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Crystal Structures of $CaNiSi_2O_6$ and $CaCoSi_2O_6$ and some crystal-chemical relations in C2/c clinopyroxenes

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To be deposited: Structure measurements

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Crystal structures of $CaNiSi_2O_6$ and $CaCoSi_2O_6$ and some crystal chemical relations in *C2/c* clinopyroxenes

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Table 5a. $CaNiSi_2O_6$: Observed and Calculated Structure Factors

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
0	0	2	200.160	213.541	-213.450	-6.209	-13.381	-11.5594	1.0000	
0	0	4	145.332	142.207	142.085	5.900	3.125	2.5125	1.0000	
0	0	6	61.177	60.275	-60.040	-5.326	.902	2.4278	1.0000	
0	0	8	63.743	64.926	64.745	4.846	-1.184	-2.5371	1.0000	
0	2	0	46.440	48.274	48.263	1.020	-1.834	-4.0056	1.0000	
0	2	1	10.945	11.798	11.022	4.206	-.853	-2.0152	1.0000	
0	2	2	49.083	42.766	42.756	-.912	6.318	19.2457	1.0000	
0	2	3	49.006	47.949	-47.766	-4.183	1.057	4.2183	1.0000	
0	2	4	27.772	27.481	27.464	.966	.291	.8022	1.0000	
0	2	5	44.833	43.669	43.480	4.062	1.164	3.3698	1.0000	
0	2	6	6.030 *	.857	-.107	-.850	5.173	3.1853	1.0000	**
0	2	7	25.898	25.506	-25.221	-3.801	.392	.6581	1.0000	
0	2	8	20.309	19.433	19.415	.853	.876	1.1138	1.0000	
0	4	0	31.539	33.333	-33.220	-2.739	-1.794	-7.6908	1.0000	
0	4	1	62.862	60.513	-60.490	1.688	2.348	5.3304	1.0000	
0	4	2	86.012	85.899	85.854	2.769	.113	.1662	1.0000	
0	4	3	19.169	18.861	18.781	-1.730	.308	.7279	1.0000	
0	4	4	30.874	29.901	-29.791	-2.560	.973	2.6188	1.0000	
0	4	5	5.235 *	2.553	-1.859	1.751	2.682	1.5838	1.0000	**
0	4	6	48.444	48.347	48.285	2.453	.097	.2333	1.0000	
0	4	7	12.275	10.239	10.100	-1.680	2.036	1.8859	1.0000	
0	4	8	20.421	21.740	-21.633	-2.149	-1.318	-1.5899	1.0000	
0	6	0	136.392	146.518	-146.452	-4.370	-10.126	-9.0169	1.0000	
0	6	1	45.991	45.018	45.018	.180	.972	3.6311	1.0000	
0	6	2	132.003	136.171	136.103	4.311	-4.168	-4.1595	1.0000	
0	6	3	31.133	29.959	-29.959	-.136	1.173	3.2339	1.0000	
0	6	4	46.829	44.618	-44.443	-3.954	2.211	6.2415	1.0000	
0	6	5	25.138	24.884	24.884	.090	.254	.4983	1.0000	
0	6	6	39.452	39.132	38.958	3.680	.320	.6730	1.0000	
0	6	7	11.541	13.213	-13.213	-.005	-1.672	-1.3351	1.0000	
0	8	0	10.962	11.169	-11.076	-1.431	-.206	-.2778	1.0000	
0	8	1	11.264	11.146	-10.288	-4.287	.119	.1620	1.0000	
0	8	2	31.729	31.013	30.978	1.459	.716	1.8838	1.0000	
0	8	3	32.817	32.075	31.790	4.269	.742	1.7901	1.0000	
0	8	4	16.067	16.089	-16.031	-1.362	-.022	-.0300	1.0000	
0	8	5	33.457	31.684	-31.415	-4.123	1.773	3.5378	1.0000	
0	8	6	33.094	32.245	32.218	1.328	.848	1.5343	1.0000	
0	8	7	28.731	27.776	27.503	3.887	.955	1.4552	1.0000	
0	10	0	97.726	98.388	98.268	4.871	-.662	-1.0798	1.0000	
0	10	1	5.537 *	7.201	6.979	-1.775	-1.664	-.9582	1.0000	**
0	10	2	81.451	79.778	-79.636	-4.752	1.674	4.7258	1.0000	
0	10	3	9.813	9.452	9.280	1.795	.362	.3171	1.0000	
0	10	4	73.504	72.947	72.806	4.541	.557	1.4009	1.0000	
0	10	5	10.591	9.958	-9.805	-1.740	.632	.4978	1.0000	
0	10	6	54.439	55.251	-55.093	-4.170	-.812	-1.6200	1.0000	
0	12	0	57.696	57.121	57.055	2.735	.575	1.3875	1.0000	
0	12	1	6.332 *	5.784	5.361	2.172	.548	.2922	1.0000	**
0	12	2	38.614	38.210	-38.119	-2.638	.404	.8198	1.0000	
0	12	3	9.234	8.065	-7.775	-2.142	1.170	.8205	1.0000	
0	12	4	16.663	14.990	14.788	2.454	1.674	1.8452	1.0000	
0	12	5	16.128	14.864	14.715	2.093	1.264	1.2509	1.0000	
0	14	-3	8.466 *	6.584	-6.181	2.267	1.882	1.0472	1.0000	**
0	14	-2	10.297	7.678	7.674	.241	2.619	1.8375	1.0000	

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
0	14	-1	20.611		17.926	17.784	-2.250	2.685	3.4159	1.0000	
0	14	0	13.735		11.602	-11.599	-.260	2.133	2.0076	1.0000	
0	14	1	19.920		17.926	-17.784	2.250	1.994	2.4822	1.0000	
0	14	2	8.241	*	7.678	7.674	.241	.563	.3104	1.0000	**
0	14	3	4.639	*	6.584	6.181	-2.267	-1.945	-.5879	1.0000	**
1	1	-8	5.399	*	3.742	-2.854	2.420	1.657	.6503	1.0000	**
1	1	-7	4.051	*	1.465	.707	1.283	2.586	.8936	1.0000	**
1	1	-6	8.060		10.367	-10.010	-2.698	-2.307	-1.8548	1.0000	
1	1	-5	9.735		8.308	-8.201	-1.328	1.427	1.6860	1.0000	
1	1	-4	30.148		29.069	-28.932	2.820	1.079	3.2014	1.0000	
1	1	-3	13.303		13.063	12.995	1.329	.240	.5453	1.0000	
1	1	-2	39.218		36.848	-36.717	-3.101	2.371	11.9322	1.0000	
1	1	-1	23.203		24.418	-24.384	-1.289	-1.215	-5.8615	1.0000	
1	1	0	50.716		51.894	51.792	3.243	-1.178	-2.4789	1.0000	
1	1	1	11.040		11.207	11.142	1.199	-.167	-.4202	1.0000	
1	1	2	106.874		106.417	-106.363	-3.378	.458	.5094	1.0000	
1	1	3	14.538		15.930	-15.891	-1.118	-1.392	-3.0979	1.0000	
1	1	4	38.545		36.315	36.167	3.284	2.229	6.9743	1.0000	
1	1	5	4.708	*	4.197	-4.078	.992	.511	.2831	1.0000	**
1	1	6	37.422		36.139	-35.998	-3.197	1.282	2.9689	1.0000	
1	1	7	17.234		15.852	15.829	-.859	1.381	1.7196	1.0000	
1	1	8	30.373		30.740	30.592	3.015	-.367	-.5823	1.0000	
