849	0.931	
5	15	0	35.122	34.701	34.701	0.0	0.421	0.503	
1	15	0	3.065	0.677	0.677	0.0	2.388	0.637	
-1	15	0	5.969	0.677	0.677	0.0	5.292	2.147	*
0	12	0	202.398	204.739	204.739	0.0	-2.342	-0.773	*
-5	15	0	35.696	34.701	34.701	0.0	0.995	1.215	*
-7	15	0	43.632	43.070	-43.070	0.0	0.562	0.634	*
-9	15	0	28.545	28.549	28.549	0.0	-0.004	-0.003	*
-10	16	0	23.716	24.576	-24.576	0.0	-0.860	-0.698	*
-6	16	0	23.108	25.251	25.251	0.0	-2.144	-2.116	*
-4	16	0	47.887	48.069	-48.069	0.0	-0.182	-0.202	*
-2	16	0	7.117	4.807	4.807	0.0	2.310	1.121	*
0	16	0	6.416	2.034	-2.034	0.0	4.383	1.997	
2	16	0	3.664	4.807	4.807	0.0	-1.143	-0.341	
4	16	0	48.183	48.069	-48.069	0.0	0.113	0.127	
6	16	0	24.298	25.251	25.251	0.0	-0.953	-0.990	
8	16	0	9.067	3.503	-3.503	0.0	5.564	2.903	
10	16	0	23.648	24.576	-24.576	0.0	-0.928	-0.704	
9	17	0	9.405	12.259	12.259	0.0	-2.854	-1.090	
7	17	0	17.198	16.361	-16.361	0.0	0.837	0.674	
5	17	0	6.476	1.468	1.468	0.0	5.008	2.205	
3	17	0	23.015	24.951	24.951	0.0	-1.936	-2.011	
1	17	0	14.142	14.690	-14.690	0.0	-0.548	-0.457	
0	12	0	202.786	204.739	204.739	0.0	-1.953	-0.643	*
-1	17	0	12.369	14.690	-14.690	0.0	-2.321	-1.646	*
-3	17	0	24.467	24.951	24.951	0.0	-0.484	-0.541	*
-7	17	0	15.281	16.361	-16.361	0.0	-1.080	-0.766	*
-9	17	0	15.746	12.259	12.259	0.0	3.487	2.415	*
-8	18	0	9.709	8.757	-8.757	0.0	0.952	0.424	*
-6	18	0	15.357	17.258	17.258	0.0	-1.900	-1.272	*
-4	18	0	5.538	0.331	-0.331	0.0	5.208	2.003	*
-2	18	0	16.919	15.124	15.124	0.0	1.795	1.586	*
0	18	0	13.542	12.574	12.574	0.0	0.968	0.770	
2	18	0	15.045	15.124	15.124	0.0	-0.079	-0.062	
4	18	0	0.701	0.331	-0.331	0.0	0.370	0.067	
6	18	0	15.678	17.258	17.258	0.0	-1.580	-1.069	
8	18	0	5.420	8.757	-8.757	0.0	-3.337	-0.969	
7	19	0	22.356	20.211	-20.211	0.0	2.145	1.854	
5	19	0	6.611	5.816	5.816	0.0	0.795	0.301	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
3	19	0	22.804	22.027	-22.027	0.0	0.777	0.844	
1	19	0	8.443	0.236	0.236	0.0	8.206	4.479	
-1	19	0	8.147	0.236	0.236	0.0	7.911	4.128	*
-3	19	0	21.267	22.027	-22.027	0.0	-0.760	-0.756	*
0	12	0	202.676	204.739	204.739	0.0	-2.063	-0.681	*
-5	19	0	7.987	5.816	5.816	0.0	2.171	0.974	*
-7	19	0	21.250	20.211	-20.211	0.0	1.039	0.837	*
-8	20	0	10.249	3.627	-3.627	0.0	6.623	3.367	*
-4	20	0	30.799	31.527	-31.527	0.0	-0.728	-0.743	*
-2	20	0	21.850	24.687	24.687	0.0	-2.837	-2.526	*
0	20	0	51.923	50.930	-50.930	0.0	0.993	1.031	
2	20	0	24.011	24.687	24.687	0.0	-0.676	-0.708	
4	20	0	31.078	31.527	-31.527	0.0	-0.449	-0.471	
7	21	0	8.536	8.058	-8.058	0.0	0.477	0.184	
5	21	0	35.637	36.204	36.204	0.0	-0.568	-0.560	
3	21	0	4.432	3.797	3.797	0.0	0.636	0.184	
1	21	0	22.534	22.393	22.393	0.0	0.141	0.134	
-1	21	0	22.145	22.393	22.393	0.0	-0.247	-0.233	*
-5	21	0	37.140	36.204	36.204	0.0	0.935	0.963	*
-7	21	0	9.304	8.058	-8.058	0.0	1.245	0.527	*
-6	22	0	9.253	7.105	7.105	0.0	2.148	0.912	*
0	12	0	202.431	204.739	204.739	0.0	-2.308	-0.761	*
-4	22	0	35.915	36.012	36.012	0.0	-0.097	-0.101	*
-2	22	0	19.140	17.393	17.393	0.0	1.747	1.500	*
0	22	0	47.440	47.047	47.047	0.0	0.393	0.401	
2	22	0	18.405	17.393	17.393	0.0	1.013	0.794	
4	22	0	35.426	36.012	36.012	0.0	-0.586	-0.584	
6	22	0	6.146	7.105	7.105	0.0	-0.959	-0.277	
5	23	0	38.524	37.419	-37.419	0.0	1.105	1.110	
3	23	0	32.640	31.311	31.311	0.0	1.328	1.417	
1	23	0	8.443	11.451	11.451	0.0	-3.008	-1.117	
-1	23	0	8.899	11.451	11.451	0.0	-2.552	-1.004	*
-3	23	0	32.116	31.311	31.311	0.0	0.805	0.801	*
-5	23	0	37.021	37.419	-37.419	0.0	-0.397	-0.396	*
-2	24	0	38.786	40.467	-40.467	0.0	-1.681	-1.645	*
0	24	0	72.945	74.255	74.255	0.0	-1.310	-1.041	
2	24	0	39.141	40.467	-40.467	0.0	-1.326	-1.331	
4	23	1	5.606	1.110	-1.110	0.0	4.495	1.299	
2	23	1	3.588	8.665	8.665	0.0	-5.077	-1.156	
0	12	0	202.355	204.739	204.739	0.0	-2.384	-0.786	*
0	23	1	17.637	17.171	17.171	0.0	0.466	0.351	
-2	23	1	7.987	6.477	-6.477	0.0	1.510	0.615	
-4	23	1	5.386	7.653	7.653	0.0	-2.267	-0.627	
-5	22	1	23.800	24.333	-24.333	0.0	-0.532	-0.464	
-3	22	1	13.289	15.719	15.719	0.0	-2.430	-1.327	
-1	22	1	10.224	5.925	-5.925	0.0	4.299	2.358	
1	22	1	17.282	17.949	-17.949	0.0	-0.667	-0.479	
3	22	1	15.138	11.620	11.620	0.0	3.517	2.620	
5	22	1	8.426	9.388	-9.388	0.0	-0.962	-0.387	
6	21	1	12.234	5.454	-5.454	0.0	6.780	3.975	
4	21	1	7.894	4.771	4.771	0.0	3.123	1.312	
2	21	1	23.454	24.052	-24.052	0.0	-0.598	-0.549	
