

## High temperature crystal chemistry of K and Na fluor-richterites

MARYELLEN CAMERON,<sup>1</sup> SHIGEHO SUENO,<sup>2</sup> J. J. PAPIKE,<sup>3</sup> AND C. T. PREWITT

*Department of Earth and Space Sciences  
State University of New York  
Stony Brook, New York 11794*

### Abstract

Crystal structure parameters have been determined for synthetic potassium richterite  $K(NaCa)Mg_5Si_8O_{22}F_2$  at 24°, 400°, 600°, and 800°C, and synthetic sodium richterite  $Na(NaCa)Mg_5Si_8O_{22}F_2$  at 24°, 400°, 600°, 800°, and 900°C. Anisotropic refinements in space group  $I2/m$  using 1150–1200 reflections resulted in  $R$  factors ranging from 0.034 to 0.063. The K atom in the A site of potassium richterite was refined at all temperatures using a half atom model with K randomly occupying two special positions (4*i*) within the (010) mirror plane. The Na atom in the A site of sodium richterite was refined using a quarter atom model in which Na randomly occupies four general positions (8*j*) off both the (010) mirror plane and the twofold axis parallel to  $b$ .

As observed in other high-temperature studies of silicate minerals, the polyhedra in these structures expand differentially. Over the temperature intervals studied, the tetrahedral distances remain statistically identical, but all other mean polyhedral distances increase significantly. Mean thermal expansion coefficients (MTEC) for mean bond lengths increase as follows:  $T_1 = T_2 \ll M_3 < M_1 < M_2 \ll ^{VIII}M_4 < ^X A$  (K richterite) and  $T_1 = T_2 \ll M_1 < M_2 < M_3 \ll ^{VIII}M_4 < ^X A$  (Na richterite). This differential polyhedral expansion is accompanied by straightening of the tetrahedral chains and by increased displacement of the double chains relative to each other. Expansion of three of the four M polyhedra in K richterite is slightly greater than for Na richterite, and the MTEC of its unit cell volume is larger (3.39 vs.  $3.10/^\circ\text{C} \times 10^{-5}$ ).

The behavior of the richterite structures at elevated temperatures is generally similar to that of tremolite. The MTEC's for structural and thermal parameters are often identical within three standard deviations. The largest difference among the three structures involves the coordination polyhedron about the A site, where the rate of expansion of the mean 10-coordinated A–O distance is significantly greater in the richterites than in tremolite.

### Introduction

Phenomena such as exsolution, solid solution, and inter- and intracrystalline equilibria are of interest to geologists because they provide information on the crystallization and cooling histories of rocks. These phenomena typically occur at elevated temperatures and/or pressures in geologic environments, and until recently they were necessarily described on an atomic level in terms of room-temperature crystal structures. Within the last ten years, however, the structures of various rock-forming

silicate minerals have been examined at temperatures up to 1050°C. Scores of refinements, on a limited number of crystals, have been published for olivines (*e.g.*, Brown and Prewitt, 1973; Hazen, 1976; Smyth and Hazen 1973; Lager and Meagher, 1978), feldspars (*e.g.*, Prewitt *et al.*, 1976; Winter *et al.*, 1979), pyroxenes (*e.g.*, Cameron *et al.*, 1973a; Sueno *et al.*, 1976), and amphiboles (*e.g.*, Sueno *et al.*, 1973). The crystals used in many of these high temperature studies have approximately end-member compositions, and thus the effects of increasing temperature on individual cations could be evaluated.

In this paper we describe the structural changes that occur in two synthetic fluor-richterites ( $KNaCaMg_5Si_8O_{22}F_2$  and  $NaNaCaMg_5Si_8O_{22}F_2$ ) at a series of temperatures between 24° and 900°C. Our primary intention is to compare the behavior of an amphibole with a filled A site (richterite) to one with a vacant A site (tremolite; Sueno *et al.*, 1973). Richterites were selected for study

<sup>1</sup> Present address: School of Geology and Geophysics, University of Oklahoma, Norman, Oklahoma 73019.

<sup>2</sup> Present address: Institute of Geoscience, The University of Tsukuba, Ibaraki, 300-31, Japan.

<sup>3</sup> Present address: Institute for the Study of Mineral Deposits, South Dakota School of Mines and Technology, Rapid City, South Dakota 57701

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
4	0	0	24.021	37.708	0.0	-13.688	-14.928	*	
0	0	0	101.346	160.235	0.0	1.511	0.914		
8	0	0	114.356	118.629	0.0	-3.673	-1.985		
10	0	0	60.937	65.760	0.0	1.176	0.835		
12	0	0	4.224	4.660	0.0	-4.660	-0.574		
-15	0	0	34.051	39.999	0.0	-5.936	-2.541	*	
-11	1	0	60.518	61.961	0.0	-1.442	-0.958	*	
-9	1	0	22.645	23.626	0.0	-1.181	-0.743	*	
-7	1	0	73.421	74.557	0.0	-1.156	-0.846	*	
-5	1	0	121.855	118.895	0.0	2.960	1.558	*	
3	1	0	140.679	136.935	0.0	1.144	0.527		
5	1	0	121.462	118.895	0.0	2.567	1.363		
7	1	0	73.372	74.557	0.0	-1.185	-0.897		
9	1	0	25.314	23.826	0.0	1.488	1.163		
11	1	0	62.424	61.561	0.0	0.473	0.331		
13	1	0	33.150	34.233	0.0	-1.143	-0.614		
-12	2	0	15.637	15.166	0.0	0.471	0.144	*	
-8	2	0	14.458	12.754	0.0	1.704	0.813	*	
0	12	0	216.358	218.344	0.0	-1.945	-0.593	*	
-6	2	0	32.666	33.811	0.0	-1.145	-1.069	*	
4	2	0	7.123	1.313	1.313	5.839	3.488		
6	2	0	33.288	33.811	0.0	-0.523	-0.502		
8	2	0	13.165	12.754	0.0	0.411	0.189		
-12	2	0	15.570	15.166	0.0	0.504	0.224		
-13	3	0	13.705	19.569	0.0	-5.863	-1.210	*	
-11	3	0	25.380	21.490	0.0	3.889	2.117	*	
-9	3	0	17.913	18.559	0.0	-6.646	-0.329	*	
-5	3	0	56.376	56.435	0.0	-0.059	-0.051	*	
-3	3	0	57.718	57.487	0.0	0.231	0.216	*	
3	3	0	87.977	91.457	0.0	-3.480	-2.507	*	
5	3	0	89.418	91.457	0.0	-2.039	-1.452		
7	3	0	55.143	57.487	0.0	1.656	1.536		
9	3	0	56.687	56.435	0.0	0.252	0.214		
11	3	0	19.103	18.559	0.0	0.549	0.358		
13	3	0	19.158	21.490	0.0	-2.333	-0.991		
-12	4	0	22.367	19.569	0.0	2.798	1.275		
0	12	0	11.871	13.243	0.0	-1.371	-0.309	*	
-10	4	0	214.100	218.344	0.0	-4.238	-1.304	*	
-8	4	0	5.600	2.355	2.355	3.245	0.689	*	
-6	4	0	6.533	8.738	8.738	-2.204	-0.549	*	
-4	4	0	17.176	17.761	0.0	-0.584	-0.407	*	
-2	4	0	14.884	11.522	11.522	3.362	3.014	*	
2	4	0	137.836	142.611	142.611	0.0	-4.775		
4	4	0	140.309	142.611	142.611	-2.302	-1.082		
6	4	0	13.345	11.522	11.522	1.822	1.357		
8	4	0	18.159	17.761	17.761	0.0	0.358	0.261	
10	4	0	14.213	8.738	8.738	5.475	3.262		
12	4	0	2.276	2.355	2.355	-0.679	-0.013		
-13	5	0	13.394	13.243	13.243	0.0	0.151	0.048	
-11	5	0	22.465	22.556	22.556	0.0	-0.131	-0.044	*
-7	5	0	17.864	20.159	20.159	0.0	-2.295	-0.741	*
5	0	10.741	7.730	7.730	0.0	3.011	1.248	*	
0	18.699	19.140	-19.140	-0.441	-0.350	*			

H	K	L	F(UBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-3	5	0	81.641	62.670	-62.676	0.0	-1.035	-0.788 *
-1	5	0	12.573	16.855	-16.855	0.0	-4.182	-3.202 *
1	5	0	12.919	16.855	-16.855	0.0	-2.936	-3.154
3	5	0	83.507	82.676	-82.676	0.0	0.831	0.623
0	12	0	214.941	218.344	-218.344	0.0	-3.403	-1.044 *
5	5	0	18.977	19.140	-19.140	0.0	-0.162	-0.145
5	5	0	7.286	5.378	-5.378	0.0	1.908	0.564
11	5	0	20.975	20.159	-20.159	0.0	6.816	3.388
13	5	0	26.509	22.596	-22.596	0.0	3.913	2.470
-10	6	0	23.349	28.098	-28.098	0.0	-4.748	-2.377 *
-8	6	0	27.001	27.654	-27.654	0.0	-0.653	-0.456 *
-6	6	0	17.831	14.217	-14.217	0.0	3.615	2.488 *
-4	6	0	4.617	3.526	-3.526	0.0	1.091	0.332 *
-2	6	0	19.354	21.541	-21.541	0.0	-2.587	-2.778 *
0	6	0	10.021	16.022	-16.022	0.0	-6.001	-3.685
4	6	0	3.471	3.526	-3.526	0.0	-0.055	-0.016
6	6	0	13.574	14.217	-14.217	0.0	-0.643	-0.289
8	6	0	26.542	27.654	-27.654	0.0	-1.112	-0.975
10	6	0	23.775	28.098	-28.098	0.0	-4.323	-2.233
-14	7	0	18.306	14.552	-14.552	0.0	3.354	1.566 *
-9	7	0	50.399	52.499	-52.499	0.0	-2.100	-1.512 *
0	12	0	215.694	218.344	-218.344	0.0	-2.649	-0.810 *
-7	7	0	37.938	36.858	-36.858	0.0	1.080	0.954 *
-5	7	0	8.776	8.945	-8.945	0.0	-0.168	-0.065 *
-3	7	0	57.64	56.459	-56.459	0.0	1.145	1.082 *
-1	7	0	15.588	17.532	-17.532	0.0	-2.343	-1.956 *
3	7	0	58.144	56.459	-56.459	0.0	1.635	1.583
5	7	0	8.158	8.945	-8.945	0.0	-0.807	-0.255
7	7	0	34.958	36.858	-36.858	0.0	-1.907	-1.459
9	7	0	52.253	52.499	-52.499	0.0	-0.201	-0.154
11	7	0	14.933	14.552	-14.552	0.0	-0.019	-0.007
-12	8	0	38.020	37.040	-37.040	0.0	0.980	0.550 *
-10	8	0	49.950	50.128	-50.128	0.0	-0.138	-0.093 *
-8	8	0	12.864	10.364	-10.364	0.0	2.440	1.067 *
-6	8	0	73.699	74.118	-74.118	0.0	-0.418	-0.315 *
-4	8	0	102.419	103.570	-103.576	0.0	-1.156	-0.703 *
-2	8	0	31.815	35.823	-35.823	0.0	-4.039	-4.481 *
0	6	0	47.812	45.256	-45.256	0.0	2.516	2.694
2	6	0	32.420	35.823	-35.823	0.0	-2.403	-3.914
4	8	0	105.154	103.576	-103.576	0.0	1.578	0.937
6	8	0	74.469	74.118	-74.118	0.0	0.351	0.260
0	12	0	214.166	218.344	-218.344	0.0	-4.238	-1.304 *
8	8	0	8.269	10.364	-10.364	0.0	-2.096	-0.763
10	8	0	50.153	50.128	-50.128	0.0	0.026	0.018
12	8	0	36.154	37.040	-37.040	0.0	-6.836	-0.502
-11	9	0	19.714	16.980	-16.980	0.0	2.734	1.023 *
-9	9	0	34.058	33.577	-33.577	0.0	0.480	0.330 *
-7	9	0	56.623	57.122	-57.122	0.0	-0.499	-0.302 *
-5	9	0	8.689	6.559	-6.559	0.0	1.130	0.386 *
-3	9	0	7.024	8.756	-8.756	0.0	-1.771	-0.686 *
1	9	0	83.491	82.829	-82.829	0.0	0.662	0.484 *
7	9	0	84.424	82.829	-82.829	0.0	1.595	1.156
9	0	98.539	97.122	-97.122	0.0	1.417	0.657	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
5	9	0	34.811	33.577	33.577	0.0	1.234	0.947
11	9	0	14.539	16.980	-16.980	0.0	-2.391	-0.818
-12	10	0	23.156	23.523	23.928	0.0	-0.742	-0.245 *
-10	10	0	28.687	29.251	29.251	0.0	-0.564	-0.296 *
-6	10	0	30.849	29.640	29.640	0.0	1.209	0.890 *
-6	10	0	17.684	17.152	17.152	0.0	0.532	0.314 *
-4	10	0	66.970	66.873	66.873	0.0	0.097	0.079 *
0	12	0	213.364	218.344	218.344	0.0	-5.040	-1.557 *
-2	10	0	45.061	48.231	48.231	0.0	-3.170	-3.130 *
0	10	0	105.039	106.257	106.257	0.0	-1.218	-0.731
2	10	0	46.305	48.231	48.231	0.0	-1.925	-1.921
4	10	0	66.883	66.873	66.873	0.0	0.015	0.012
6	10	0	17.618	17.152	17.152	0.0	0.466	0.264
3	10	0	30.668	29.640	29.640	0.0	1.029	0.755
10	10	0	28.956	29.251	29.251	0.0	-0.253	-0.164
12	10	0	27.819	23.928	23.928	0.0	3.892	2.437
-11	11	0	66.937	67.488	67.488	0.0	-0.551	-0.323 *
-9	11	0	11.183	5.876	5.876	0.0	5.307	1.902 *
-7	11	0	136.755	137.991	137.991	0.0	-1.235	-0.563 *
-5	11	0	41.704	42.967	42.967	0.0	-1.263	-1.062 *
-3	11	0	80.653	83.120	83.120	0.0	-2.462	-1.759 *
-1	11	0	124.278	122.962	122.962	0.0	1.316	0.676 *
1	11	0	126.243	122.962	122.962	0.0	3.281	1.664
5	11	0	81.379	83.120	83.120	0.0	-1.742	-1.240
3	11	0	39.887	42.967	42.967	0.0	-3.081	-2.589
7	11	0	137.181	137.991	137.991	0.0	-0.810	-0.368
11	11	0	65.950	67.438	67.438	0.0	-2.461	1.551
0	12	0	215.924	218.344	218.344	0.0	-2.420	-0.739 *
-10	12	0	56.965	57.775	57.775	0.0	-6.810	-0.523 *
-8	12	0	53.232	55.295	55.295	0.0	-2.064	-1.484 *
-6	12	0	33.665	34.085	-34.085	0.0	-6.420	-0.313 *
-4	12	0	59.847	59.575	59.575	0.0	0.272	0.222
-2	12	0	40.902	39.801	-39.801	0.0	1.101	1.016 *
0	12	0	214.712	218.344	218.344	0.0	-3.632	-1.115 *
2	12	0	40.869	39.801	-39.801	0.0	1.068	1.005
4	12	0	60.109	59.575	59.575	0.0	0.534	0.446
6	12	0	34.713	34.685	-34.685	0.0	0.628	0.504
8	12	0	54.667	55.295	55.295	0.0	-0.683	-0.521
10	12	0	59.241	57.775	57.775	0.0	1.466	0.987
-11	13	0	17.799	23.247	23.247	0.0	-5.449	-1.484 *
-9	13	0	24.528	27.413	-27.413	0.0	-2.385	-1.322 *
-7	13	0	38.905	39.823	39.823	0.0	-5.919	-0.657 *
-5	13	0	69.557	67.942	-67.942	0.0	1.615	1.225 *
-3	13	0	21.303	20.648	-20.648	0.0	0.655	0.454 *
1	13	0	8.121	6.228	6.228	0.0	1.893	0.649 *
3	13	0	18.865	20.648	-20.648	0.0	-0.006	-0.002
5	13	0	70.031	67.942	-67.942	0.0	1.785	-1.059
0	12	0	24.565	28.344	28.344	0.0	-2.089	1.589 *
7	13	0	40.919	39.823	39.823	0.0	-3.779	-1.161 *
9	13	0	24.102	27.413	-27.413	0.0	-5.310	-1.687
11	13	0	21.565	23.247	23.247	0.0	-1.683	-0.710
14	0		9.988	6.730	-0.730	*	2.022	9.258

H	K	L	F(OBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
-6	14	0	4.503	1.201	-1.201	0.0	3.302	C.660 *
-4	14	0	15.080	12.766	12.766	0.0	2.314	1.395 *
-2	14	0	36.563	36.154	36.154	0.0	0.409	0.361 *
0	14	0	6.582	7.704	-7.704	0.0	-1.122	-0.303
2	14	0	37.087	36.154	36.154	0.0	6.933	C.853
4	14	0	11.658	12.766	12.766	0.0	-1.108	-0.518
-9	15	C	37.349	36.150	36.150	0.0	1.199	0.636 *
-7	15	C	53.257	53.867	-53.867	0.0	-0.570	-0.378 *
-5	15	C	31.856	32.619	-32.019	0.0	-0.123	-0.090 *
-3	15	C	8.589	1.048	-1.048	0.0	7.942	3.032 *
-1	15	C	10.414	13.487	-13.487	0.0	-3.073	-1.203 *
1	15	C	16.783	13.487	-13.487	0.0	3.296	2.868
0	12	0	214.450	218.344	218.344	0.0	-3.894	-1.157 *
3	15	0	10.332	1.048	-1.048	0.0	9.284	4.150
5	15	0	32.944	32.019	32.019	0.0	6.925	0.765
7	15	0	57.391	53.867	-53.867	0.0	3.524	2.710
9	15	0	38.184	36.150	36.150	0.0	2.034	1.369
-10	16	0	28.736	27.569	-27.569	0.0	1.167	0.508 *
-3	16	0	11.871	11.713	-11.713	0.0	0.158	0.044 *
-6	16	0	32.437	35.641	0.0	-3.204	-2.130 *	
-4	16	0	52.258	53.231	-53.231	0.0	-0.935	-0.741 *
-2	16	0	8.776	4.698	4.698	0.0	4.079	1.441 *
0	16	0	9.481	6.540	6.940	0.0	2.540	1.162
4	16	0	50.743	53.231	-53.231	0.0	-2.488	-1.871
6	16	0	36.629	35.641	35.641	0.0	6.983	0.813
8	16	0	12.608	11.713	-11.713	0.0	0.895	0.323
10	17	0	30.581	27.569	-27.569	0.0	3.312	2.173
-9	17	0	8.133	16.451	16.451	0.0	-8.313	-1.288 *
-7	17	0	15.948	12.235	-12.235	0.0	3.714	1.343 *
-5	17	0	8.531	8.345	-8.345	0.0	0.186	0.058 *
-3	17	0	27.066	26.309	26.309	0.0	0.757	0.604 *
-1	17	C	17.471	17.459	-17.459	0.0	0.012	0.007 *
0	12	0	214.843	218.344	218.344	0.0	-3.501	-1.074 *
1	17	0	12.650	17.459	-17.459	0.0	-4.769	-1.759
3	17	0	22.416	26.309	26.309	0.0	-3.893	-2.024
5	17	0	7.630	8.345	-8.345	0.0	-0.715	-0.199
7	17	0	13.361	12.235	-12.235	0.0	1.127	0.356
9	17	0	15.441	16.451	16.451	0.0	-1.010	-0.312
-8	18	0	5.756	10.243	-10.243	0.0	-4.447	-0.674 *
-6	18	0	24.725	25.296	25.296	0.0	-0.572	-0.252 *
-2	18	0	25.651	24.923	24.923	0.0	0.767	0.511 *
0	13	0	19.756	15.655	19.655	0.0	0.101	0.058
2	13	0	25.298	24.923	24.923	0.0	0.374	0.236
4	18	0	10.856	8.804	8.804	0.0	2.052	0.777
6	18	0	26.853	25.296	25.296	0.0	1.557	0.917
8	18	0	16.669	10.243	-10.243	0.0	6.425	3.118
-7	19	0	31.422	26.123	-26.123	0.0	5.299	2.888 *
-5	19	0	2.325	3.390	3.390	0.0	-1.065	-0.135 *
-3	19	0	32.813	32.033	-32.033	0.0	0.781	0.524 *
-1	19	0	7.434	6.689	-6.689	0.0	0.745	0.156 *
1	19	0	7.286	6.689	-6.689	0.0	0.597	0.151
3	19	0	31.946	32.033	-32.033	0.0	-0.087	-0.064 *
0	12	0	214.852	218.344	-218.344	0.0	-3.452	-1.059 *

H	K	L	F (UBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
3	19	0	8.007	3.390	0.0	4.617	1.223	
7	19	0	25.509	26.123	-26.123	0.0	-0.154	-0.076
-6	20	0	13.512	1.843	1.843	0.0	1.469	3.902 *
-4	20	0	34.025	34.091	-34.091	0.0	-0.066	-0.039 *
-2	20	0	30.718	31.473	31.473	0.0	-0.756	-0.494 *
0	20	0	56.441	56.842	-56.842	0.0	-0.401	-0.292
2	20	0	32.289	31.473	31.473	0.0	0.816	0.583
4	20	0	36.556	34.691	-34.691	0.0	2.505	1.746
-5	21	0	11.937	1.843	1.843	0.0	0.0	3.573 *
-1	21	0	38.708	39.257	39.257	0.0	-0.549	-0.354 *
1	21	0	21.941	25.643	25.643	0.0	-3.702	-1.549 *
3	21	0	24.594	25.643	25.643	0.0	-1.049	-0.548
5	21	0	6.910	5.512	5.512	0.0	1.397	1.299
-6	22	0	41.672	39.257	39.257	0.0	2.415	1.689
-4	22	0	50.022	48.089	48.089	0.0	-2.533	-0.458 *
-2	22	0	22.989	19.564	19.564	0.0	1.934	1.223 *
0	22	0	215.236	218.344	218.344	0.0	-3.025	1.553 *
6	22	0	67.788	67.471	67.471	0.0	-3.108	-0.952 *
2	22	0	15.845	19.564	19.564	0.0	0.317	0.208
4	22	0	50.153	48.089	48.089	0.0	-0.118	-0.050
6	22	0	15.113	11.441	11.441	0.0	2.065	1.264
-5	23	0	49.269	49.553	-49.553	0.0	3.672	1.279
-3	23	0	32.633	36.393	36.393	0.0	-0.283	-0.143 *
-1	23	0	15.375	9.223	9.223	0.0	-3.760	-1.765 *
1	23	0	10.189	9.223	9.223	0.0	6.153	2.238 *
3	23	0	37.644	36.393	36.393	0.0	0.962	0.232
5	23	0	50.939	49.553	-49.553	0.0	1.251	0.843
-2	24	0	59.552	43.812	-43.812	0.0	1.387	0.777
0	24	0	92.067	90.611	90.611	0.0	-4.220	-2.054 *
2	24	0	42.310	43.812	-43.812	0.0	1.476	0.821
-13	0	1	21.050	17.216	-17.216	0.0	-1.502	-0.854
-9	0	1	5.653	12.961	-12.961	0.0	3.873	1.552
-7	0	1	4.585	4.805	-4.805	0.0	-3.268	-1.158
-3	0	1	12.821	11.234	-11.234	0.0	-0.220	-0.055
3	0	1	27.918	26.359	-26.359	0.0	1.587	1.208
0	12	0	215.154	218.344	218.344	0.0	1.559	1.898
-7	0	1	17.679	2.723	2.723	0.0	-3.190	-0.977 *
11	0	1	11.314	6.190	-6.190	0.0	4.950	1.752
-12	1	1	4.274	6.056	-6.056	0.0	5.125	2.074
-10	1	1	6.157	8.776	-8.776	0.0	-1.823	-0.294
-8	1	1	4.012	8.284	-8.284	0.0	-2.619	-0.640
-4	1	1	20.369	19.642	19.642	0.0	-4.273	-0.885
2	1	1	64.841	67.452	-67.452	0.0	0.728	0.830
4	1	1	9.448	10.562	-10.562	0.0	-2.611	-2.417
6	1	1	12.264	11.854	-11.854	0.0	-1.114	-0.581
8	1	1	14.553	16.008	-16.008	0.0	0.410	0.190
10	1	1	10.790	11.507	-11.507	0.0	-1.615	-0.809
12	1	1	6.861	8.865	-8.865	0.0	0.717	0.236
-13	2	1	18.486	21.660	-21.660	0.0	-2.004	-0.419
-11	2	1	27.476	26.714	-26.714	0.0	3.174	-0.953
-9	2	1	24.807	25.304	-25.304	0.0	0.702	0.407
-7	2	1	55.737	54.385	-54.385	0.0	-6.497	-0.388
						0.0	1.352	1.269

H	K	L	F(UBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-5	2	1	44.570	44.685	-44.089	0.0	0.481	0.542
0	12	0	214.712	218.344	218.344	0.0	-3.632	-1.115 *
-3	2	1	137.263	140.860	140.860	0.0	-3.597	-1.723
3	2	1	115.617	116.611	116.611	0.0	-1.064	-0.555
5	2	1	24.037	23.518	23.518	0.0	0.519	0.437
7	2	1	47.173	45.969	45.969	0.0	-1.204	1.058
4	2	1	19.682	20.189	20.189	0.0	-0.508	-0.288
11	2	1	35.401	37.538	37.538	0.0	-2.538	-1.450
-12	3	1	44.439	42.898	42.898	0.0	1.541	1.025
-6	3	1	26.755	27.740	27.740	0.0	-0.985	-0.654
-9	3	1	12.641	10.549	10.549	0.0	2.091	1.304
-4	3	1	25.369	26.120	26.120	0.0	1.189	1.456
-2	3	1	150.149	155.981	153.981	0.0	-3.832	-1.688
2	3	1	134.571	138.521	138.521	0.0	-3.550	-1.726
4	3	1	25.625	25.789	25.789	0.0	-0.164	-0.155
6	3	1	43.214	40.288	40.288	0.0	-0.073	-0.066
8	3	1	19.763	16.369	16.369	0.0	3.394	2.586
10	3	1	7.663	7.843	7.843	0.0	-0.180	-0.051
12	3	1	35.057	32.780	32.780	0.0	2.277	1.621
-13	4	1	26.493	24.879	24.879	0.0	1.614	0.805
-11	4	1	20.418	18.792	18.792	0.0	1.626	0.823
0	12	0	214.139	218.344	218.344	0.0	-4.205	-1.294 *
-7	4	1	11.822	15.019	15.019	0.0	-3.197	-1.317
-5	4	1	27.148	26.272	26.272	0.0	0.876	0.886
-3	4	1	13.951	16.815	16.815	0.0	-2.864	-2.183
-1	4	1	22.760	24.906	24.906	0.0	-2.146	-2.573
1	4	1	15.375	16.925	16.925	0.0	-1.250	-1.086
3	4	1	6.893	9.936	9.936	0.0	-3.042	-1.439
5	4	1	8.858	6.281	6.281	0.0	2.577	1.159
7	4	1	25.553	26.783	26.783	0.0	-1.190	-0.913
9	4	1	21.188	19.945	19.945	0.0	1.243	0.764
11	4	1	21.056	21.673	21.673	0.0	0.022	0.013
-12	5	1	83.442	81.739	81.739	0.0	1.703	1.010
-10	5	1	7.679	11.855	11.855	0.0	-4.175	-0.952
-3	5	1	9.775	12.080	12.080	0.0	-2.305	-0.823
-6	5	1	100.192	102.377	102.377	0.0	-2.184	-1.344
-4	5	1	93.856	93.139	93.139	0.0	0.716	0.478
3	5	1	213.127	212.549	212.549	0.0	-2.822	-0.893
2	5	1	84.113	83.620	83.620	0.0	0.493	0.370
4	5	1	124.737	123.763	123.763	0.0	0.974	0.508
0	12	0	215.662	218.344	218.344	0.0	1.104	0.722
5	1		155.520	157.814	157.814	0.0	-2.682	-0.820 *
8	1		28.720	28.820	28.820	0.0	-2.294	-0.949
12	5		44.930	45.852	45.852	0.0	-0.100	-0.072
-13	6	1	57.456	57.913	57.913	0.0	-0.921	-0.533
-9	6	1	109.083	111.516	111.516	0.0	-0.457	-0.255
-7	6	1	94.592	96.280	96.280	0.0	-2.433	-1.327
-5	9	1	261.907	267.507	267.507	0.0	-1.687	-1.063
-3	6	1	171.812	168.859	168.859	0.0	-5.599	-1.828
-1	6	1	140.358	145.682	145.682	0.0	-4.725	-2.210
3	6	1	54.509	41.635	41.635	0.0	12.574	12.795 *
1	74.141		72.693	72.693	72.693	1.444	1.150	