1	3	-8	4.483	*	7.418	7.412	.299	-2.935	-.9157	1.0000	**
1	3	-7	71.966		72.476	72.313	4.848	-.509	-1.2277	1.0000	
1	3	-6	30.908		30.402	-30.400	-.413	.506	1.0841	1.0000	
1	3	-5	122.821		128.827	-128.720	-5.251	-6.006	-6.8838	1.0000	
1	3	-4	13.726		12.962	12.956	.387	.764	1.3208	1.0000	
1	3	-3	145.427		166.040	165.952	5.399	-20.613	-18.2151	1.0000	
1	3	-2	57.955		58.583	-58.581	-.454	-.628	-1.5472	1.0000	
1	3	-1	127.460		144.737	-144.639	-5.329	-17.277	-14.8154	1.0000	
1	3	0	8.163		8.675	8.667	.379	-.512	-.8980	1.0000	
1	3	1	29.828		33.801	33.419	5.069	-3.973	-17.0322	1.0000	
1	3	2	42.268		40.714	-40.712	-.390	1.554	6.6621	1.0000	
1	3	3	58.396		57.324	-57.119	-4.835	1.072	4.1362	1.0000	
1	3	4	6.194	*	8.037	8.031	.300	-1.843	-1.4714	1.0000	**
1	3	5	46.526		46.939	46.724	4.486	-.413	-1.1376	1.0000	
1	3	6	13.813		14.897	-14.894	-.269	-1.084	-1.2676	1.0000	
1	3	7	40.108		40.204	-39.998	-4.070	-.096	-.1957	1.0000	
1	3	8	6.738	*	5.717	5.714	.184	1.021	.4563	1.0000	**
1	5	-8	32.895		36.149	-35.928	-3.997	-3.254	-5.3059	1.0000	
1	5	-7	4.190	*	1.100	.334	1.048	3.090	1.0337	1.0000	**
1	5	-6	21.466		22.720	22.300	4.351	-1.254	-2.0443	1.0000	
1	5	-5	10.064		11.939	-11.884	-1.144	-1.875	-1.9381	1.0000	
1	5	-4	40.056		42.244	-41.977	-4.746	-2.188	-6.3327	1.0000	
1	5	-3	6.712		9.941	9.872	1.169	-3.229	-3.0642	1.0000	
1	5	-2	49.187		50.426	50.175	5.017	-1.239	-4.7798	1.0000	
1	5	-1	42.440		42.872	-42.854	-1.219	-.431	-1.7824	1.0000	
1	5	0	133.627		141.940	-141.841	-5.313	-8.313	-8.2251	1.0000	
1	5	1	19.367		19.605	19.571	1.154	-.238	-.6565	1.0000	
1	5	2	112.627		112.572	112.445	5.337	.056	.0672	1.0000	
1	5	3	37.637		39.030	-39.013	-1.147	-1.392	-4.2415	1.0000	
1	5	4	91.170		90.397	-90.245	-5.236	.773	1.4663	1.0000	
1	5	5	7.256	*	7.820	7.755	1.010	-.564	-.4241	1.0000	**

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
1	5	6	60.633	60.996	60.795	4.952	-.363	-.8756	1.0000	
1	5	7	4.345 *	5.972	-5.900	-.919	-1.626	-.5230	1.0000	**
1	5	8	60.538	60.269	-60.091	-4.626	.269	.5456	1.0000	
1	7	-7	42.535	43.722	-43.575	-3.575	-1.186	-2.2515	1.0000	
1	7	-6	17.424	17.806	-17.755	1.347	-.382	-.4807	1.0000	
1	7	-5	51.174	51.521	51.381	3.796	-.347	-.8736	1.0000	
1	7	-4	16.171	16.694	16.630	-1.459	-.523	-.8295	1.0000	
1	7	-3	83.231	85.423	-85.331	-3.977	-2.192	-4.3014	1.0000	
1	7	-2	24.041	23.532	-23.482	1.540	.508	1.2523	1.0000	
1	7	-1	70.178	70.686	70.576	3.928	-.507	-1.3659	1.0000	
1	7	0	24.058	23.756	-23.695	-1.712	.302	.7757	1.0000	
1	7	1	84.967	85.964	-85.877	-3.857	-.997	-1.7750	1.0000	
1	7	2	15.022	15.108	15.007	1.745	-.086	-.1464	1.0000	
1	7	3	46.976	46.307	46.168	3.592	.668	1.9342	1.0000	
1	7	4	13.796	12.391	-12.266	-1.756	1.404	1.8472	1.0000	
1	7	5	45.611	44.894	-44.769	-3.345	.717	1.6933	1.0000	
1	7	6	4.172 *	2.181	1.374	1.694	1.991	.6680	1.0000	**
1	7	7	8.440 *	9.404	8.942	2.911	-.965	-.5527	1.0000	**
1	9	-7	28.092	29.197	-29.069	-2.734	-1.105	-1.5990	1.0000	
1	9	-6	9.485	5.030	4.945	-.920	4.455	3.0883	1.0000	
1	9	-5	41.637	42.010	41.911	2.880	-.373	-.7856	1.0000	
1	9	-4	12.267	13.622	-13.587	.976	-1.355	-1.4391	1.0000	
1	9	-3	62.559	62.607	-62.537	-2.961	-.048	-.1326	1.0000	
1	9	-2	3.524 *	1.240	.589	-1.091	2.284	.9086	1.0000	**
1	9	-1	14.754	13.779	13.496	2.776	.976	1.5061	1.0000	
1	9	0	3.438 *	1.189	.281	1.155	2.249	.9135	1.0000	**
1	9	1	3.481 *	3.019	-1.461	-2.642	.462	.1857	1.0000	**
1	9	2	16.577	14.258	-14.204	-1.236	2.319	3.6781	1.0000	
1	9	3	18.167	18.510	-18.350	2.427	-.343	-.5300	1.0000	
1	9	4	7.800 *	8.014	7.918	1.236	-.213	-.1419	1.0000	**
1	9	5	12.733	12.844	-12.629	-2.336	-.111	-.1050	1.0000	
1	9	6	14.297	11.852	-11.787	-1.237	2.445	2.3196	1.0000	
1	11	-6	7.265 *	6.318	-5.593	-2.939	.947	.4454	1.0000	**
1	11	-5	4.431 *	2.430	2.287	.821	2.002	.6331	1.0000	**
1	11	-4	4.812 *	4.634	-3.402	3.146	.178	.0667	1.0000	**
1	11	-3	22.702	22.769	-22.749	-.961	-.067	-.1069	1.0000	
1	11	-2	10.228	11.483	-10.973	-3.387	-1.255	-1.1094	1.0000	
1	11	-1	14.253	15.031	14.999	.977	-.777	-.9471	1.0000	
1	11	0	31.858	31.481	31.277	3.580	.378	.8096	1.0000	
1	11	1	39.693	39.325	-39.311	-1.069	.368	.8352	1.0000	
1	11	2	43.054	42.338	-42.178	-3.673	.716	1.6246	1.0000	
1	11	3	22.037	22.091	22.068	1.000	-.054	-.0811	1.0000	
1	11	4	30.632	29.427	29.206	3.605	1.205	2.1127	1.0000	
1	11	5	31.979	32.729	-32.714	-.998	-.750	-1.2225	1.0000	
1	13	-4	13.899	12.955	12.802	1.987	.944	.8345	1.0000	
1	13	-3	46.958	47.451	47.270	4.141	-.493	-.9843	1.0000	
1	13	-2	21.000	18.714	-18.595	-2.105	2.286	3.1129	1.0000	
1	13	-1	59.683	60.238	-60.092	-4.186	-.555	-1.2601	1.0000	
1	13	0	32.558	30.928	30.850	2.197	1.630	2.9956	1.0000	
1	13	1	39.218	38.320	38.111	4.000	.898	1.7625	1.0000	
1	13	2	33.577	32.409	-32.335	-2.197	1.168	2.1126	1.0000	
1	13	3	47.839	47.793	-47.639	-3.834	.046	.0923	1.0000	
1	13	4	23.203	21.793	21.692	2.099	1.410	1.8759	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
1	15	-1	24.239	23.584	-23.446	-2.553	.655	.8615	1.0000	