0	21	1	29.752	29.100	29.100	0.0	0.652	0.715	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-2	21	1	35.932	34.939	-34.939	0.0	0.994	1.132	
-4	21	1	9.836	11.493	11.493	0.0	-1.657	-0.770	
-6	21	1	9.658	2.745	2.745	0.0	6.914	3.342	
-7	20	1	15.788	13.362	13.362	0.0	2.425	1.830	
-5	20	1	3.732	3.428	-3.428	0.0	0.303	0.081	
-3	20	1	11.558	11.140	11.140	0.0	0.418	0.246	
0	12	0	201.959	204.739	204.739	0.0	-2.781	-0.920	*
1	20	1	3.521	6.355	6.355	0.0	-2.834	-0.736	
3	20	1	10.334	10.546	10.546	0.0	-0.212	-0.113	
7	20	1	14.327	14.097	14.097	0.0	0.231	0.128	
6	19	1	24.222	24.041	24.041	0.0	0.181	0.154	
4	19	1	16.674	15.423	-15.423	0.0	1.251	1.051	
2	19	1	11.719	10.722	10.722	0.0	0.997	0.605	
0	19	1	37.038	36.448	-36.448	0.0	0.590	0.660	
-2	19	1	37.334	38.006	38.006	0.0	-0.672	-0.737	
-4	19	1	10.596	13.689	-13.689	0.0	-3.094	-1.651	
-6	19	1	5.074	6.529	6.529	0.0	-1.455	-0.441	
-9	18	1	34.294	35.099	35.099	0.0	-0.804	-0.807	
-7	18	1	73.545	74.681	-74.681	0.0	-1.136	-0.922	
-5	18	1	74.245	72.877	72.877	0.0	1.368	1.117	
-3	18	1	1.849	0.958	0.958	0.0	0.891	0.155	
-1	18	1	8.975	5.689	5.689	0.0	3.286	1.802	
1	18	1	23.175	23.155	-23.155	0.0	0.020	0.021	
3	18	1	19.756	19.391	-19.391	0.0	0.365	0.327	
5	18	1	66.968	67.466	67.466	0.0	-0.498	-0.434	
0	12	0	202.406	204.739	204.739	0.0	-2.333	-0.770	*
7	18	1	41.648	40.873	-40.873	0.0	0.775	0.792	
8	17	1	8.451	8.209	8.209	0.0	0.242	0.095	
6	17	1	71.544	69.621	69.621	0.0	1.922	1.615	
2	17	1	70.016	69.182	69.182	0.0	0.833	0.720	
0	17	1	44.898	44.744	-44.744	0.0	0.154	0.181	
-2	17	1	110.726	110.257	110.257	0.0	0.470	0.275	
-4	17	1	17.434	17.238	17.238	0.0	0.196	0.164	
-6	17	1	44.721	43.340	43.340	0.0	1.381	1.528	
-8	17	1	10.140	9.795	9.795	0.0	0.345	0.166	
-10	17	1	3.706	5.140	-5.140	0.0	-1.434	-0.336	
-9	16	1	28.452	29.048	29.048	0.0	-0.596	-0.588	
-7	16	1	20.001	18.676	18.676	0.0	1.325	1.216	
-5	16	1	52.227	51.880	51.880	0.0	0.347	0.370	
-3	16	1	43.750	44.159	44.159	0.0	-0.409	-0.470	
-1	16	1	53.941	54.138	54.138	0.0	-0.197	-0.209	
1	16	1	43.294	43.044	43.044	0.0	0.250	0.291	
3	16	1	35.561	35.134	35.134	0.0	0.427	0.516	
5	16	1	45.844	46.399	46.399	0.0	-0.555	-0.603	
7	16	1	25.801	24.788	24.788	0.0	1.013	0.984	
0	12	0	202.499	204.739	204.739	0.0	-2.240	-0.739	*
9	16	1	29.946	28.967	28.967	0.0	0.979	0.886	
8	15	1	14.243	9.404	9.404	0.0	4.839	3.980	
6	15	1	3.791	4.351	-4.351	0.0	-0.560	-0.158	
4	15	1	1.959	2.613	2.613	0.0	-0.654	-0.148	
2	15	1	22.525	22.266	-22.266	0.0	0.259	0.295	
0	15	1	56.600	57.372	57.372	0.0	-0.772	-0.795	
-2	15	1	51.467	51.304	-51.304	0.0	0.163	0.177	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-4	15	1	17.620	17.390	17.390	0.0	0.230	0.221	
-6	15	1	19.072	20.645	20.645	0.0	-1.573	-1.433	
-8	15	1	10.866	8.444	-8.444	0.0	2.422	1.427	
-10	15	1	15.543	13.197	13.197	0.0	2.346	1.579	
-11	14	1	5.310	5.342	5.342	0.0	-0.031	-0.009	
-9	14	1	27.270	27.029	-27.029	0.0	0.241	0.255	
-7	14	1	27.844	27.802	27.802	0.0	0.042	0.047	
-5	14	1	74.853	75.205	-75.205	0.0	-0.352	-0.293	
-3	14	1	35.029	36.446	36.446	0.0	-1.417	-1.749	
-1	14	1	35.831	35.789	-35.789	0.0	0.042	0.053	
1	14	1	53.291	54.482	-54.482	0.0	-1.191	-1.283	
3	14	1	20.364	21.255	21.255	0.0	-0.891	-0.951	
5	14	1	45.076	43.128	-43.128	0.0	1.948	2.307	
0	12	0	202.153	204.739	204.739	0.0	-2.586	-0.856	*
7	14	1	7.489	9.646	9.646	0.0	-2.158	-0.900	
9	14	1	31.306	31.189	-31.189	0.0	0.117	0.108	
10	13	1	4.399	5.794	-5.794	0.0	-1.395	-0.360	
8	13	1	13.610	11.559	11.559	0.0	2.051	1.509	
6	13	1	10.292	5.423	-5.423	0.0	4.869	3.222	
4	13	1	19.258	19.385	19.385	0.0	-0.127	-0.130	
2	13	1	25.784	25.320	-25.320	0.0	0.464	0.567	
0	13	1	39.107	40.585	40.585	0.0	-1.478	-1.824	
-2	13	1	35.054	33.951	-33.951	0.0	1.103	1.420	
-4	13	1	35.595	35.292	35.292	0.0	0.303	0.386	
-6	13	1	6.357	2.840	-2.840	0.0	3.517	1.666	
-8	13	1	7.067	3.378	-3.378	0.0	3.688	1.680	
-11	12	1	7.582	9.021	9.021	0.0	-1.439	-0.531	
-9	12	1	9.312	5.232	-5.232	0.0	4.080	2.269	
-7	12	1	11.102	11.753	11.753	0.0	-0.651	-0.414	
-5	12	1	13.635	11.646	11.646	0.0	1.989	1.530	
-3	12	1	9.557	8.688	8.688	0.0	0.869	0.528	
-1	12	1	16.514	17.273	17.273	0.0	-0.759	-0.749	
1	12	1	16.531	18.504	18.504	0.0	-1.974	-1.841	
0	12	0	201.739	204.739	204.739	0.0	-3.000	-0.993	*
3	12	1	7.227	6.461	6.461	0.0	0.766	0.356	
5	12	1	10.199	9.003	9.003	0.0	1.196	0.753	
7	12	1	8.519	9.070	9.070	0.0	-0.552	-0.269	
9	12	1	4.990	3.618	3.618	0.0	1.372	0.428	