H	K	L	F(UIS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
5	0	1	242.679	247.317	0.0	-4.639	-1.264	
7	0	1	30.275	30.297	0.0	-0.022	-0.018	
9	3	1	89.517	89.693	0.0	0.418	0.256	
11	0	1	25.371	28.356	-28.356	0.0	-2.485	-1.175
-12	7	1	47.746	45.501	45.901	0.0	1.845	1.172
-10	7	1	15.193	18.437	-18.437	0.0	0.754	0.338
-8	7	1	30.881	33.313	-33.313	0.0	-2.432	-1.786
6	12	0	212.770	218.344	218.344	0.0	-2.563	-0.784 *
-6	7	1	32.336	32.360	32.060	0.0	0.246	0.216
-4	7	1	8.056	3.401	-3.401	0.0	4.655	2.285
-2	7	1	61.599	60.663	60.063	0.0	1.539	1.447
0	7	1	137.050	138.232	-138.232	0.0	-1.181	-0.563
2	7	1	15.326	12.555	13.555	0.0	1.771	1.465
4	7	1	64.022	64.484	-64.484	0.0	-0.461	-0.385
6	7	1	63.394	66.715	66.715	0.0	1.679	1.325
8	7	1	7.827	10.345	-10.345	0.0	-2.518	-0.659
10	7	1	25.527	24.897	-24.897	0.0	0.630	0.353
12	7	1	11.642	11.490	11.490	0.0	0.152	0.044
-11	8	1	16.570	18.472	-18.472	0.0	-1.902	-0.678
-9	8	1	17.864	14.400	-14.400	0.0	3.458	1.946
-7	8	1	16.980	17.862	-17.862	0.0	-0.882	-0.489
-5	8	1	16.987	16.132	-16.132	0.0	-5.145	-2.582
-3	8	1	11.626	11.329	11.329	0.0	0.297	0.188
1	8	1	3.651	5.362	5.362	0.0	-1.710	-0.496
3	6	1	6.107	2.753	2.753	0.0	3.354	1.189
5	8	1	23.480	23.464	-23.464	0.0	0.016	0.011
0	12	0	215.431	218.344	218.344	0.0	-2.862	-6.376 *
7	8	1	27.033	28.497	-28.497	0.0	-1.464	-1.177
-11	8	1	17.373	15.212	-15.212	0.0	2.161	1.052
-12	9	1	25.249	27.750	-27.750	0.0	-2.501	-1.017
-10	9	1	16.439	16.004	16.004	0.0	0.436	0.184
-3	9	1	10.652	2.141	-2.141	0.0	8.551	3.695
-6	9	1	17.389	15.683	15.683	0.0	1.706	1.014
-4	9	1	20.435	18.168	18.168	0.0	2.267	1.657
-2	9	1	59.503	61.357	-61.357	0.0	-1.854	-1.677
0	9	1	94.134	93.431	93.431	0.0	0.703	0.463
2	9	1	67.395	68.437	-68.437	0.0	-1.042	-0.370
4	9	1	34.827	33.353	33.353	0.0	1.474	1.295
6	9	1	14.409	10.903	-10.903	0.0	3.506	2.035
8	9	1	4.650	1.097	1.097	0.0	3.554	0.779
10	9	1	22.285	22.814	22.314	0.0	-0.529	-0.311
-11	10	1	18.650	21.710	21.710	0.0	-3.060	-1.086
-9	10	1	22.612	22.326	-22.326	0.0	0.287	0.178
-7	10	1	21.155	19.426	19.426	0.0	1.729	1.253
-5	10	1	24.938	29.765	-29.765	0.0	-4.828	-3.293
-3	10	1	52.503	59.559	59.559	0.0	-0.056	-0.050
0	12	0	214.548	218.344	218.344	0.0	-3.796	-1.166 *
-1	10	1	37.807	36.098	-36.098	0.0	1.710	1.854
5	10	1	5.305	0.730	0.730	0.0	4.575	1.455
5	10	1	51.807	52.798	52.798	0.0	-0.990	-0.922
7	10	1	36.907	35.746	-35.746	0.0	1.161	1.024
9	10	1	22.743	22.130	22.130	0.0	0.613	0.352
10	1		15.735	14.318	-14.318	0.0	1.417	0.678

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-11	10	1	23.022	20.339	0.0	2.683	1.539	1.539
-12	11	1	4.661	0.951	0.951	3.650	0.495	0.495
-10	11	1	16.816	18.006	-18.006	-1.190	-0.527	-0.527
-8	11	1	11.642	11.467	11.467	0.175	0.671	0.671
-6	11	1	15.359	21.805	-21.805	-6.447	-2.840	-2.840
-4	11	1	11.953	17.112	-17.112	0.0	-5.159	-2.041
-2	11	1	28.163	29.374	-29.374	0.0	-1.211	-0.956
0	11	1	9.219	9.758	-9.758	0.0	-0.539	-0.241
2	11	1	58.717	58.614	-58.614	0.0	0.103	0.089
4	11	1	9.666	8.630	-8.630	0.0	0.376	0.136
6	11	1	16.112	17.397	-17.397	0.0	-1.285	-0.657
10	11	1	17.116	17.469	-17.469	0.0	-0.292	-0.108
-11	12	1	14.819	11.784	11.784	0.0	3.034	0.884
0	12	C	214.556	218.344	-218.344	0.0	-3.648	-1.120 *
-7	12	1	16.243	19.000	-19.000	0.0	-2.757	-1.253
-5	12	1	23.120	22.589	-22.589	0.0	6.632	0.544
-3	12	1	22.514	20.083	-20.083	0.0	2.431	1.892
-1	12	1	27.312	29.240	-29.240	0.0	-1.928	-1.739
1	12	1	34.765	35.876	-35.876	0.0	-1.081	-1.050
3	12	1	16.603	16.223	-16.223	0.0	0.380	0.207
5	12	1	19.845	20.515	-20.515	0.0	-0.670	-0.429
7	12	1	14.966	17.555	-17.555	0.0	-2.589	-1.064
9	12	1	6.089	13.201	-13.201	0.0	-5.113	-1.205
-10	13	1	5.976	3.389	-3.389	0.0	2.587	0.463
-6	13	1	6.893	3.952	-3.952	0.0	3.411	1.050
-4	13	1	32.764	34.153	-34.153	0.0	-1.388	-1.081
-2	13	1	47.485	47.159	-47.159	0.0	0.325	0.286
0	13	1	3.9150	39.680	-39.680	0.0	-0.530	-0.503
-8	13	1	33.354	35.248	-35.248	0.0	-1.894	-1.605
-4	13	1	18.175	15.891	-15.891	0.0	2.284	1.347
6	13	1	8.465	11.331	-11.331	0.0	-2.866	-0.756
0	12	O	215.743	218.344	-218.344	0.0	-2.600	-0.795 *
8	13	1	16.751	15.882	-15.882	0.0	0.888	0.421
10	13	1	16.135	9.562	-9.562	0.0	0.574	0.180
-11	14	1	6.028	2.511	-2.511	0.0	4.317	0.726
-9	14	1	29.833	33.031	-33.031	0.0	-3.198	-1.610
-7	14	1	32.535	31.780	-31.780	0.0	0.755	0.613
-5	14	1	82.394	84.798	-84.798	0.0	-2.404	-1.631
-3	14	1	41.197	42.441	-42.441	0.0	-1.244	-1.374
-1	14	1	34.909	33.050	-33.050	0.0	1.859	1.752
1	14	1	52.004	51.515	-51.515	0.0	0.489	0.428
3	14	1	22.056	24.908	-24.908	0.0	-2.853	-1.889
5	14	1	43.358	43.065	-43.065	0.0	0.353	0.311
7	14	1	11.216	9.172	-9.172	0.0	2.045	0.687
9	14	1	37.218	38.650	-38.650	0.0	-1.432	-0.931
-10	15	1	10.643	14.478	-14.478	0.0	-3.835	-0.835
-8	15	1	17.225	14.018	-14.018	0.0	3.208	1.469
-6	15	1	20.828	18.915	-18.915	0.0	1.913	1.106
-4	15	1	18.241	17.668	-17.668	0.0	0.573	0.333
-2	15	1	55.852	58.208	-58.208	0.0	-2.356	-1.927
0	15	1	25.511	27.947	-27.947	0.0	-1.259	-1.047
2	15	1	48.631	49.890	-49.890	0.0	-2.437	-1.551
0	12	O	213.926	218.344	-218.344	0.0	-4.418	-1.361 *

## STRUCTURE FACTORS PAGE 5

H	K	L	F(UBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
-8	15	1	12.673	10.577	10.577	0.0	1.696	0.658	
-9	16	1	41.917	39.765	39.765	0.0	2.015	1.330	
-7	16	1	23.415	24.592	24.592	0.0	-1.277	-0.727	
-5	16	1	67.674	68.515	68.515	0.0	-1.242	-0.895	
-3	16	1	51.873	53.821	53.821	0.0	-1.949	-1.458	
-1	16	1	70.293	71.495	71.495	0.0	-1.202	-0.873	
1	16	1	53.494	54.159	54.159	0.0	-0.665	-0.521	
3	16	1	40.273	46.234	46.234	0.0	0.039	0.031	
5	16	1	61.222	62.458	62.458	0.0	-1.235	-0.852	
7	16	1	36.448	36.274	36.274	0.0	0.175	0.132	
9	16	1	45.045	42.708	42.708	0.0	-0.337	1.528	
-10	17	1	7.166	4.563	4.563	-4.563	2.543	0.412	
-6	17	1	11.233	9.623	9.623	0.0	1.609	0.447	
-6	17	1	48.434	49.509	49.509	0.0	-1.075	-0.762	
-4	17	1	13.256	14.652	14.652	0.0	-0.756	-0.522	
-2	17	1	119.628	119.809	119.809	0.0	-0.180	-0.092	
0	17	1	57.227	57.402	57.402	0.0	-0.175	-0.134	
2	17	1	70.932	76.841	76.841	0.0	0.091	0.065	
0	12	6	214.041	218.344	218.344	0.0	-4.303	-1.325 *	
6	17	1	86.176	87.364	87.364	0.0	-1.187	-0.725	
8	17	1	4.814	2.612	2.612	0.0	2.802	0.477	
-9	18	1	36.170	38.539	38.539	0.0	-2.369	-1.206	
-7	18	1	84.064	86.065	86.065	0.0	-2.001	-1.177	
-5	18	1	83.917	84.180	84.180	0.0	-0.264	-0.166	
-3	18	1	4.044	5.218	5.218	0.0	-1.173	-0.216	
-1	18	1	11.265	8.917	8.917	0.0	2.348	0.953	
1	18	1	21.843	22.585	22.585	0.0	-0.742	-0.412	
3	18	1	11.020	11.057	11.057	0.0	-0.038	-0.014	
5	18	1	69.802	69.701	69.701	0.0	0.101	0.066	
7	18	1	38.299	39.531	39.531	-39.531	-1.232	-0.745	
-6	19	1	13.492	9.591	9.591	0.0	3.901	1.388	
-4	19	1	13.689	16.109	16.109	-16.109	0.0	-2.421	-0.930
-2	19	1	36.825	37.836	37.836	-37.836	0.0	-1.011	-0.723
0	19	1	38.266	36.706	36.706	-36.706	0.0	1.560	1.174
4	19	1	20.549	16.176	16.176	-16.176	0.0	4.374	2.670
6	19	1	30.013	31.523	31.523	0.0	-1.510	-0.850	
0	12	6	214.892	218.344	218.344	0.0	-3.452	-1.059 *	
-3	20	1	22.400	17.459	17.459	0.0	4.940	3.373	
1	20	1	18.028	14.322	14.322	0.0	3.706	2.260	
3	20	1	12.788	18.097	18.097	0.0	-5.309	-1.563	
5	20	1	14.156	15.668	15.668	-15.668	-1.472	-0.532	
7	20	1	27.476	26.348	26.348	0.0	1.128	0.553	
-6	21	1	10.954	1.593	1.593	-1.593	0.0	9.361	2.567
-2	21	1	48.811	45.369	45.369	-49.369	0.0	-0.558	-0.383
2	21	1	26.837	29.245	29.245	0.0	-2.408	-1.346	
4	21	1	36.023	34.391	34.391	-34.391	1.631	1.084	
6	21	1	4.650	0.891	0.891	-0.891	3.759	0.694	
-5	22	1	13.787	15.630	15.630	-15.630	-1.843	-0.533	
-3	22	1	26.771	28.347	28.347	-28.347	0.0	-1.576	-0.712
1	22	1	19.436	19.258	19.258	-19.258	0.0	0.178	0.069
3	22	1	17.466	18.239	18.239	-18.239	0.0	-0.834	-0.326
0	22	1	13.967	13.082	13.082	-13.082	0.0	0.385	0.287
12	0	214.073	218.344	218.344	0.0	-4.270	-1.315 *		

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
5	22	1	2.0085	2.0508	-2.0568	0.0	0.117	0.015
-4	23	1	10.004	15.055	15.055	0.0	-5.051	-1.103
0	23	1	11.282	16.603	16.603	0.0	-5.322	-1.221
2	23	1	16.751	13.614	13.614	0.0	3.136	1.703
4	23	1	6.026	0.443	0.443	0.0	5.583	1.058
-3	24	1	15.244	4.345	4.345	0.0	10.899	3.977 *
-1	24	1	8.940	4.525	4.925	0.0	4.015	0.895
1	24	1	3.832	3.898	3.898	0.0	-0.067	-0.010
-12	0	2	48.050	49.843	-49.843	0.0	-1.752	-1.074
-10	0	2	86.667	86.823	86.823	0.0	-0.156	-0.059
-8	0	2	79.266	80.732	80.732	0.0	-1.465	-1.036
-6	0	2	114.520	112.859	113.859	0.0	0.661	0.364
-4	0	2	167.571	170.519	170.919	0.0	-3.347	-1.314
-2	0	2	103.942	97.335	-97.335	0.0	6.607	4.084
0	0	2	278.227	281.931	281.931	0.0	-3.704	-0.889
2	0	2	144.779	143.809	143.809	0.0	0.969	0.437
4	0	2	218.904	226.503	226.503	0.0	-7.599	-2.292
6	0	2	54.509	56.602	-56.602	0.0	-2.293	-1.910
8	0	2	78.644	80.654	80.654	0.0	-1.409	-0.962
10	0	2	214.155	213.344	218.344	0.0	-4.189	-1.289 *
-13	1	2	82.017	61.353	81.353	0.0	0.664	0.409
-11	1	2	10.168	0.865	0.865	0.0	9.303	2.540
-9	1	2	32.748	31.573	31.573	0.0	1.175	0.928
-7	1	2	33.125	33.389	-33.389	0.0	-0.264	-0.247
-5	1	2	31.520	32.112	-32.112	0.0	-3.561	-1.368
-3	1	2	11.216	3.551	-3.551	0.0	-6.592	-0.572
-1	1	2	20.320	22.203	-22.203	0.0	7.666	6.274
1	1	2	168.563	172.524	172.524	0.0	-1.883	-1.849
3	1	2	66.888	65.325	65.325	0.0	7.975	4.295
5	1	2	36.579	35.729	-35.729	0.0	1.563	1.323
7	1	2	56.743	52.816	52.816	0.0	6.851	0.749
9	1	2	37.546	34.580	-34.580	0.0	-2.073	-1.664
11	1	2	62.336	63.551	63.551	0.0	-2.565	2.222
-10	2	2	4.257	2.047	-2.047	0.0	-1.216	-0.809
-8	2	2	3.471	6.404	6.404	0.0	2.211	0.478
-6	2	2	29.162	29.143	-29.143	0.0	-2.932	-0.559
-4	2	2	14.376	13.238	-13.238	0.0	0.019	0.017
-2	2	2	12.166	11.694	-11.694	0.0	1.138	0.892
0	12	0	214.050	218.344	218.344	0.0	-4.254	-1.310 *
0	2	2	24.021	21.867	-21.867	0.0	2.154	2.194
4	2	2	16.832	18.268	18.268	0.0	0.750	0.373
8	2	2	16.177	18.509	-18.509	0.0	-1.436	-0.908
10	2	2	18.339	17.588	-17.588	0.0	2.331	-1.169
-13	3	2	19.632	16.630	-16.630	0.0	3.003	1.200
-11	3	2	10.159	12.774	-12.774	0.0	5.384	2.975
-9	3	2	64.350	64.840	64.840	0.0	-0.491	-0.376
-7	3	2	91.133	91.689	-91.689	0.0	-0.551	-0.359
-5	3	2	17.635	21.366	21.366	0.0	-3.731	-2.678
-3	3	2	17.045	13.389	13.389	0.0	3.657	3.536
1	3	2	82.061	80.144	-80.144	0.0	1.856	1.396
3	3	2	8.580	6.244	6.244	0.0	2.336	0.983
5	3	2	32.666	32.476	32.476	0.0	0.190	0.165

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-1	7	3	2	70.670	71.911	-71.911	0.0	-1.241	-0.909
9	3	2	39.936	40.932	40.932	0.0	-1.046	-0.750	
11	3	2	29.309	29.629	29.629	0.0	-0.319	-0.159	
-12	4	2	48.254	48.423	48.423	0.0	-0.169	-0.110	
0	12	6	214.237	218.344	218.344	0.0	-4.107	-1.264 *	
-10	4	2	42.523	41.998	41.998	0.0	-0.525	0.414	
-8	4	2	9.530	6.543	6.543	0.0	2.987	1.192	
-6	4	2	89.336	89.403	89.403	0.0	-0.067	-0.044	
-4	4	2	66.455	65.761	65.761	0.0	0.734	0.633	
-2	4	2	21.417	25.418	25.418	0.0	-4.001	-3.857	
0	4	2	100.602	95.506	95.506	0.0	5.096	3.213	
2	4	2	72.488	74.215	74.215	0.0	-1.723	-1.399	
4	4	2	77.678	76.987	76.987	0.0	0.691	0.508	
6	4	2	94.118	95.606	95.606	0.0	-1.488	-0.938	
8	4	2	4.339	8.531	8.531	0.0	-4.192	-0.343	
10	4	2	23.104	24.486	24.486	0.0	-1.382	-0.742	
-13	5	2	10.971	2.923	2.923	0.0	8.048	2.103	
-11	5	2	21.253	21.163	21.163	0.0	0.090	0.047	
-9	5	2	36.727	37.667	37.667	0.0	-0.940	-0.730	
-7	5	2	46.053	46.905	46.905	0.0	-0.812	-0.723	
-5	5	2	25.985	25.193	25.193	0.0	0.792	0.669	
-3	5	2	26.166	22.932	22.932	0.0	3.233	3.406	
-1	5	2	64.710	64.812	64.812	0.0	-0.102	-0.092	
1	5	2	82.296	81.084	81.084	0.0	1.211	0.897	
3	5	2	32.109	29.507	29.507	0.0	2.602	2.663	
0	12	6	24.4565	218.344	218.344	0.0	-3.779	-1.161 *	
5	5	2	31.9465	32.135	32.135	0.0	-0.190	-0.169	
7	5	2	43.719	41.776	41.776	0.0	1.943	1.528	
9	5	2	12.837	14.712	14.712	0.0	-1.875	-0.638	
11	5	2	15.670	14.466	14.466	0.0	1.204	0.433	
-10	6	2	19.387	20.644	20.644	0.0	-1.257	-0.748	
-8	6	2	15.600	21.067	21.067	0.0	-1.467	-0.841	
-6	6	2	16.800	18.818	18.818	0.0	-2.019	-1.117	
-4	6	2	9.988	6.854	6.854	0.0	3.134	1.684	
-2	6	2	4.053	4.591	4.591	0.0	-0.598	-0.158	
0	6	2	10.021	9.514	9.514	0.0	0.506	0.297	
2	6	2	11.036	11.561	11.561	0.0	-0.524	-0.257	
4	6	2	15.359	13.889	13.889	0.0	1.469	0.975	
6	6	2	23.971	24.678	24.678	0.0	-0.706	-0.528	
8	6	2	28.065	29.635	29.635	0.0	-1.570	-1.047	
10	6	2	17.857	19.613	19.613	0.0	-1.716	-0.747	
-15	7	2	22.940	26.089	26.089	0.0	-3.149	-1.071	
-11	7	2	20.271	20.463	20.463	0.0	-0.192	-0.055	
-9	7	2	24.381	24.160	24.160	0.0	0.221	0.155	
0	12	6	213.173	218.344	218.344	0.0	-5.174	-1.598 *	
-5	7	2	35.630	36.026	36.026	0.0	-0.396	-0.383	
-3	7	2	40.034	59.587	59.587	0.0	0.047	0.048	
-1	7	2	44.062	41.941	41.941	0.0	2.121	2.242	
1	7	2	19.51	18.236	18.236	0.0	1.265	0.979	
3	7	2	6.15	9.306	9.306	0.0	-2.751	-0.750	
5	7	2	18.142	14.699	17.059	0.0	1.044	0.689	
9	7	2	15.228	13.898	13.898	0.0	1.330	0.560	
11	7	2	16.849	12.910	12.910	0.0	3.939	1.505	

## K-RICHTERITE 4000 1/15/73

## STRUCTURE FACTORS

PAGE 12

H	K	L	F(CUBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-1	6	2	13.480	18.579	18.579	0.0	-0.993	-0.038
-10	3	2	13.650	14.617	14.617	0.0	-1.222	-0.461
-6	8	2	17.857	20.435	20.435	0.0	-2.588	-1.653
-4	6	2	18.568	15.774	15.774	0.0	-2.794	-2.020
-2	8	2	56.664	56.335	56.335	0.0	-3.270	-0.246
0	8	2	85.664	88.574	88.574	0.0	-1.090	0.742
2	6	2	35.914	85.429	85.429	0.0	-6.518	-6.350
4	6	4	49.013	42.022	42.022	0.0	-1.991	1.871
6	8	2	14.566	15.447	15.447	0.0	-0.481	-0.232
0	12	6	214.368	218.344	218.344	0.0	-3.976	-1.222 *
10	8	2	1.294	5.658	5.658	0.0	-4.365	-0.574
-11	9	2	12.624	11.576	11.576	0.0	0.648	0.197
-9	9	2	10.381	13.517	13.517	0.0	-2.136	-0.927
-7	9	2	46.649	47.625	47.625	0.0	-0.975	-0.818
-5	9	2	15.293	16.074	16.074	0.0	-0.780	-0.466
-3	9	2	88.780	89.865	89.865	0.0	-1.085	-0.732
-1	9	2	11.282	8.501	8.501	0.0	2.381	1.208
1	9	2	42.046	42.004	42.004	0.0	0.045	0.042
3	9	2	75.353	78.515	78.515	0.0	-3.562	-2.811
5	9	2	23.448	22.020	22.020	0.0	1.428	1.164
7	9	2	43.424	44.347	44.347	0.0	-0.923	-0.704
9	9	2	5.764	2.163	2.163	0.0	3.601	6.778
-10	10	2	29.801	30.654	30.654	0.0	-0.854	-0.609
-8	10	2	46.034	40.117	40.117	0.0	-0.083	-0.066
-6	10	2	25.560	23.382	23.382	0.0	2.178	1.803
-4	10	2	54.280	53.573	53.573	0.0	0.307	0.267
-2	10	2	29.850	21.347	21.347	0.0	-1.497	-1.267
0	10	2	68.067	69.066	69.066	0.0	-0.999	-0.757
2	10	2	42.228	44.093	44.093	0.0	-1.865	-1.655
4	10	2	77.400	77.854	77.854	0.0	-0.454	-0.326
6	10	2	21.630	18.625	18.625	0.0	3.005	2.072
8	10	2	18.241	18.518	18.518	0.0	-0.278	-0.137
10	10	2	10.103	11.633	11.633	0.0	-1.530	-0.453
-11	11	2	41.655	43.506	43.506	0.0	-1.351	-0.771
-7	11	2	14.531	14.3624	14.3624	0.0	-2.693	-1.193
-5	11	2	19.141	17.857	17.857	0.0	1.284	1.006
-3	11	2	121.413	124.416	124.416	0.0	-3.003	-1.551
-1	11	2	3.193	4.642	4.642	0.0	-1.449	-0.304
1	11	2	95.444	53.570	53.570	0.0	1.474	0.924
3	11	2	143.370	146.316	146.316	0.0	-2.945	-1.304
5	11	2	13.509	15.422	15.422	0.0	-1.913	-0.884
7	11	2	51.201	52.865	52.865	0.0	-1.664	-1.212
9	11	2	12.166	5.603	5.603	0.0	6.563	2.800
-12	12	2	32.306	27.551	27.551	0.0	4.355	2.791
-8	12	2	15.211	14.593	14.593	0.0	0.618	0.271
-6	12	2	22.465	21.359	21.359	0.0	1.106	0.636
-4	12	2	26.182	26.635	26.635	0.0	-0.372	-0.234
-10	12	0	213.304	218.344	218.344	0.0	-0.453	-0.319
-2	12	2	130.681	131.587	131.587	0.0	-5.040	-1.558 *
0	12	2	203.365	208.090	208.090	0.0	-1.307	-0.632
2	12	2	12.684	12.865	12.865	0.0	-6.725	-2.521
4	12	2	71.996	73.038	73.038	0.0	-0.781	-0.328
6	12	2				-1.041	-0.741	