1	15	0	30.986	29.441	-29.286	-3.010	1.545	2.3851	1.0000	
1	15	1	4.630 *	5.241	-4.672	2.375	-.611	-.1846	1.0000	**
2	0	-8	63.682	63.495	63.316	4.759	.187	.4093	1.0000	
2	0	-6	65.332	63.900	-63.701	-5.028	1.433	4.0449	1.0000	
2	0	-4	36.730	35.436	35.063	5.130	1.294	4.2807	1.0000	
2	0	-2	17.087	18.152	-17.394	-5.191	-1.066	-3.4270	1.0000	
2	0	0	67.760	66.191	65.986	5.206	1.569	2.4210	1.0000	
2	0	2	131.934	138.606	-138.510	-5.171	-6.672	-4.9829	1.0000	
2	0	4	56.219	53.932	53.711	4.878	2.287	7.7861	1.0000	
2	0	6	33.301	33.791	-33.484	-4.548	-.490	-1.0321	1.0000	
2	0	8	14.746	15.255	14.689	4.115	-.509	-.4753	1.0000	
2	2	-8	6.436 *	3.578	-3.502	.735	2.857	1.3179	1.0000	**
2	2	-7	38.985	40.265	40.053	4.131	-1.280	-2.6947	1.0000	
2	2	-6	3.697 *	1.274	-1.040	-.736	2.423	.9167	1.0000	**
2	2	-5	72.329	73.081	-72.936	-4.593	-.751	-2.1749	1.0000	
2	2	-4	4.570 *	2.655	-2.563	.693	1.915	1.2739	1.0000	**
2	2	-3	146.248	160.332	160.254	5.008	-14.084	-9.2639	1.0000	
2	2	-2	4.397 *	5.238	5.197	-.650	-.841	-.7848	1.0000	**
2	2	-1	160.458	193.151	-193.081	-5.177	-32.692	-30.7687	1.0000	
2	2	0	45.032	43.345	-43.341	.579	1.687	5.0075	1.0000	
2	2	1	141.799	161.665	161.581	5.185	-19.865	-16.9093	1.0000	
2	2	2	27.945	26.044	26.038	-.563	1.901	7.0989	1.0000	
2	2	3	108.922	111.947	-111.834	-5.024	-3.025	-3.1270	1.0000	
2	2	4	50.327	49.293	-49.291	.482	1.034	3.3243	1.0000	
2	2	5	100.655	101.459	101.346	4.786	-.805	-1.1943	1.0000	
2	2	6	24.594	23.526	23.521	-.516	1.067	1.9006	1.0000	
2	2	7	69.340	68.913	-68.775	-4.354	.427	.9892	1.0000	
2	2	8	18.581	18.101	-18.094	.511	.480	.5290	1.0000	
2	4	-8	12.215	11.544	-11.360	-2.053	.671	.5395	1.0000	
2	4	-7	4.164 *	3.535	2.950	1.948	.628	.2115	1.0000	**
2	4	-6	20.153	19.670	19.552	2.150	.484	.8000	1.0000	
2	4	-5	11.627	11.837	-11.640	-2.147	-.209	-.2633	1.0000	
2	4	-4	19.091	20.568	-20.453	-2.169	-1.477	-3.1094	1.0000	
2	4	-3	68.243	70.433	70.393	2.396	-2.190	-5.5113	1.0000	
2	4	-2	4.587 *	5.102	4.641	2.121	-.515	-.4355	1.0000	**
2	4	-1	55.268	54.963	-54.909	-2.447	.305	.8031	1.0000	
2	4	0	11.791	11.115	-10.918	-2.086	.676	1.4764	1.0000	
2	4	1	55.536	53.139	53.081	2.471	2.398	7.9303	1.0000	
2	4	2	24.127	22.747	-22.661	1.973	1.380	4.0957	1.0000	
2	4	3	26.796	26.064	-25.955	-2.381	.732	1.9713	1.0000	
2	4	4	18.313	17.766	17.665	-1.891	.547	1.0384	1.0000	
2	4	5	42.924	42.860	42.796	2.329	.065	.1623	1.0000	
2	4	6	25.786	24.976	-24.915	1.752	.809	1.4198	1.0000	
2	4	7	24.049	23.739	-23.644	-2.126	.310	.4540	1.0000	
2	6	-8	32.126	32.156	-31.992	-3.244	-.029	-.0467	1.0000	
2	6	-7	16.646	17.693	17.693	-.080	-1.047	-1.2124	1.0000	
2	6	-6	24.974	24.584	24.354	3.354	.390	.6736	1.0000	
2	6	-5	3.637 *	.940	.927	.158	2.696	1.0405	1.0000	**
2	6	-4	3.412 *	5.872	4.827	-3.345	-2.460	-1.0099	1.0000	**
2	6	-3	13.804	15.241	15.240	-.135	-1.436	-2.3754	1.0000	
2	6	-2	33.344	33.591	-33.428	3.308	-.247	-.7727	1.0000	
2	6	-1	16.586	15.440	15.438	.214	1.146	2.5506	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
2	6	0	9.243	8.865	-8.211	-3.341	.378	.5149	1.0000	
2	6	1	16.603	16.431	16.430	-.171	.172	.3694	1.0000	
2	6	2	26.753	25.825	25.614	3.289	.929	2.4429	1.0000	
2	6	3	10.141	9.293	9.290	.232	.849	1.0345	1.0000	
2	6	4	20.222	19.824	-19.571	-3.159	.399	.7324	1.0000	
2	6	5	6.392 *	7.654	7.651	-.191	-1.261	-.7229	1.0000	**
2	6	6	5.848 *	7.237	-6.630	2.902	-1.389	-.6330	1.0000	**
2	6	7	4.414 *	1.899	1.886	.223	2.515	.7977	1.0000	**
2	8	-7	26.148	26.355	-26.022	-4.172	-.206	-.3060	1.0000	
2	8	-6	23.574	25.457	25.424	1.294	-1.883	-2.8676	1.0000	
2	8	-5	68.191	71.136	70.979	4.721	-2.944	-7.4096	1.0000	
2	8	-4	34.908	35.135	-35.107	-1.399	-.227	-.5266	1.0000	
2	8	-3	88.595	90.713	-90.572	-5.053	-2.118	-3.4050	1.0000	
2	8	-2	34.597	34.534	34.504	1.437	.063	.1690	1.0000	
2	8	-1	124.816	134.793	134.688	5.316	-9.977	-8.7497	1.0000	
2	8	0	36.316	36.646	-36.617	-1.452	-.330	-.9548	1.0000	
2	8	1	90.781	90.974	-90.823	-5.241	-.193	-.3235	1.0000	
2	8	2	19.220	19.236	19.186	1.387	-.015	-.0292	1.0000	
2	8	3	99.367	99.589	99.456	5.159	-.222	-.3834	1.0000	
2	8	4	12.189	14.127	-14.066	-1.312	-1.938	-2.0214	1.0000	
2	8	5	73.876	73.210	-73.050	-4.841	.665	1.6380	1.0000	
2	8	6	4.362 *	6.029	5.910	1.190	-1.666	-.5343	1.0000	**
2	10	-6	43.382	43.829	-43.659	-3.864	-.447	-.8487	1.0000	
2	10	-5	27.453	27.481	27.408	2.005	-.028	-.0467	1.0000	
2	10	-4	40.402	41.316	41.122	3.991	-.914	-1.9591	1.0000	
2	10	-3	26.097	25.317	-25.229	-2.107	.780	1.4563	1.0000	
2	10	-2	37.663	37.580	-37.363	-4.033	.083	.1963	1.0000	
2	10	-1	51.848	51.504	51.455	2.247	.344	.9257	1.0000	
2	10	0	30.459	30.383	30.120	3.987	.076	.1695	1.0000	
2	10	1	18.089	16.162	-16.018	-2.151	1.927	3.0557	1.0000	
2	10	2	26.667	25.043	-24.742	-3.871	1.624	3.2408	1.0000	
2	10	3	33.379	32.313	32.241	2.156	1.066	2.1649	1.0000	
2	10	4	12.958	11.621	11.032	3.653	1.337	1.3340	1.0000	
2	10	5	19.203	18.953	-18.846	-2.011	.250	.2989	1.0000	