10	11	1	4.517	7.595	-7.595	0.0	-3.078	-0.800	
6	11	1	10.216	9.893	-9.893	0.0	0.322	0.217	
4	11	1	8.375	6.897	-6.897	0.0	1.478	0.803	
2	11	1	44.333	43.047	-43.047	0.0	1.286	1.603	
0	11	1	10.325	5.458	5.458	0.0	4.868	4.148	
-2	11	1	25.607	24.752	-24.752	0.0	0.855	1.164	
-4	11	1	7.886	10.364	-10.364	0.0	-2.478	-1.288	
-6	11	1	11.634	10.250	-10.250	0.0	1.384	0.948	
-8	11	1	15.315	12.227	12.227	0.0	3.088	2.974	
-10	11	1	6.467	9.007	-9.007	0.0	-2.540	-0.917	
-12	11	1	5.986	2.397	-2.397	0.0	3.589	1.181	
-11	10	1	14.066	14.753	14.753	0.0	-0.688	-0.397	
-9	10	1	21.723	19.324	-19.324	0.0	2.399	2.607	
-7	10	1	22.280	21.686	21.686	0.0	0.594	0.651	
-5	10	1	33.847	33.767	-33.767	0.0	0.080	0.105	

A RICHTERITE 800 C, JUNE, 1973 STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	12	0	198.100	204.739	204.739	0.0	-6.639	-2.240	*
-3	10	1	53.299	53.181	53.181	0.0	0.118	0.133	
-1	10	1	35.848	36.428	-36.428	0.0	-0.580	-0.818	
1	10	1	12.968	12.597	-12.597	0.0	0.371	0.382	
3	10	1	45.996	47.668	47.668	0.0	-1.672	-2.020	
5	10	1	37.503	39.395	-39.395	0.0	-1.892	-2.264	
7	10	1	19.106	20.336	20.336	0.0	-1.230	-1.129	
9	10	1	16.261	13.757	-13.757	0.0	2.503	2.017	
11	10	1	15.898	15.431	15.431	0.0	0.467	0.282	
10	9	1	20.254	20.050	20.050	0.0	0.204	0.171	
8	9	1	7.404	0.387	0.387	0.0	7.017	3.325	
4	9	1	32.986	32.480	32.480	0.0	0.506	0.652	
2	9	1	51.273	51.083	-51.083	0.0	0.190	0.220	
0	9	1	95.606	97.333	97.333	0.0	-1.727	-1.189	
-2	9	1	51.957	51.259	-51.259	0.0	0.698	0.826	
-4	9	1	25.869	25.461	25.461	0.0	0.408	0.555	
-6	9	1	16.565	19.138	19.138	0.0	-2.573	-2.162	
-8	9	1	2.237	4.710	-4.710	0.0	-2.473	-0.598	
-10	9	1	9.743	12.743	12.743	0.0	-3.000	-1.433	
-12	9	1	24.990	23.969	-23.969	0.0	1.021	0.923	
0	12	0	198.978	204.739	204.739	0.0	-5.761	-1.933	*
-13	8	1	1.461	4.374	4.374	0.0	-2.914	-0.507	
-11	8	1	12.124	12.692	-12.692	0.0	-0.568	-0.328	
-9	8	1	9.160	10.254	-10.254	0.0	-1.094	-0.578	
-7	8	1	2.803	6.329	6.329	0.0	-3.526	-0.879	
-5	8	1	15.915	16.598	-16.598	0.0	-0.684	-0.638	
-3	8	1	6.273	0.250	0.250	0.0	6.023	3.567	
-1	8	1	10.190	11.312	-11.312	0.0	-1.122	-1.117	
1	8	1	10.013	10.571	-10.571	0.0	-0.557	-0.532	
3	8	1	9.219	9.409	-9.409	0.0	-0.189	-0.140	
5	8	1	19.748	20.267	-20.267	0.0	-0.520	-0.535	
7	8	1	14.150	13.229	13.229	0.0	0.921	0.758	
11	8	1	11.119	10.566	-10.566	0.0	0.553	0.269	
12	7	1	20.229	19.181	19.181	0.0	1.048	0.761	
10	7	1	26.848	26.401	-26.401	0.0	0.447	0.430	
8	7	1	9.431	3.162	3.162	0.0	6.269	3.788	
6	7	1	58.736	59.699	59.699	0.0	-0.963	-0.967	
4	7	1	47.575	47.738	-47.738	0.0	-0.163	-0.201	
2	7	1	27.810	28.272	28.272	0.0	-0.461	-0.759	
0	7	1	128.059	128.130	-128.130	0.0	-0.071	-0.037	
0	12	0	199.029	204.739	204.739	0.0	-5.710	-1.916	*
-2	7	1	77.167	77.284	77.284	0.0	-0.117	-0.099	
-4	7	1	6.492	3.498	3.498	0.0	2.995	1.791	
-6	7	1	30.808	32.589	32.589	0.0	-1.781	-2.244	
-8	7	1	15.062	16.825	-16.825	0.0	-1.763	-1.431	
-10	7	1	19.097	18.027	-18.027	0.0	1.071	0.899	
-12	7	1	45.278	45.267	45.267	0.0	0.011	0.011	
-13	6	1	38.558	38.652	38.652	0.0	-0.094	-0.089	
-11	6	1	7.328	1.382	1.382	0.0	5.946	2.524	
-9	6	1	94.913	96.942	96.942	0.0	-2.029	-1.373	
-7	6	1	96.602	99.177	-99.177	0.0	-2.575	-1.723	
-5	6	1	184.609	194.136	194.136	0.0	-9.527	-3.451	
-3	6	1	157.204	154.571	154.571	0.0	2.632	1.118	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-1	6	1	123.306	126.106	126.106	0.0	-2.800	-1.514	
1	6	1	52.497	43.244	-43.244	0.0	9.253	11.071	
3	6	1	52.784	51.581	51.581	0.0	1.203	1.397	
5	6	1	225.472	235.489	235.489	0.0	-10.018	-2.966	*
7	6	1	41.108	40.961	-40.961	0.0	0.146	0.173	
9	6	1	69.838	70.550	70.550	0.0	-0.712	-0.611	
11	6	1	22.432	21.046	-21.046	0.0	1.386	1.181	
12	5	1	40.863	41.097	41.097	0.0	-0.235	-0.222	
0	12	0	199.645	204.739	204.739	0.0	-5.094	-1.704	*
10	5	1	12.056	11.414	-11.414	0.0	0.642	0.382	
8	5	1	32.986	32.868	32.868	0.0	0.118	0.140	
6	5	1	133.058	136.967	136.967	0.0	-3.909	-1.937	
4	5	1	25.126	25.797	25.797	0.0	-0.671	-0.947	
2	5	1	124.750	130.918	130.918	0.0	-6.168	-3.291	
0	5	1	72.835	71.144	-71.144	0.0	1.691	1.517	
-2	5	1	212.504	220.179	220.179	0.0	-7.675	-2.418	
-4	5	1	94.820	94.979	94.979	0.0	-0.159	-0.111	
-6	5	1	89.940	93.214	93.214	0.0	-3.274	-2.364	
-8	5	1	16.210	16.752	16.752	0.0	-0.542	-0.436	
-10	5	1	4.213	4.596	4.596	0.0	-0.383	-0.117	
-12	5	1	68.884	67.991	67.991	0.0	0.893	0.745	