H	K	L	F(OBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
0	12	2	26.302	27.255	-27.255	0.0	-0.893	-0.523
0	12	2	29.031	32.016	32.016	0.0	-2.985	-1.629
10	12	2	15.164	17.644	17.644	0.0	-2.481	-0.829
-9	13	2	17.176	11.696	-11.696	0.0	5.480	3.541
-7	13	2	36.317	38.688	38.688	0.0	-2.370	-1.686
-5	13	2	55.672	55.889	-55.889	0.0	-0.218	0.174
-3	13	2	28.905	30.426	30.426	0.0	-1.526	-1.234
-1	13	2	67.662	67.204	-67.204	0.0	-0.202	-0.155
1	13	2	13.918	13.450	-13.450	0.0	0.468	0.238
3	13	2	42.736	44.129	44.129	0.0	-1.393	-1.151
5	13	2	46.322	46.622	-46.622	0.0	-0.300	-0.231
7	13	2	15.539	15.470	-13.470	0.0	-2.069	0.963
9	13	2	16.423	17.320	-17.320	0.0	-0.897	-0.350
-6	14	2	15.359	11.404	11.404	0.0	3.955	1.952
0	12	0	213.951	218.344	218.344	0.0	-4.352	-1.341 *
-6	14	2	5.715	2.304	-2.304	0.0	3.410	0.956
-4	14	2	11.757	3.117	3.117	0.0	6.639	5.129
-2	14	2	26.346	25.855	25.855	0.0	0.491	0.402
2	14	2	25.063	24.918	24.918	0.0	0.086	0.064
4	14	2	10.381	11.587	11.587	0.0	-1.206	-0.436
6	14	2	16.210	19.663	19.663	0.0	-3.453	-1.321
8	14	2	7.459	4.437	-4.437	0.0	3.063	0.752
-11	15	2	16.194	11.196	-11.196	0.0	4.997	1.693
-9	15	2	25.527	24.670	24.670	0.0	0.857	0.419
-7	15	2	30.636	31.547	-31.547	0.0	-0.911	-0.556
-5	15	2	30.767	32.476	32.476	0.0	-1.709	-1.251
-3	15	2	37.693	39.132	-39.132	0.0	-1.439	-1.068
-1	15	2	27.721	28.395	28.395	0.0	-0.674	-0.506
1	15	2	12.100	7.154	-7.154	0.0	4.947	2.428
3	15	2	29.178	29.389	-29.389	0.0	-0.211	-0.159
5	15	2	30.079	29.844	29.844	0.0	0.235	0.155
7	15	2	23.693	23.258	-23.258	0.0	0.435	0.234
-10	16	2	5.043	4.553	-4.553	0.0	0.490	0.079
0	12	0	214.990	218.344	218.344	0.0	-3.353	-1.029 *
-4	16	2	14.254	14.895	-14.895	0.0	0.600	-0.248
-2	16	2	12.919	14.233	14.233	0.0	-1.314	-0.544
6	16	2	41.023	40.591	-40.591	0.0	0.442	0.373
2	16	2	29.047	28.456	-28.456	0.0	0.591	0.451
4	16	2	25.560	28.206	-28.206	0.0	-2.640	-1.569
6	16	2	11.085	4.515	4.515	0.0	6.570	2.370
-5	17	2	7.778	3.262	3.262	0.0	4.516	1.332
-3	17	2	11.855	7.856	-7.856	0.0	3.959	1.840
-1	17	2	5.120	5.758	5.758	0.0	3.362	1.176
3	17	2	9.906	3.501	-3.501	0.0	6.406	2.855
5	17	2	5.502	2.521	-2.521	0.0	2.980	0.666
7	17	2	11.134	7.727	7.727	0.0	3.407	1.093
-6	18	2	17.946	17.114	17.114	0.0	0.831	0.390
-4	18	2	11.855	8.003	8.003	0.0	3.852	1.566
0	12	0	212.567	218.344	218.344	0.0	-5.777	-1.790 *
-2	18	2	20.746	22.369	22.369	0.0	-1.623	-0.804
2	18	2	5.497	10.911	10.911	0.0	-1.414	-0.474
4	18	2	22.460	22.697	22.697	0.0	-0.298	-0.168
18			11.560	14.281	14.281	0.0	-2.721	-0.857

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
6	18	2	24.135	24.355	24.355	0.0	-0.220	-0.106
-7	19	2	37.415	35.583	-35.583	0.0	1.832	1.266
-5	19	2	4.659	5.738	5.738	0.0	-1.038	-0.189
-3	19	2	21.122	19.378	-19.378	0.0	1.744	1.035
-1	19	2	7.941	7.365	-7.365	0.0	0.577	0.157
1	19	2	22.973	26.558	-26.558	0.0	-3.585	-1.643
-8	20	2	8.220	2.310	-2.310	0.0	5.910	1.247
-6	20	2	15.910	13.011	-13.011	0.0	2.905	1.260
-4	20	2	37.583	39.381	-39.381	0.0	-1.393	-0.960
-2	20	2	14.310	8.724	-8.724	0.0	5.630	2.987
0	20	2	24.315	23.871	-23.871	0.0	0.444	0.260
-2	20	2	24.364	25.504	-25.504	0.0	-1.139	-0.530
4	20	2	55.058	56.489	-56.489	0.0	-1.390	-0.954
0	20	2	28.573	27.744	-27.744	0.0	0.829	0.462
0	12	0	214.679	218.344	-218.344	0.0	-3.665	-1.125 *
-7	21	2	16.194	11.099	-11.099	0.0	5.095	1.870
-5	21	2	26.149	26.725	-26.725	0.0	-0.576	-0.322
-3	21	2	14.344	20.257	-20.257	0.0	-5.913	-1.773
-1	21	2	25.462	24.944	-24.944	0.0	0.517	0.315
3	21	2	18.175	20.117	-20.117	0.0	-1.942	-0.722
5	21	2	33.583	33.471	-33.471	0.0	0.112	0.054
-6	22	2	23.710	24.128	-24.128	0.0	-0.419	-0.178
-4	22	2	39.510	38.715	-38.715	0.0	0.795	0.474
-2	22	2	10.496	11.376	-11.376	0.0	-6.880	-0.249
0	22	2	59.978	57.951	-57.951	0.0	2.027	1.514
2	22	2	19.567	18.018	-18.018	0.0	1.549	0.718
4	22	2	51.955	52.232	-52.232	0.0	-0.278	-0.181
-3	23	2	23.644	25.133	-25.133	0.0	-1.489	-0.654
-1	23	2	21.434	19.515	-19.515	0.0	1.918	0.820
1	23	2	25.904	27.796	-27.796	0.0	-1.892	-0.864
-13	0	3	13.590	13.070	-13.070	0.0	0.521	0.172
-11	0	3	6.943	10.659	-10.659	0.0	-3.716	-0.974
-9	0	3	18.846	20.003	-20.003	0.0	-1.157	-0.678
0	12	0	213.959	218.344	-218.344	0.0	-4.385	-1.351 *
-5	0	3	12.870	12.425	-12.425	0.0	0.445	0.219
-3	0	3	17.848	18.274	-18.274	0.0	-0.426	-0.306
-1	0	3	4.421	2.318	-2.318	0.0	2.103	0.614
1	0	3	12.624	14.687	-14.687	0.0	-1.463	-0.752
3	0	3	16.046	15.515	-15.515	0.0	0.532	0.300
7	0	3	11.118	11.103	-11.103	0.0	0.015	0.005
9	0	3	14.606	16.259	-16.259	0.0	-1.654	-0.678
-12	1	3	9.169	1.657	-1.657	0.0	7.473	2.306
-2	1	3	27.410	27.514	-27.514	0.0	-0.104	-0.096
0	1	3	31.624	31.013	-31.013	0.0	0.622	0.579
2	1	3	31.520	32.196	-32.196	0.0	-0.676	-0.524
4	1	3	5.976	0.137	-0.137	0.0	5.840	1.593
6	1	3	18.273	17.588	-17.588	0.0	0.685	0.398
8	1	3	16.652	15.618	-15.618	0.0	1.035	0.541
10	1	3	18.552	16.007	-16.007	0.0	2.545	1.225
0	12	0	213.271	218.344	-218.344	0.0	-5.073	-1.568 *

H	K	L	F (QS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA
-11	2	3	17.340	13.022	0.0	4.318	2.7C8	
-9	2	3	25.134	24.521	-24.521	C.C	0.613	0.450
-7	2	3	50.645	51.675	51.675	0.0	-0.430	=C.380
-5	2	3	61.632	63.074	-63.074	0.0	-1.442	-1.208
-3	2	3	105.055	104.624	104.624	0.0	0.452	0.258
-1	2	3	3.029	4.418	-4.418	0.0	-1.389	-0.308
1	2	3	5.927	7.839	7.839	0.0	-1.912	-0.523
3	2	3	52.626	53.925	53.925	0.0	-1.299	-1.152
5	2	3	6.173	8.503	8.503	0.0	-2.330	-0.685
7	2	3	28.065	28.856	28.856	0.0	-0.791	-0.481
-16	3	3	8.711	12.215	12.215	0.0	-3.504	-0.953
-8	3	3	53.281	53.252	-53.252	0.0	0.029	0.025
-6	3	3	10.479	9.358	9.358	0.0	1.121	C.471
-4	3	3	7.401	6.772	6.772	0.0	6.629	2.380
-2	3	3	103.467	102.361	-102.361	0.0	1.106	0.667
0	3	3	28.474	26.024	26.024	0.0	2.451	2.239
2	3	3	77.924	76.972	-76.972	0.0	0.952	0.693
0	12	0	214.237	218.344	218.344	0.0	-4.107	-1.264 *
6	3	3	54.149	54.404	-54.404	0.0	-0.256	-0.209
10	3	3	9.857	2.406	2.406	0.0	7.451	2.379
-13	4	3	21.630	22.178	22.178	0.0	-0.548	-0.242
-9	4	3	4.028	9.832	9.832	0.0	-5.804	-1.059
-5	4	3	10.872	11.947	11.947	0.0	-1.074	-0.457
-3	4	3	13.476	9.877	9.877	0.0	3.599	2.058
-1	4	3	23.693	23.848	23.848	0.0	-C.155	-0.135
1	4	3	18.306	20.903	20.903	0.0	-2.597	-1.477
3	4	3	14.294	12.954	12.954	0.0	1.341	C.7C9
5	4	3	16.070	12.258	-12.258	0.0	-2.188	-0.788
7	4	3	14.835	14.921	14.921	0.0	-C.086	-0.045
9	4	3	24.037	21.631	21.631	0.0	2.406	1.420
-12	5	3	78.317	76.298	76.298	0.0	2.019	1.290
-10	5	3	22.416	21.371	21.371	0.0	1.045	0.665
-8	5	3	60.682	59.838	59.838	0.0	C.844	0.667
-6	5	3	27.148	28.529	28.529	0.0	-1.381	-1.050
0	12	0	212.894	218.344	218.344	0.0	-5.449	-1.687 *
-4	5	3	23.358	26.655	26.655	0.0	-3.256	-2.275
-2	5	3	184.486	187.532	187.532	0.0	-2.046	-1.382
0	5	3	23.480	22.548	22.548	0.0	C.932	0.735
2	5	3	99.472	58.780	58.780	0.0	0.691	0.420
4	5	3	47.485	48.839	-48.839	0.0	-1.354	-1.125
6	5	3	106.414	106.278	106.278	0.0	0.136	0.076
8	5	3	26.804	28.249	28.249	0.0	-1.445	-0.811
10	5	3	19.452	22.659	22.659	0.0	-3.207	-1.208
-13	6	3	20.238	20.755	20.755	0.0	-0.517	-0.213
-11	6	3	19.354	19.119	19.119	0.0	0.235	0.107
-9	6	3	132.465	134.108	134.108	0.0	-1.643	-0.763
-7	6	3	82.083	84.521	-84.521	0.0	-2.439	-1.648
-5	6	3	110.566	112.835	112.835	0.0	-1.868	-1.041
-3	6	3	44.292	42.547	42.547	0.0	1.745	1.704
1	6	3	214.925	214.131	214.131	0.0	C.794	0.243
3	6	3	23.513	24.851	24.851	0.0	-1.338	-0.957

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
3	6	3	2.129	10.212	0.0	-8.033	-1.218		
5	6	3	108.232	110.658	0.0	-2.426	-1.539		
7	6	3	15.211	13.665	0.0	1.546	0.732		
9	6	3	92.349	93.638	0.0	-1.289	-0.721	*	
12	6	3	213.853	218.344	0.0	-4.451	-1.372	*	
12	7	3	37.358	39.438	0.0	-2.040	-1.140		
-8	7	3	17.438	15.499	0.0	1.939	1.269		
-6	7	3	19.976	20.535	0.0	-0.959	-0.579		
-4	7	3	34.385	35.557	0.0	-1.212	-1.049		
-2	7	3	80.806	81.814	0.0	-1.008	-0.723		
0	7	3	38.757	39.269	0.0	-0.512	-0.465		
2	7	3	14.425	15.222	0.0	-6.797	-0.368		
16	7	3	8.629	10.0442	0.0	8.187	2.158		
-11	8	3	16.823	7.741	0.0	3.082	1.682		
-9	8	3	11.380	16.348	0.0	-4.968	-1.472		
-5	3	3	15.850	13.522	0.0	2.328	1.404		
-3	6	3	7.450	4.728	0.0	2.723	0.882		
1	8	3	9.644	13.051	0.0	-3.407	-1.171		
3	8	3	13.509	12.735	0.0	0.772	0.382		
12	0	3	213.598	218.344	0.0	-4.745	-1.464	*	
5	8	3	26.853	29.427	0.0	-2.574	-1.943		
7	8	3	4.445	12.082	0.0	-7.677	-1.390		
9	8	3	13.623	7.803	0.0	5.821	2.566		
-12	9	3	19.272	19.143	0.0	0.129	0.061		
-10	9	3	26.182	25.564	0.0	0.618	0.386		
-8	9	3	33.583	33.736	0.0	-0.153	-0.115		
-6	9	3	25.756	25.858	0.0	-0.102	-0.079		
-4	9	3	35.466	35.072	0.0	0.394	0.328		
-2	9	3	56.277	56.757	0.0	-0.480	-0.408		
0	9	3	57.636	60.087	0.0	-2.450	-2.052		
2	9	3	35.220	35.278	0.0	-0.058	-0.052		
4	9	3	31.667	30.187	0.0	1.481	1.156		
6	9	3	24.446	23.275	0.0	1.171	0.829		
8	9	3	1C.692	7.574	0.0	3.118	1.048		
-11	10	3	6.651	2.276	0.0	3.015	0.762		
-9	10	3	13.902	14.643	0.0	-0.741	-0.306		
-7	10	3	31.847	31.060	0.0	0.788	0.592		
-5	10	3	60.027	60.622	0.0	-0.595	-0.456		
-3	10	3	57.718	58.071	0.0	-0.352	-0.285		
-1	10	3	1C.987	9.009	-9.009	0.0	1.978	0.919	
0	12	0	214.155	218.344	218.344	0.0	-4.189	-1.289	*
1	1C	3	22.170	19.679	-19.679	0.0	2.491	1.808	
3	10	3	23.055	23.418	23.418	0.0	-0.363	-0.254	
5	10	3	12.854	7.154	7.154	0.0	-5.699	3.063	
7	10	3	11.478	3.308	3.308	0.0	8.170	3.415	
9	10	3	25.920	21.769	-21.769	0.0	4.151	2.524	
-10	11	3	10.643	8.399	-8.399	0.0	2.244	0.695	
-4	11	3	9.006	1.320	1.320	0.0	7.679	3.310	
-2	11	3	39.625	39.900	-39.900	0.0	-0.275	-0.237	
0	11	3	8.547	0.647	0.647	0.0	7.900	2.966	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
2	11	3	19.308	18.558	-18.558	0.0	-2.249	-1.100
4	11	3	24.921	23.279	-23.279	0.0	1.642	1.163
6	11	3	21.057	24.172	-24.172	0.0	-3.115	-1.403
-11	12	3	12.690	14.465	14.465	0.0	-1.775	-0.558
-9	12	3	10.594	3.789	-3.789	0.0	6.805	2.383
-7	12	3	16.914	15.757	15.757	0.0	1.153	0.638
-5	12	3	6.206	6.802	6.802	0.0	-0.597	-0.161
0	12	0	214.057	218.344	218.344	0.0	-4.287	-1.320 *
-3	12	3	15.408	15.443	15.443	0.0	-0.035	-0.018
-1	12	3	14.737	20.745	20.745	0.0	-6.008	-2.487
1	12	3	30.488	31.426	31.426	0.0	-0.938	-0.750
3	12	3	9.448	9.295	9.295	0.0	0.153	0.051
5	12	3	18.699	17.603	17.603	0.0	1.096	0.620
7	12	3	9.300	6.883	6.883	0.0	2.417	0.736
-8	13	3	4.716	0.897	-0.897	0.0	3.319	0.782
-4	13	3	10.365	13.001	13.001	0.0	-2.696	-1.022
-2	13	3	16.046	15.285	-15.285	0.0	0.762	0.443
0	13	3	32.273	32.470	32.470	0.0	-0.197	-0.153
2	13	3	35.597	36.250	-36.250	0.0	-0.659	-0.494
4	13	3	20.533	22.211	22.211	0.0	-1.678	-0.81
6	13	3	17.062	15.215	-15.215	0.0	1.747	0.828
8	13	3	9.955	9.938	9.938	0.0	0.017	0.006
-9	14	3	37.456	39.412	-39.412	0.0	-1.915	-1.139
-7	14	3	16.882	19.817	19.817	0.0	-2.935	-1.270
-5	14	3	58.864	57.437	-57.437	0.0	1.427	1.102
0	12	0	213.942	218.344	218.344	0.0	-4.401	-1.356 *
-3	14	3	37.251	36.193	36.193	0.0	1.053	0.689
-1	14	3	53.739	54.311	-54.311	0.0	-0.572	-0.467
3	14	3	11.102	7.357	7.357	0.0	5.705	1.555
5	14	3	32.715	35.382	-35.382	0.0	-2.667	-1.784
7	14	3	14.409	12.685	12.685	0.0	1.724	0.674
-10	15	3	16.652	15.046	15.046	0.0	1.607	0.626
-8	15	3	13.689	11.680	-11.680	0.0	2.009	0.808
-6	15	3	14.147	13.964	13.964	0.0	0.183	0.085
-4	15	3	9.071	8.517	8.517	0.0	0.554	0.188
-2	15	3	22.907	21.729	-21.729	0.0	1.178	0.760
0	15	3	28.540	31.582	31.582	0.0	-3.042	-2.059
2	15	3	35.351	35.185	-35.185	0.0	0.167	0.132
4	15	3	21.859	21.180	21.180	0.0	0.680	0.455
6	15	3	21.712	16.544	-16.544	0.0	4.768	2.968
-9	16	3	33.730	35.636	-35.636	0.0	-1.905	-0.964
-7	16	3	7.778	11.679	11.679	0.0	-3.301	-0.731
-5	16	3	57.194	57.288	57.288	0.0	-0.093	-0.068
-1	16	3	67.264	64.865	64.865	0.0	2.399	1.752
0	12	0	213.156	218.344	-218.344	0.0	-5.187	-1.604 *
-3	16	3	48.008	48.148	48.148	0.0	-0.140	-0.111
3	16	3	40.738	41.406	41.406	0.0	-0.667	-0.462
5	16	3	31.454	29.785	29.785	0.0	1.669	1.255
7	16	3	29.735	28.539	28.539	0.0	1.167	0.762
-3	17	3	27.561	26.625	26.625	0.0	0.736	0.411
-6	17	3	5.453	12.821	12.821	0.0	-7.369	-1.368
-2	17	3	91.252	91.729	91.729	0.0	-0.477	-0.284

H	K	L	F (UBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA
0	17	3	11.020	10.535	-10.535	0.0	0.485	0.154
2	17	5	70.146	70.197	70.197	0.0	-0.051	-0.036
4	17	3	51.676	50.142	-50.142	0.0	1.534	1.052
6	17	3	70.352	69.057	69.057	0.0	1.295	0.836
7	18	3	63.416	62.153	-62.153	0.0	1.263	0.830
-5	18	3	20.826	23.053	23.053	0.0	-2.225	-1.072
-3	18	3	12.952	17.415	-17.415	0.0	-4.463	-1.544
-1	18	3	78.775	76.468	76.468	0.0	0.367	0.236
1	18	3	34.713	36.340	-36.340	0.0	-1.627	-0.985
3	18	3	24.283	23.721	-23.721	0.0	0.562	0.297
5	18	3	44.865	44.571	44.571	0.0	0.294	0.189
0	12	0	212.043	218.344	218.344	0.0	-6.301	-1.957 *
-6	19	3	9.579	1.500	1.500	0.0	8.079	2.529
-4	19	3	8.711	8.618	-8.618	0.0	0.693	0.158
-2	19	3	13.394	15.335	15.335	0.0	-1.941	-0.656
0	19	3	15.361	9.569	-9.569	0.0	3.772	1.723
2	19	3	20.828	21.724	21.724	0.0	-0.896	-0.398
4	19	3	42.933	42.741	-42.741	0.0	0.191	0.122
-7	20	3	11.724	16.566	16.566	0.0	-4.842	-1.171
-3	20	3	19.223	18.324	18.324	0.0	0.899	0.397
1	20	3	10.450	12.475	12.475	0.0	-1.980	-0.547
3	20	3	17.242	17.383	17.383	0.0	-6.141	-0.057
-4	21	3	3.291	2.065	2.065	0.0	1.226	0.195
-2	21	3	28.523	28.750	-28.750	0.0	-0.226	-0.126
0	21	3	18.715	17.171	17.171	0.0	1.544	0.766
2	21	3	37.464	35.267	-35.267	0.0	2.197	1.368
-3	22	3	16.063	13.705	13.705	0.0	2.358	0.909
-1	22	3	18.241	17.674	-17.674	0.0	0.566	0.241
1	22	3	7.254	0.604	0.604	0.0	6.649	1.517
0	12	0	212.501	218.344	218.344	0.0	-5.342	-1.812 *
-10	0	4	41.295	40.576	40.576	0.0	0.319	0.243
-8	0	4	21.843	22.098	-22.098	0.0	-0.255	-0.175
-6	0	4	158.598	163.570	163.570	0.0	-4.979	-2.003
-4	0	4	121.790	122.287	122.287	0.0	-0.497	-0.254
-2	0	4	56.146	56.851	-56.851	0.0	6.704	-0.585
0	0	4	175.742	174.716	174.716	0.0	1.026	0.379
2	0	4	4.421	1.545	1.545	0.0	2.876	0.669
4	0	4	154.423	158.137	158.137	0.0	-3.714	-1.514
6	0	4	14.082	15.645	15.645	0.0	-5.563	-2.126
8	0	4	53.215	52.414	52.414	0.0	0.801	0.567
-11	1	4	28.605	27.727	27.727	0.0	0.878	0.524
-9	1	4	17.759	19.362	-19.362	0.0	-1.564	-0.766
-7	1	4	75.992	76.521	76.521	0.0	-0.529	-0.378
-5	1	4	11.233	12.849	-12.849	0.0	-1.617	-0.649
-3	1	4	131.860	136.226	136.226	0.0	-4.366	-2.054
-1	1	4	73.208	72.708	-72.708	0.0	0.500	0.379
1	1	4	5.564	5.274	5.274	0.0	0.310	0.077
3	1	4	68.410	70.879	70.879	0.0	-2.468	-1.815
0	12	0	213.051	218.344	218.344	0.0	-5.253	-1.625 *
5	1	4	12.788	10.741	10.741	0.0	2.047	0.979
7	1	4	14.065	13.326	13.326	0.0	0.739	0.252
9	1	4	24.774	22.816	-22.816	0.0	1.958	1.064
2	4		3.875	5.781	-5.781	0.0	3.094	0.875

H	K	L	F(U(B))	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-10	2	4	9.038	9.098	-9.098	0.0	-0.659	-0.183
-6	2	4	3.439	5.677	5.677	0.0	-2.238	-0.430
-6	2	4	8.809	12.521	-12.521	0.0	-3.712	-1.166
-2	2	4	4.159	5.576	-5.576	0.0	-1.417	-0.306
0	2	4	17.209	16.718	-16.718	0.0	0.491	0.305
2	2	4	-16.603	16.506	-16.506	0.0	0.097	0.054
4	2	4	8.564	2.090	2.090	0.0	6.473	2.305
6	2	4	9.464	12.216	12.216	0.0	-2.752	-0.800
8	2	4	5.289	4.939	-4.939	0.0	-0.069	0.069
-11	3	4	16.079	16.437	-16.437	0.0	-0.358	-0.146
-9	3	4	21.712	18.151	18.151	0.0	3.561	2.442
-7	3	4	16.914	19.346	-19.346	0.0	-2.432	-1.405
-5	3	4	36.556	37.624	37.624	0.0	-1.029	-0.856
-3	3	4	76.810	78.056	-78.056	0.0	-1.246	-0.898
0	12	0	213.615	218.344	-218.344	0.0	-1.246	0.203
-1	3	4	50.743	53.357	53.357	0.0	-1.459	*
1	3	4	14.753	13.838	-13.838	0.0	-2.614	-2.218
3	3	4	42.441	42.196	-42.196	0.0	0.915	0.441
5	3	4	15.555	18.607	18.607	0.0	0.246	0.203
7	3	4	17.193	20.541	-20.541	0.0	-3.051	-1.253
-12	4	4	11.964	14.111	14.111	0.0	-2.207	-0.672
-10	4	4	11.658	4.085	-4.085	0.0	7.573	3.222
-8	4	4	15.211	18.539	18.539	0.0	-3.727	-1.672
-6	4	4	15.670	14.444	-14.444	0.0	1.226	0.874
-4	4	4	22.580	22.798	22.798	0.0	-0.219	-0.144
-2	4	4	38.774	38.405	38.405	0.0	0.369	0.349
0	4	4	44.865	45.574	-45.574	0.0	-0.709	-0.590
2	4	4	85.112	87.380	-87.380	0.0	-2.268	-1.476
4	4	4	15.015	15.781	-15.781	0.0	-0.766	-0.355
6	4	4	19.829	19.604	19.604	0.0	0.825	0.419
8	4	4	11.969	11.069	11.069	0.0	0.900	0.292
-11	5	4	26.660	19.789	-19.789	0.0	1.071	0.572
-7	5	4	5.338	2.451	-2.451	0.0	2.887	0.743
-5	5	4	9.628	7.480	7.480	0.0	2.148	0.867
0	12	0	213.500	218.344	218.344	0.0	-4.843	-1.495 *
-3	5	4	41.639	43.953	-43.953	0.0	-2.314	-1.904
-1	5	4	8.514	6.767	6.767	0.0	1.747	0.653
1	5	4	25.380	24.265	-24.265	0.0	1.114	0.762
3	5	4	25.871	26.776	-26.776	0.0	-0.905	-0.644
5	5	4	16.308	14.020	-14.020	0.0	2.288	1.157
-12	6	4	9.104	4.503	-4.503	0.0	4.201	1.377
-10	6	4	13.312	12.757	12.757	0.0	0.555	0.221
-8	6	4	13.836	13.757	-13.757	0.0	0.079	0.036
-6	6	4	2.161	6.866	6.866	0.0	-4.705	-0.794
-2	6	4	9.350	7.375	7.375	0.0	1.974	0.710
0	6	4	5.976	1.564	-1.564	0.0	4.413	1.206
2	6	4	6.975	5.706	-5.706	0.0	1.269	0.365
4	6	4	11.102	9.420	-9.420	0.0	1.682	0.681
6	6	4	23.169	22.911	22.911	0.0	0.258	0.134
8	6	4	16.800	15.873	-15.873	0.0	0.927	0.462
-11	7	4	8.269	15.751	-15.751	0.0	-7.482	-1.692
-9	7	4	39.003	40.625	40.625	0.0	-1.622	-1.115
-7	7	4	24.446	26.098	-26.098	0.0	-1.651	-0.927