2	10	6	12.940	11.641	-11.128	-3.417	1.299	1.0668	1.0000	
2	12	-5	21.622	19.947	-19.802	-2.402	1.675	2.0624	1.0000	
2	12	-4	18.702	16.996	-16.879	1.989	1.706	2.0574	1.0000	
2	12	-3	52.729	49.886	49.815	2.676	2.842	6.2083	1.0000	
2	12	-2	27.375	26.520	26.448	-1.950	.855	1.4772	1.0000	
2	12	-1	40.264	36.713	-36.611	-2.724	3.551	7.6125	1.0000	
2	12	0	14.461	13.486	-13.343	1.960	.975	1.0851	1.0000	
2	12	1	57.877	55.076	55.005	2.807	2.801	6.6168	1.0000	
2	12	2	8.060 *	3.959	-3.441	-1.958	4.101	2.6374	1.0000	**
2	12	3	34.545	32.344	-32.233	-2.669	2.201	3.9207	1.0000	
2	12	4	4.492 *	1.906	.378	1.868	2.586	.8048	1.0000	**
2	14	-3	37.845	39.090	38.976	2.984	-1.245	-2.1513	1.0000	
2	14	-2	15.411	15.485	-15.485	-.039	-.074	-.0742	1.0000	
2	14	-1	24.654	26.347	-26.172	-3.040	-1.693	-2.3907	1.0000	
2	14	0	14.789	13.605	13.605	.053	1.184	1.1515	1.0000	
2	14	1	33.983	34.688	34.550	3.097	-.705	-1.2176	1.0000	
2	14	2	7.818 *	7.454	-7.454	-.041	.364	.1922	1.0000	**
2	14	3	17.856	17.491	-17.237	-2.969	.365	.3772	1.0000	
3	1	-8	52.496	49.910	49.803	3.259	2.586	5.5428	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
3	1	-7	18.806	17.781	-17.761	.848	1.025	1.4468	1.0000	
3	1	-6	64.676	62.126	-62.028	-3.498	2.549	7.1975	1.0000	
3	1	-5	34.579	32.331	32.320	-.847	2.248	6.1962	1.0000	
3	1	-4	110.986	109.630	109.568	3.707	1.356	1.5388	1.0000	
3	1	-3	54.586	51.101	-51.094	.866	3.485	10.6170	1.0000	
3	1	-2	36.005	37.662	-37.487	-3.627	-1.658	-7.6758	1.0000	
3	1	-1	66.101	62.120	62.113	-.913	3.981	6.7772	1.0000	
3	1	0	121.542	126.312	126.260	3.650	-4.770	-4.3826	1.0000	
3	1	1	57.903	55.157	-55.149	.955	2.746	6.6230	1.0000	
3	1	2	59.095	59.024	-58.925	-3.426	.071	.1832	1.0000	
3	1	3	19.151	17.613	17.583	-1.024	1.538	3.6340	1.0000	
3	1	4	70.904	70.029	69.954	3.245	.875	2.4695	1.0000	
3	1	5	7.282 *	6.760	6.670	1.099	.523	.4088	1.0000	**
3	1	6	4.976 *	4.563	-3.606	-2.796	.412	.1815	1.0000	**
3	1	7	14.789	13.103	-13.054	-1.125	1.686	1.7122	1.0000	
3	1	8	9.606 *	10.387	10.082	2.501	-.781	-.4735	1.0000	**
3	3	-8	13.865	13.137	13.136	.180	.727	.6737	1.0000	
3	3	-7	7.369 *	5.666	-4.107	3.904	1.703	1.0373	1.0000	**
3	3	-6	3.758 *	3.709	3.705	-.164	.049	.0182	1.0000	**
3	3	-5	10.211	11.520	-10.709	-4.245	-1.309	-1.4858	1.0000	
3	3	-4	26.053	26.503	26.501	.275	-.449	-1.1825	1.0000	
3	3	-3	66.110	65.569	65.410	4.561	.541	1.1810	1.0000	
3	3	-2	13.018	10.556	10.553	-.241	2.462	5.5886	1.0000	
3	3	-1	136.867	143.855	-143.775	-4.786	-6.988	-5.4294	1.0000	
3	3	0	60.141	57.759	57.758	.351	2.381	5.7426	1.0000	
3	3	1	89.848	86.045	85.912	4.789	3.803	5.3688	1.0000	
3	3	2	8.232	7.022	7.016	-.283	1.210	1.5742	1.0000	
3	3	3	43.555	40.564	-40.292	-4.693	2.991	9.8914	1.0000	
3	3	4	31.677	30.429	30.427	.364	1.248	3.2111	1.0000	
3	3	5	42.302	40.451	40.194	4.551	1.851	4.6582	1.0000	
3	3	6	5.624 *	3.768	-3.757	-.277	1.856	.8915	1.0000	**
3	3	7	49.368	47.324	-47.125	-4.335	2.044	4.2254	1.0000	
3	5	-8	61.713	62.919	-62.733	-4.831	-1.206	-2.5394	1.0000	
3	5	-7	5.805 *	1.976	1.755	.908	3.829	1.7590	1.0000	**
3	5	-6	109.751	113.216	113.089	5.371	-3.465	-4.9526	1.0000	
3	5	-5	4.561 *	3.308	-3.162	-.972	1.253	.6198	1.0000	**
3	5	-4	110.805	115.677	-115.542	-5.594	-4.873	-5.3723	1.0000	
3	5	-3	13.580	13.104	-13.067	.982	.475	.7976	1.0000	
3	5	-2	138.715	149.134	149.024	5.741	-10.419	-8.9343	1.0000	
3	5	-1	5.105 *	3.461	3.303	-1.035	1.644	1.3693	1.0000	**
3	5	0	107.531	112.798	-112.658	-5.621	-5.267	-6.7008	1.0000	
3	5	1	12.241	10.919	-10.871	1.033	1.321	2.3172	1.0000	
3	5	2	138.707	146.417	146.314	5.498	-7.711	-7.5008	1.0000	
3	5	3	7.775	8.179	-8.110	-1.058	-.405	-.3936	1.0000	
3	5	4	76.692	74.995	-74.826	-5.040	1.697	5.0359	1.0000	
3	5	5	17.648	18.048	18.017	1.061	-.400	-.5714	1.0000	
3	5	6	53.843	53.400	53.205	4.564	.443	1.0055	1.0000	
3	5	7	17.925	18.950	-18.923	-1.019	-1.026	-1.1309	1.0000	
3	7	-7	18.754	18.926	-18.698	-2.931	-.172	-.2099	1.0000	
3	7	-6	36.566	36.863	36.809	1.978	-.296	-.6016	1.0000	
3	7	-5	3.810 *	3.438	1.511	3.088	.372	.1366	1.0000	**
3	7	-4	23.082	23.003	-22.918	-1.974	.079	.1574	1.0000	
3	7	-3	17.484	17.570	-17.257	-3.301	-.086	-.1572	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
3	7	-2	30.027	29.629	29.562	1.987	.398	1.0722	1.0000	
3	7	-1	14.547	13.997	13.577	3.403	.550	.9361	1.0000	
3	7	0	3.265 *	5.749	-5.431	-1.885	-2.484	-1.0650	1.0000	**
3	7	1	30.053	27.659	-27.439	-3.482	2.393	6.4436	1.0000	
3	7	2	38.242	37.820	37.774	1.869	.422	1.1912	1.0000	
3	7	3	32.454	31.235	31.042	3.469	1.219	2.9405	1.0000	
3	7	4	9.157	7.366	-7.174	-1.669	1.791	1.5472	1.0000	
3	7	5	46.310	44.801	-44.671	-3.417	1.509	3.3596	1.0000	
3	7	6	5.209 *	3.978	3.681	1.509	1.231	.4640	1.0000	**
3	7	7	47.865	45.477	45.361	3.252	2.388	4.5323	1.0000	
3	9	-7	20.007	19.508	19.406	-1.990	.499	.5833	1.0000	
3	9	-6	16.093	15.993	-15.934	-1.374	.100	.1083	1.0000	
3	9	-5	30.243	30.631	-30.560	2.081	-.388	-.7130	1.0000	