-13	4	1	16.573	18.606	18.606	0.0	-2.033	-1.241	
-11	4	1	9.388	10.913	-10.913	0.0	-1.525	-0.689	
-9	4	1	3.208	3.090	3.090	0.0	0.118	0.034	
-7	4	1	11.735	11.514	11.514	0.0	0.222	0.156	
-5	4	1	20.170	19.494	19.494	0.0	0.675	1.000	
-3	4	1	6.754	7.030	7.030	0.0	-0.276	-0.222	
-1	4	1	8.603	10.277	10.277	0.0	-1.674	-1.537	
1	4	1	8.738	4.365	4.365	0.0	4.373	4.504	
0	12	0	199.173	204.739	204.739	0.0	-5.567	-1.868	*
3	4	1	4.289	1.050	1.050	0.0	3.238	1.835	
5	4	1	5.859	3.552	3.552	0.0	2.307	1.076	
7	4	1	15.864	15.352	15.352	0.0	0.512	0.427	
9	4	1	15.915	16.378	16.378	0.0	-0.464	-0.361	
11	4	1	10.410	13.448	-13.448	0.0	-3.038	-1.390	
12	3	1	24.788	26.310	-26.310	0.0	-1.522	-1.202	
10	3	1	3.242	12.144	12.144	0.0	-8.902	-2.035	
8	3	1	12.816	11.015	-11.015	0.0	1.801	1.359	
6	3	1	26.316	28.394	-28.394	0.0	-2.078	-2.564	
4	3	1	22.500	21.606	-21.606	0.0	0.894	1.340	
2	3	1	111.681	116.973	-116.973	0.0	-5.293	-3.150	
-2	3	1	140.369	143.313	-143.313	0.0	-2.944	-1.400	
-4	3	1	17.299	16.753	-16.753	0.0	0.546	0.840	
-8	3	1	21.301	20.510	-20.510	0.0	0.791	0.852	
-10	3	1	9.929	8.547	8.547	0.0	1.382	0.758	
-12	3	1	34.446	34.615	-34.615	0.0	-0.168	-0.171	
-13	2	1	16.624	16.973	-16.973	0.0	-0.350	-0.223	
-11	2	1	17.392	17.851	17.851	0.0	-0.459	-0.351	
-9	2	1	25.945	27.684	-27.684	0.0	-1.740	-2.040	
0	12	0	198.311	204.739	204.739	0.0	-6.428	-2.163	*
-7	2	1	44.738	46.081	46.081	0.0	-1.343	-1.640	
-5	2	1	51.501	51.715	-51.715	0.0	-0.214	-0.256	
-3	2	1	121.820	125.158	125.158	0.0	-3.337	-1.830	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
1	2	1	7.877	6.753	-6.753	0.0	1.124	0.993	
3	2	1	102.951	104.449	104.449	0.0	-1.498	-0.965	
5	2	1	33.045	32.142	-32.142	0.0	0.903	1.273	
7	2	1	38.440	37.808	37.808	0.0	0.632	0.764	
9	2	1	23.699	22.817	-22.817	0.0	0.882	0.976	
11	2	1	29.026	26.823	26.823	0.0	2.203	2.309	
12	1	1	8.316	1.004	1.004	0.0	7.312	2.946	
10	1	1	3.377	4.748	-4.748	0.0	-1.371	-0.357	
8	1	1	9.127	14.246	14.246	0.0	-5.120	-2.671	
6	1	1	7.919	5.637	-5.637	0.0	2.282	1.269	
4	1	1	11.609	12.369	12.369	0.0	-0.760	-0.797	
2	1	1	49.432	50.924	-50.924	0.0	-1.492	-1.900	
-4	1	1	24.138	25.162	25.162	0.0	-1.024	-1.810	
-6	1	1	5.361	5.007	5.007	0.0	0.354	0.179	
-8	1	1	8.240	8.300	8.300	0.0	-0.060	-0.029	
-10	1	1	3.402	4.580	-4.580	0.0	-1.178	-0.318	
0	12	0	199.485	204.739	204.739	0.0	-5.254	-1.758	*
-13	0	1	16.083	14.835	-14.835	0.0	1.249	0.865	
-11	0	1	9.658	6.523	6.523	0.0	3.135	1.760	
-9	0	1	5.386	7.523	-7.523	0.0	-2.137	-0.784	
-7	0	1	2.288	5.046	-5.046	0.0	-2.758	-0.699	
-5	0	1	9.988	9.488	-9.488	0.0	0.500	0.489	
-3	0	1	18.709	18.991	-18.991	0.0	-0.282	-0.457	
3	0	1	30.293	31.116	-31.116	0.0	-0.824	-1.394	
5	0	1	8.189	4.206	-4.206	0.0	3.984	2.913	
7	0	1	3.630	0.674	-0.674	0.0	2.956	0.860	
9	0	1	8.789	6.353	-6.353	0.0	2.436	1.294	
11	0	1	1.697	2.533	2.533	0.0	-0.836	-0.160	
-12	0	2	46.030	46.542	-46.542	0.0	-0.512	-0.514	
-10	0	2	74.988	74.871	74.871	0.0	0.117	0.096	
-8	0	2	62.392	64.492	64.492	0.0	-2.101	-2.023	
-6	0	2	97.691	99.492	99.492	0.0	-1.801	-1.205	
-4	0	2	152.223	159.341	159.341	0.0	-7.118	-3.123	
-2	0	2	109.916	107.263	-107.263	0.0	2.653	1.603	
0	0	2	247.972	268.786	268.786	0.0	-20.815	-5.629	*
2	0	2	124.446	124.213	124.213	0.0	0.233	0.125	
4	0	2	188.383	197.022	197.022	0.0	-8.639	-3.064	
0	12	0	199.299	204.739	204.739	0.0	-5.440	-1.825	*
6	0	2	45.608	46.186	-46.186	0.0	-0.578	-0.671	
8	0	2	47.913	48.037	48.037	0.0	-0.125	-0.137	
10	0	2	76.449	75.737	75.737	0.0	0.712	0.555	
11	1	2	49.187	48.692	48.692	0.0	0.496	0.477	
9	1	2	25.489	25.514	-25.514	0.0	-0.026	-0.026	
7	1	2	59.260	59.152	59.152	0.0	0.108	0.106	
5	1	2	41.623	42.582	-42.582	0.0	-0.959	-1.159	
3	1	2	77.454	79.190	79.190	0.0	-1.737	-1.449	
1	1	2	116.771	115.241	115.241	0.0	1.531	0.872	
-1	1	2	6.780	4.569	-4.569	0.0	2.210	1.757	
-5	1	2	21.031	21.184	-21.184	0.0	-0.153	-0.211	
-7	1	2	160.049	164.974	164.974	0.0	-4.925	-2.047	
-9	1	2	30.065	30.610	-30.610	0.0	-0.546	-0.659	
-11	1	2	23.606	26.327	26.327	0.0	-2.721	-2.558	
-13	1	2	5.091	4.390	4.390	0.0	0.701	0.194	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-6	2	2	26.696	25.844	-25.844	0.0	0.852	1.160	
0	12	0	199.755	204.739	204.739	0.0	-4.984	-1.668	*
-4	2	2	17.029	17.512	-17.512	0.0	-0.483	-0.673	
-2	2	2	21.445	21.016	-21.016	0.0	0.428	0.746	
0	2	2	30.174	30.049	-30.049	0.0	0.125	0.211	
2	2	2	10.325	10.052	-10.052	0.0	0.273	0.257	