<i>h</i>	<i>k</i>	<i>l</i>	F(CALC)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
0	12	0	214.172	213.344	0.0	-4.172	-1.284	*	
-5	7	4	26.362	24.749	0.0	1.613	1.195		
-3	7	4	17.242	17.365	0.0	-0.123	-0.673		
-1	7	4	11.495	13.312	0.0	-1.817	-0.677		
1	7	4	24.004	24.985	-24.585	0.0	-0.981	-0.682	
3	7	4	36.399	35.155	35.155	0.0	1.244	1.001	
7	7	4	13.410	14.749	0.0	-1.339	-0.430		
-12	8	4	34.451	37.312	0.0	-2.861	-1.630		
-10	6	4	50.334	49.359	0.0	0.975	0.694		
-8	6	4	13.278	9.628	0.0	4.349	2.216		
-6	6	4	25.609	25.506	0.0	0.103	0.070		
-4	6	4	39.772	40.206	0.0	-0.433	-0.359		
4	6	4	70.195	70.397	0.0	-0.202	-0.142		
6	8	4	45.617	47.284	47.284	0.0	-0.667	-0.456	
3	8	4	3.651	1.829	0.0	1.822	0.299		
-11	9	4	13.705	13.045	-13.045	0.0	0.660	0.232	
-9	9	4	35.843	35.219	0.0	0.624	0.426		
0	12	0	214.384	218.344	0.0	-3.959	-1.217	*	
-7	9	4	49.810	48.650	-48.650	0.0	1.159	0.920	
-3	9	4	30.308	29.311	0.0	0.998	0.795		
-5	9	4	51.889	51.545	-51.945	0.0	-0.056	-0.042	
3	9	4	15.113	15.569	-15.569	0.0	-0.455	-0.208	
5	9	4	5.534	1.862	-1.862	0.0	3.672	0.789	
7	9	4	46.142	45.210	0.0	0.932	0.637		
-10	10	4	13.738	16.923	0.0	-3.185	-1.010		
-9	10	4	21.843	23.059	0.0	-1.216	-0.683		
-6	10	4	29.244	30.473	0.0	-1.229	-0.873		
-4	10	4	39.085	39.289	0.0	-0.204	-0.156		
-2	10	4	23.611	22.963	0.0	0.648	0.462		
2	10	4	12.348	12.379	0.0	-0.131	-0.058		
4	10	4	48.925	49.781	49.781	0.0	-0.855	-0.613	
6	10	4	29.801	28.482	28.482	0.0	1.319	0.901	
-11	11	4	33.272	32.571	32.571	0.0	0.301	0.183	
-9	11	4	32.633	32.215	-32.215	0.0	0.418	0.319	
-7	11	4	116.550	117.119	117.119	0.0	-0.569	-0.289	
0	12	0	213.156	218.344	218.344	0.0	-5.187	-1.604	*
-5	11	4	2.754	12.209	12.209	0.0	-9.474	-1.429	
-3	11	4	105.530	104.706	104.706	0.0	0.824	0.466	
-1	11	4	14.311	14.850	-14.850	0.0	-0.539	-0.238	
1	11	4	65.171	63.040	63.040	0.0	0.131	0.100	
3	11	4	54.443	56.626	56.626	0.0	-2.183	-1.571	
5	11	4	33.812	31.970	31.970	0.0	1.842	1.262	
7	11	4	48.107	50.538	50.538	0.0	-2.432	-1.570	
-10	12	4	44.695	44.304	44.304	0.0	-0.209	-0.145	
-8	12	4	32.813	31.793	-31.793	0.0	1.020	0.628	
-6	12	4	45.847	44.379	44.379	0.0	-0.151	-0.094	
0	12	4	43.162	42.183	42.183	0.0	-1.065	-0.848	
2	12	4	23.169	20.424	-20.424	0.0	0.979	0.770	
4	12	4	113.750	113.395	113.395	0.0	2.745	1.948	
6	12	4	40.591	40.758	-40.758	0.0	-0.207	-0.139	
8	12	4	38.937	43.327	-43.327	0.0	-4.390	-2.498	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-7	13	4	42.621	43.347	0.0	-0.725	-0.520	
-5	13	4	20.467	20.812	-20.812	0.0	-0.344	-0.220
-3	13	4	21.499	20.013	20.013	0.0	-1.486	-1.020
0	12	6	213.336	218.344	218.344	0.0	-5.007	-1.547 *
-1	13	4	43.653	41.698	-41.698	0.0	1.955	1.480
1	13	4	10.450	3.776	-3.776	0.0	6.654	2.621
3	13	4	15.572	10.025	-10.025	0.0	5.546	2.944
-10	14	4	13.553	6.275	-6.275	0.0	7.282	2.848
-8	14	4	10.581	15.331	15.331	0.0	-4.950	-1.317
-6	14	4	8.067	7.259	-7.259	0.0	0.748	0.155
-4	14	4	6.910	4.205	4.205	0.0	2.704	0.761
-2	14	4	20.435	20.157	-20.157	0.0	0.278	0.160
0	14	4	7.941	5.913	-5.913	0.0	2.029	0.621
2	14	4	13.394	14.110	14.110	0.0	-0.716	-0.251
4	14	4	5.534	1.854	1.854	0.0	3.681	0.702
6	14	4	22.318	23.295	23.295	0.0	-0.977	-0.454
-9	15	4	32.488	31.578	-31.578	0.0	0.907	0.548
-7	15	4	28.884	29.858	-29.858	0.0	-0.974	-0.609
-5	15	4	22.727	21.110	21.110	0.0	1.617	0.865
-3	15	4	20.811	19.813	-19.813	0.0	0.998	0.523
-1	15	4	24.168	23.718	-23.718	0.0	0.450	0.274
1	15	4	22.563	20.078	-20.078	0.0	2.485	1.677
3	15	4	6.288	1.418	1.418	0.0	4.870	1.113
0	12	0	212.714	218.344	-218.344	0.0	-5.629	-1.744 *
5	15	4	10.987	10.801	-10.801	0.0	0.186	0.053
-8	16	4	8.673	4.308	-4.308	0.0	4.370	1.177
-4	16	4	13.132	15.650	15.650	0.0	-2.518	-0.764
-2	16	4	16.587	13.441	-13.441	0.0	-1.724	-0.962
2	16	4	13.803	17.308	17.308	0.0	-3.505	-1.122
4	16	4	21.843	23.567	-23.567	0.0	0.201	0.139
-7	17	4	12.854	10.855	-10.855	0.0	1.598	0.714
-5	17	4	6.304	3.540	-3.540	0.0	2.764	0.607
-3	17	4	13.738	16.755	16.755	0.0	-3.017	-1.085
-1	17	4	8.662	1.420	-1.420	0.0	7.242	2.282
1	17	4	18.437	18.426	-18.426	0.0	0.011	0.065
3	17	4	11.151	16.380	16.380	0.0	-5.230	-1.536
-6	18	4	12.477	12.564	12.564	0.0	-1.087	-0.362
-4	18	4	9.038	4.681	-4.681	0.0	4.358	1.407
-2	18	4	13.918	15.060	15.060	0.0	-1.142	-0.425
0	18	4	15.031	11.799	-11.799	0.0	3.233	1.421
2	18	4	4.257	8.919	8.919	0.0	-4.661	-0.706
-5	19	4	18.028	13.596	-13.596	0.0	4.031	1.886
0	12	0	213.648	218.344	-218.344	0.0	-4.696	-1.449 *
-3	19	4	33.513	33.020	-33.020	0.0	0.498	0.343
-1	19	4	12.149	8.966	-8.966	0.0	3.183	1.302
1	19	4	19.370	17.130	-17.130	0.0	2.240	1.162
-4	20	4	9.710	9.530	-9.530	0.0	0.221	0.061
-2	20	4	7.647	9.255	9.255	0.0	-1.608	-0.407
0	20	4	37.513	39.295	-39.295	0.0	-1.782	-1.151
-1	0	5	13.771	11.637	-11.637	0.0	2.133	0.787
-9	0	5	18.044	14.584	-14.584	0.0	3.460	1.967
-5	0	5	8.416	6.570	-6.570	0.0	1.847	0.615

H	K	L	F(CUBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-3	0	5	13.427	13.324	-13.324	0.0	0.103	0.049
-1	0	5	14.294	14.373	-14.373	0.0	-0.078	-0.033
1	0	5	18.421	17.793	-17.793	0.0	0.623	0.284
-12	1	5	16.840	5.519	-5.519	0.0	5.321	2.032
-10	1	5	9.059	7.327	7.327	0.0	1.727	0.457
0	12	0	214.522	218.344	218.344	0.0	-3.812	-1.172 *
-4	1	5	11.003	12.572	-12.572	0.0	-1.569	-0.573
3	1	5	15.621	16.111	16.111	0.0	-0.490	-0.234
2	1	5	12.768	10.633	-10.633	0.0	2.155	0.909
5	1	5	16.701	16.004	-16.004	0.0	0.698	0.293
-11	2	5	9.595	9.329	9.329	0.0	0.266	0.072
-9	2	5	13.322	16.808	-16.808	0.0	-0.872	-0.639
-7	2	5	33.910	34.783	34.783	0.0	-0.049	-0.038
-5	2	5	43.951	49.040	-49.040	0.0	-0.494	-0.001
-3	2	5	59.028	61.257	61.257	0.0	-2.228	-1.717
-1	2	5	14.655	13.592	-13.592	0.0	1.062	0.558
1	2	5	23.382	18.022	18.022	0.0	5.360	4.109
3	2	5	15.375	11.282	11.282	0.0	4.093	2.080
5	2	5	14.687	15.574	15.574	0.0	-1.286	-0.490
7	2	5	25.265	25.359	25.359	0.0	-0.094	-0.047
-12	3	5	21.556	20.753	-20.753	0.0	0.943	0.484
-10	3	5	28.523	26.362	26.362	0.0	2.162	1.311
-8	3	5	42.900	42.745	-42.745	0.0	0.155	0.121
-6	3	5	3.668	1.712	1.712	0.0	1.896	0.366
0	12	0	212.960	218.344	218.344	0.0	-5.384	-1.667 *
-2	3	5	37.284	38.494	-38.494	0.0	-1.211	-0.888
0	3	5	11.757	11.938	11.938	0.0	-0.182	-0.069
2	3	5	55.279	54.783	-54.783	0.0	0.495	0.375
4	3	5	15.408	17.481	17.481	0.0	-2.073	-0.818
6	3	5	33.632	34.283	-34.283	0.0	-0.651	-0.390
-9	4	5	11.707	13.205	13.205	0.0	-1.497	-0.535
-5	4	5	8.269	8.461	8.461	0.0	-0.192	-0.055
-3	4	5	5.665	4.921	-4.921	0.0	0.745	0.179
1	4	5	15.916	10.263	10.263	0.0	5.652	3.223
3	4	5	25.134	23.203	23.203	0.0	1.926	1.200
5	4	5	12.159	10.214	-10.214	0.0	1.984	0.727
-8	5	5	76.286	76.118	76.118	0.0	0.168	0.110
-6	5	5	20.584	23.865	23.865	0.0	2.219	1.510
-4	5	5	7.376	12.208	12.208	0.0	-4.332	-1.155
-2	5	5	64.759	66.440	66.440	0.0	-1.681	-1.235
0	12	6	213.828	218.344	218.344	0.0	-4.516	-1.352 *
5	5	30.252	28.538	28.538	0.0	1.754	1.414	
2	5	103.484	104.595	104.595	0.0	-0.444	-0.298	
4	5	42.785	42.160	-42.160	0.0	-1.112	-0.616	
6	5	50.284	50.729	50.729	0.0	0.617	0.484	
-11	6	5	10.971	8.396	-8.396	0.0	2.575	0.893
-7	6	5	10.332	10.317	-10.317	0.0	0.015	0.005
-5	6	5	70.403	70.657	70.657	0.0	-0.289	-0.209
-3	6	5	48.401	46.469	-49.409	0.0	-1.007	-0.835
-1	6	5	146.039	144.446	144.446	0.0	1.593	0.682
1	6	5	25.625	25.811	25.811	0.0	-0.186	-0.112
3	6	5	35.974	36.975	36.975	0.0	-1.601	-0.647

B	K	L	F(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
5	6	5	38.055	40.463	40.463	0.0
-10	7	5	13.370	13.195	-13.195	-1.607
-8	7	5	33.223	35.665	35.665	0.0
-4	7	5	20.369	22.452	-22.452	-2.452
-2	7	5	11.904	9.347	9.347	-2.083
0	7	5	15.735	16.757	-16.757	-2.083
2	7	5	50.694	50.576	50.576	0.0
0	8	5	214.024	213.344	213.344	0.0
4	7	5	64.628	62.293	-62.293	-1.614
6	7	5	12.552	9.507	9.507	0.0
-14	8	5	11.511	2.926	-2.926	-2.926
-1	3	5	14.294	14.516	-14.516	0.0
1	3	5	5.682	5.109	5.109	0.0
3	8	5	11.691	15.535	15.535	0.0
5	8	5	12.935	13.320	-13.320	-3.320
-10	9	5	28.229	27.527	27.527	0.0
-6	9	5	21.679	26.492	-26.492	-6.492
-6	9	5	10.381	13.743	13.743	0.0
-4	9	5	9.481	13.175	13.175	0.0
-2	9	5	12.264	12.601	-12.601	0.0
0	9	5	30.226	30.782	-30.782	0.0
2	9	5	34.516	33.590	-33.590	0.0
4	9	5	36.121	37.505	-37.505	0.0
-9	10	5	18.241	17.320	-17.320	-1.320
0	12	0	213.533	218.344	-218.344	0.0
-7	10	5	15.469	17.924	17.924	0.0
-5	10	5	31.569	32.823	-32.823	-1.254
-3	10	5	30.406	31.453	31.453	-1.047
-1	10	5	21.106	19.514	-19.514	-1.593
1	10	5	11.413	7.879	7.879	0.0
3	10	5	5.518	2.470	-2.470	-2.470
5	10	5	9.202	4.335	4.335	0.0
-10	11	5	5.289	2.578	-2.578	-2.578
-6	11	5	12.510	9.787	-9.787	0.0
-4	11	5	9.415	5.222	-5.222	-5.222
-2	11	5	7.794	10.532	-10.532	-2.788
0	11	5	4.954	6.160	-6.160	-0.658
2	11	5	15.768	15.365	-15.365	0.0
4	11	5	8.072	5.546	-5.546	0.0
-9	12	5	2.407	9.318	-9.318	0.0
-7	12	5	16.505	14.641	14.641	0.0
-5	12	5	12.063	6.582	6.582	0.0
-1	12	5	6.271	2.676	2.676	0.0
0	12	0	213.058	218.344	218.344	-5.286
1	12	5	22.924	22.723	22.723	0.0
3	12	5	3.373	10.815	10.815	0.0
-8	13	5	11.883	13.649	-13.649	0.0
-6	13	5	10.234	6.431	6.431	0.0
4	13	5	7.876	10.790	10.790	-2.914

H	K	L	F(OBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
-2	13	5	19.501	17.242	-17.242	0.0	2.260	1.198
2	13	5	14.475	10.638	-10.638	0.0	3.837	1.819
4	13	5	12.257	9.043	-9.043	0.0	3.254	1.247
-7	14	5	18.535	20.962	-20.962	0.0	-4.426	-1.016
-5	14	5	64.088	63.603	-63.603	0.0	0.485	0.328
-3	14	5	35.875	36.114	-36.114	0.0	-0.239	-0.159
-1	14	5	27.809	27.251	-27.251	0.0	0.552	0.328
1	14	5	5.715	15.477	-15.477	0.0	-5.762	-1.636
3	14	5	10.725	8.599	-8.599	0.0	2.126	0.536
-8	15	5	21.728	25.550	-25.550	0.0	-3.822	-1.664
-6	15	5	20.746	17.736	-17.736	0.0	3.010	1.463
-4	15	5	11.364	12.471	-12.471	0.0	-1.107	-0.362
-2	15	5	18.977	21.327	-21.327	0.0	-2.350	-1.020
0	15	5	23.398	20.356	-20.356	0.0	3.042	1.776
0	12	0	214.673	218.344	-218.344	0.0	-4.270	-1.315 *
2	15	5	11.855	14.361	-14.361	0.0	-2.500	-0.719
-7	16	5	7.139	10.187	-10.187	0.0	-3.048	-0.594
-5	16	5	36.956	36.052	-36.052	0.0	0.904	0.671
-3	16	5	16.587	14.483	-14.483	0.0	2.104	0.964
-1	16	5	43.931	44.064	-44.064	0.0	-0.132	-0.090
1	15	5	30.154	28.673	-28.673	0.0	1.520	0.928
-4	17	5	8.482	3.774	-3.774	0.0	4.708	1.212
-2	17	5	47.075	47.433	-47.433	0.0	-0.357	-0.232
0	17	5	10.348	4.645	-4.645	0.0	5.704	1.950
-3	18	5	57.680	55.634	-55.634	0.0	1.445	1.039
-10	0	6	91.432	91.239	-91.239	0.0	0.193	0.167
-8	0	6	41.803	39.865	-39.865	0.0	1.938	1.385
-6	0	6	32.912	34.489	-34.489	0.0	-1.574	-0.995
-4	0	6	91.285	90.513	-90.513	0.0	0.772	0.461
-2	0	6	38.593	39.403	-39.403	0.0	-0.809	-0.504
0	6	51.169	49.640	-49.640	0.0	1.529	1.185	
2	0	6	19.239	19.044	-19.044	0.0	0.196	0.092
4	0	6	108.625	108.004	-108.004	0.0	0.621	0.317
-2	1	6	27.836	26.421	-26.421	0.0	1.414	0.944
-7	1	6	53.919	50.610	-50.610	0.0	3.310	2.485
0	12	0	212.600	218.344	-218.344	0.0	-5.744	-1.780 *
-5	1	6	22.514	19.644	-19.644	0.0	2.870	1.877
-3	1	6	71.276	72.609	-72.609	0.0	-1.333	-0.886
1	1	6	26.166	25.348	-25.348	0.0	0.818	0.466
3	1	6	19.027	18.058	-18.058	0.0	0.969	0.430
-10	2	6	9.448	6.043	-6.043	0.0	3.404	0.899
-2	2	6	4.044	0.339	-0.339	0.0	2.533	0.439
0	2	6	5.240	4.565	-4.565	0.0	0.675	0.138
-6	2	6	10.004	11.050	-11.050	0.0	-1.046	-0.275
4	2	6	16.407	12.790	-12.790	0.0	3.617	1.723
-9	3	6	21.925	20.471	-20.471	0.0	1.453	0.741
-7	3	6	27.263	27.287	-27.287	0.0	-0.024	-0.013
-5	3	6	25.265	25.578	-25.578	0.0	-0.313	-0.157
-3	3	6	25.871	24.056	-24.056	0.0	1.774	1.257
-1	3	6	18.159	20.736	-20.736	0.0	-2.577	-1.105

H	K	L	F(CUBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	3	6	21.843	23.514	-23.914	0.0	-2.071	-0.955
3	3	9	11.250	12.084	12.084	0.0	-0.885	-0.300
0	12	3	212.731	218.344	218.344	0.0	-5.613	-1.739 *
-10	4	6	35.777	35.284	-35.284	0.0	0.494	0.291
-6	4	6	17.045	20.122	20.122	0.0	-2.077	-1.324
-4	4	6	12.477	3.432	-3.432	0.0	5.045	4.735
6	4	6	11.544	8.426	8.426	0.0	3.118	1.160
-5	5	6	3.177	2.538	-2.538	0.0	6.737	-1.250
-3	5	9	5.010	4.567	4.567	0.0	-2.650	0.554
4	4	8	26.280	28.531	-28.531	0.0	0.592	-0.366
-9	5	6	22.678	21.521	21.521	0.0	1.157	0.554
-7	5	6	23.726	24.317	-24.317	0.0	6.444	0.090
3	5	6	6.615	9.930	9.930	0.0	6.556	0.312
-8	6	6	5.747	5.440	-5.440	0.0	0.308	0.062
-6	6	9	5.799	1.697	1.697	0.0	2.102	0.370
-2	6	9	2.390	4.210	4.210	0.0	5.025	1.701
0	6	14.589	7.535	7.935	0.0	6.655	3.355	
12	0	213.975	218.344	218.344	0.0	-4.369	-1.687 *	
2	6	6	7.548	11.652	-11.662	0.0	4.114	-1.032
-5	7	6	24.809	24.058	24.058	0.0	-1.249	-0.742
-3	7	6	17.733	19.453	-19.453	0.0	-1.720	-0.737
-1	7	6	30.898	30.502	30.502	0.0	0.396	0.267
-8	6	6	15.616	15.311	15.311	0.0	4.305	2.749
-6	8	6	28.605	26.486	-26.486	0.0	2.119	1.331
-4	8	6	10.463	13.794	13.794	0.0	-3.531	-0.914
-2	8	6	13.492	6.475	6.475	0.0	7.017	3.154
0	8	6	43.244	43.587	-43.587	0.0	-0.343	-0.214
2	8	6	44.701	45.119	45.119	0.0	-0.418	-0.274
-7	9	6	8.556	7.223	-7.223	0.0	1.373	0.356
-3	9	6	16.325	20.784	20.784	0.0	-4.459	-1.554
-3	9	6	50.388	52.161	-52.161	0.0	-2.073	-1.312
-1	9	6	20.304	20.808	20.808	0.0	-0.504	-0.229
1	9	6	17.700	15.547	-15.547	0.0	2.153	0.572
-8	10	6	16.456	8.898	8.898	0.0	7.558	4.179
0	12	0	213.189	218.344	218.344	0.0	-5.155	-1.593 *
-6	10	6	8.334	15.043	15.043	0.0	-6.709	-1.593
-4	10	6	24.332	22.754	22.754	0.0	1.577	0.923
-2	10	6	22.252	21.693	21.693	0.0	0.559	0.270
0	10	6	25.216	24.531	24.531	0.0	0.685	0.357
2	10	6	10.840	3.481	3.481	0.0	7.359	2.413
-1	11	6	5.191	8.980	-8.980	0.0	-3.790	-0.685
1	11	6	25.258	27.714	27.714	0.0	-2.416	-1.160
-6	12	6	39.559	40.161	40.161	0.0	-0.601	-0.381
-4	12	6	32.289	28.560	28.560	0.0	3.329	2.223
0	12	6	50.432	48.753	48.753	0.0	1.679	1.317
-5	13	6	32.830	31.744	-31.744	0.0	1.086	0.684
-3	13	6	47.615	48.956	48.956	0.0	-1.381	-0.881
-1	13	6	24.037	24.858	-24.858	0.0	-0.821	-0.434

## K-KICHLERITE 4000C 1/15/73

## STRUCTURE FACTORS

PAGE 26

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	12	0	212.960	218.344	0.0	-5.384	-1.667	*
-5	0	7	9.153	1.162	0.0	7.992	2.583	
-1	0	7	16.014	13.670	-1.162	0.0	2.343	0.984
-7	2	7	20.975	23.592	23.592	0.0	-2.617	-1.116
-5	2	7	34.338	34.730	-34.730	0.0	-0.393	-0.237
-3	2	7	36.039	23.636	0.0	2.403	1.822	
-1	2	7	11.429	8.697	-8.697	0.0	3.332	1.152
-6	3	7	7.925	6.681	6.681	0.0	1.244	0.302
-4	3	7	14.000	13.927	-13.927	0.0	0.073	0.023
-2	3	7	5.109	8.835	-8.835	0.0	-3.720	-0.633
-2	4	7	10.965	9.530	9.530	0.0	1.375	0.437
-6	5	7	19.943	18.711	18.711	0.0	1.232	0.565
-4	5	7	26.706	25.610	25.610	0.0	1.096	0.601
-2	5	7	15.682	18.892	18.892	0.0	0.790	0.380
0	12	C	213.975	218.344	218.344	0.0	-4.309	-1.346 *
-5	6	7	75.566	76.700	76.700	0.0	-1.134	-0.701

## ALL REFLECTIONS

NUMERATOR DENOMINATOR NUMBER R

WEIGHTED R 2525.64 1280358.00 1341 0.044

UNWEIGHTED R 2874.29 57003.69 1341 C.050

## RANGES OF FIGURES

2052.05	15393.93	856	0.133
288.79	12059.66	244	0.024
55.65	6430.04	75	C.015
62.28	3802.62	32	C.016
41.05	2122.90	14	C.019
14.40	765.50	4	C.015
319.36	16085.41	75	0.020
3.70	278.23	1	0.013

RANGES OF  $(\sin(\theta)/\lambda\cos\alpha)^{1/2}$ 

212.19	5443.54	84	0.039
495.06	20863.98	193	0.024
251.28	5776.36	142	0.044
246.36	5499.59	155	0.045
293.24	4910.48	166	C.066
353.57	4727.74	185	C.083
445.52	4835.75	157	0.092
535.56	4947.87	215	C.105

## UNREJECTED REFLECTIONS

WEIGHTED R 1765.57 872174.94 1156 C.045

UNWEIGHTED R 2291.12 37862.79 1156 C.061

## RANGES OF F(OBS)

1832.27	14012.61	821	0.131
247.69	10629.46	217	0.023
84.80	5756.13	67	C.015
52.00	3341.85	28	C.016
41.05	2122.90	14	C.019
14.40	765.50	4	0.019
15.85	866.63	4	C.018
3.70	278.23	1	0.013

RANGES OF  $(\sin(\theta)/\lambda\cos\alpha)^{1/2}$ 

154.67	4637.98	69	0.033
170.57	5013.25	107	0.034
236.60	5389.13	130	0.044
217.01	4885.73	138	C.044
273.43	4544.77	154	0.060
364.22	4261.63	175	C.084
390.25	4421.68	182	C.088
485.27	4610.32	201	C.105