3	9	-4	30.001	28.839	28.802	1.455	1.162	2.3197	1.0000	
3	9	-3	3.723 *	5.530	-5.029	-2.299	-1.806	-.6789	1.0000	**
3	9	-2	16.577	16.713	-16.653	-1.415	-.136	-.2192	1.0000	
3	9	-1	14.046	12.782	12.557	2.392	1.264	1.8515	1.0000	
3	9	0	27.859	26.917	26.881	1.404	.942	2.1372	1.0000	
3	9	1	6.133 *	7.352	-6.940	-2.425	-1.219	-.7969	1.0000	**
3	9	2	10.366	10.046	-9.964	-1.285	.320	.3221	1.0000	
3	9	3	11.411	13.221	-13.006	2.375	-1.810	-1.7908	1.0000	
3	9	4	14.919	13.655	13.602	1.199	1.264	1.4344	1.0000	
3	9	5	4.354 *	3.656	2.782	-2.371	.698	.2245	1.0000	**
3	9	6	4.570 *	2.382	2.151	-1.022	2.188	.6701	1.0000	**
3	11	-6	49.973	50.625	-50.481	-3.817	-.652	-1.2579	1.0000	
3	11	-5	13.847	15.067	15.037	.955	-1.220	-1.1206	1.0000	
3	11	-4	58.888	59.093	58.958	3.998	-.205	-.4661	1.0000	
3	11	-3	23.479	24.115	-24.092	-1.037	-.636	-1.0218	1.0000	
3	11	-2	45.956	46.936	-46.765	-3.997	-.979	-2.2678	1.0000	
3	11	-1	13.934	13.722	13.684	1.022	.212	.2479	1.0000	
3	11	0	51.908	51.536	51.384	3.951	.372	.9164	1.0000	
3	11	1	19.981	20.712	-20.686	-1.030	-.731	-1.0850	1.0000	
3	11	2	48.470	47.110	-46.958	-3.780	1.361	3.0882	1.0000	
3	11	3	18.823	18.898	18.872	.978	-.074	-.0958	1.0000	
3	11	4	38.760	37.829	37.666	3.506	.932	1.7395	1.0000	
3	11	5	24.585	24.554	-24.536	-.929	.031	.0427	1.0000	
3	13	-4	31.167	30.308	30.228	2.206	.859	1.3622	1.0000	
3	13	-3	7.749 *	8.654	7.936	3.452	-.906	-.4877	1.0000	**
3	13	-2	25.077	23.935	-23.831	-2.237	1.142	1.7168	1.0000	
3	13	-1	21.164	20.634	-20.314	-3.620	.530	.7217	1.0000	
3	13	0	27.824	26.085	25.989	2.240	1.739	2.8761	1.0000	
3	13	1	16.612	17.284	16.893	3.657	-.672	-.7413	1.0000	
3	13	2	33.120	31.495	-31.419	-2.197	1.624	2.8062	1.0000	
3	13	3	28.671	27.834	-27.591	-3.668	.837	1.2748	1.0000	
3	15	-1	25.829	25.021	-24.915	-2.306	.808	1.0871	1.0000	
3	15	0	44.876	42.625	-42.498	-3.281	2.252	4.0725	1.0000	
4	0	-8	29.474	29.232	28.888	4.466	.243	.3955	1.0000	
4	0	-6	99.108	97.211	-97.075	-5.143	1.897	2.9278	1.0000	
4	0	-4	110.407	108.996	108.857	5.502	1.412	1.5865	1.0000	
4	0	-2	150.334	160.839	-160.734	-5.820	-10.505	-8.0005	1.0000	
4	0	0	68.762	70.508	70.266	5.846	-1.747	-3.3151	1.0000	
4	0	2	143.043	158.510	-158.399	-5.940	-15.467	-14.0985	1.0000	
4	0	4	121.404	122.542	122.408	5.720	-1.138	-1.2313	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
4	0	6	105.371	104.671	-104.533	-5.375	.700	1.5009	1.0000	
4	2	-8	28.265	27.555	-27.549	.599	.709	1.1249	1.0000	
4	2	-7	53.385	52.781	52.608	4.275	.604	1.4273	1.0000	
4	2	-6	3.671 *	2.258	2.128	-.754	1.413	.5382	1.0000	**
4	2	-5	52.012	51.525	-51.335	-4.420	.486	1.4817	1.0000	
4	2	-4	26.356	24.762	-24.750	.762	1.594	4.1936	1.0000	
4	2	-3	67.276	66.599	66.447	4.493	.677	1.6682	1.0000	
4	2	-2	37.793	36.123	-36.112	-.912	1.670	6.9041	1.0000	
4	2	-1	110.952	109.528	-109.436	-4.488	1.423	1.8725	1.0000	
4	2	0	8.189	4.696	-4.610	.894	3.493	5.6956	1.0000	
4	2	1	67.319	66.163	66.023	4.302	1.156	3.4326	1.0000	
4	2	2	55.977	55.886	-55.877	-1.001	.091	.3632	1.0000	
4	2	3	21.276	20.977	-20.586	-4.028	.299	.6934	1.0000	
4	2	4	11.826	11.303	11.266	.917	.523	.6953	1.0000	
4	2	5	5.572 *	5.946	4.643	3.714	-.374	-.2081	1.0000	**
4	2	6	7.230 *	8.900	-8.855	-.884	-1.669	-.9661	1.0000	**
4	2	7	16.301	18.764	-18.447	-3.437	-2.464	-2.5240	1.0000	
4	4	-8	4.501 *	3.344	-2.739	-1.918	1.157	.3600	1.0000	**
4	4	-7	11.670	10.260	10.049	2.072	1.410	1.2560	1.0000	
4	4	-6	7.507 *	6.658	-6.320	2.095	.849	.5885	1.0000	**
4	4	-5	6.271 *	2.054	.158	-2.048	4.218	3.0516	1.0000	**
4	4	-4	41.317	40.945	-40.875	-2.389	.372	1.1343	1.0000	
4	4	-3	13.407	5.285	-4.890	2.004	8.122	14.2451	1.0000	
4	4	-2	25.803	25.745	25.625	2.482	.058	.1759	1.0000	
4	4	-1	22.235	22.259	-22.172	-1.970	-.024	-.0721	1.0000	
4	4	0	89.787	91.331	-91.292	-2.657	-1.543	-3.1341	1.0000	
4	4	1	13.122	11.398	-11.252	1.817	1.724	3.2709	1.0000	
4	4	2	62.041	61.284	61.228	2.626	.757	2.7369	1.0000	
4	4	3	25.760	24.939	24.883	-1.673	.821	2.0222	1.0000	
4	4	4	67.725	65.757	-65.705	-2.598	1.968	5.8428	1.0000	
4	4	5	34.597	32.647	-32.611	1.518	1.950	4.1808	1.0000	
4	4	6	23.082	22.838	22.717	2.349	.243	.3613	1.0000	
4	4	7	7.161 *	8.700	8.575	-1.468	-1.539	-.7547	1.0000	**
4	6	-8	19.747	20.042	-19.807	-3.062	-.295	-.3378	1.0000	
4	6	-7	8.267 *	6.558	6.556	-.176	1.708	1.0691	1.0000	**
4	6	-6	32.368	33.199	33.022	3.418	-.831	-1.6298	1.0000	
4	6	-5	15.117	16.085	-16.085	.086	-.968	-1.3179	1.0000	
4	6	-4	71.655	72.211	-72.113	-3.770	-.556	-1.6931	1.0000	
4	6	-3	14.469	14.884	14.884	-.030	-.414	-.6851	1.0000	
4	6	-2	36.774	34.894	34.680	3.855	1.880	5.7268	1.0000	
4	6	-1	33.042	31.947	-31.947	-.060	1.095	3.3362	1.0000	
4	6	0	53.627	51.040	-50.884	-3.986	2.587	9.0759	1.0000	
4	6	1	20.689	20.077	20.077	.079	.612	1.3630	1.0000	
4	6	2	54.646	52.470	52.319	3.982	2.176	6.8095	1.0000	
4	6	3	36.454	35.453	-35.453	-.145	1.001	2.5740	1.0000	
4	6	4	84.000	80.522	-80.424	-3.964	3.478	9.8198	1.0000	