6	2	2	14.648	12.089	-12.089	0.0	2.559	2.150	
8	2	2	14.631	13.356	-13.356	0.0	1.276	1.001	
10	2	2	15.011	12.443	-12.443	0.0	2.568	1.810	
11	3	2	17.831	17.048	-17.048	0.0	0.783	0.579	
9	3	2	29.617	29.778	29.778	0.0	-0.161	-0.172	
7	3	2	62.451	62.726	-62.726	0.0	-0.275	-0.261	
5	3	2	45.608	46.944	46.944	0.0	-1.336	-1.567	
1	3	2	69.754	67.594	-67.594	0.0	2.160	1.999	
-1	3	2	5.885	7.263	7.263	0.0	-1.378	-0.949	
-3	3	2	23.918	20.200	20.200	0.0	3.719	6.292	
-5	3	2	16.413	20.323	20.323	0.0	-3.910	-4.211	
-7	3	2	83.119	84.272	-84.272	0.0	-1.153	-0.887	
-9	3	2	57.031	58.326	58.326	0.0	-1.295	-1.311	
-11	3	2	11.043	10.058	-10.058	0.0	0.985	0.578	
0	12	0	198.911	204.739	204.739	0.0	-5.828	-1.956	*
-13	3	2	16.624	15.582	-15.582	0.0	1.041	0.743	
-12	4	2	42.036	39.913	39.913	0.0	2.123	2.328	
-10	4	2	39.115	39.835	-39.835	0.0	-0.719	-0.804	
-8	4	2	11.026	4.762	4.762	0.0	6.264	4.122	
-6	4	2	76.863	76.908	76.908	0.0	-0.045	-0.037	
-4	4	2	71.375	69.889	-69.889	0.0	1.486	1.343	
-2	4	2	9.355	11.432	11.432	0.0	-2.077	-2.034	
0	4	2	82.570	76.646	76.646	0.0	5.924	4.709	
2	4	2	73.654	75.490	75.490	0.0	-1.836	-1.611	
4	4	2	78.121	79.545	-79.545	0.0	-1.424	-1.163	
6	4	2	65.752	68.048	68.048	0.0	-2.296	-2.109	
8	4	2	15.256	14.942	14.942	0.0	0.314	0.231	
10	4	2	30.065	30.035	-30.035	0.0	0.030	0.031	
11	5	2	1.781	8.032	-8.032	0.0	-6.250	-1.079	
9	5	2	15.518	14.266	14.266	0.0	1.252	0.909	
7	5	2	38.718	39.149	-39.149	0.0	-0.430	-0.515	
5	5	2	5.049	5.618	-5.618	0.0	-0.569	-0.201	
3	5	2	29.018	26.608	26.608	0.0	2.409	3.357	
1	5	2	73.612	72.118	-72.119	0.0	1.494	1.311	
-1	5	2	45.557	44.722	-44.722	0.0	0.835	1.099	
0	12	0	198.742	204.739	204.739	0.0	-5.997	-2.012	*
-3	5	2	39.917	37.490	37.490	0.0	2.427	3.422	
-5	5	2	15.526	16.006	-16.006	0.0	-0.480	-0.455	
-7	5	2	39.402	41.110	-41.110	0.0	-1.708	-2.086	
-9	5	2	37.410	37.682	37.682	0.0	-0.272	-0.326	
-11	5	2	11.617	11.418	-11.418	0.0	0.199	0.114	
-12	6	2	6.788	0.994	-0.994	0.0	5.794	2.125	
-10	6	2	16.159	14.114	14.114	0.0	2.045	1.730	
-8	6	2	17.924	18.422	-18.422	0.0	-0.498	-0.487	
-6	6	2	14.294	15.416	15.416	0.0	-1.122	-0.943	
-4	6	2	8.130	11.571	-11.571	0.0	-3.441	-2.111	
-2	6	2	5.108	6.902	-6.902	0.0	-1.794	-0.924	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
2	6	2	6.535	4.704	4.704	0.0	1.831	1.079	
6	6	2	14.657	13.712	13.712	0.0	0.944	0.788	
8	6	2	20.060	21.376	-21.376	0.0	-1.316	-1.181	
10	6	2	9.211	8.117	8.117	0.0	1.094	0.468	
11	7	2	12.647	13.493	-13.493	0.0	-0.845	-0.417	
9	7	2	14.378	14.916	14.916	0.0	-0.538	-0.354	
0	12	0	199.021	204.739	204.739	0.0	-5.719	-1.919	*
7	7	2	2.507	2.933	-2.933	0.0	-0.426	-0.104	
5	7	2	19.638	21.172	21.172	0.0	-1.534	-1.356	
3	7	2	5.488	6.242	-6.242	0.0	-0.754	-0.308	
1	7	2	31.415	32.030	32.030	0.0	-0.614	-0.899	
-1	7	2	41.378	40.493	40.493	0.0	0.885	1.218	
-3	7	2	31.702	32.856	-32.856	0.0	-1.153	-1.570	
-5	7	2	35.502	36.113	36.113	0.0	-0.611	-0.787	
-9	7	2	19.722	18.878	18.878	0.0	0.844	0.827	
-11	7	2	16.143	18.329	-18.329	0.0	-2.187	-1.480	
-13	7	2	18.321	18.009	18.009	0.0	0.312	0.224	
-12	8	2	17.282	17.615	17.615	0.0	-0.333	-0.214	
-10	8	2	11.212	14.177	-14.177	0.0	-2.965	-1.554	
-6	8	2	20.415	21.372	-21.372	0.0	-0.957	-0.961	
-4	8	2	26.240	25.166	-25.166	0.0	1.074	1.430	
-2	8	2	54.464	52.320	52.320	0.0	2.144	2.396	
0	8	2	95.327	93.974	-93.974	0.0	1.353	0.932	
2	8	2	72.498	72.188	72.188	0.0	0.310	0.272	
4	8	2	38.592	38.583	-38.583	0.0	0.009	0.011	
0	12	0	199.384	204.739	204.739	0.0	-5.356	-1.792	*
6	8	2	6.053	6.068	6.068	0.0	-0.014	-0.006	
8	8	2	6.923	3.164	-3.164	0.0	3.759	1.596	
7	9	2	31.601	32.830	-32.830	0.0	-1.229	-1.373	
5	9	2	29.566	29.605	29.605	0.0	-0.039	-0.048	
3	9	2	68.876	70.730	-70.730	0.0	-1.854	-1.677	
1	9	2	23.724	24.698	-24.698	0.0	-0.974	-1.131	
-1	9	2	16.320	16.616	16.616	0.0	-0.296	-0.303	
-3	9	2	75.512	76.290	-76.290	0.0	-0.778	-0.654	
-5	9	2	26.223	25.764	25.764	0.0	0.459	0.533	
-7	9	2	42.079	41.696	-41.696	0.0	0.383	0.453	
-9	9	2	19.460	18.319	18.319	0.0	1.142	1.136	
-11	9	2	5.446	6.496	-6.496	0.0	-1.051	-0.331	
-12	10	2	9.042	4.408	4.408	0.0	4.634	2.071	
-10	10	2	23.369	23.026	23.026	0.0	0.344	0.351	
-8	10	2	32.952	33.978	33.978	0.0	-1.026	-1.179	
-6	10	2	14.733	14.817	14.817	0.0	-0.084	-0.064	
-4	10	2	43.235	44.592	44.592	0.0	-1.357	-1.624	
-2	10	2	25.058	26.350	26.350	0.0	-1.292	-1.545	
0	12	0	199.561	204.739	204.739	0.0	-5.178	-1.733	*