SUM FCAL STANDARD DEV OF UNIT WEIGHT OBS 56966.46 1.30

## K-KICHTERFILE 400C 1/15/73

PARAMETER

OLD

CHANGE

NEW

ERROR SHIFT/ERROR

ATOM 1 O(1) EQUIPOINT FRACTION = 1.000

EXTINCTION CORRECTION 0.0

SCALE FACTOR 1 0.6167

0.0

0.00000 0.00000 0.00000

ATOM 2 O(2) EQUIPOINT FRACTION = 1.000

EXTINCTION CORRECTION 0.0

SCALE FACTOR 1 0.6167

0.0

0.00000 0.00000 0.00000

ATOM 3 F(3) EQUIPOINT FRACTION = 0.500

EXTINCTION CORRECTION 0.0

SCALE FACTOR 1 0.6167

0.0

0.00000 0.00000 0.00000

ATOM 4 O(4) EQUIPOINT FRACTION = 1.000

EXTINCTION CORRECTION 0.0

SCALE FACTOR 1 0.6167

0.0

0.00000 0.00000 0.00000

ATOM 5 O(5) EQUIPOINT FRACTION = 1.000

EXTINCTION CORRECTION 0.0

SCALE FACTOR 1 0.6167

0.0

0.00000 0.00000 0.00000

ATOM 1 O(1) EQUIPOINT FRACTION = 1.000

EXTINCTION CORRECTION 0.0

SCALE FACTOR 1 0.6167

0.0

0.00000 0.00000 0.00000

ATOM 2 O(2) EQUIPOINT FRACTION = 1.000

EXTINCTION CORRECTION 0.0

SCALE FACTOR 1 0.6167

0.0

0.00000 0.00000 0.00000

ATOM 3 F(3) EQUIPOINT FRACTION = 0.500

EXTINCTION CORRECTION 0.0

SCALE FACTOR 1 0.6167

0.0

0.00000 0.00000 0.00000

ATOM 4 O(4) EQUIPOINT FRACTION = 1.000

EXTINCTION CORRECTION 0.0

SCALE FACTOR 1 0.6167

0.0

0.00000 0.00000 0.00000

ATOM 5 O(5) EQUIPOINT FRACTION = 1.000

EXTINCTION CORRECTION 0.0

SCALE FACTOR 1 0.6167

0.0

0.00000 0.00000 0.00000

BETA2	0.0011744	-0.000004	0.0311740	0.0000716	-0.01
BETA3	0.0104220	0.000058	0.0104278	0.0000805	0.01
BETA12	-0.0000302	-0.000002	-0.0000304	0.0000169	-0.00
BETA13	0.00011476	0.000001	0.00011478	0.00004121	0.00
BETA23	0.00011214	-0.000002	0.00011212	0.00002177	-0.00

ATOM 6 U(6) EQUIFLUID FRACTION = 1.000

EQUIFLUID FRACTION = 1.000

EQUIFLUID FRACTION = 0.500

OCCUPANCY SPECIES = 1

OCCUPANCY SPECIES = 1

X 0.3403810 0.000056 0.3403866 C.0002711 0.02

Y 0.8820383 0.000003 C.8820386 C.0001486 0.02

Z 0.7502497 0.000005 C.7502552 C.0004558 0.02

BETA1 0.0025100 -0.0000054 C.0035046 C.0002833 -0.02

BETA2 0.0014322 0.0000054 C.0014326 C.0002836 0.00

BETA3 0.0101775 -0.0000051 C.000251 0.0101724 C.0005751 -0.01

BETA12 -0.0000234 0.000005 -C.000229 C.0001154 0.00

BETA13 0.0016805 -0.0000050 C.0016756 C.0004143 -0.01

BETA23 -0.0014274 0.000001 -0.0014273 C.0002260 0.00

ATOM 7 U(7) EQUIFLUID FRACTION = 0.500

EQUIFLUID FRACTION = 0.500

OCCUPANCY SPECIES = 1

OCCUPANCY SPECIES = 1

X 0.3342318 0.000025 0.3343343 C.000446SC 0.01

Y 0.0 0.0 0.0

Z 0.0257128 -0.000018 C.0297110 0.0008164 -0.00

BETA1 0.0044380 -0.000011 0.0044268 C.0004157 -0.03

BETA2 0.0005448 0.0000010 0.0005453 -C.00010C2 0.01

BETA3 0.0198772 -0.0000167 0.0198605 C.0016317 -0.01

BETA12 0.0 0.0 0.0

BETA13 0.0004159 -0.0000090 C.0004669 C.00066414 -0.01

BETA23 0.0 0.0 0.0

ATOM 8 T(1) EQUIFLUID FRACTION = 1.000

EQUIFLUID FRACTION = 1.000

OCCUPANCY SPECIES = 3

OCCUPANCY SPECIES = 3

X 1.00000 1.00000 1.00000 C.00010C60 0.02

Y 0.2761747 0.000023 0.2761770 C.0000482 0.01

Z 0.9155470 0.000004 0.9155473 C.000155G 0.00

BETA1 0.9770015 0.000008 C.5770023 C.000155G 0.00

BETA2 0.0021535 -0.000019 0.0021516 C.0000561 -0.02

BETA22 0.0006101 -0.000000 C.0006101 C.000272 0.00

BETA3 0.0073681 0.000000 0.0073754 C.0003479 0.02

BETA2 0.0000654 -0.000001 0.0000653 C.0000410 -0.00

BETA13 0.0012482 0.000010 0.0012492 C.0001359 0.01

BETA23 0.0000038 0.000003 C.0000041 C.0000746 0.00

ATOM 9 T(2) EQUIFLUID FRACTION = 1.000

EQUIFLUID FRACTION = 1.000

OCCUPANCY SPECIES = 3

OCCUPANCY SPECIES = 3

X 1.00000 1.00000 1.00000 C.0001030 -0.01

Y 0.2842419 -0.000012 0.284267 C.0001030 -0.01

Z 0.8288965 0.000001 0.8288966 C.0000489 0.00

BETA1 0.4806901 -0.000005 C.4806896 C.0001584 -0.00

BETA2 0.0020597 0.000028 C.0021025 C.0000962 0.03

BETA22 0.0006513 -0.000001 C.0006511 C.0000266 -0.00

BETA3 0.0070307 -0.000009 0.0070298 C.0003426 -0.00

BETA2 0.0001543 0.000003 0.0001546 C.0000411 0.01

BETA13 0.0006437 0.000012 0.0006449 C.0001380 0.01

BETA23 0.0000755 0.000004 0.0000759 C.0000746 0.01

ATOM 10 M(1) EQUIFLUID FRACTION = 0.500

EQUIFLUID FRACTION = 0.500

OCCUPANCY SPECIES = 4

OCCUPANCY SPECIES = 4

X 1.00000 1.00000 1.00000 0.0

Y 0.0 0.0 0.0

Z 0.9102094 0.0000002 C.9102094 C.0000000 -0.00

BETA11 0.5000000 0.0000002 C.5000000 0.0000000 -0.00

BETA2 0.0000000 0.0000002 C.0000000 0.0000000 -0.00

BETA22 0.0007700 0.0000001 C.0007700 C.0000001 -0.00

BETA33	0.0006871	0.0000122	0.0006992	0.0006548	0.02	
BETA12	0.0	0.0	0.0	0.0		
BETA13	0.0	0.0012404	0.0000012	0.0012416	0.0002856	0.00
BETA23	0.0	0.0	0.0	0.0		

ATOM 11 N(2) EQUIPOINT FRACTION = 0.500

OCCUPANCY SPECIES	4	1.00000	1.00000		
X	0.0	0.0	0.0		
Y	0.0	0.8201564	-0.0000002	0.8201562	0.0000000
Z	0.0	0.0	0.0	0.0	
BETA11	0.0029367	0.0000050	0.0029417	0.00001845	0.003
BETA22	0.0008500	0.0000005	0.0008505	0.00000528	0.01
BETA33	0.0107502	-0.0000209	0.0107293	0.00006875	-0.03
BETA12	0.0	0.0	0.0		
BETA13	0.0	0.0005623	0.0000009	0.0005631	0.0000000
BETA23	0.0	0.0	0.0	0.0	

ATOM 12 N(3) EQUIPOINT FRACTION = 0.250

OCCUPANCY SPECIES	4	1.00000	1.00000		
X	0.0	0.0	0.0		
Y	0.0	0.0	0.0		
Z	0.0	0.0	0.0		
BETA11	0.0003277C	0.0000018	0.0032787	0.00002597	0.01
BETA22	0.0006645	0.0000001	0.0006646	0.00000689	0.00
BETA33	0.0008375	-0.0000132	0.0083644	0.00005166	-0.01
BETA12	0.0	0.0	0.0		
BETA13	0.0012677	0.0000005	0.0012682	0.0003809	0.00
BETA23	0.0	0.0	0.0		

ATOM 13 N(4) EQUIPOINT FRACTION = 0.500

OCCUPANCY SPECIES	5	0.50000	0.50000		
OCCUPANCY SPECIES	6	0.50000	0.50000		
TOTAL OCCUPANCY (FIXED)	1.0000	1.0000			
X	0.0	0.0	0.0		
Y	0.7221957	0.0000009	0.7221966	0.0000000	0.01
Z	0.500000	0.000000	0.500000	0.000000	
BETA11	0.0067588	0.0000047	0.0067635	0.00001554	0.02
BETA22	0.0010529	0.0000006	0.0010529	0.00000448	0.00
BETA33	0.00135702	-0.0000205	0.0135497	0.0000551	-0.03
BETA12	0.0	0.0	0.0		
BETA13	-0.0018457	-0.0000018	-0.0018474	0.0002636	-0.01
BETA23	0.0	0.0	0.0		

ATOM 14 A EQUIPOINT FRACTION = 0.500

OCCUPANCY SPECIES	7	0.50000	0.50000		
X	0.4807048	0.0015101	0.4822149	0.0037013	0.41
Y	0.0	0.0	0.0		
Z	0.5223573	0.0025569	0.52253143	0.0068161	0.34
BETA11	0.0180053	0.0013781	0.0193834	0.0034837	0.46
BETA22	0.0030230	-0.0000031	0.0030198	0.0001070	-0.03
BETA33	0.04006162	-0.0030441	0.0375722	0.0092046	-0.33
BETA12	0.0	0.0	0.0		
BETA13	-0.0150404	0.0004607	-0.0145797	0.0036493	0.13
BETA23	0.0	0.0	0.0		

MAXIMUM SHIFT/ERROR = C.41

AVERAGE SHIFT/ERROR = C.02

H	K	L	F(UBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-3	4	7	6.200	C 491	U 481	0.0	5.709	1.256
-1	4	7	9.217	2.147	-2.147	0.0	7.070	2.578
-6	5	7	15.713	17.218	17.218	0.0	-3.500	-1.150
-4	5	7	21.814	21.476	21.476	0.0	0.339	0.146
-2	5	7	16.159	16.583	16.583	0.0	-0.424	-0.154
-5	6	7	17.538	19.690	19.690	0.0	0.848	0.542
-3	6	7	47.981	46.343	-46.343	0.0	1.638	1.152
-4	7	7	6.678	6.119	6.119	0.0	0.559	0.110
0	12	0	206.156	210.970	210.970	0.0	-4.814	-1.537 *
4	6	0	26.612	39.826	39.826	0.0	-13.213	-15.276 *
6	0	0	95.600	93.788	93.788	0.0	1.813	1.156
8	0	0	108.313	111.475	111.475	0.0	-3.162	-1.781
10	0	0	59.672	58.032	58.032	0.0	1.640	1.154
12	0	J	4.233	3.601	-3.601	0.0	C 636	0.108
-13	1	C	30.075	31.081	-31.081	0.0	-1.006	-0.377 *
-11	1	0	58.511	57.616	57.616	0.0	0.901	C 603 *
-9	1	0	20.264	22.741	22.741	0.0	-2.477	-1.371 *
-7	1	0	73.275	73.728	73.728	0.0	-0.453	-0.339 *
-5	1	0	119.591	116.565	-116.565	0.0	3.026	1.624 *
-3	1	J	137.761	137.833	137.833	0.0	-0.072	-0.034 *
3	1	C	138.635	137.833	137.833	0.0	C 802	0.381
5	1	0	118.519	116.565	-116.565	0.0	1.954	1.055
7	1	0	73.093	73.728	73.728	0.0	-0.635	-0.482
9	1	0	19.555	22.741	22.741	0.0	-3.186	-1.787
11	1	0	56.572	57.616	57.616	0.0	-1.044	-0.754
13	1	0	32.263	31.081	-31.081	0.0	1.187	0.746
-12	2	0	14.345	14.681	14.681	0.0	-0.336	-0.090 *
-10	2	0	3.199	4.769	-4.769	0.0	-1.571	-0.250 *
-8	2	0	13.982	11.504	-11.504	0.0	2.478	1.185 *
0	12	0	205.321	210.970	210.970	0.0	-5.639	-1.806 *
-6	2	0	29.960	31.211	-31.211	0.0	-1.251	-1.019 *
6	2	0	30.256	31.211	-31.211	0.0	-0.954	-0.837 *
8	2	0	11.542	11.504	-11.504	0.0	0.038	0.016
10	2	0	5.6C6	4.769	-4.769	0.0	0.837	0.205
12	2	0	17.7C9	14.681	14.681	0.0	3.027	1.456
-13	3	0	11.8C6	18.857	18.857	0.0	-7.051	-1.274 *
-11	3	0	21.758	19.582	-19.582	0.0	2.216	0.951 *
-9	3	0	16.076	17.120	17.120	0.0	-1.044	-0.460 *
-7	3	0	54.956	54.37	-54.37	0.0	0.919	0.780 *
-5	3	0	57.314	57.645	57.645	0.0	0.269	0.251 *
-3	3	0	86.136	90.062	-90.062	0.0	-3.926	-2.886 *
3	3	0	87.801	90.062	-90.062	0.0	-2.261	-1.631 *
5	3	0	58.485	57.645	57.645	0.0	1.439	1.350
7	3	0	52.829	54.037	-54.037	0.0	-1.208	-1.003
9	3	0	17.049	17.120	17.120	0.0	-0.071	-0.035
11	3	0	18.721	19.582	-19.582	0.0	-0.851	-0.369
13	3	0	22.309	18.857	18.857	0.0	3.052	1.741
-12	4	0	7.024	10.118	10.118	0.0	-3.094	-0.493 *
0	12	0	206.040	210.970	210.970	0.0	-4.930	-1.574 *
-10	4	0	12.333	2.398	2.398	0.0	9.936	4.055 *
-8	4	0	10.124	5.638	5.638	0.0	4.486	1.625 *
-6	4	0	13.999	15.889	15.889	0.0	-1.891	-0.975 *
-4	4	0	12.201	9.953	9.953	0.0	2.248	1.801 *

H	K	L	F(UBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-2	4	0	137.135	142.601	142.601	0.0	-5.466	-2.026 *
2	4	0	139.427	142.601	142.601	0.0	-3.174	-1.201
4	4	0	9.794	9.553	9.553	0.0	-0.159	-0.351
6	4	0	16.010	15.889	15.889	0.0	0.121	0.075
10	4	0	3.941	2.398	2.398	0.0	1.543	0.295
12	4	0	6.595	10.118	10.118	0.0	-3.523	-0.629
-13	5	0	23.958	21.293	21.293	0.0	2.665	0.969 *
-11	5	0	15.648	19.211	19.211	0.0	-3.563	-1.033 *
-7	5	0	13.422	5.160	5.160	0.0	8.261	4.458 *
-5	5	0	13.603	16.712	16.712	0.0	-3.109	-1.810 *
-3	5	0	79.343	81.710	81.710	0.0	-2.367	-1.841 *
1	5	0	12.861	17.384	17.384	0.0	-4.523	-3.589 *
1	5	0	13.075	17.384	17.384	0.0	-4.309	-3.466
3	5	0	81.354	81.710	81.710	0.0	-0.355	-0.270
0	12	0	206.914	210.570	210.570	0.0	-4.056	-1.290 *
5	5	0	13.191	16.712	16.712	0.0	-3.522	-1.974
7	5	0	6.299	5.160	5.160	0.0	1.138	0.311
11	5	0	21.567	19.211	19.211	0.0	2.356	1.231
13	5	0	20.759	21.293	21.293	0.0	-0.534	-0.211
-10	0	0	28.155	25.272	25.272	0.0	2.923	2.137 *
-8	6	0	25.903	26.223	26.223	0.0	-0.320	-0.224 *
-6	6	0	17.939	17.435	17.435	0.0	0.504	0.310 *
-2	6	0	19.852	21.343	21.343	0.0	-1.491	-1.659 *
0	6	0	14.147	15.097	15.097	0.0	-0.950	-0.873
2	6	0	19.407	21.343	21.343	0.0	-1.937	-2.026
6	6	0	14.923	17.435	17.435	0.0	-2.612	-1.255
3	6	0	22.193	26.223	26.223	0.0	-4.030	-2.344
10	6	0	24.683	25.272	25.272	0.0	-0.589	-0.369
12	6	0	6.161	11.631	11.631	0.0	-5.530	-1.039
-11	7	0	18.434	17.631	17.631	0.0	0.803	0.303 *
-9	7	0	48.245	48.564	48.564	0.0	-0.719	-0.540 *
0	12	0	205.859	210.570	210.570	0.0	-5.111	-1.633 *
-7	7	0	32.647	32.420	32.420	0.0	0.227	0.181 *
-5	7	0	11.954	6.521	6.521	0.0	5.433	2.857 *
-3	7	0	57.034	53.705	53.705	0.0	3.329	3.220 *
-1	7	0	18.401	16.815	16.815	0.0	1.586	1.961 *
1	7	0	15.334	16.815	16.815	0.0	-1.481	-1.271
3	7	0	56.803	53.705	53.705	0.0	3.098	3.014
5	7	0	10.800	6.521	6.521	0.0	4.279	1.925
7	7	0	35.318	32.420	32.420	0.0	2.898	2.424
9	7	0	47.619	48.564	48.564	0.0	-1.346	-1.028
11	7	0	18.319	17.631	17.631	0.0	0.687	0.308
-12	8	0	34.058	31.806	31.806	0.0	2.292	1.029
-10	8	0	41.749	44.023	44.023	0.0	-2.274	-1.461 *
-3	8	0	15.878	14.550	14.550	0.0	1.328	0.696 *
-6	8	0	69.657	71.577	71.577	0.0	-2.280	-1.747 *
-4	8	0	95.788	101.253	101.253	0.0	-1.465	-0.906 *
-2	8	0	31.229	33.498	33.498	0.0	-2.269	-2.684 *
0	8	0	45.854	43.196	43.196	0.0	2.689	2.990
2	8	0	32.581	33.498	33.498	0.0	-0.917	-1.174
4	8	0	102.031	101.253	101.253	0.0	0.717	0.475
6	8	0	72.170	71.577	71.577	0.0	0.193	0.146 *
0	12	0	206.469	210.570	210.570	0.0	-4.501	-1.435 *

H	K	L	F(LUSS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
3	8	0	14.157	14.550	-14.550	0.0	-0.353	-0.173
15	8	0	44.535	44.023	-44.023	0.0	0.512	0.384
12	6	0	28.772	31.806	-31.806	0.0	-3.033	-1.356
-11	9	0	19.011	14.151	-14.151	0.0	4.860	1.828 *
-9	9	0	32.070	33.283	-33.283	0.0	-1.213	-0.832 *
-7	9	0	89.120	90.517	-90.517	0.0	-1.397	-0.885 *
-5	9	0	10.124	8.245	-8.245	0.0	1.379	0.851 *
-1	9	0	80.728	81.501	-81.501	0.0	-0.774	-0.582 *
1	9	0	81.766	81.501	-81.501	0.0	0.265	0.199
5	9	0	10.074	8.245	-8.245	0.0	1.829	0.778
7	9	0	89.928	90.517	-90.517	0.0	-0.539	-0.373
9	9	0	31.928	33.283	-33.283	0.0	-1.344	-0.689
11	9	0	14.114	14.151	-14.151	0.0	-0.037	-0.012 *
-12	10	0	27.157	21.889	-21.889	0.0	5.268	2.377 *
-10	10	0	23.150	24.053	-24.053	0.0	-0.903	-0.375 *
-8	10	0	25.953	29.170	-29.170	0.0	-3.223	-1.645 *
-6	10	0	17.033	17.075	-17.075	0.0	-0.043	-0.022 *
-4	10	0	63.035	65.222	-65.222	0.0	-2.187	-1.818 *
0	12	0	205.908	210.570	-210.570	0.0	-5.061	-1.617 *
-2	10	0	45.080	47.907	-47.907	0.0	-2.828	-2.783 *
0	10	0	105.361	106.890	-106.890	0.0	-1.528	-0.913
2	10	0	43.513	47.907	-47.907	0.0	-4.394	-4.106
4	10	0	63.580	65.222	-65.222	0.0	-1.643	-1.331
6	10	0	16.241	17.075	-17.075	0.0	-0.834	-0.410
8	10	0	32.416	29.176	-29.176	0.0	3.240	2.567
10	10	0	24.053	24.053	-24.053	0.0	0.004	0.002
12	10	0	23.546	21.889	-21.889	0.0	1.657	0.773
-11	11	0	59.342	61.656	-61.656	0.0	-1.714	-1.004 *
-7	11	0	125.098	129.180	-129.180	0.0	-4.082	-1.992 *
-5	11	0	41.758	41.444	-41.444	0.0	0.355	0.303 *
-3	11	0	75.659	79.062	-79.062	0.0	-3.363	-2.462 *
-1	11	0	120.557	119.866	-119.866	0.0	0.730	0.384 *
1	11	0	121.009	119.866	-119.866	0.0	0.599	0.234
3	11	0	78.386	79.062	-79.062	0.0	-0.675	-0.492
5	11	0	40.288	41.444	-41.444	0.0	-1.146	-1.004
7	11	0	127.407	129.180	-129.180	0.0	-1.713	-0.858
9	11	0	2.968	3.667	-3.667	0.0	-0.699	-0.117
11	11	0	62.254	61.056	-61.056	0.0	1.233	0.792
0	12	0	206.485	210.570	-210.570	0.0	-4.484	-1.429 *
-10	12	0	52.450	50.420	-50.420	0.0	2.030	1.383 *
-8	12	0	49.878	51.446	-51.446	0.0	-1.563	-1.145 *
-6	12	0	35.578	35.075	-35.075	0.0	0.903	0.703 *
-4	12	0	55.682	57.553	-57.553	0.0	-2.273	-1.862 *
-2	12	0	40.446	42.004	-42.004	0.0	-1.558	-1.343 *
0	12	0	205.677	210.570	-210.570	0.0	-5.292	-1.693 *
2	12	0	42.013	42.004	-42.004	0.0	0.008	0.007
4	12	0	55.912	57.555	-57.555	0.0	-2.042	-1.710
6	12	0	35.417	35.075	-35.075	0.0	0.342	0.282
8	12	0	50.785	51.446	-51.446	0.0	-0.661	-0.492
10	12	0	50.834	50.420	-50.420	0.0	0.414	0.295
-11	13	0	22.128	21.559	-21.559	0.0	0.529	0.175 *
-9	13	0	25.277	25.682	-25.682	0.0	-0.405	-0.183 *
-7	13	0	36.835	38.883	-38.883	0.0	-2.048	-1.421 *

H	K	L	F(LBSI)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-5	13	0	63.349	63.775	0.0	-0.426	-0.327 *	
-3	13	0	16.439	18.121	-18.121	0.0	-1.682	-0.885 *
-1	13	0	8.162	4.571	4.571	0.0	3.591	1.186 *
1	13	0	4.848	4.571	4.571	0.0	0.277	0.368
3	13	0	19.654	18.121	-18.121	0.0	1.533	1.017
5	13	0	63.662	63.775	-63.775	0.0	-0.113	-0.086
0	12	0	206.848	210.970	210.970	0.0	-4.122	-1.312 *
7	13	0	39.721	38.883	38.883	0.0	0.837	0.661
9	13	0	24.255	25.682	-25.682	0.0	-1.427	-0.682
11	13	0	19.671	21.599	21.599	0.0	-1.923	-0.664 *
0	14	0	13.257	8.289	-8.289	0.0	4.963	2.647
2	14	0	35.203	33.425	33.425	0.0	1.777	1.547
4	14	0	9.563	12.656	12.656	0.0	-3.093	-1.022
6	14	0	6.358	1.825	-1.825	0.0	4.573	1.241
8	14	0	1.814	0.992	0.992	0.0	0.822	0.109
-9	15	0	32.647	32.447	32.447	0.0	0.200	0.108 *
-7	15	0	50.566	48.936	-48.936	0.0	2.030	1.454 *
-5	15	0	20.650	29.872	-29.872	0.0	-1.182	-0.777 *
-1	15	0	9.926	10.795	-10.795	0.0	-0.869	-0.292 *
1	15	0	8.442	10.755	-10.755	0.0	-2.353	-0.729 *
0	12	0	206.172	210.970	-210.970	0.0	-4.798	-1.531 *
3	15	0	11.954	3.838	-3.838	0.0	8.117	4.767
5	15	0	28.047	29.872	-29.872	0.0	-1.826	-1.204
7	15	0	48.427	48.936	-48.936	0.0	-0.509	-0.378
9	15	0	34.164	32.447	32.447	0.0	1.717	1.141
-10	16	0	23.628	22.847	-22.847	0.0	0.781	0.255 *
-8	16	0	8.904	9.559	-9.559	0.0	-1.055	-0.222 *
-6	16	0	32.449	33.275	-33.275	0.0	-0.926	-0.527 *
-4	16	0	48.311	48.944	-48.944	0.0	-0.632	-0.458 *
0	16	0	5.722	5.303	-5.303	0.0	0.418	0.106
4	16	0	48.262	48.944	-48.944	0.0	-0.682	-0.528
6	16	0	32.433	33.275	-33.275	0.0	-0.842	-0.556
8	16	0	12.543	9.559	-9.559	0.0	2.589	0.892
10	16	0	19.127	22.847	-22.847	0.0	-3.720	-1.204
-9	17	0	15.878	16.783	-16.783	0.0	-0.904	-0.244 *
-3	17	0	25.293	26.499	-26.499	0.0	-1.205	-0.736 *
-1	17	0	15.136	15.651	-15.651	0.0	-0.514	-0.238 *
0	12	0	206.353	210.570	-210.570	0.0	-4.616	-1.472 *
1	17	0	19.054	15.651	-15.651	0.0	3.443	2.369
3	17	0	23.654	26.499	-26.499	0.0	-2.805	-1.580
5	17	0	4.089	5.438	-5.438	0.0	-1.348	-0.246
7	17	0	12.234	11.108	-11.108	0.0	1.126	0.405
9	17	0	18.401	16.783	-16.783	0.0	1.618	0.655
-8	18	0	6.991	10.882	-10.882	0.0	-3.891	-0.616 *
-6	18	0	22.523	24.804	-24.804	0.0	-2.281	-0.942 *
-4	18	0	10.750	4.832	-4.832	0.0	5.919	2.064 *
-2	18	0	22.424	21.686	-21.686	0.0	0.739	0.356 *
2	18	0	15.648	18.266	-18.266	0.0	-2.618	-1.119
4	18	0	22.012	21.686	-21.686	0.0	0.327	0.167
			9.052	4.832	-4.832	0.0	4.221	1.345