4	6	5	19.246	18.792	18.791	.105	.455	.6497	1.0000	
4	6	6	53.610	51.645	51.514	3.677	1.965	4.1354	1.0000	
4	6	7	23.358	22.356	-22.355	-.111	1.002	1.2894	1.0000	
4	8	-7	46.906	48.121	-47.923	-4.361	-1.215	-2.3838	1.0000	
4	8	-6	6.971 *	7.231	7.127	1.223	-.260	-.1427	1.0000	**
4	8	-5	39.547	39.422	39.165	4.494	.124	.2716	1.0000	
4	8	-4	27.427	28.622	-28.589	-1.377	-1.195	-2.3855	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
4	8	-3	54.681	54.184	-53.989	-4.596	.497	1.4370	1.0000	
4	8	-2	23.108	23.647	23.605	1.410	-.540	-1.1360	1.0000	
4	8	-1	53.964	52.522	52.325	4.546	1.442	4.3918	1.0000	
4	8	0	47.157	47.331	-47.308	-1.484	-.174	-.5168	1.0000	
4	8	1	49.239	49.208	-49.010	-4.407	.031	.0890	1.0000	
4	8	2	33.500	34.045	34.015	1.429	-.545	-1.3142	1.0000	
4	8	3	7.291 *	8.111	7.012	4.076	-.820	-.5583	1.0000	**
4	8	4	34.260	34.246	-34.218	-1.377	.014	.0291	1.0000	
4	8	5	15.765	15.216	-14.729	-3.817	.549	.5997	1.0000	
4	8	6	11.437	10.880	10.813	1.202	.557	.4190	1.0000	
4	10	-6	33.837	34.962	-34.750	-3.840	-1.125	-1.8878	1.0000	
4	10	-5	4.259 *	4.398	3.979	1.873	-.139	-.0457	1.0000	**
4	10	-4	47.839	47.950	47.767	4.191	-.111	-.2519	1.0000	
4	10	-3	13.726	15.923	-15.805	-1.933	-2.196	-2.4685	1.0000	
4	10	-2	72.252	71.732	-71.592	-4.475	.520	1.3988	1.0000	
4	10	-1	13.657	14.006	13.876	1.905	-.348	-.4246	1.0000	
4	10	0	78.981	77.811	77.675	4.592	1.170	3.3027	1.0000	
4	10	1	20.110	19.817	-19.729	-1.866	.293	.4650	1.0000	
4	10	2	90.885	90.594	-90.476	-4.618	.291	.7654	1.0000	
4	10	3	4.172 *	8.106	-7.929	1.686	-3.934	-1.3199	1.0000	**
4	10	4	73.694	72.540	72.406	4.420	1.154	2.6712	1.0000	
4	10	5	6.237 *	3.467	-3.071	-1.608	2.770	1.2148	1.0000	**
4	12	-5	24.386	23.882	-23.767	-2.343	.504	.6860	1.0000	
4	12	-4	22.391	20.338	20.208	2.301	2.052	2.8284	1.0000	
4	12	-3	17.933	17.023	16.861	2.340	.910	1.0866	1.0000	
4	12	-2	9.908	9.710	-9.415	-2.375	.198	.1498	1.0000	
4	12	-1	25.846	25.003	-24.893	-2.338	.843	1.3748	1.0000	
4	12	0	4.155 *	2.643	1.094	2.406	1.512	.5087	1.0000	**
4	12	1	11.316	9.077	8.805	2.204	2.239	1.9062	1.0000	
4	12	2	16.646	16.707	-16.525	-2.461	-.061	-.0682	1.0000	
4	12	3	16.767	14.607	-14.454	-2.105	2.161	2.3159	1.0000	
4	12	4	28.256	26.944	26.834	2.438	1.312	1.9473	1.0000	
4	14	-3	4.639 *	2.819	1.196	2.553	1.819	.5485	1.0000	**
4	14	-2	4.535 *	2.544	-2.540	.136	1.991	.6147	1.0000	**
4	14	-1	14.176	12.205	-11.941	-2.527	1.970	1.8247	1.0000	
4	14	0	7.593 *	6.663	6.661	-.145	.930	.4766	1.0000	**
4	14	1	9.796	5.674	-5.163	2.351	4.122	2.6660	1.0000	
4	14	2	4.613 *	5.697	-5.695	.167	-1.085	-.3295	1.0000	**
5	1	-8	4.328 *	2.792	-1.107	2.562	1.536	.4968	1.0000	**
5	1	-7	21.708	21.840	21.795	1.396	-.132	-.2031	1.0000	
5	1	-6	8.025	6.477	5.896	-2.681	1.548	1.2272	1.0000	
5	1	-5	31.280	30.858	-30.823	-1.467	.422	1.0851	1.0000	
5	1	-4	19.756	18.144	17.923	2.822	1.612	3.5893	1.0000	
5	1	-3	46.768	45.183	45.158	1.507	1.585	5.9199	1.0000	
5	1	-2	6.159	3.376	1.840	-2.831	2.783	3.1278	1.0000	
5	1	-1	41.974	39.807	-39.779	-1.477	2.167	9.6498	1.0000	
5	1	0	28.291	25.654	-25.499	2.818	2.637	9.8456	1.0000	
5	1	1	25.829	25.036	24.997	1.401	.792	2.5480	1.0000	
5	1	2	8.379	7.632	7.092	-2.818	.748	.9111	1.0000	
5	1	3	7.230	4.506	4.329	-1.250	2.724	2.6061	1.0000	
5	1	4	14.564	14.578	14.306	2.803	-.014	-.0202	1.0000	
5	1	5	9.787	6.969	-6.878	1.126	2.818	2.5689	1.0000	
5	1	6	22.823	22.723	-22.559	-2.722	.100	.1466	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
5	1	7	4.527 *	2.680	2.480	-1.014	1.847	.5717	1.0000	**
5	3	-8	19.091	18.642	18.640	.296	.449	.5468	1.0000	
5	3	-7	78.160	77.811	77.658	4.870	.349	.8789	1.0000	
5	3	-6	15.463	15.494	-15.490	-.337	-.031	-.0426	1.0000	
5	3	-5	75.707	74.605	-74.426	-5.165	1.102	3.4477	1.0000	
5	3	-4	30.986	29.871	29.869	.414	1.114	3.0717	1.0000	
5	3	-3	109.630	110.977	110.844	5.430	-1.347	-1.7325	1.0000	
5	3	-2	30.329	29.352	-29.349	-.432	.978	3.2331	1.0000	
5	3	-1	147.734	157.657	-157.560	-5.541	-9.923	-11.3739	1.0000	
5	3	0	36.610	36.973	36.970	.449	-.364	-1.3582	1.0000	
5	3	1	167.585	192.132	192.053	5.501	-24.547	-26.0702	1.0000	
5	3	2	29.336	29.288	-29.285	-.427	.048	.1397	1.0000	
5	3	3	106.598	111.547	-111.429	-5.135	-4.949	-13.0207	1.0000	
5	3	4	18.426	17.447	17.444	.370	.978	1.7158	1.0000	
5	3	5	64.201	64.883	64.715	4.667	-.682	-1.7556	1.0000	
5	3	6	15.480	16.059	-16.055	-.321	-.579	-.6380	1.0000	
5	3	7	32.135	33.529	-33.277	-4.107	-1.394	-2.2419	1.0000	
5	5	-8	16.473	16.147	-15.634	-4.038	.326	.3339	1.0000	
5	5	-7	24.766	25.075	25.049	1.148	-.309	-.4827	1.0000	
5	5	-6	31.331	32.026	31.727	4.371	-.695	-1.3870	1.0000	
5	5	-5	19.911	20.340	-20.306	-1.190	-.429	-.7523	1.0000	
5	5	-4	42.423	42.581	-42.332	-4.594	-.158	-.4453	1.0000	
5	5	-3	44.393	44.898	44.879	1.277	-.505	-1.5796	1.0000	
5	5	-2	47.373	46.768	46.530	4.711	.605	2.0608	1.0000	
5	5	-1	20.914	20.845	-20.809	-1.228	.069	.1688	1.0000	