0	10	2	49.610	49.570	49.570	0.0	0.040	0.046	
2	10	2	34.261	34.145	34.145	0.0	0.116	0.144	
4	10	2	56.533	57.676	57.676	0.0	-1.144	-1.178	
6	10	2	11.001	11.579	11.579	0.0	-0.578	-0.351	
8	10	2	13.500	13.037	13.037	0.0	0.463	0.308	
10	10	2	8.975	7.421	7.421	0.0	1.554	0.646	
9	11	2	2.845	1.708	1.708	0.0	1.138	0.255	
7	11	2	51.408	50.810	50.810	0.0	0.598	0.632	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
5	11	2	14.716	13.324	-13.324	0.0	1.391	1.239	
3	11	2	138.047	141.504	141.504	0.0	-3.457	-1.651	
1	11	2	85.348	85.475	85.475	0.0	-0.128	-0.096	
-1	11	2	14.260	15.838	15.838	0.0	-1.578	-1.255	
-3	11	2	113.335	114.029	114.029	0.0	-0.694	-0.401	
-5	11	2	11.592	13.952	-13.952	0.0	-2.360	-1.426	
-7	11	2	125.636	128.183	128.183	0.0	-2.547	-1.329	
-9	11	2	6.518	4.915	4.915	0.0	1.602	0.626	
-11	11	2	32.673	32.479	32.479	0.0	0.194	0.195	
-12	12	2	25.109	25.153	-25.153	0.0	-0.045	-0.037	
-10	12	2	14.766	16.574	16.574	0.0	-1.808	-1.139	
-8	12	2	15.796	15.244	15.244	0.0	0.553	0.436	
0	12	0	199.325	204.739	204.739	0.0	-5.415	-1.812	*
-6	12	2	80.797	81.943	81.943	0.0	-1.146	-0.893	
-4	12	2	30.580	29.708	29.708	0.0	0.872	1.022	
-2	12	2	133.024	136.810	-136.810	0.0	-3.787	-1.877	
0	12	2	187.598	190.998	190.998	0.0	-3.401	-1.210	
2	12	2	10.815	10.528	-10.528	0.0	0.287	0.166	
4	12	2	50.884	51.387	51.387	0.0	-0.503	-0.541	
6	12	2	25.531	24.104	-24.104	0.0	1.427	1.496	
8	12	2	22.795	20.910	20.910	0.0	1.885	1.876	
9	13	2	18.093	16.111	-16.111	0.0	1.981	1.565	
5	13	2	40.584	41.206	-41.206	0.0	-0.622	-0.722	
3	13	2	50.268	51.630	51.630	0.0	-1.362	-1.508	
1	13	2	11.803	15.504	-15.504	0.0	-3.701	-2.260	
-1	13	2	50.699	51.620	-51.620	0.0	-0.921	-1.010	
-3	13	2	35.042	36.734	36.734	0.0	-0.692	-0.854	
-5	13	2	50.260	51.715	-51.715	0.0	-1.456	-1.596	
-7	13	2	40.821	41.024	41.024	0.0	-0.204	-0.232	
-9	13	2	9.760	10.879	-10.879	0.0	-1.119	-0.537	
-11	13	2	7.894	7.815	7.815	0.0	0.079	0.030	
-10	14	2	6.560	4.459	-4.459	0.0	2.101	0.743	
0	12	0	199.173	204.739	204.739	0.0	-5.567	-1.868	*
-8	14	2	6.374	6.192	6.192	0.0	0.183	0.068	
-6	14	2	7.818	1.611	-1.611	0.0	6.207	3.210	
-4	14	2	6.957	4.320	-4.320	0.0	2.637	1.280	
-2	14	2	10.832	10.523	10.523	0.0	0.309	0.192	
2	14	2	14.547	14.497	14.497	0.0	0.050	0.040	
6	14	2	5.091	7.907	7.907	0.0	-2.816	-0.847	
8	14	2	8.916	2.881	-2.881	0.0	6.034	2.657	
7	15	2	19.292	18.356	-18.356	0.0	0.936	0.775	
5	15	2	31.534	32.768	32.768	0.0	-1.234	-1.341	
3	15	2	21.723	21.201	-21.201	0.0	0.522	0.562	
1	15	2	7.776	6.786	6.786	0.0	0.990	0.508	
-1	15	2	27.633	28.677	28.677	0.0	-1.044	-1.275	
-3	15	2	28.477	28.824	-28.824	0.0	-0.346	-0.419	
-5	15	2	33.062	31.795	31.795	0.0	1.266	1.531	
-7	15	2	25.885	26.019	-26.019	0.0	-0.134	-0.142	
-9	15	2	22.770	22.363	22.363	0.0	0.407	0.368	
-11	15	2	9.346	7.555	-7.555	0.0	1.792	0.745	
-10	16	2	4.838	3.985	-3.985	0.0	0.853	0.233	
0	12	0	198.615	204.739	204.739	0.0	-6.124	-2.061	*
-8	16	2	5.665	0.377	-0.377	0.0	5.288	1.815	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-6	16	2	5.277	6.653	-6.653	0.0	-1.377	-0.452	
-4	16	2	14.530	15.535	-15.535	0.0	-1.005	-0.739	
-2	16	2	16.649	16.231	16.231	0.0	0.418	0.406	
0	16	2	39.605	41.630	-41.630	0.0	-2.025	-2.352	
2	16	2	21.951	21.294	21.294	0.0	0.657	0.676	
4	16	2	24.349	24.409	-24.409	0.0	-0.060	-0.063	
6	16	2	4.036	1.083	1.083	0.0	2.952	0.808	
8	16	2	3.858	1.320	-1.320	0.0	2.538	0.630	
7	17	2	7.463	3.232	3.232	0.0	4.232	1.586	
5	17	2	6.796	4.598	4.598	0.0	2.198	0.865	
3	17	2	5.479	5.259	-5.259	0.0	0.221	0.078	
1	17	2	3.825	0.863	0.863	0.0	2.962	0.358	
-1	17	2	6.746	6.546	6.546	0.0	0.200	0.080	
-3	17	2	5.099	5.046	-5.046	0.0	0.054	0.018	
-5	17	2	6.079	5.504	5.504	0.0	0.575	0.214	
-9	17	2	5.648	3.806	3.806	0.0	1.842	0.574	
-8	18	2	8.460	6.574	-6.574	0.0	1.886	0.778	
-6	18	2	10.266	9.647	9.647	0.0	0.619	0.311	
0	12	0	198.624	204.739	204.739	0.0	-6.115	-2.058	*
-2	18	2	15.138	14.950	14.950	0.0	0.188	0.147	
0	18	2	6.501	1.163	1.163	0.0	5.338	2.165	
2	18	2	15.163	14.668	14.668	0.0	0.495	0.369	
6	18	2	13.627	13.753	13.753	0.0	-0.126	-0.074	
5	19	2	1.621	4.168	4.168	0.0	-2.547	-0.451	
3	19	2	4.753	2.060	-2.060	0.0	2.694	0.818	
1	19	2	11.440	13.998	-13.998	0.0	-2.558	-1.377	
-1	19	2	6.450	1.851	-1.851	0.0	4.599	1.840	
-3	19	2	13.686	14.699	-14.699	0.0	-1.014	-0.671	
-5	19	2	2.862	6.584	6.584	0.0	-3.722	-0.824	
-7	19	2	24.475	25.133	-25.133	0.0	-0.658	-0.541	