H	K	L	F(UBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
6	15	C	21.798	24.654	24.654	0.0	-3.006	-1.328
6	16	C	11.355	10.832	-10.382	0.0	0.973	0.275
-7	19	C	21.781	22.277	-22.277	0.0	-0.496	-0.175 *
-5	19	C	12.531	1.357	1.357	0.0	11.134	3.651 *
-3	19	C	28.245	28.508	-28.508	0.0	-0.663	-0.358 *
-1	19	0	4.386	7.321	-7.321	0.0	-2.935	-0.549 *
1	19	0	7.799	7.321	-7.321	0.0	0.478	0.129
3	19	C	29.168	28.908	-28.908	0.0	0.260	0.166
0	12	0	205.958	210.570	-210.570	0.0	-5.012	-1.601 *
5	19	C	8.558	1.397	1.397	0.0	7.160	1.967
7	19	C	21.880	22.277	-22.277	0.0	-0.397	-0.163
-8	20	0	5.820	7.567	-7.567	0.0	-1.747	-0.231 *
-6	20	0	13.471	4.625	4.625	0.0	-1.362	-0.656
-4	20	C	29.953	30.514	-30.514	0.0	-0.521	-0.263 *
-2	20	0	30.467	29.557	29.557	0.0	0.930	0.556 *
0	20	0	51.131	50.803	-50.803	0.0	0.328	0.250
2	20	0	28.476	29.557	-29.557	0.0	-1.082	-0.589
4	20	0	29.152	30.514	-30.514	0.0	1.154	0.634 *
8	20	C	10.586	7.567	-7.567	0.0	3.018	0.665
-7	21	0	6.480	4.078	-4.078	0.0	2.402	0.352 *
-5	21	C	37.050	35.895	-35.895	0.0	2.605	1.669
-3	21	0	5.959	6.202	-6.202	0.0	-3.940	-1.253 *
-1	21	C	27.957	23.960	-23.960	0.0	3.757	0.981 *
1	21	0	24.617	23.950	-23.950	0.0	4.037	2.441 *
3	21	C	38.501	35.895	-35.895	0.0	0.657	0.367
0	12	0	207.030	210.570	-210.570	0.0	1.154	0.634 *
-4	22	0	44.371	42.718	-42.718	0.0	1.001	*
-2	22	C	20.363	16.849	-16.849	0.0	3.514	1.945 *
0	22	C	59.177	58.756	-58.756	0.0	0.421	0.265
2	22	0	16.769	16.849	-16.849	0.0	-0.080	-0.026
4	22	C	42.260	42.718	-42.718	0.0	-0.458	-0.258
6	22	C	14.774	7.394	7.394	0.0	7.380	2.613
-5	23	C	42.969	43.787	-43.787	0.0	-0.818	-0.403 *
-3	23	C	29.547	30.358	-30.358	0.0	2.315	1.267
1	23	C	11.344	8.577	8.577	0.0	-0.811	-0.358 *
3	23	C	29.755	30.358	-30.358	0.0	2.767	0.677
5	23	0	46.102	42.787	-43.787	0.0	-0.564	-0.268
-2	24	C	38.068	40.592	-40.592	0.0	2.315	1.267
0	24	0	78.040	80.117	-80.117	0.0	-2.504	-1.211 *
2	24	C	40.545	40.592	-40.592	0.0	-2.077	-1.157
-13	0	1	16.851	17.182	-17.182	0.0	-0.047	-0.027
-9	0	1	7.957	8.792	-8.792	0.0	-0.331	-0.103
0	12	0	206.040	210.570	-210.570	0.0	-0.795	-0.241
-3	0	1	12.359	9.589	-9.589	0.0	-4.930	-1.574 *
3	0	1	24.964	24.248	-24.248	0.0	0.715	0.764
5	0	1	6.678	4.255	4.255	0.0	4.912	2.749
7	0	1	9.168	0.090	0.090	0.0	6.588	2.013
9	0	1	10.421	4.170	-4.170	0.0	6.250	2.859
11	0	1	7.172	1.056	-1.056	0.0	6.117	1.495
-12	1	1	12.854	3.000	8.060	0.0	4.834	1.524
-10	1	1	9.811	7.432	-7.432	0.0	2.379	0.826
-8	1	1	6.183	9.223	-9.223	0.0	-3.040	-0.795
-4	1	1	19.522	20.542	-20.542	0.0	-1.020	-1.117

H	K	L	F(OBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
2	1	1	65.327	66.786	-0.676	0.0	-1.459	-1.358
4	1	1	12.312	13.031	0.0	0.0	0.291	0.211
5	1	1	12.949	13.740	-13.740	0.0	-0.756	-0.375
8	1	1	13.306	15.920	15.920	0.0	-2.614	-1.222
10	1	1	11.311	11.550	-11.550	0.0	-0.259	-0.083
12	1	1	14.757	9.871	9.871	0.0	4.886	2.013
13	2	1	25.036	20.386	-20.386	0.0	4.143	1.946
-11	2	1	18.930	23.011	23.011	0.0	-4.182	-1.560
-9	2	1	22.358	26.102	-26.102	0.0	-3.747	-2.125
0	12	6	206.469	210.970	210.970	0.0	-4.501	-1.434 *
-7	2	1	50.290	51.866	51.866	0.0	-1.577	-1.365
-5	2	1	44.057	45.124	-45.124	0.0	-1.067	-1.138
-3	2	1	133.771	137.511	137.511	0.0	-3.740	-1.836
3	2	1	112.550	113.074	113.074	0.0	-0.524	-0.300
5	2	1	25.903	24.157	-24.157	0.0	1.746	1.513
7	2	1	41.947	43.471	43.471	0.0	-0.525	-1.202
9	2	1	20.165	20.854	-20.854	0.0	-0.688	-0.366
11	2	1	33.966	32.878	-32.878	0.0	1.089	0.745
-12	3	1	35.368	37.846	-37.846	0.0	-2.478	-1.306
-10	3	1	13.240	7.622	7.622	0.0	6.218	2.658
-8	3	1	23.694	23.238	-23.238	0.0	0.456	0.303
-4	3	1	27.157	25.730	-25.730	0.0	1.426	1.729
-2	3	1	148.347	154.021	-154.021	0.0	-5.674	-2.530
2	3	1	133.606	137.040	-137.040	0.0	-3.433	-1.683
4	3	1	22.474	24.885	-24.885	0.0	-2.412	-1.610
6	3	1	38.616	39.678	-39.678	0.0	-1.062	-0.946
8	3	1	10.685	14.259	-14.259	0.0	-3.575	-1.295
10	3	1	4.732	8.854	-8.854	0.0	-4.122	-0.827
12	3	1	27.585	27.392	-27.392	0.0	0.193	0.054
0	12	0	205.414	210.570	-210.570	0.0	-5.556	-1.779 *
-13	4	1	23.364	22.531	-22.531	0.0	0.833	0.294
-11	4	1	17.256	16.243	-16.243	0.0	1.054	0.456
-9	4	1	6.694	2.297	-2.297	0.0	4.397	1.227
-7	4	1	17.175	16.237	-16.237	0.0	0.927	0.614
-5	4	1	27.091	25.201	-25.201	0.0	1.889	1.978
-3	4	1	16.769	17.959	-17.959	0.0	-1.190	-1.143
-1	4	1	24.156	26.258	-26.258	0.0	-2.152	-2.685
1	4	1	17.329	17.029	-17.029	0.0	0.300	0.277
3	4	1	5.738	11.206	-11.206	0.0	-5.468	-2.079
5	4	1	4.501	5.173	-5.173	0.0	-0.671	-0.161
7	4	1	27.519	25.439	-25.439	0.0	2.080	1.548
9	4	1	17.560	20.357	-20.357	0.0	-2.797	-1.282
11	4	1	16.554	19.479	-19.479	0.0	-2.924	-1.003
12	5	1	71.708	71.241	-71.241	0.0	0.468	0.287
-10	5	1	8.327	14.187	-14.187	0.0	-5.860	-1.535
-8	5	1	11.328	9.554	-9.554	0.0	1.733	0.763
-6	5	1	97.843	100.177	-100.177	0.0	-2.335	-1.461
-4	5	1	92.946	92.202	-92.202	0.0	0.743	0.501
-2	5	1	208.546	213.473	-213.473	0.0	-4.926	-1.571
0	5	1	82.129	83.496	-83.496	0.0	-1.367	-1.052
2	5	1	206.255	210.570	-210.570	0.0	-4.715	-1.505 *
4	5	1	121.124	121.576	-121.576	0.0	-0.451	-0.241
			13.042	13.087	-13.087	0.0	-0.044	-0.023

H	K	L	F(OBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
0	5	1	150.227	155.240	155.240	0.0	-5.020	-2.143
3	5	1	23.249	22.920	22.920	0.0	0.329	0.423
10	5	1	5.160	6.552	6.552	0.0	2.613	0.407
12	5	1	42.600	43.307	43.307	0.0	-0.555	1.558
-13	6	1	51.065	53.529	53.529	0.0	-2.464	-1.256
-11	6	1	10.470	5.555	5.555	0.0	4.915	1.379
-9	6	1	102.756	103.171	103.171	0.0	-0.414	-0.236
-7	6	1	92.204	93.191	93.191	0.0	-0.987	-0.634
-5	6	1	194.103	200.928	200.928	0.0	-6.825	-2.315
-3	6	1	167.622	164.463	164.463	0.0	3.159	1.241
-1	6	1	135.321	140.228	140.228	0.0	-4.907	-2.575
1	6	1	53.868	41.848	41.848	0.0	-0.881	-0.567
3	6	1	71.355	72.022	72.022	0.0	-0.042	-0.023
9	6	1	231.460	235.139	235.139	0.0	-0.627	-0.505
7	6	1	30.784	29.496	29.496	0.0	-3.739	-1.068
9	6	1	82.871	83.752	83.752	0.0	1.288	0.972
11	6	1	25.960	30.602	30.602	0.0	-3.002	-12.382 *
-12	7	1	41.304	41.622	41.622	0.0	-0.319	-0.168
0	12	6	206.485	210.970	210.970	0.0	-4.484	-1.429 *
-10	7	1	16.653	13.251	13.251	0.0	-3.402	1.447
-8	7	1	25.399	30.410	30.410	0.0	-5.011	-0.741
-6	7	1	30.863	33.325	33.325	0.0	-2.442	-1.890
-4	7	1	11.311	5.853	5.853	0.0	-5.458	3.431
-2	7	1	61.552	60.732	60.732	0.0	0.819	0.760
0	7	1	133.854	135.501	135.501	0.0	-1.647	-0.802
2	7	1	13.108	12.451	12.451	0.0	0.657	0.451
4	7	1	65.509	65.321	65.321	0.0	0.188	0.157
6	7	1	65.525	66.366	66.366	0.0	-0.841	-0.659
10	7	1	21.689	20.426	20.426	0.0	0.663	0.293
-13	8	1	7.816	5.757	5.757	0.0	-2.059	0.323
-11	8	1	16.488	16.564	16.564	0.0	-0.476	-0.161
-9	8	1	13.834	11.189	11.189	0.0	2.645	1.056
-7	8	1	13.267	16.571	16.571	0.0	-3.364	-1.359
-5	8	1	14.807	17.053	17.053	0.0	-2.246	-1.150
-3	8	1	16.225	11.660	11.660	0.0	4.505	4.261
-1	8	1	7.832	1.219	1.219	0.0	6.613	3.731
0	12	0	207.310	210.970	210.970	0.0	-3.660	-1.162 *
3	6	1	6.942	2.854	2.854	0.0	4.087	1.554
5	6	1	22.424	24.682	24.682	0.0	-0.250	-0.179
7	8	1	23.018	24.557	24.557	0.0	-1.539	-0.938
11	8	1	11.587	12.236	12.236	0.0	-0.248	-0.067
-12	9	1	24.222	24.713	24.713	0.0	-0.491	-0.156
-10	9	1	13.207	14.493	14.493	0.0	-1.286	-0.415
-6	9	1	13.900	15.408	15.408	0.0	-1.508	-0.749
-4	9	1	20.775	19.422	19.422	0.0	1.354	1.016
-2	9	1	60.546	61.149	61.149	0.0	-0.603	-0.536
0	9	1	93.242	90.574	90.574	0.0	2.668	1.775
2	9	1	66.300	66.516	66.516	0.0	-0.215	-0.181
4	9	1	34.527	33.198	33.198	0.0	1.329	1.156
6	9	1	14.180	12.457	12.457	0.0	1.723	0.877
8	9	1	5.464	1.406	1.406	0.0	7.998	2.768
10	9	1	22.523	21.306	21.306	0.0	1.217	0.689
-11	10	1	16.785	18.678	18.678	0.0	-1.892	-0.605

H	K	L	F(OBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
-2	10	1	19.755	20.708	-20.788	0.0	-1.035	-0.525
-7	10	1	19.011	19.725	19.723	0.0	-0.712	-0.405
0	14	0	207.046	210.570	210.570	0.0	-3.924	-1.247 *
-5	10	1	29.828	31.177	-31.177	0.0	-1.350	-1.201
-3	10	1	55.359	58.991	58.991	0.0	0.368	0.328
-1	10	1	34.857	34.121	-34.121	0.0	0.730	0.723
1	10	1	5.474	1.029	-1.029	0.0	4.446	1.563
3	10	1	47.701	49.674	49.674	0.0	-1.973	-1.843
5	10	1	34.923	34.566	-34.566	0.0	0.357	0.260
7	10	1	24.964	23.052	23.052	0.0	1.911	1.338
9	10	1	14.230	15.535	-15.535	0.0	-1.306	-0.475
11	10	1	18.731	17.664	17.664	0.0	1.067	0.436
-12	11	1	11.427	3.733	3.733	0.0	7.693	1.804
-10	11	1	11.575	14.439	-14.439	0.0	-2.864	-0.744
-8	11	1	16.027	12.218	12.218	0.0	3.809	1.966
-6	11	1	19.935	18.7C	-18.7C	0.0	1.227	0.826
-4	11	1	13.6E5	13.716	-13.716	0.0	-0.030	-0.016
-2	11	1	30.636	29.357	-29.357	0.0	1.239	1.133
0	11	1	2.490	5.810	-5.810	0.0	-3.320	-0.616
2	11	1	54.473	54.701	-54.701	0.0	-0.223	-0.200
6	11	1	16.423	16.528	-16.528	0.0	-0.505	-0.262
0	12	C	207.277	210.570	210.570	0.0	-3.693	-1.173 *
10	11	1	16.043	14.344	-14.344	0.0	1.699	0.716
-11	12	1	9.745	12.600	12.600	0.0	-2.856	-0.591
-7	12	1	16.868	15.713	15.713	0.0	1.155	0.571
-5	12	1	18.764	19.861	19.861	0.0	-1.097	-0.613
-3	12	1	19.176	18.941	18.941	0.0	0.235	0.158
-1	12	1	26.678	29.374	29.374	0.0	-2.696	-2.160
1	12	1	32.532	34.843	34.843	0.0	-2.312	-1.920
3	12	1	19.500	15.884	15.884	0.0	3.621	2.590
5	12	1	16.983	19.824	19.824	0.0	-2.841	-1.353
7	12	1	18.451	14.555	14.555	0.0	3.896	2.441
9	12	1	13.059	9.445	9.445	0.0	3.614	1.357
-10	13	1	13.042	2.523	2.523	0.0	10.520	3.332 *
-8	13	1	8.228	2.077	-2.077	0.0	6.150	1.840
-6	13	1	7.321	8.252	-8.252	0.0	-0.931	-0.253
-4	13	1	33.950	32.812	32.812	0.0	1.138	1.035
-2	13	1	42.920	44.443	-44.443	0.0	-1.524	-1.333
0	13	1	35.450	35.435	35.435	0.0	0.015	0.013
2	13	1	35.434	36.117	-36.117	0.0	-0.683	-0.611
0	12	0	207.359	210.570	210.570	0.0	-3.610	-1.146 *
4	13	1	19.061	17.292	17.292	0.0	1.769	1.115
6	13	1	14.477	13.170	-13.170	0.0	1.307	0.557
8	13	1	13.224	13.576	13.576	0.0	-0.353	-0.120
10	13	1	15.268	10.547	-10.547	0.0	4.322	1.811
-9	14	1	28.063	30.997	-30.997	0.0	-2.934	-1.386
-7	14	1	31.328	30.886	30.886	0.0	0.442	0.323
-5	14	1	74.257	77.662	-77.662	0.0	-3.365	-2.319
-3	14	1	36.418	38.789	38.789	0.0	-0.371	-0.318
-1	14	1	31.542	33.526	-33.526	0.0	-1.984	-1.496
1	14	1	45.650	47.220	-47.220	0.0	-1.531	-1.274
3	14	1	20.973	23.704	23.704	0.0	-2.730	-1.633
5	14	1	42.695	41.889	-41.889	0.0	0.206	0.158

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
7	14	1	9.052	8.054	0.0	0.0	0.598	0.270
9	14	1	32.532	32.884	-32.884	0.0	-0.352	-0.157
-13	15	1	7.502	14.507	14.507	0.0	-7.005	-1.127
-8	15	1	11.014	9.709	9.709	0.0	1.306	0.370
-6	15	1	19.605	19.445	19.445	0.0	0.159	0.081
-9	15	1	14.703	17.555	17.555	0.0	-2.848	-1.249
-2	15	1	51.642	52.883	52.883	0.0	-1.241	-1.031
0	12	3	20.5879	210.970	210.970	0.0	-5.094	-1.528 *
0	15	1	51.741	51.606	51.606	0.0	0.135	0.113
2	15	1	25.640	26.676	-26.676	0.0	-1.036	-0.733
6	19	1	5.787	5.543	5.543	0.0	0.244	0.053
8	15	1	11.097	10.815	10.815	0.0	0.281	0.085
13	15	1	11.971	11.659	11.659	0.0	0.311	0.084
-9	10	1	35.022	35.604	35.604	0.0	-0.583	-0.335
-7	16	1	24.403	21.320	21.320	0.0	2.577	1.531
-5	16	1	60.480	62.759	62.759	0.0	-2.279	-1.631
-3	16	1	50.603	51.446	51.446	0.0	-0.843	-0.680
-1	16	1	66.416	66.356	66.356	0.0	0.060	0.045
1	16	1	50.438	50.296	50.296	0.0	0.143	0.123
3	16	1	45.014	44.379	44.379	0.0	0.635	0.509
5	10	1	55.451	59.337	59.337	0.0	-0.886	-0.643
7	16	1	30.586	32.021	32.021	0.0	-1.435	-0.816
9	16	1	38.830	37.650	37.650	0.0	1.150	0.697
-9	17	1	44.858	46.389	46.389	0.0	-1.991	-1.384
-4	17	1	10.206	11.875	11.875	0.0	-1.669	-0.509
3	12	3	206.716	210.970	210.970	0.0	-4.254	-1.355 *
-2	17	1	112.550	110.586	110.586	0.0	1.645	0.879
0	17	1	55.253	56.699	-56.699	0.0	-1.446	-1.132
2	17	1	64.454	66.795	66.795	0.0	-2.341	-1.630
-5	13	1	74.356	75.553	75.553	0.0	-1.157	-0.745
6	17	1	81.437	79.375	79.375	0.0	2.062	1.302
-9	18	1	34.576	37.184	37.184	0.0	-2.607	-1.325
-7	18	1	74.116	77.698	-77.698	0.0	-3.583	-2.188
-5	13	1	74.356	75.553	75.553	0.0	-1.157	-0.745
-3	18	1	6.991	3.519	3.519	0.0	3.472	0.965
-1	18	1	13.356	9.601	9.601	0.0	3.754	1.722
1	18	1	21.237	22.274	-22.274	0.0	-1.037	-0.560
3	18	1	10.355	12.319	-12.319	0.0	-1.964	-0.582
5	18	1	65.492	63.957	63.957	0.0	1.535	1.054
7	18	1	39.325	36.148	-36.148	0.0	3.177	2.037
-4	19	1	6.002	10.353	-16.353	0.0	-10.351	-1.903 *
-2	19	1	33.637	34.432	34.432	0.0	-0.796	-0.544
0	19	1	35.351	34.344	-34.344	0.0	1.007	0.776
6	12	0	267.837	210.970	210.970	0.0	-3.132	-0.952 *
4	19	1	18.286	17.618	-17.618	0.0	0.668	0.311
6	19	1	25.020	27.579	27.579	0.0	1.441	0.870
-7	20	1	15.714	20.113	20.113	0.0	-4.400	-1.248
-5	20	1	6.777	7.874	-7.874	0.0	-1.097	-0.234
-3	20	1	15.730	14.858	14.858	0.0	0.872	0.339
-1	20	1	2.984	2.132	2.132	0.0	0.853	0.141
1	20	1	12.628	11.638	11.638	0.0	1.190	0.456
3	20	1	16.571	15.147	15.147	0.0	1.424	0.626
5	20	1	13.191	14.410	-14.410	0.0	-1.219	-0.428
7	20	1	26.950	21.281	21.281	0.0	-0.291	-0.113

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-6	21	1	11.460	1.628	-1.628	0.0	3.832	2.769
-4	21	1	1.929	8.911	8.911	0.0	-6.982	-0.355
-2	21	1	45.956	45.299	45.299	0.0	1.791	1.269
0	21	1	26.448	27.168	27.168	0.0	-0.720	-0.427
2	21	1	33.406	32.604	32.604	0.0	0.802	0.562
4	21	1	10.701	3.180	3.180	0.0	7.521	2.338
6	21	1	16.439	12.347	12.347	0.0	-23.562	1.589
8	22	1	25.739	23.562	23.562	0.0	2.177	0.928
-5	22	1	19.127	19.324	19.324	0.0	-0.197	-0.079
6	14	0	207.837	210.970	210.970	0.0	-3.132	-0.952 *
-1	22	1	15.021	1.895	1.895	0.0	13.126	5.672 *
1	22	1	10.272	14.128	14.128	0.0	-3.856	-0.985
3	24	1	20.833	14.741	14.741	0.0	0.067	4.112
-4	23	1	9.695	12.716	12.716	0.0	-3.020	-0.641
-2	23	1	4.897	5.014	5.014	0.0	-0.117	-0.019
0	23	1	18.434	17.411	17.411	0.0	1.023	0.417
2	23	1	1.500	9.665	9.665	0.0	-6.164	-0.917
-1	24	1	7.436	2.689	2.689	0.0	4.748	0.890
-12	0	2	48.427	46.315	46.315	0.0	1.611	1.128
-10	0	2	80.167	77.510	77.510	0.0	-2.356	-0.569
-4	0	2	163.549	166.529	166.529	0.0	-2.979	-1.196
-2	0	2	102.650	97.451	97.451	0.0	5.240	3.278
0	0	2	276.660	279.617	279.617	0.0	-0.810	-0.564
2	0	2	141.158	139.469	139.469	0.0	1.689	0.780
0	12	0	208.349	213.970	213.970	0.0	-2.621	-0.828 *
4	3	2	214.120	222.703	222.703	0.0	-8.584	-2.643
6	0	2	56.424	57.833	57.833	0.0	-1.409	-1.155
8	0	2	75.188	75.597	75.597	0.0	-0.810	-0.564
10	0	2	71.560	70.463	70.463	0.0	1.077	0.715
-11	1	2	34.543	31.502	31.502	0.0	2.642	2.214
-9	1	2	32.565	32.282	32.282	0.0	0.283	0.239
-7	1	2	103.929	167.854	167.854	0.0	-3.926	-1.550
-5	1	2	29.432	28.054	28.054	0.0	1.378	1.349
-3	1	2	5.877	3.592	3.592	0.0	6.285	4.222
-1	1	2	26.957	22.394	22.394	0.0	-1.437	-1.521
1	1	2	115.212	112.376	112.376	0.0	6.834	3.710
3	1	2	65.155	63.748	63.748	0.0	1.447	1.231
5	1	2	34.148	33.805	33.805	0.0	0.342	0.281
0	12	0	209.404	210.570	210.570	0.0	-1.566	-0.492 *
-6	2	2	28.146	27.328	27.328	0.0	0.818	0.757
-4	2	2	11.047	10.631	10.631	0.0	0.416	0.245
-2	2	2	13.867	11.923	11.923	0.0	1.943	1.632
0	2	2	25.013	23.075	23.075	0.0	1.938	2.193
2	2	2	7.222	3.962	3.962	0.0	3.260	1.438
4	2	2	18.566	17.826	17.826	0.0	0.740	0.504
-13	3	2	9.234	13.605	13.605	0.0	-4.372	-0.872
-11	3	2	14.048	12.125	12.125	0.0	1.924	0.742
-9	3	2	61.106	63.349	63.349	0.0	-2.242	-1.738
-7	3	2	86.383	87.543	87.543	0.0	-1.159	-0.785
-5	3	2	15.318	20.662	20.662	0.0	-5.344	-3.267
-3	3	2	19.226	13.325	13.325	0.0	5.900	6.543
-1	3	2	3.034	6.464	6.464	0.0	-3.430	-0.915
1	3	2	79.524	77.739	77.739	0.0	1.785	1.372

H	K	L	F(UVS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
3	3	2	8.063	c.014	6.014	0.0	2.049	0.713
5	3	2	23.452	30.474	30.474	0.0	-1.982	-1.382
7	3	2	66.119	66.331	66.331	0.0	-0.212	-0.161
6	12	3	207.953	210.570	210.570	0.0	-3.017	-0.954 *
-12	4	2	44.882	43.158	43.158	0.0	1.723	1.058
-10	4	2	39.688	38.554	38.554	0.0	1.134	0.903
-8	4	2	5.778	2.422	2.422	0.0	7.356	3.053
-6	4	2	84.565	86.618	86.618	0.0	-1.053	-0.721
-4	4	2	67.108	66.172	66.172	0.0	0.930	0.803
4	4	2	75.517	75.628	75.628	0.0	-0.788	-0.607
6	4	2	90.044	91.596	91.596	0.0	-1.553	-0.581
8	4	2	5.457	3.570	3.570	0.0	5.527	1.923
10	4	2	21.583	21.559	21.559	0.0	0.024	0.012
-9	5	2	36.506	37.293	37.293	0.0	-0.489	0.363
-7	5	2	41.386	42.105	42.105	0.0	-0.719	-0.581
-5	5	2	24.386	23.232	23.232	0.0	-2.32	-0.952
-3	5	2	29.432	26.502	26.502	0.0	2.930	3.286
0	12	0	207.590	210.570	210.570	0.0	-3.380	-1.071 *
-1	5	2	63.646	63.124	63.124	0.0	0.522	0.476
1	5	2	81.354	79.687	79.687	0.0	1.607	1.241
3	5	2	33.818	28.504	28.504	0.0	4.214	4.134
5	5	2	31.559	30.848	30.848	0.0	0.711	0.558
7	5	2	58.072	38.925	38.925	0.0	-0.853	-0.632
9	5	2	19.308	16.864	16.864	0.0	2.444	1.403
11	5	2	5.959	13.761	13.761	0.0	-3.742	-0.959
-8	6	2	17.247	18.423	18.423	0.0	-1.176	-0.538
-6	6	2	22.128	23.154	23.154	0.0	-2.026	-0.672
-6	6	2	19.044	22.446	22.446	0.0	-3.402	-2.262
0	6	2	5.540	10.341	10.341	0.0	-4.801	-1.581
2	6	2	9.464	12.261	12.261	0.0	-2.797	-1.366
4	6	2	5.276	10.075	10.075	0.0	-4.798	-1.204
6	6	2	25.449	24.940	24.940	0.0	0.469	0.384
3	6	2	23.743	27.077	27.077	0.0	-3.334	-1.946
10	6	2	15.351	15.575	19.875	0.0	-4.524	-1.631
-15	7	2	27.948	25.378	25.378	0.0	2.570	1.399
0	12	3	208.431	210.970	210.970	0.0	-2.539	-0.802 *
-11	7	2	26.957	26.369	26.369	0.0	0.588	0.287
-9	7	2	19.638	20.558	20.558	0.0	-0.921	-0.493
-5	7	2	34.355	34.844	34.844	0.0	-0.449	-0.386
-3	7	2	38.187	38.459	38.459	0.0	-0.272	-0.252
-1	7	2	41.815	40.666	40.666	0.0	1.749	1.813
1	7	2	18.813	18.350	18.350	0.0	0.463	0.316
3	7	2	9.451	8.098	-8.098	0.0	1.333	0.540
5	7	2	8.393	13.512	13.512	0.0	-5.119	-1.416
9	7	2	18.137	14.228	14.228	0.0	3.909	2.168
11	7	2	15.351	13.653	13.653	0.0	1.597	0.720
-12	8	2	15.400	15.253	15.253	0.0	0.148	0.046
-10	8	2	5.613	11.544	11.544	0.0	-1.931	-0.531
-6	8	2	21.237	20.587	20.587	0.0	0.657	0.458
-4	8	2	18.599	17.845	17.845	0.0	0.754	0.454
-2	8	2	56.577	55.564	55.564	0.0	1.013	0.934
0	8	2	90.011	87.043	-87.043	0.0	2.968	2.015
2	8	2	86.152	84.241	84.241	0.0	1.912	1.318