5	5	0	25.812	25.831	-25.399	-4.705	-.020	-.0545	1.0000	
5	5	1	28.956	30.294	30.269	1.222	-1.338	-3.6880	1.0000	
5	5	2	32.351	33.490	33.163	4.671	-1.139	-3.0676	1.0000	
5	5	3	7.973	6.051	5.954	-1.078	1.922	1.6985	1.0000	
5	5	4	50.923	50.990	-50.784	-4.581	-.067	-.1711	1.0000	
5	5	5	5.252 *	6.066	5.978	1.029	-.814	-.3582	1.0000	**
5	5	6	47.252	45.614	45.407	4.334	1.638	3.2700	1.0000	
5	5	7	4.613 *	2.937	-2.790	-.916	1.676	.5080	1.0000	**
5	7	-7	49.403	49.721	-49.591	-3.596	-.318	-.6571	1.0000	
5	7	-6	10.236	9.437	-9.330	1.418	.800	.6565	1.0000	
5	7	-5	80.743	83.113	83.020	3.941	-2.370	-6.3807	1.0000	
5	7	-4	9.753	8.085	7.954	-1.449	1.668	1.6791	1.0000	
5	7	-3	79.603	79.989	-79.886	-4.056	-.386	-1.2090	1.0000	
5	7	-2	15.091	14.768	-14.698	1.443	.323	.5338	1.0000	
5	7	-1	109.829	112.717	112.640	4.160	-2.888	-6.3083	1.0000	
5	7	0	31.573	31.541	31.510	-1.406	.032	.0845	1.0000	
5	7	1	68.416	70.206	-70.093	-3.979	-1.790	-5.5997	1.0000	
5	7	2	21.829	21.831	-21.785	1.417	-.002	-.0038	1.0000	
5	7	3	60.495	60.367	60.249	3.774	.128	.3441	1.0000	
5	7	4	4.034 *	2.248	1.716	-1.452	1.786	.6191	1.0000	**
5	7	5	23.540	25.019	-24.789	-3.385	-1.479	-2.1955	1.0000	
5	7	6	4.958 *	2.486	2.039	1.422	2.472	.8621	1.0000	**
5	9	-7	19.937	18.959	-18.760	-2.738	.978	1.1325	1.0000	
5	9	-6	8.906 *	8.353	8.301	-.929	.553	.3537	1.0000	**
5	9	-5	27.176	26.958	26.799	2.923	.219	.3721	1.0000	
5	9	-4	7.299 *	8.771	-8.720	.950	-1.472	-.9111	1.0000	**
5	9	-3	15.463	14.258	-13.948	-2.958	1.205	1.6410	1.0000	
5	9	-2	12.405	13.233	13.198	-.951	-.828	-.9879	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
5	9	-1	64.539	64.374	64.299	3.103	.215	.6070	1.0000	
5	9	0	12.811	14.143	-14.111	.956	-1.332	-1.6586	1.0000	
5	9	1	52.133	51.945	-51.859	-2.987	.187	.4930	1.0000	
5	9	2	10.219	10.303	10.258	-.966	-.084	-.0758	1.0000	
5	9	3	49.947	49.375	49.293	2.838	.572	1.3253	1.0000	
5	9	4	4.224 *	4.166	-4.050	.975	.058	.0193	1.0000	**
5	9	5	5.382 *	6.521	-6.034	-2.473	-1.140	-.4255	1.0000	**
5	11	-6	5.857 *	4.690	-3.640	-2.957	1.167	.4503	1.0000	**
5	11	-5	28.610	29.260	29.246	.886	-.650	-1.0025	1.0000	
5	11	-4	7.697 *	8.476	7.895	3.085	-.779	-.4532	1.0000	**
5	11	-3	13.942	11.875	-11.844	-.868	2.067	2.1953	1.0000	
5	11	-2	4.077 *	3.140	-.303	-3.126	.937	.3219	1.0000	**
5	11	-1	28.619	30.019	30.004	.956	-1.400	-2.5320	1.0000	
5	11	0	10.461	9.616	-9.098	3.114	.846	.7093	1.0000	
5	11	1	4.129 *	2.895	-2.763	-.864	1.234	.4191	1.0000	**
5	11	2	7.438 *	3.238	.901	-3.110	4.200	2.4556	1.0000	**
5	11	3	14.504	15.452	15.426	.886	-.948	-.9298	1.0000	
5	11	4	16.949	15.902	15.600	3.087	1.046	1.1012	1.0000	
5	13	-4	24.403	22.786	22.700	1.975	1.618	2.1776	1.0000	
5	13	-3	70.809	71.359	71.228	4.327	-.550	-1.2016	1.0000	
5	13	-2	22.581	20.717	-20.618	-2.023	1.864	2.5387	1.0000	
5	13	-1	58.473	57.522	-57.361	-4.308	.951	2.0383	1.0000	
5	13	0	14.055	12.780	12.622	2.005	1.275	1.1999	1.0000	
5	13	1	66.801	66.313	66.176	4.254	.488	1.0651	1.0000	
5	13	2	15.359	14.131	-13.992	-1.976	1.228	1.2150	1.0000	
5	13	3	32.800	31.933	-31.691	-3.919	.867	1.3754	1.0000	
6	0	-8	60.503	59.809	59.595	5.053	.694	1.5159	1.0000	
6	0	-6	76.752	75.454	-75.262	-5.373	1.298	3.6663	1.0000	
6	0	-4	143.346	151.083	150.977	5.674	-7.738	-7.1660	1.0000	
6	0	-2	147.362	150.360	-150.255	-5.628	-2.998	-2.7114	1.0000	
6	0	0	133.506	130.350	130.236	5.458	3.156	3.5470	1.0000	
6	0	2	25.656	25.423	-24.921	-5.029	.233	.6125	1.0000	
6	0	4	39.011	41.087	40.815	4.725	-2.076	-5.2254	1.0000	
6	0	6	20.706	20.040	-19.587	-4.240	.666	.9071	1.0000	
6	2	-8	12.802	12.474	12.436	.965	.328	.2858	1.0000	
6	2	-7	28.386	28.593	28.340	3.791	-.207	-.3683	1.0000	
6	2	-6	3.801 *	4.643	4.556	-.898	-.843	-.3106	1.0000	**
6	2	-5	39.529	38.941	-38.722	-4.127	.588	1.5824	1.0000	
6	2	-4	10.893	8.920	8.874	.901	1.973	2.6556	1.0000	
6	2	-3	40.557	38.798	38.552	4.363	1.759	5.8193	1.0000	
6	2	-2	39.054	35.640	35.631	-.769	3.415	11.9782	1.0000	
6	2	-1	84.622	85.435	-85.311	-4.597	-.813	-2.4774	1.0000	
6	2	0	6.911	7.399	-7.361	.750	-.489	-.5386	1.0000	
6	2	1	97.787	109.181	109.080	4.696	-11.394	-45.4839	1.0000	
6	2	2	30.511	32.557	32.551	-.623	-2.046	-5.6392	1.0000	
6	2	3	87.991	94.366	-94.253	-4.623	-6.376	-20.5019	1.0000	
6	2	4	7.282 *	8.414	8.388	.658	-1.132	-.8507	1.0000	**
6	2	5	57.808	59.979	59.821	4.355	-2.171	-5.2361	1.0000	
6	2	6	11.342	9.575	9.560	-.538	1.767	1.4308	1.0000	
6	2	7	44.401	44.912	-44.733	-4.012	-.511	-.9386	1.0000	
6	4	-8	23.937	24.070	-23.955	-2.352	-.133	-.1815	1.0000	
6	4	-7	7.144 *	6.826	-6.600	1.742	.318	.1730	1.0000	**
6	4	-6	35.020	35.044	34.958	2.461	-.024	-.0518	1.0000	

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
6	4	-5	3.930	*	3.157	2.532	-1.886	.773	.3303	1.0000	**
6	4	-4	20.706		20.074	-19.927	-2.426	.632	1.3070	1.0000	
6	4	-3	21.510		22.001	-21.914	1.952	-.492	-1.1157	1.0000	
6	4	-2	34.657		35.123	35.040	2.410	-.466	-1.4568	1.0000	