-8	20	2	9.186	0.885	-0.885	0.0	8.301	3.796	
-6	20	2	8.747	12.684	12.684	0.0	-3.937	-1.509	
-4	20	2	33.703	33.233	-33.233	0.0	0.471	0.526	
-2	20	2	9.084	6.540	6.540	0.0	2.544	1.205	
0	20	2	26.096	25.416	-25.416	0.0	0.681	0.645	
2	20	2	23.327	23.277	23.277	0.0	0.050	0.048	
4	20	2	48.504	48.259	-48.259	0.0	0.244	0.249	
0	12	0	198.666	204.739	204.739	0.0	-6.073	-2.044	*
6	20	2	17.536	16.672	16.672	0.0	0.864	0.591	
5	21	2	34.978	33.639	33.639	0.0	1.339	1.367	
3	21	2	10.435	12.735	12.735	0.0	-2.300	-1.032	
1	21	2	2.997	2.058	2.058	0.0	0.939	0.217	
-1	21	2	25.472	24.005	24.005	0.0	1.467	1.424	
-3	21	2	14.522	16.222	16.222	0.0	-1.701	-1.049	
-5	21	2	23.294	23.482	23.482	0.0	-0.189	-0.158	
-7	21	2	15.509	14.620	-14.620	0.0	0.890	0.573	
-6	22	2	18.101	16.723	16.723	0.0	1.378	0.971	
-4	22	2	28.925	28.399	28.399	0.0	0.526	0.510	
-2	22	2	10.098	9.012	9.012	0.0	1.085	0.516	
0	22	2	41.935	43.116	43.116	0.0	-1.180	-1.205	
2	22	2	14.834	15.067	15.067	0.0	-0.233	-0.134	
4	22	2	32.960	33.702	33.702	0.0	-0.741	-0.676	
1	23	2	18.920	20.972	20.972	0.0	-2.052	-1.335	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-1	23	2	7.793	10.160	-10.160	0.0	-2.368	-0.868	
-3	23	2	22.863	21.881	21.881	0.0	0.982	0.843	
-2	24	2	47.364	48.495	-48.495	0.0	-1.131	-1.072	
0	24	2	41.792	42.267	42.267	0.0	-0.476	-0.462	
-3	22	3	10.477	11.640	11.640	0.0	-1.163	-0.514	
0	12	0	198.480	204.739	204.739	0.0	-6.259	-2.106	*
-1	22	3	11.541	12.655	-12.655	0.0	-1.113	-0.538	
1	22	3	10.233	5.502	-5.502	0.0	4.731	2.180	
2	21	3	24.872	22.992	-22.992	0.0	1.880	1.662	
0	21	3	19.680	18.777	18.777	0.0	0.904	0.709	
-2	21	3	21.487	21.231	-21.231	0.0	0.255	0.213	
-7	20	3	9.768	8.403	8.403	0.0	1.365	0.565	
-5	20	3	5.201	6.883	-6.883	0.0	-1.682	-0.473	
-3	20	3	14.277	11.532	11.532	0.0	2.745	1.837	
1	20	3	8.105	5.568	5.568	0.0	2.537	0.992	
3	20	3	13.069	8.805	8.805	0.0	4.264	2.645	
4	19	3	32.884	33.927	-33.927	0.0	-1.042	-1.029	
2	19	3	24.383	23.248	23.248	0.0	1.135	1.084	
0	19	3	13.669	13.986	-13.986	0.0	-0.317	-0.196	
-2	19	3	20.524	20.285	20.285	0.0	0.240	0.200	
-4	19	3	6.366	11.069	-11.069	0.0	-4.703	-1.522	
-6	19	3	4.652	0.480	0.480	0.0	4.172	1.131	
-8	19	3	4.888	0.400	-0.400	0.0	4.488	1.211	
0	12	0	198.413	204.739	204.739	0.0	-6.327	-2.129	*
-9	18	3	56.018	56.402	56.402	0.0	-0.385	-0.351	
-7	18	3	52.683	53.033	-53.033	0.0	-0.351	-0.332	
-5	18	3	25.227	23.758	23.758	0.0	1.469	1.392	
-3	18	3	14.876	15.674	-15.674	0.0	-0.798	-0.528	
-1	18	3	60.729	61.096	61.096	0.0	-0.367	-0.343	
1	18	3	24.053	25.232	-25.232	0.0	-1.179	-1.058	
3	18	3	33.982	33.463	-33.463	0.0	0.519	0.544	
5	18	3	42.374	43.726	43.726	0.0	-1.352	-1.323	
6	17	3	51.256	51.756	51.756	0.0	-0.500	-0.478	
4	17	3	32.673	32.343	-32.343	0.0	0.330	0.343	
2	17	3	62.358	62.582	62.582	0.0	-0.224	-0.206	
0	17	3	10.646	9.681	-9.681	0.0	0.966	0.542	
-2	17	3	86.817	86.899	86.899	0.0	-0.083	-0.059	
-4	17	3	8.679	7.252	7.252	0.0	1.427	0.640	
-6	17	3	12.521	14.472	14.472	0.0	-1.952	-1.075	
-8	17	3	19.688	20.984	20.984	0.0	-1.295	-0.935	
-9	16	3	26.595	25.223	25.223	0.0	1.372	1.250	
-7	16	3	9.110	9.845	9.845	0.0	-0.735	-0.325	
-5	16	3	41.623	42.688	42.688	0.0	-1.065	-1.147	
-3	16	3	30.900	29.011	29.011	0.0	1.889	2.260	
0	12	0	198.945	204.739	204.739	0.0	-5.795	-1.944	*
-1	16	3	46.638	46.712	46.712	0.0	-0.074	-0.080	
1	16	3	37.731	37.273	37.273	0.0	0.457	0.521	
3	16	3	29.144	27.992	27.992	0.0	1.152	1.197	
5	16	3	22.238	22.553	22.553	0.0	-0.315	-0.248	
7	16	3	13.795	16.061	16.061	0.0	-2.266	-1.203	
6	15	3	11.896	11.161	-11.161	0.0	0.735	0.405	
4	15	3	19.300	20.416	20.416	0.0	-1.116	-0.847	
2	15	3	24.298	24.724	-24.724	0.0	-0.426	-0.424	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	15	3	34.455	33.906	33.906	0.0	0.548	0.670	
-2	15	3	24.357	23.880	-23.880	0.0	0.478	0.529	
-4	15	3	15.670	15.017	15.017	0.0	0.653	0.523	
-6	15	3	15.340	14.780	14.780	0.0	0.561	0.431	
-8	15	3	11.398	10.457	-10.457	0.0	0.941	0.521	
-10	15	3	16.252	15.015	15.015	0.0	1.237	0.797	
-11	14	3	11.727	9.402	9.402	0.0	2.325	1.162	
-9	14	3	31.745	32.031	-32.031	0.0	-0.286	-0.287	
-7	14	3	23.361	22.187	22.187	0.0	1.174	1.140	
-5	14	3	49.660	51.888	-51.888	0.0	-2.228	-2.356	
-3	14	3	30.149	29.936	29.936	0.0	0.213	0.261	
-1	14	3	43.007	43.263	-43.263	0.0	-0.255	-0.300	
0	12	0	198.050	204.739	204.739	0.0	-6.690	-2.257	*
1	14	3	16.261	18.153	-18.153	0.0	-1.892	-1.474	