H	K	L	F(OBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
0	12	0	208.052	210.970	0.0	-2.918	-0.923	*
4	3	2	43.343	42.446	-42.446	0.0	1.397	1.277
6	9	2	16.291	15.759	15.759	0.0	0.532	0.295
8	8	2	12.234	6.086	-6.086	0.0	6.149	3.143
10	8	2	11.971	3.804	-3.804	0.0	8.167	3.346
-9	9	2	17.066	15.740	15.740	0.0	1.326	0.688
-7	9	2	43.480	43.416	-43.416	0.0	0.064	0.057
-5	9	2	17.841	19.085	19.085	0.0	-1.245	-0.755
-3	9	2	85.328	84.661	-84.661	0.0	0.467	0.323
-1	9	2	12.251	13.430	10.430	0.0	1.821	0.960
1	9	2	42.573	39.569	-39.569	0.0	2.604	2.394
3	9	2	71.527	74.566	-74.566	0.0	-3.039	-2.302
5	9	2	20.110	21.589	21.589	0.0	-1.473	-0.780
7	9	2	41.551	39.555	-39.555	0.0	2.046	1.520
-12	10	2	8.838	5.420	5.420	0.0	3.418	0.712
-10	10	2	26.662	27.018	27.018	0.0	-0.356	-0.210
-8	10	2	38.682	38.664	38.664	0.0	-0.018	0.015
-6	10	2	22.787	21.113	21.113	0.0	1.675	1.193
-4	10	2	53.439	53.601	53.601	0.0	-0.162	-0.139
0	12	0	208.563	210.970	210.970	0.0	-2.407	-0.760
-2	10	2	31.879	31.803	31.803	0.0	-0.524	-0.460
0	10	2	64.486	66.210	66.210	0.0	-1.724	-1.395
2	10	2	43.216	43.622	43.622	0.0	-0.406	-0.352
4	10	2	75.089	75.873	75.873	0.0	-0.784	-0.565
6	10	2	17.000	16.316	16.316	0.0	0.684	0.335
8	10	2	21.946	19.994	19.994	0.0	2.853	1.638
10	10	2	12.004	8.661	8.661	0.0	3.343	1.061
-11	11	2	38.006	38.840	38.840	0.0	-0.834	-0.471
-9	11	2	9.552	7.338	7.338	0.0	1.714	0.557
-7	11	2	134.348	135.927	135.927	0.0	-1.578	-0.730
-5	11	2	17.851	17.720	17.720	0.0	0.137	0.051
-3	11	2	115.941	116.138	116.138	0.0	-0.191	-0.103
1	11	2	95.238	93.072	93.072	0.0	2.166	1.354
3	11	2	136.475	137.054	137.054	0.0	-0.579	-0.267
5	11	2	16.307	14.693	-14.693	0.0	1.614	0.927
7	11	2	46.844	49.540	49.540	0.0	-2.696	-2.042
9	11	2	6.315	3.713	3.713	0.0	2.602	0.557
-12	12	2	26.497	23.643	-23.643	0.0	2.854	1.155
-10	12	2	14.263	12.919	12.919	0.0	1.343	0.498
0	12	0	267.788	210.970	210.970	0.0	-3.182	-1.008 *
-8	12	2	17.890	19.648	19.648	0.0	-1.758	-0.851
-6	12	2	82.904	83.487	83.487	0.0	-0.583	-0.395
-4	12	2	29.399	26.783	26.783	0.0	1.616	2.216
-2	12	2	127.440	129.635	-129.635	0.0	-2.196	-1.080
0	12	2	195.504	198.645	198.645	0.0	-3.140	-1.049
2	12	2	15.763	16.026	-16.026	0.0	-0.263	-0.130
4	12	2	65.565	70.491	70.491	0.0	-0.927	-0.687
6	12	2	29.844	28.585	-28.585	0.0	1.259	0.925
8	12	2	30.042	29.523	29.523	0.0	0.519	0.337
10	12	2	15.516	13.673	13.673	0.0	1.843	0.670
-11	13	2	2.193	8.551	8.551	0.0	-6.358	-0.728
-9	13	2	17.263	10.047	-10.047	0.0	7.216	4.142
-7	13	2	36.769	37.136	37.136	0.0	-0.366	-0.257

H	K	L	F(OBS)	F(CALC)	A1CALC	B1CALC	DELTA F	DELTA/SIGMA
-5	13	2	54.874	52.897	-52.897	0.0	1.977	1.645
-3	13	2	31.856	32.922	32.922	0.0	-1.067	-0.843
-1	13	2	62.376	64.515	-64.515	0.0	-2.139	-1.739
1	13	2	12.185	14.745	-14.745	0.0	-2.560	-1.068
3	13	2	42.540	42.630	42.630	0.0	-0.089	-0.074
5	13	2	43.579	43.265	-43.265	0.0	0.314	0.263
7	13	2	14.850	10.847	-10.847	0.0	4.009	1.957
0	12	0	407.667	210.570	210.570	0.0	-3.363	-1.066 *
9	13	2	14.757	16.142	-16.142	0.0	-1.384	-0.495
-8	14	2	8.426	8.495	8.495	0.0	-0.070	-0.020
-4	14	2	1.955	2.365	2.365	0.0	-0.369	-0.065
-2	14	2	24.617	22.216	22.216	0.0	2.402	1.924
6	14	2	4.563	2.329	-2.329	0.0	2.634	0.646
2	14	2	22.655	21.870	21.870	0.0	0.735	0.583
4	14	2	8.129	9.647	9.647	0.0	-1.519	-0.488
8	14	2	10.140	3.505	-3.505	0.0	6.635	2.438
-11	15	2	3.083	10.010	-10.010	0.0	-6.927	-0.751
-9	15	2	25.475	23.159	23.159	0.0	2.316	1.232
-7	15	2	28.773	29.623	-29.623	0.0	0.155	0.104
-5	15	2	28.772	31.123	31.123	0.0	-2.352	-1.467
-3	15	2	38.080	37.487	-37.487	0.0	0.601	0.513
-1	15	2	27.272	26.029	26.029	0.0	1.243	0.938
1	15	2	3.578	5.894	-5.894	0.0	-2.316	-0.442
3	15	2	27.404	27.217	-27.217	0.0	0.187	0.125
5	15	2	26.744	27.219	27.219	0.0	-0.475	-0.306
0	12	0	2.085	210.970	210.970	0.0	-2.885	-0.912 *
7	15	2	18.643	21.559	-21.559	0.0	-2.910	-1.237
9	15	2	14.361	16.525	16.525	0.0	-2.165	-0.737
-4	16	2	16.472	13.571	-13.571	0.0	2.501	1.499
-2	16	2	10.324	15.898	15.898	0.0	-0.425	0.232
0	16	2	38.022	38.325	-38.325	0.0	-0.302	-0.231
2	16	2	28.393	28.021	28.021	0.0	0.372	0.279
4	16	2	24.073	25.704	-25.704	0.0	-1.631	-0.867
6	16	2	8.558	5.786	5.786	0.0	2.771	0.866
8	16	2	6.490	4.732	-4.732	0.0	1.764	0.384
-7	17	2	11.130	5.134	5.134	0.0	5.995	2.306
-5	17	2	9.481	5.363	5.363	0.0	4.118	1.379
-3	17	2	7.568	5.629	-5.629	0.0	1.939	0.541
-1	17	2	7.865	6.068	6.068	0.0	1.197	0.373
0	17	2	207.161	210.970	210.970	0.0	-1.210 *	-1.210 *
-2	18	2	20.611	19.995	19.995	0.0	0.616	0.331
2	18	2	22.350	20.610	20.610	0.0	1.742	1.057
4	18	2	8.656	10.533	10.533	0.0	-1.877	-0.495
6	18	2	21.682	21.625	21.625	0.0	0.058	0.028
-7	19	2	29.820	30.166	-30.166	0.0	-0.339	-0.181
-5	19	2	6.315	5.078	5.078	0.0	1.237	0.268
-3	19	2	19.654	19.329	-19.329	0.0	0.325	0.165
1	19	2	23.162	23.981	-23.981	0.0	4.182	3.618
3	19	2	1.253	3.650	-3.650	0.0	-2.397	-0.310
5	19	2	13.069	5.220	-5.220	0.0	7.790	3.394
-8	20	2	5.870	2.310	-2.310	0.0	3.560	0.550
-6	20	2	14.939	13.139	13.139	0.0	1.800	0.680

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-4	20	2	36.110	34.258	-34.258	0.0	1.852	1.271
-2	26	2	12.878	9.445	9.445	0.0	3.433	1.305
0	12	0	269.058	210.570	210.570	0.0	-1.912	-0.602 *
0	20	2	21.386	21.409	-21.409	0.0	-0.024	-0.011
2	20	2	20.644	24.186	24.186	0.0	-3.543	-1.382
4	20	2	49.350	50.541	-50.541	0.0	-1.191	-0.716
6	20	2	24.634	26.173	26.173	0.0	-1.539	-0.636
-7	21	2	12.861	16.495	-10.455	0.0	2.366	0.674
-3	21	2	25.253	24.281	24.281	0.0	1.012	0.473
3	21	2	18.325	19.136	19.136	0.0	-0.801	-0.325
5	21	2	28.047	30.758	30.758	0.0	-2.711	-1.160
-6	22	2	17.379	19.581	19.581	0.0	-2.602	-0.773
-4	22	2	32.103	32.735	32.735	0.0	-0.631	-0.333
-2	22	2	9.102	8.159	8.159	0.0	0.942	0.232
0	22	2	53.258	51.660	51.660	0.0	1.597	1.163
2	22	2	15.054	14.651	14.651	0.0	4.443	2.307
4	22	2	44.305	44.523	44.523	0.0	-0.219	-0.130
-3	23	2	26.283	22.683	22.683	0.0	3.600	1.840
-1	23	2	18.071	18.342	-18.342	0.0	-0.271	-0.104
1	23	2	22.226	24.619	24.619	0.0	-2.392	-1.055
0	12	0	267.359	210.570	210.570	0.0	-3.610	-1.146 *
-13	6	3	17.313	13.540	-13.540	0.0	3.773	1.741
-9	0	3	15.862	14.953	-14.953	0.0	0.909	0.478
-7	0	3	0.214	4.187	4.187	0.0	-3.973	-0.520
-3	6	3	18.721	20.570	-20.570	0.0	-1.839	-1.357
-1	0	3	3.149	6.423	6.423	0.0	2.726	0.600
1	0	3	17.181	14.309	14.309	0.0	2.873	2.150
3	0	3	14.345	16.516	-16.516	0.0	-2.571	-1.146
7	0	3	10.454	8.512	-8.512	0.0	1.942	0.683
9	0	3	5.474	11.566	11.566	0.0	-6.092	-1.058
-12	1	3	7.238	1.338	-1.338	0.0	5.901	1.338
-10	1	3	6.991	5.521	5.521	0.0	1.470	0.410
-8	1	3	7.050	3.047	3.047	0.0	4.043	1.215
-2	1	3	25.722	25.220	-25.220	0.0	0.502	0.428
0	1	3	31.345	30.918	30.918	0.0	0.427	0.411
2	1	3	32.829	32.132	-32.132	0.0	0.697	0.646
0	12	0	207.376	210.570	210.570	0.0	-3.594	-1.140 *
6	1	3	19.638	17.104	-17.104	0.0	2.533	1.455
8	1	3	5.392	15.260	15.260	0.0	-9.868	-1.722
10	1	3	19.110	16.175	-16.175	0.0	2.935	1.430
-11	2	3	4.4139	11.512	11.512	0.0	-7.373	-1.241
-9	2	3	28.921	26.210	-26.210	0.0	2.710	2.112
-7	2	3	47.685	47.644	47.644	0.0	0.041	0.036
-5	2	3	61.815	62.074	-62.074	0.0	-0.259	-0.219
-3	2	3	106.267	100.645	100.645	0.0	-0.379	-0.234
1	2	3	16.783	7.251	7.251	0.0	3.533	1.769
5	2	3	49.218	50.735	50.735	0.0	-1.486	-1.312
7	2	3	7.865	6.623	6.623	0.0	1.842	0.649
9	2	3	28.838	25.569	25.569	0.0	3.269	2.357
5	2	3	26.990	21.745	-21.745	0.0	-0.750	-0.367

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-12	3	3	21.831	22.096	-22.096	0.0	-0.265	-0.117
-10	3	3	14.906	12.803	12.803	0.0	2.103	1.115
-8	3	3	47.784	48.143	-48.143	0.0	-0.359	-0.362
-6	3	3	9.184	12.531	12.531	0.0	-3.347	-1.183
6	12	0	207.541	210.970	210.970	0.0	-3.429	-1.087 *
-4	3	3	9.943	2.647	2.647	0.0	7.295	3.282
2	3	3	100.217	99.090	-99.090	0.0	1.127	0.700
0	3	3	29.056	27.807	27.807	0.0	1.829	1.731
2	3	3	75.089	75.002	-75.002	0.0	0.087	0.054
4	3	3	8.920	1.160	1.160	0.0	7.760	2.791
6	3	3	56.719	51.219	-51.219	0.0	7.760	2.791
8	3	3	9.910	10.304	-10.304	0.0	-0.394	-0.118
-15	4	3	23.463	26.713	26.713	0.0	-2.750	1.410
-9	4	3	6.513	11.878	11.878	0.0	-5.365	-1.538
-7	4	3	8.739	5.534	-5.534	0.0	3.205	1.130
-5	4	3	7.140	11.467	11.467	0.0	-4.327	-1.228
-3	4	3	14.873	12.128	12.128	0.0	2.744	1.681
-1	4	3	22.968	23.347	23.347	0.0	-0.378	-0.289
1	4	3	19.902	19.801	19.801	0.0	0.101	0.066
3	4	3	15.021	12.593	12.593	0.0	2.029	1.045
5	4	3	14.180	11.547	-11.547	0.0	2.633	1.348
7	4	3	12.845	12.477	12.477	0.0	0.368	0.146
9	4	3	23.117	18.889	18.889	0.0	4.228	2.920
0	12	0	209.338	210.570	210.570	0.0	-1.632	-0.513 *
-12	3	3	68.526	67.711	67.711	0.0	0.815	0.524
-10	5	3	20.924	20.939	20.939	0.0	-0.015	-0.005
-8	5	3	54.593	54.311	54.311	0.0	0.282	0.231
-6	5	3	30.190	29.657	29.657	0.0	1.094	0.862
-4	5	3	24.419	25.120	25.120	0.0	-0.701	-0.563
-2	5	3	181.753	184.924	184.924	0.0	-3.172	-1.143
0	5	3	22.441	22.532	22.532	0.0	-0.091	-0.066
2	5	3	97.414	57.526	97.526	0.0	0.388	0.238
4	5	3	45.426	47.244	-47.344	0.0	-1.913	-1.561
6	5	3	100.029	102.124	102.124	0.0	-1.495	-0.864
8	5	3	35.557	23.493	23.493	0.0	2.064	1.311
10	5	3	23.826	22.644	22.644	0.0	1.182	0.713
-13	6	3	18.747	19.449	19.449	0.0	-0.702	-0.231
-11	6	3	14.256	14.395	14.395	0.0	-0.100	-0.039
-9	6	3	124.043	125.145	125.145	0.0	-1.102	-0.541
-7	6	3	38.2426	82.427	-82.427	0.0	-0.001	-0.001
-5	6	3	105.295	106.336	106.336	0.0	-1.090	-0.632
-3	6	3	38.995	39.307	39.307	0.0	-0.312	-0.274
-1	6	3	206.139	208.124	208.124	0.0	-1.985	-0.634
1	6	3	22.292	21.997	21.997	0.0	0.295	0.239
0	12	0	208.134	210.570	210.570	0.0	-2.836	-0.857 *
3	6	3	84.530	84.127	84.127	0.0	0.410	0.242
-12	7	3	36.621	35.599	35.599	0.0	1.022	0.611
-10	7	3	11.410	0.522	0.522	0.0	10.388	4.907 *
-8	7	3	14.246	15.562	15.562	0.0	-1.716	-0.717
-6	7	3	16.686	16.503	16.503	0.0	0.183	0.101

H	K	L	F(UBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
-4	7	3	31.839	33.356	-33.356	0.0	-1.516	-1.350
-2	7	3	81.024	80.308	80.308	0.0	0.717	0.515
0	7	3	38.731	39.018	-39.018	0.0	-0.287	-0.263
2	7	3	18.500	17.729	17.729	0.0	0.771	0.444
4	7	3	85.267	83.920	-83.920	0.0	-0.654	-0.439
6	7	3	42.145	41.573	41.573	0.0	0.572	0.430
0	7	3	16.685	16.829	-16.829	0.0	1.355	0.617
10	7	3	3.083	1.585	1.585	0.0	1.093	0.162
-2	3	3	16.324	14.756	-14.756	0.0	1.563	0.755
-7	3	3	9.151	6.803	6.803	0.0	2.343	0.957
-5	8	3	16.684	13.527	-13.527	0.0	2.957	1.770
0	12	0	258.069	210.570	-210.570	0.0	-2.901	-0.918 *
-3	6	3	8.772	2.740	2.740	0.0	6.024	2.334
1	6	3	15.532	12.665	-12.665	0.0	2.867	1.326
3	6	3	3.887	10.520	10.520	0.0	-1.640	-0.500
5	6	3	26.002	28.063	-28.063	0.0	-2.061	-1.262
7	8	3	12.729	9.686	9.686	0.0	3.043	1.523
-12	9	3	14.345	18.630	-18.630	0.0	-4.285	-1.317
-15	9	3	24.304	24.163	-24.163	0.0	0.136	0.089
-8	9	3	32.750	31.793	-31.793	0.0	1.002	0.655
-6	9	3	19.489	22.856	-22.856	0.0	-3.367	-1.756
-4	9	3	33.604	34.590	-34.590	0.0	-0.986	-0.798
-2	9	3	52.954	53.829	-53.829	0.0	-0.835	-0.656
0	9	3	57.363	58.372	-58.372	0.0	-1.008	-0.862
2	9	3	35.450	35.527	-35.527	0.0	-0.076	-0.063
4	9	3	30.982	29.548	-29.548	0.0	1.034	0.779
6	9	3	18.731	21.499	-21.499	0.0	-2.768	-1.263
-9	10	3	14.510	14.905	-14.905	0.0	-0.395	-0.155
0	12	0	268.035	210.570	-210.570	0.0	-2.934	-0.928 *
-7	10	3	29.152	29.933	-29.933	0.0	-0.781	-0.538
-5	10	3	56.143	57.182	-57.182	0.0	-1.039	-0.860
-3	10	3	56.852	56.441	-56.441	0.0	0.411	0.347
-1	10	3	6.282	16.901	-16.901	0.0	-4.619	-1.186
1	10	3	18.055	18.457	-18.457	0.0	-0.402	-0.241
3	10	3	20.973	23.751	-23.751	0.0	-2.778	-1.655
5	10	3	4.716	2.703	2.703	0.0	2.013	0.464
9	10	3	16.175	18.560	-18.560	0.0	-2.391	-0.800
-12	11	3	11.057	6.250	6.250	0.0	4.847	1.295
-10	11	3	2.539	5.983	-5.983	0.0	-3.444	-0.506
-4	11	3	5.129	2.380	2.380	0.0	2.748	0.667
-2	11	3	35.005	36.431	-36.431	0.0	-1.426	-1.111
2	11	3	15.367	18.571	-18.571	0.0	-3.203	-1.654
4	11	3	17.775	19.254	-19.254	0.0	-1.450	-0.684
6	11	3	17.577	20.532	-20.532	0.0	-2.955	-1.201
8	11	3	1.179	9.566	9.566	0.0	1.213	0.416
0	12	0	207.310	210.970	-210.970	0.0	-3.660	-1.162 *
-7	12	3	12.713	13.381	-13.381	0.0	-0.669	-0.267
-5	12	3	9.283	5.650	5.650	0.0	3.634	1.344
-3	12	3	15.603	13.782	-13.782	0.0	-0.179	-0.090
-1	12	3	20.017	19.212	19.212	0.0	0.805	0.554
1	12	3	28.551	29.576	-29.576	0.0	-0.985	-0.731
3	12	3	6.654	7.518	-7.518	0.0	-1.223	-0.314
5	12	3	15.073	17.425	-17.425	0.0	-2.354	-0.958

H	K	L	F(UBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
7	12	3	8.079	6.111	6.111	0.0	1.968	0.541
-8	13	3	4.055	6.806	6.806	0.0	3.453	0.618
-6	13	3	7.167	5.273	5.273	0.0	1.853	0.547
-4	13	3	13.867	12.242	12.242	0.0	1.625	0.720
-2	13	3	16.142	14.769	14.769	0.0	1.433	0.829
0	12	3	25.969	28.543	28.543	0.0	-2.574	-1.579
2	15	3	37.544	35.092	35.092	0.0	2.452	1.092
4	13	3	22.210	22.381	22.381	0.0	-0.171	-0.114
6	13	3	15.202	16.850	16.850	0.0	-1.594	-0.673
8	13	3	12.630	10.374	10.374	0.0	2.256	0.842
0	12	0	20.8.233	21.0.570	21.0.570	0.0	-2.737	-0.865 *
-9	14	3	34.340	34.543	34.543	0.0	-0.598	-0.349
-7	14	3	17.659	20.312	20.312	0.0	-2.653	-1.242
-5	14	3	53.175	53.213	53.213	0.0	-0.938	-0.076
-3	14	3	34.923	34.347	34.347	0.0	0.575	0.438
-1	14	3	56.191	50.576	50.576	0.0	-0.385	-0.306
1	14	3	6.843	8.297	8.297	0.0	-1.454	-0.387
5	14	3	28.822	30.801	30.801	0.0	-1.979	-1.043
7	14	3	14.032	10.877	10.877	0.0	3.155	1.326
-10	15	3	12.366	14.664	14.664	0.0	-2.498	-0.644
-8	15	3	11.031	10.025	10.025	0.0	1.006	0.318
-6	15	3	16.291	15.928	15.928	0.0	0.363	0.165
-4	15	3	14.263	11.520	11.520	0.0	2.742	1.440
2	15	3	31.444	29.686	29.686	0.0	1.753	1.328
4	15	3	23.183	20.860	20.860	0.0	2.310	1.087
6	15	3	18.517	15.511	15.511	0.0	3.005	1.387
-9	16	3	31.312	30.546	30.546	0.0	0.366	0.205
6	12	0	208.002	210.570	210.570	0.0	-2.967	-0.939 *
-7	16	3	13.883	9.765	9.765	0.0	4.118	2.071
-5	16	3	49.820	50.752	50.752	0.0	-0.924	-0.668
-3	16	3	30.383	31.081	31.081	0.0	-0.198	-0.130
-1	16	3	59.853	60.417	60.417	0.0	-0.564	-0.410
1	16	3	42.375	43.175	43.175	0.0	-0.799	-0.574
3	16	3	38.555	37.633	37.633	0.0	0.917	0.650
5	16	3	29.119	25.594	25.594	0.0	3.125	2.368
7	16	3	24.354	25.076	25.076	0.0	-0.723	-0.340
-6	17	3	22.325	22.281	22.281	0.0	0.044	0.022
-6	17	3	9.580	10.926	10.926	0.0	-1.346	-0.366
-2	17	3	88.312	85.947	85.947	0.0	2.365	1.471
0	17	3	11.723	11.781	11.781	0.0	-0.058	-0.020
2	17	3	63.259	63.071	63.071	0.0	0.228	0.164
4	17	3	46.839	46.532	46.532	0.0	2.307	1.728
0	17	3	61.782	63.556	63.556	0.0	-1.813	-1.084
-9	18	3	59.678	58.336	58.336	0.0	0.742	0.453
-7	18	3	57.557	56.043	56.043	0.0	1.914	1.294
-5	18	3	22.589	23.544	23.544	0.0	-0.955	-0.511
-3	18	3	20.017	17.579	17.579	0.0	2.438	1.265
0	12	0	208.085	210.570	210.570	0.0	-2.885	-0.913 *
1	18	3	76.439	70.141	70.141	0.0	0.298	0.202
3	18	3	34.444	33.020	33.020	0.0	1.425	1.035
5	18	3	18.302	20.254	20.254	0.0	-1.951	-0.750
-8	19	3	36.786	36.991	36.991	0.0	-0.206	-0.111
			4.0831	3.571	3.571	0.0	1.260	0.214

H	K	L	F(UFS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-4	19	3	11.476	9.747	-9.747	0.0	1.729	0.653
-5	20	3	6.909	5.944	-5.944	0.0	-3.035	-1.000
-3	20	3	14.329	15.329	-15.329	0.0	-1.000	-0.623
1	20	3	7.519	10.150	-10.150	0.0	-2.631	-0.351
3	20	3	6.991	14.560	-14.560	0.0	-7.569	-0.557
-4	21	3	6.282	3.831	-3.831	0.0	2.451	-1.357
-2	21	3	22.490	25.338	-25.338	0.0	-2.846	0.465
0	21	3	10.513	12.070	-12.070	0.0	-2.450	-1.232
2	21	3	10.439	16.814	-16.814	0.0	-0.375	-0.770 *
-3	22	3	18.863	14.521	-14.521	0.0	0.097	0.177
-1	22	3	12.267	13.264	-13.264	0.0	0.055	0.055
-12	0	4	5.557	2.317	-2.317	0.0	3.239	-0.303
-10	0	4	35.665	35.275	-35.275	0.0	0.390	0.663
-8	0	4	22.820	24.760	-24.760	0.0	0.060	0.295
-6	0	4	149.254	153.840	-153.840	0.0	-4.587	0.036
-4	0	4	116.425	117.650	-117.650	0.0	-1.225	-1.953
-2	0	4	57.627	58.771	-58.771	0.0	-1.144	-0.652
0	0	4	169.254	167.103	-167.103	0.0	2.071	-0.949
2	0	4	6.332	1.994	-1.994	0.0	4.338	0.792
4	0	4	149.287	151.441	-151.441	0.0	-2.154	1.148
6	0	4	15.499	14.680	-14.680	0.0	0.819	-0.900
8	0	4	47.256	47.721	-47.721	0.0	-0.465	0.392
-13	1	4	9.382	5.747	-5.747	0.0	3.635	-0.511
-11	1	4	23.941	26.634	-26.634	0.0	-2.693	0.935
-9	1	4	17.906	16.732	-16.732	0.0	1.125	-1.359
-7	1	4	73.324	74.100	-74.100	0.0	0.615	-0.776
0	12	0	207.804	210.970	-210.970	0.0	-3.165	-0.561 *
-5	1	4	7.601	11.594	-11.594	0.0	-3.992	-1.002 *
-3	1	4	130.638	133.751	-133.751	0.0	-3.113	-1.105
-1	1	4	69.268	69.532	-69.532	0.0	-0.664	-1.502
1	1	4	8.656	6.375	-6.375	0.0	2.282	-0.507
3	1	4	65.278	67.051	-67.051	0.0	-1.773	0.742
5	1	4	3.050	11.109	-11.109	0.0	-8.059	-1.345
7	1	4	12.284	13.294	-13.294	0.0	-1.010	-1.311
9	1	4	19.176	20.642	-20.642	0.0	-1.460	-0.343
-12	2	4	3.347	1.691	-1.691	0.0	1.656	-0.599
-10	2	4	11.624	7.431	-7.431	0.0	4.193	0.255
-8	2	4	6.810	7.315	-7.315	0.0	-0.505	1.709
-6	2	4	3.347	10.574	-10.574	0.0	-7.627	-0.133
-4	2	4	8.244	3.801	-3.801	0.0	4.444	-1.421
-2	2	4	8.360	4.830	-4.830	0.0	3.530	1.565
0	2	4	18.813	16.534	-16.534	0.0	1.879	1.156
-11	3	4	13.537	14.378	-14.378	0.0	-0.841	-0.944 *
-9	3	4	16.951	18.203	-18.203	0.0	-1.026	1.346
-7	3	4	18.269	18.538	-18.538	0.0	-5.042	-0.916
-5	3	4	36.637	38.473	-38.473	0.0	-0.268	-0.571
-3	3	4	74.561	75.709	-75.709	0.0	-1.835	-0.138
-1	3	4	50.318	51.646	-51.646	0.0	-1.148	-1.532
				0.0	0.0	0.0	0.829	-0.720

H	K	L	F(OBS)	F(CALC)	A(CALC)	E(CALC)	DELTA_F	DELTA/SIGMA
1	3	4	14.301	12.632	-12.632	0.0	1.730	0.804
3	3	4	40.252	39.345	-39.345	0.0	0.887	0.735
3	3	4	16.142	16.750	-16.750	0.0	-0.603	-0.291
7	3	4	10.932	18.029	-18.029	0.0	-7.098	-1.772
-12	4	4	11.443	10.244	10.244	0.0	1.199	0.341
-8	4	4	15.450	18.202	18.202	0.0	-2.752	-1.184
-6	4	4	15.779	15.370	-15.370	0.0	0.409	0.235
-4	4	4	16.538	18.649	18.649	0.0	-2.107	-1.112
-2	4	4	16.767	18.635	18.635	0.0	0.076	0.061
0	4	4	20.429	17.221	-17.221	0.0	-2.700	-2.114
0	4	4	16.767	18.481	18.481	0.0	-1.812	-1.218
0	12	0	208.134	210.570	210.570	0.0	-2.830	-0.896 *
-11	5	4	17.082	15.274	-15.274	0.0	1.808	0.868
-9	5	4	4.501	0.040	-0.040	0.0	4.461	0.939
-5	5	4	5.013	10.469	10.469	0.0	-5.456	-1.250
-3	5	4	39.490	39.213	-39.213	0.0	0.177	0.158
-1	5	4	9.662	7.780	-7.780	0.0	1.870	0.657
1	5	4	23.150	21.470	-21.470	0.0	1.673	1.047
3	5	4	23.826	23.170	-23.170	0.0	0.656	0.358
5	5	4	17.395	12.691	-12.691	0.0	5.304	2.887
-12	6	4	11.146	13.564	-13.564	0.0	7.582	2.524
-10	6	4	13.207	14.978	-14.978	0.0	-1.771	-0.579
-6	6	4	12.410	15.728	-15.728	0.0	-3.312	-1.249
-4	6	4	4.914	1.304	-1.304	0.0	3.809	0.843
-2	6	4	12.020	8.545	-8.545	0.0	3.475	1.718
0	6	4	5.754	3.035	-3.035	0.0	2.719	0.704
4	6	4	2.341	7.813	-7.813	0.0	-5.471	-0.637
0	12	0	207.854	210.570	210.570	0.0	-3.116	-0.986 *
6	0	4	19.308	21.242	-21.242	0.0	-1.934	-0.991
8	6	4	0.975	16.777	-16.777	0.0	-5.802	-1.715
-11	7	4	19.341	15.265	-15.265	0.0	4.076	2.153
-9	7	4	36.324	36.578	-36.578	0.0	-0.254	-0.180
-7	7	4	23.776	24.023	-24.023	0.0	-0.247	-0.150
-5	7	4	23.166	22.149	-22.149	0.0	1.017	0.721
-3	7	4	16.917	16.250	-16.250	0.0	0.667	0.380
-1	7	4	13.784	12.854	-12.854	0.0	0.930	0.424
1	7	4	25.178	23.147	-23.147	0.0	2.031	1.538
3	7	4	35.417	34.514	-34.514	0.0	0.903	0.741
7	7	4	12.360	12.881	-12.881	0.0	-0.515	-0.165
-12	8	4	30.714	33.362	-33.362	0.0	-2.644	-1.258
-10	8	4	46.556	43.083	-43.083	0.0	3.513	2.698
-8	8	4	4.419	7.114	-7.114	0.0	-2.695	-0.548
-6	8	4	23.513	24.768	-24.768	0.0	-1.256	-0.816
-4	8	4	37.313	39.347	-39.347	0.0	-2.034	-1.671
-2	8	4	1.658	6.393	-6.393	0.0	-4.695	-0.747
0	8	4	8.056	3.414	-3.414	0.0	4.682	1.668
2	8	4	45.045	44.188	-44.188	0.0	0.958	0.761
0	12	0	208.810	210.570	210.570	0.0	-2.159	-0.681 *
4	8	4	66.300	67.656	-67.656	0.0	-1.396	-1.009
6	8	4	44.502	43.099	-43.099	0.0	1.404	1.031
-11	9	4	14.526	16.750	-16.750	0.0	3.776	1.430

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-9	9	4	36.374	37.519	37.519	0.0	-1.205	-0.869
-7	9	4	41.950	42.156	-43.156	0.0	-1.159	-0.835
-5	9	4	12.662	8.820	8.820	0.0	2.838	1.958
-3	9	4	27.124	25.178	-25.178	0.0	1.946	1.433
-1	9	4	7.304	4.023	4.023	0.0	3.281	1.034
1	9	4	47.751	48.791	-48.791	0.0	-1.041	-0.862
3	9	4	11.591	13.167	-13.167	0.0	-1.575	-0.565
5	9	4	5.210	1.337	-1.337	0.0	4.173	0.859
7	9	4	39.952	39.285	-39.285	0.0	0.660	0.436
-13	10	4	16.142	14.058	14.058	0.0	2.084	0.937
-8	10	4	22.935	22.279	22.279	0.0	0.656	0.379
-6	10	4	30.026	29.166	29.166	0.0	0.860	0.654
-4	10	4	38.863	37.486	37.486	0.0	-2.456	-0.775 *
-2	10	4	18.849	21.203	21.203	0.0	-1.754	-1.159
0	10	4	38.860	39.409	39.409	0.0	-0.526	-0.389
2	10	4	14.230	11.658	11.658	0.0	2.571	1.133
0	12	0	26.513	210.970	210.970	0.0	-2.456	-0.775 *
4	10	4	44.387	46.141	46.141	0.0	-1.754	-1.159
6	10	4	25.656	23.639	23.639	0.0	1.967	1.051
-11	11	4	26.399	29.928	29.928	0.0	-0.529	-0.252
-9	11	4	32.202	31.436	-31.436	0.0	0.766	0.502
0	11	4	107.719	107.718	107.718	0.0	0.001	0.001
-5	11	4	13.488	11.512	11.512	0.0	1.976	1.018
-3	11	4	57.760	98.027	98.027	0.0	-0.267	-0.157
-1	11	4	14.790	16.604	-16.604	0.0	-1.314	-0.813
3	11	4	60.958	60.436	60.436	0.0	0.521	0.400
5	11	4	51.675	52.030	52.030	0.0	-0.355	-0.270
-5	11	4	32.021	29.480	29.480	0.0	2.540	1.732
-3	11	4	45.244	44.736	44.736	0.0	0.508	0.338
-1	11	4	14.790	16.604	-16.604	0.0	-1.314	-0.813
-8	12	4	28.954	27.409	-27.409	0.0	1.545	0.938
-6	12	4	41.732	39.440	39.440	0.0	2.293	1.805
-4	12	4	80.431	80.721	80.721	0.0	-0.290	-0.191
-2	12	4	43.216	46.574	-46.574	0.0	-3.757	-2.694
0	12	4	40.199	39.961	39.961	0.0	0.238	0.168
2	12	4	23.348	23.658	-23.658	0.0	-0.310	-0.181
4	12	4	105.345	104.556	104.556	0.0	0.439	0.239
6	12	4	40.549	210.570	210.570	0.0	-2.671	-0.844 *
-9	13	4	32.449	38.980	-38.980	0.0	1.565	1.007
-7	13	4	40.661	40.916	40.916	0.0	-0.255	-0.185
-5	13	4	20.950	18.421	-18.421	0.0	2.569	1.445
-3	13	4	21.435	21.149	21.149	0.0	0.280	0.175
-1	13	4	41.403	38.809	-38.809	0.0	2.594	2.038
3	13	4	11.344	9.168	-9.168	0.0	2.176	0.759
5	13	4	4.600	2.551	-2.551	0.0	2.049	0.383
-10	14	4	10.619	5.283	-5.283	0.0	5.336	1.457
-8	14	4	18.500	13.202	-13.202	0.0	5.298	3.458
-6	14	4	16.324	9.033	-9.033	0.0	7.291	4.904
-2	14	4	18.187	18.615	18.615	0.0	-0.428	-0.219
2	14	4	11.156	10.868	10.868	0.0	0.307	0.057
6	14	4	22.359	18.491	18.491	0.0	3.818	2.067
-9	15	4	27.783	28.260	28.260	0.0	-0.477	-0.241

H	K	L	F(UBS)	F(CALC)	A(CALC)	E(CALC)	DELTA F	DELTA/SIGMA
-7	15	4	26.365	26.546	-26.546	0.0	-0.181	-0.110
0	12	3	207.557	210.570	210.570	0.0	-3.413	-1.082 *
-5	15	4	20.248	20.863	20.863	0.0	-0.612	-0.283
-3	15	4	20.182	20.343	20.343	0.0	-0.161	-0.087
-1	15	4	22.259	22.423	22.423	0.0	-0.163	-0.097
1	15	4	14.675	17.227	17.227	0.0	-2.552	-0.948
5	15	4	3.891	5.713	9.713	0.0	-5.821	-0.856
-6	10	4	17.360	15.908	15.908	0.0	1.092	0.517
-4	16	4	18.559	20.015	20.015	0.0	-1.416	-0.602
2	15	4	19.902	17.735	17.735	0.0	2.166	1.187
4	16	4	46.578	39.640	-39.640	0.0	0.938	0.608
-7	17	4	9.365	5.259	-9.259	0.0	0.106	0.025
-3	17	4	14.807	17.819	17.819	0.0	-3.012	-1.104
1	17	4	19.704	16.689	-16.689	0.0	3.014	1.454
3	17	4	16.266	16.649	16.649	0.0	-5.843	-1.445
-5	18	4	13.570	12.610	12.610	0.0	0.960	0.369
0	12	3	209.288	210.570	210.570	0.0	-1.681	-0.528 *
-4	16	4	6.051	2.755	2.755	0.0	3.296	0.644
-2	13	4	13.290	11.795	11.795	0.0	1.495	0.533
0	18	4	7.502	9.910	9.910	0.0	-2.414	-0.548
2	18	4	6.084	8.038	8.038	0.0	-2.004	-0.397
-5	19	4	13.554	12.619	12.619	0.0	0.935	0.337
-3	19	4	30.240	29.677	-29.677	0.0	1.163	0.738
1	19	4	18.451	15.891	-15.891	0.0	2.560	1.063
-2	20	4	15.038	9.553	9.553	0.0	5.454	2.679
0	20	4	33.043	33.496	-33.496	0.0	-0.453	-0.243
-11	0	5	3.970	10.475	10.475	0.0	-1.506	-0.377
-9	0	5	13.125	10.109	-10.109	0.0	3.016	1.108
-7	0	5	11.888	4.500	4.500	0.0	7.389	3.689
-5	0	5	8.689	2.700	-2.700	0.0	5.989	1.962
-3	0	5	14.625	12.731	-12.731	0.0	1.395	1.007
-1	0	5	16.948	13.127	-13.127	0.0	-2.179	-0.775
3	0	5	7.552	6.418	-6.418	0.0	1.133	0.257
5	0	5	1.863	1.682	1.682	0.0	0.181	0.026
0	12	0	207.590	210.970	210.970	0.0	-3.380	-1.371 *
7	0	5	15.763	14.863	-14.863	0.0	0.900	0.320
-10	1	5	3.562	4.423	4.423	0.0	-0.861	-0.139
-8	1	5	8.768	1.450	1.450	0.0	7.558	2.403
-6	1	5	4.758	4.016	4.016	0.0	0.782	0.160
-4	1	5	1.830	6.106	6.106	0.0	-4.276	-0.650
-2	1	5	13.933	10.559	-10.559	0.0	2.974	1.427
0	1	5	16.587	17.422	17.422	0.0	-0.835	-0.436
2	1	5	13.521	10.264	-10.264	0.0	3.257	1.469
4	1	5	12.037	7.151	7.151	0.0	4.886	1.927
6	1	5	17.857	15.115	-15.115	0.0	2.742	1.197
-11	2	5	13.191	9.246	9.246	0.0	3.945	1.841
-9	2	5	19.935	17.234	-17.234	0.0	2.701	1.489
-7	2	5	32.449	31.238	31.238	0.0	1.211	0.899
-5	2	5	45.871	47.841	-47.841	0.0	-1.970	-1.460
-3	2	5	57.677	57.241	57.241	0.0	0.430	0.345
-1	2	5	15.516	15.320	-15.320	0.0	0.196	0.100
1	2	5	20.215	16.182	16.182	0.0	4.033	2.257
3	2	5	2.678	7.585	7.585	0.0	-5.907	-0.835

H	K	L	F(UBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
5	2	3	5.161	13.125	13.155	0.0	-7.994	-1.226
0	12	3	208.316	210.570	210.570	0.0	-2.654	-0.338 *
7	2	5	42.128	40.934	40.934	0.0	1.194	0.203
-12	3	5	13.059	17.283	-17.283	0.0	-4.224	-1.116
-10	3	5	28.371	27.470	27.470	0.0	1.401	0.829
-8	3	5	37.699	38.992	-38.992	0.0	-1.893	-1.283
-6	3	5	4.050	3.084	3.084	0.0	0.972	0.190
-4	3	5	10.437	1.264	1.264	0.0	9.173	3.821
-2	3	5	36.637	35.302	35.302	0.0	1.336	1.139
0	3	5	10.388	11.639	11.639	0.0	-1.251	-0.398
2	3	5	50.719	50.487	-50.487	0.0	0.232	0.166
4	3	5	16.324	17.619	17.619	0.0	-1.556	-0.600
6	3	5	30.850	31.624	-31.624	0.0	-0.174	-0.101
-9	4	5	13.257	13.065	13.065	0.0	0.192	0.065
-5	4	5	7.321	8.137	8.137	0.0	-0.316	-0.218
-3	4	5	4.848	4.773	-4.773	0.0	0.074	0.016
-1	4	5	3.512	7.569	7.569	0.0	-4.057	-0.701
1	4	5	5.352	10.063	10.063	0.0	-4.671	-0.957
3	4	5	22.721	20.536	20.536	0.0	2.185	1.165
5	4	5	8.492	10.438	-10.438	0.0	-1.947	-0.488
0	12	0	209.025	210.570	210.570	0.0	-1.945	-0.613 *
-10	5	5	12.795	5.433	5.433	0.0	7.363	3.524
-8	5	5	68.444	69.055	69.055	0.0	-0.611	-0.408
-6	5	5	24.700	21.575	21.575	0.0	2.725	1.939
-4	5	5	11.591	10.364	10.364	0.0	1.227	0.514
-2	5	5	61.935	63.783	63.783	0.0	-2.253	-1.040
6	5	5	23.925	26.529	26.529	0.0	-3.015	-1.735
2	5	5	56.919	58.658	58.658	0.0	-1.738	-1.002
4	5	5	38.435	39.216	-39.216	0.0	-0.781	-0.541
0	5	5	45.409	48.725	48.725	0.0	-3.315	-2.134
-11	6	5	8.261	9.229	-9.229	0.0	-0.968	-0.228
-9	6	5	97.051	56.619	56.619	0.0	0.433	0.244
-7	6	5	11.591	11.630	-11.630	0.0	-0.039	-0.013
-5	6	5	65.674	65.942	65.942	0.0	-0.269	-0.195
-3	6	5	47.899	48.934	-48.934	0.0	-1.035	-0.800
-1	6	5	133.260	134.562	134.562	0.0	-1.302	-0.600
1	6	5	23.727	22.183	22.183	0.0	1.544	1.050
3	6	5	34.609	35.260	35.260	0.0	-0.650	-0.416
5	6	5	32.202	32.722	32.722	0.0	-0.550	-0.328
-10	7	5	7.914	10.741	-10.741	0.0	-2.826	-0.573
-8	7	5	35.137	34.027	34.027	0.0	1.110	0.801 *
0	12	6	208.645	210.570	210.570	0.0	-2.324	-0.733 *
-4	7	5	20.060	21.611	-21.611	0.0	-1.544	-0.742
-2	7	5	7.205	10.320	10.320	0.0	-3.114	-0.750
0	7	5	6.463	8.569	8.569	0.0	-2.505	-0.570
2	7	5	48.723	48.789	48.789	0.0	-0.065	-0.050
4	7	5	58.930	58.356	-58.356	0.0	0.573	0.401
6	7	5	12.910	11.527	11.527	0.0	1.384	0.467
-11	6	5	15.681	1.570	-1.570	0.0	13.711	10.927 *
-7	8	5	3.759	0.338	-0.338	0.0	3.421	0.644
-5	8	5	10.107	9.511	-9.511	0.0	0.536	0.163
-1	8	5	8.508	15.605	-15.605	0.0	-6.498	-1.713
3	8	5	10.289	13.714	13.714	0.0	-3.425	-0.900

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-1	6	9	5	26.942	24.873	24.873	0.0	2.069
-6	9	5	22.210	25.040	-25.040	0.0	-2.830	1.176
-9	9	5	5.837	12.340	12.340	0.0	-6.503	-1.307
-4	9	5	9.943	11.927	11.927	0.0	-1.984	-1.363
0	12	6	209.437	210.570	210.570	0.0	-0.614	-0.614 *
-2	9	5	7.123	11.772	11.772	0.0	-1.533	-0.482 *
0	9	5	26.975	28.838	28.838	0.0	-4.649	-1.158
2	9	5	33.966	34.549	34.549	0.0	-1.862	-1.039
4	9	5	34.148	35.260	35.260	0.0	-1.112	-1.755
-9	16	5	14.510	15.179	15.179	0.0	-2.389	-0.689
-1	10	5	15.285	17.674	17.674	0.0	-0.223	-0.920
-7	10	5	4.501	7.440	7.440	0.0	-2.938	-0.513
-5	10	5	32.021	36.846	36.846	0.0	-1.174	-0.810
-3	10	5	26.711	29.780	29.780	0.0	-3.069	-1.983
-1	16	5	19.473	18.195	18.195	0.0	1.368	0.354
1	10	5	4.501	7.440	7.440	0.0	0.402	0.070
-10	11	5	10.025	1.607	1.607	0.0	3.693	1.763
-6	11	5	2.623	6.004	6.004	0.0	-0.711	-0.135
-6	11	5	2.688	7.110	7.110	0.0	-4.423	-0.693
-2	11	5	12.037	9.101	9.101	0.0	2.930	1.122
0	11	5	3.743	3.341	3.341	0.0	0.402	0.070
2	11	5	15.862	12.169	12.169	0.0	3.693	1.763
0	12	0	208.035	210.970	210.970	0.0	-2.934	-0.928 *
-9	12	5	10.503	8.526	8.526	0.0	1.977	0.544
-7	12	5	14.032	14.285	14.285	0.0	-0.253	-0.103
-5	12	5	8.053	6.372	6.372	0.0	1.724	0.467
-3	12	5	9.332	2.779	2.779	0.0	6.554	2.091
1	12	5	24.045	21.800	21.800	0.0	0.246	0.136
3	12	5	4.963	6.960	6.960	0.0	-1.997	-0.356
-8	13	5	12.680	10.925	10.925	0.0	1.545	0.647
-6	13	5	22.853	19.780	19.780	0.0	3.073	1.804
-4	13	5	3.413	3.840	3.840	0.0	-0.427	-0.613
-2	13	5	7.222	9.208	9.208	0.0	-2.046	-0.490
0	13	5	16.571	15.020	15.020	0.0	0.0	0.0
2	13	5	22.853	19.780	19.780	0.0	1.755	0.427
4	13	5	10.142	11.932	11.932	0.0	4.211	1.745
-1	14	5	16.713	9.073	9.073	0.0	1.644	0.479
-3	14	5	12.130	19.814	19.814	0.0	-7.678	-2.059
-3	14	5	54.544	50.231	50.231	0.0	-1.687	-1.083
-1	14	5	37.577	34.757	34.757	0.0	2.700	2.143
1	14	5	26.358	20.641	20.641	0.0	-0.243	-0.143
3	14	5	8.294	13.022	13.022	0.0	-4.728	-0.942
0	12	0	207.590	210.570	210.570	0.0	7.036	3.693
-3	15	5	21.501	21.720	21.720	0.0	-3.380	-1.071 *
-6	15	5	18.665	18.197	18.197	0.0	-0.227	-0.094
-4	15	5	16.241	11.539	11.539	0.0	4.468	0.210
-2	15	5	20.083	17.838	17.838	0.0	4.302	2.217
0	15	5	21.237	21.328	21.328	0.0	2.245	1.160
2	15	5	12.680	12.840	12.840	0.0	-0.091	-0.045
-7	10	5	13.290	7.618	7.618	0.0	-0.160	-0.046
-5	10	5	29.415	33.628	33.628	0.0	5.672	2.015
-3	16	5	15.747	12.932	12.932	0.0	-1.212	-0.660
-1	16	5	38.863	38.790	38.790	0.0	2.844	1.185
1	16	5	22.886	24.253	24.253	0.0	0.073	0.046
							-1.367	-0.735

H	K	L	F(UBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-6	17	5	11.740	3.349	3.349	0.0	8.350	2.706
-4	17	5	14.050	4.061	-4.067	0.0	5.431	4.758
-2	17	5	42.304	44.035	42.765	0.0	0.019	0.012
0	17	5	8.442	2.640	2.848	0.0	5.594	1.467
-3	18	5	49.037	50.753	-50.753	0.0	-1.716	-1.054
-10	0	6	82.113	60.617	80.617	0.0	1.496	0.685
-8	0	6	36.951	30.233	-36.233	0.0	0.717	0.471
-6	0	6	31.361	28.724	28.724	0.0	2.637	1.854
-4	0	6	31.381	28.572	28.572	0.0	-1.185	-0.747
4	0	6	20.627	21.922	-21.922	0.0	-1.292	-0.578
4	6	6	95.129	57.368	97.369	0.0	1.760	0.946
-9	1	6	24.700	24.433	-24.433	0.0	0.266	0.137
-7	1	6	47.470	47.022	47.022	0.0	0.448	0.319
-5	1	6	17.544	17.130	-17.130	0.0	0.413	0.178
-3	1	6	66.856	69.329	69.329	0.0	-0.473	-0.322
-1	1	6	8.508	7.478	-7.478	0.0	1.030	0.276
1	1	6	26.101	24.570	24.570	0.0	1.131	0.620
3	1	6	7.420	10.796	-16.756	0.0	-9.376	-1.675
-6	2	6	15.262	8.405	-8.405	0.0	6.797	3.016
-2	2	6	8.327	1.901	1.901	0.0	6.425	1.842
0	2	6	6.727	4.305	-4.368	0.0	2.359	0.588
2	2	6	15.021	11.350	-11.350	0.0	3.085	1.020
4	2	6	15.741	11.265	-11.265	0.0	4.481	2.201
-9	3	6	22.375	19.955	19.955	0.0	2.420	1.407
0	12	0	267.722	210.570	210.570	0.0	-3.248	-1.029 *
-7	3	6	26.283	24.564	-24.964	0.0	1.318	0.789
-5	3	6	23.859	24.722	24.722	0.0	-0.863	-0.460
-3	3	6	24.321	23.534	-23.534	0.0	0.787	0.468
-1	3	6	20.314	20.072	20.072	0.0	0.242	0.125
1	3	6	22.259	21.596	-21.596	0.0	0.664	0.323
3	3	6	9.778	10.850	10.850	0.0	-1.072	-0.287
-10	4	6	30.504	31.906	-31.906	0.0	-1.402	-0.751
-8	4	6	37.099	35.638	35.638	0.0	-0.792	-0.208
-6	4	6	9.267	10.053	10.053	0.0	0.0	0.0
-4	4	6	15.885	19.090	19.090	0.0	0.795	0.457
0	4	6	9.382	4.404	-4.404	0.0	4.978	1.522
2	4	6	9.168	5.558	5.558	0.0	3.209	0.923
4	4	6	25.503	28.190	-28.190	0.0	1.461	0.957
-9	5	6	29.155	26.701	-26.701	0.0	-2.682	-1.389
-7	5	6	22.523	22.133	22.133	0.0	0.391	0.224
-5	5	6	20.677	20.458	-20.458	0.0	0.218	0.103
-1	5	6	10.789	7.405	7.405	0.0	-3.645	-0.629
1	5	6	29.155	1.222	-1.222	0.0	9.561	3.257
0	12	0	208.019	210.570	210.570	0.0	1.494	0.814 *
3	5	6	13.059	10.667	10.667	0.0	-2.951	-0.934 *
-10	0	6	8.046	8.457	8.457	0.0	2.391	0.929
-8	0	6	9.670	6.243	-6.243	0.0	0.411	0.102
-6	0	6	7.453	3.127	3.127	0.0	0.435	0.057
-4	0	6	4.386	5.288	-5.288	0.0	4.326	1.066
0	6	6	13.107	7.332	7.332	0.0	-0.902	-0.163
				2.775	2.775	0.0	2.775	0.803