3	14	3	2.296	6.543	6.543	0.0	-4.247	-0.926	
5	14	3	34.978	33.851	-33.851	0.0	1.127	1.296	
7	14	3	8.519	10.987	10.987	0.0	-2.468	-0.911	
8	13	3	13.779	8.532	8.532	0.0	5.246	3.655	
6	13	3	10.967	9.279	-9.279	0.0	1.688	0.943	
4	13	3	21.360	21.015	21.015	0.0	0.345	0.338	
2	13	3	25.615	25.946	-25.946	0.0	-0.331	-0.366	
0	13	3	33.003	32.972	32.972	0.0	0.030	0.038	
-2	13	3	11.482	11.881	-11.881	0.0	-0.399	-0.254	
-4	13	3	17.662	15.937	15.937	0.0	1.725	1.584	
-6	13	3	7.843	6.531	-6.531	0.0	1.312	0.602	
-11	12	3	11.550	9.115	9.115	0.0	2.435	1.249	
-9	12	3	9.304	4.028	-4.028	0.0	5.276	2.729	
-7	12	3	10.300	10.453	10.453	0.0	-0.153	-0.085	
-5	12	3	3.267	2.568	2.568	0.0	0.699	0.195	
-3	12	3	3.402	5.517	5.517	0.0	-2.114	-0.591	
-1	12	3	13.551	13.653	13.653	0.0	-0.102	-0.074	
0	12	0	198.134	204.739	204.739	0.0	-6.605	-2.229	*
1	12	3	14.944	16.728	16.728	0.0	-1.784	-1.409	
5	12	3	6.805	6.370	6.370	0.0	0.435	0.173	
7	12	3	4.644	3.257	3.257	0.0	1.386	0.377	
8	11	3	8.595	7.827	7.827	0.0	0.768	0.307	
6	11	3	17.806	17.966	-17.966	0.0	-0.160	-0.136	
4	11	3	13.576	14.060	-14.060	0.0	-0.485	-0.356	
2	11	3	6.839	9.738	-9.738	0.0	-2.899	-1.235	
0	11	3	9.051	8.121	8.121	0.0	0.929	0.489	
-2	11	3	33.298	34.511	-34.511	0.0	-1.213	-1.437	
-4	11	3	7.430	7.492	7.492	0.0	-0.063	-0.028	
-6	11	3	7.632	1.452	1.452	0.0	6.180	3.128	
-8	11	3	7.793	2.638	-2.638	0.0	5.155	2.366	
-11	10	3	3.538	2.919	2.919	0.0	0.619	0.150	
-9	10	3	12.993	13.664	-13.664	0.0	-0.671	-0.434	
-7	10	3	29.127	30.322	30.322	0.0	-1.194	-1.334	
-5	10	3	53.020	54.310	-54.310	0.0	-1.289	-1.364	
-3	10	3	50.167	50.410	50.410	0.0	-0.243	-0.269	
0	12	0	198.497	204.739	204.739	0.0	-6.242	-2.100	*
-1	10	3	8.738	7.325	-7.325	0.0	1.414	0.734	
1	10	3	27.278	27.295	-27.295	0.0	-0.016	-0.018	
3	10	3	21.917	22.490	22.490	0.0	-0.572	-0.665	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
5	10	3	7.843	5.338	-5.338	0.0	2.505	1.236	
9	10	3	21.326	20.753	-20.753	0.0	0.573	0.482	
8	9	3	2.558	3.216	3.216	0.0	-0.658	-0.135	
6	9	3	14.471	12.610	-12.610	0.0	1.861	1.499	
4	9	3	29.187	28.586	28.586	0.0	0.600	0.748	
2	9	3	24.298	23.933	-23.933	0.0	0.365	0.386	
0	9	3	59.395	60.125	60.125	0.0	-0.730	-0.727	
-2	9	3	49.508	49.768	-49.768	0.0	-0.260	-0.296	
-4	9	3	38.887	40.194	40.194	0.0	-1.307	-1.579	
-6	9	3	18.253	19.023	19.023	0.0	-0.770	-0.702	
-8	9	3	30.554	30.840	-30.840	0.0	-0.286	-0.325	
-10	9	3	19.359	19.928	19.928	0.0	-0.569	-0.484	
-12	9	3	15.315	16.815	-16.815	0.0	-1.500	-0.893	
-11	8	3	4.323	4.408	-4.408	0.0	-0.085	-0.024	
-9	8	3	11.946	12.386	-12.386	0.0	-0.439	-0.278	
-7	8	3	2.220	1.021	1.021	0.0	1.200	0.288	
0	12	0	198.421	204.739	204.739	0.0	-6.318	-2.126	*
-5	8	3	16.404	13.488	-13.488	0.0	2.916	2.636	
-3	8	3	5.336	3.301	-3.301	0.0	2.034	0.801	
-1	8	3	10.275	10.920	-10.920	0.0	-0.646	-0.407	
3	8	3	5.589	0.223	-0.223	0.0	5.366	2.044	
5	8	3	23.842	23.791	-23.791	0.0	0.051	0.057	
9	8	3	1.672	3.458	3.458	0.0	-1.786	-0.319	
8	7	3	7.117	6.957	6.957	0.0	0.160	0.060	
6	7	3	37.173	37.545	37.545	0.0	-0.372	-0.420	
4	7	3	67.061	68.604	-68.604	0.0	-1.544	-1.406	
2	7	3	26.806	26.914	26.914	0.0	-0.108	-0.125	
0	7	3	38.423	38.264	-38.264	0.0	0.159	0.202	
-2	7	3	93.444	92.191	92.191	0.0	1.253	0.873	
-4	7	3	30.436	29.639	-29.639	0.0	0.797	1.027	
-6	7	3	9.912	11.787	-11.787	0.0	-1.875	-0.966	
-8	7	3	20.609	20.904	20.904	0.0	-0.296	-0.299	
-10	7	3	5.750	1.841	-1.841	0.0	3.908	1.366	
-12	7	3	33.712	36.359	36.359	0.0	-2.647	-2.431	
-13	6	3	14.277	12.924	12.924	0.0	1.352	0.774	
0	12	0	198.193	204.739	204.739	0.0	-6.546	-2.203	*
-11	6	3	12.461	12.839	12.839	0.0	-0.377	-0.216	
-9	6	3	118.097	119.433	119.433	0.0	-1.336	-0.736	
-7	6	3	77.952	79.810	-79.810	0.0	-1.858	-1.487	
-5	6	3	99.987	100.781	100.781	0.0	-0.793	-0.516	
-3	6	3	38.431	37.617	37.617	0.0	0.815	1.049	
-1	6	3	188.222	188.400	188.400	0.0	-0.178	-0.063	
1	6	3	26.248	27.807	27.807	0.0	-1.558	-1.828	
3	6	3	15.357	17.467	-17.467	0.0	-2.110	-1.622	
5	6	3	107.780	110.562	110.562	0.0	-2.782	-1.672	
7	6	3	0.431	1.408	-1.408	0.0	-0.978	-0.164	
9	6	3	71.789	70.562	70.562	0.0	1.226	0.995	
8	5	3	34.590	33.742	33.742	0.0	0.848	0.948	
6	5	3	85.989	86.549	86.549	0.0	-0.560	-0.412	
4	5	3	31.052	32.510	-32.510	0.0	-1.457	-1.726	
2	5	3	97.091	98.972	98.972	0.0	-1.881	-1.258	
0	5	3	19.697	19.319	19.319	0.0	0.378	0.453	
-2	5	3	187.513	188.112	188.112	0.0	-0.599	-0.213	