6	4	-1	13.683		14.720	-14.568	-2.110	-1.037	-1.8750	1.0000	
6	4	0	12.716		11.368	11.150	-2.218	1.347	2.2603	1.0000	
6	4	1	28.800		31.575	31.499	2.186	-2.775	-7.6477	1.0000	
6	4	2	13.096		16.639	16.502	2.135	-3.544	-5.2591	1.0000	
6	4	3	33.552		35.653	-35.585	-2.200	-2.101	-5.1757	1.0000	
6	4	4	3.784	*	2.015	-.585	-1.928	1.769	.6541	1.0000	**
6	4	5	15.178		13.601	13.441	2.081	1.577	1.8436	1.0000	
6	4	6	16.085		17.429	17.335	1.804	-1.344	-1.4276	1.0000	
6	6	-8	21.631		21.389	-21.096	-3.529	.242	.2978	1.0000	
6	6	-7	8.310	*	10.129	10.129	-.042	-1.819	-1.0854	1.0000	**
6	6	-6	44.876		45.835	45.680	3.762	-.958	-2.1333	1.0000	
6	6	-5	25.699		26.595	-26.595	-.008	-.895	-1.6991	1.0000	
6	6	-4	65.280		65.142	-65.028	-3.855	.138	.4097	1.0000	
6	6	-3	13.666		12.313	12.313	-.048	1.353	2.0343	1.0000	
6	6	-2	89.166		90.082	89.999	3.854	-.916	-3.1191	1.0000	
6	6	-1	24.369		24.763	-24.763	.041	-.394	-.9494	1.0000	
6	6	0	26.036		27.467	-27.233	-3.575	-1.431	-3.5234	1.0000	
6	6	1	3.343	*	2.557	2.554	-.121	.786	.3286	1.0000	**
6	6	2	7.982		9.397	8.787	3.331	-1.415	-1.2410	1.0000	
6	6	3	7.818		9.173	-9.172	.133	-1.355	-1.0455	1.0000	
6	6	4	10.288		11.407	11.001	-3.016	-1.119	-.9664	1.0000	
6	6	5	4.276	*	2.140	2.132	-.183	2.136	.6986	1.0000	**
6	6	6	7.343	*	9.758	9.349	2.797	-2.416	-1.1849	1.0000	**
6	8	-7	33.949		35.468	-35.253	-3.893	-1.519	-2.5118	1.0000	
6	8	-6	20.896		21.198	21.161	1.259	-.302	-.4061	1.0000	
6	8	-5	23.177		22.651	22.264	4.170	.526	.8341	1.0000	
6	8	-4	11.601		12.428	-12.360	-1.299	-.827	-.8395	1.0000	
6	8	-3	42.449		43.064	-42.830	-4.482	-.615	-1.5824	1.0000	
6	8	-2	21.734		22.251	22.209	1.366	-.516	-.9799	1.0000	
6	8	-1	49.887		50.488	50.273	4.655	-.601	-1.6576	1.0000	
6	8	0	11.645		9.713	-9.621	-1.331	1.932	2.3295	1.0000	
6	8	1	84.034		87.115	-86.982	-4.807	-3.080	-8.9147	1.0000	
6	8	2	26.036		27.855	27.822	1.351	-1.819	-3.4518	1.0000	
6	8	3	65.755		69.173	69.014	4.688	-3.417	-8.5994	1.0000	
6	8	4	22.054		23.355	-23.321	-1.272	-1.302	-1.9072	1.0000	
6	8	5	51.303		55.203	-55.024	-4.450	-3.900	-7.9204	1.0000	
6	10	-6	47.909		48.121	-47.943	-4.140	-.213	-.4178	1.0000	
6	10	-5	5.399	*	1.774	-.224	1.759	3.625	1.4778	1.0000	**
6	10	-4	56.754		57.854	57.695	4.284	-1.099	-2.4953	1.0000	
6	10	-3	12.543		11.562	-11.405	-1.897	.981	.9876	1.0000	
6	10	-2	47.468		47.594	-47.404	-4.248	-.126	-.2972	1.0000	
6	10	-1	5.088	*	7.013	6.740	1.938	-1.925	-.8672	1.0000	**
6	10	0	41.672		42.054	41.850	4.128	-.382	-.8669	1.0000	
6	10	1	32.221		33.536	-33.474	-2.039	-1.315	-2.4950	1.0000	
6	10	2	30.485		29.904	-29.649	-3.892	.581	1.0679	1.0000	
6	10	3	21.397		20.967	20.875	1.964	.430	.5857	1.0000	
6	10	4	36.307		37.055	36.875	3.648	-.747	-1.3110	1.0000	
6	12	-5	21.674		20.210	-20.095	-2.158	1.464	1.8023	1.0000	
6	12	-4	28.541		29.250	29.149	2.421	-.709	-1.0792	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
6	12	-3	13.502	10.318	10.067	2.263	3.184	2.9721	1.0000	
6	12	-2	27.496	27.272	-27.170	-2.359	.224	.3552	1.0000	
6	12	-1	32.083	30.609	-30.512	-2.431	1.474	2.6659	1.0000	
6	12	0	9.200	7.674	7.356	2.187	1.525	1.0266	1.0000	
6	12	1	26.710	25.444	25.326	2.447	1.266	1.9281	1.0000	
6	12	2	11.472	13.391	13.245	-1.972	-1.920	-1.4815	1.0000	
6	12	3	37.197	35.263	-35.178	-2.455	1.934	3.2917	1.0000	
6	14	-2	4.656 *	3.432	3.429	.146	1.224	.3681	1.0000	**
6	14	-1	14.633	14.938	-14.696	-2.678	-.304	-.2774	1.0000	
6	14	0	4.647 *	1.154	-1.150	-.098	3.493	1.0531	1.0000	**
7	1	-8	12.569	13.716	13.391	2.970	-1.147	-.9766	1.0000	
7	1	-7	14.521	14.723	-14.688	1.016	-.202	-.2223	1.0000	
7	1	-6	49.420	47.736	-47.619	-3.334	1.684	4.2391	1.0000	
7	1	-5	20.395	20.066	20.042	-.977	.329	.6142	1.0000	
7	1	-4	53.463	51.329	51.209	3.507	2.134	6.6775	1.0000	
7	1	-3	28.973	26.596	-26.580	.929	2.377	6.5513	1.0000	
7	1	-2	132.893	132.209	-132.156	-3.746	.684	.6886	1.0000	
7	1	-1	22.494	20.360	20.340	-.901	2.135	5.7468	1.0000	
7	1	0	77.426	73.609	73.520	3.626	3.817	6.4981	1.0000	
7	1	1	13.001	11.170	-11.135	.884	1.831	3.0719	1.0000	
7	1	2	78.359	76.867	-76.786	-3.533	1.492	3.3205	1.0000	
7	1	3	14.167	14.350	14.325	-.849	-.183	-.2686	1.0000	
7	1	4	31.539	32.391	32.230	3.226	-.852	-1.8266	1.0000	
7	1	5	24.283	24.091	-24.078	.785	.192	.3128	1.0000	
7	1	6	43.555	44.106	-44.003	-3.006	-.551	-1.0629	1.0000	
7	3	-8	4.518 *	.356	-.334	.126	4.161	1.2881	1.0000	**
7	3	-7	51.252	50.655	50.477	4.242	.597	1.3292	1.0000	
7	3	-6	22.183	21.585	-21.584	-.225	.598	1.0184	1.0000	
7	3	-5	44.781	43.750	-43.532	-4.359	1.032	2.7781	1.0000	
7	3	-4	7.299	7.244	-7.242	.164	.056	.0472	1.0000	
7	3	-3	11.394	8.977	7.860	4.337	2.417	3.4124	1.0000	
7	3	-2	29.250	28.342	-28.341	-.257	.908	2.5628	1.0000	
7	3	-1	11.169	11.880	11.076	-4.294	-.710	-1.0406	1.0000	
7	3	0	12.854	11.048	-11.047	.186	1.806	2.9863	1.0000	
7	3	1	14.167	12.640	11.901	4.259	1.527	2.5621	1.0000	
7	3	2	23.350	23.155	-23.154	-.266	.194	.4247	1.0000	
7	3	3	37.447	35.078	-34.829	-4.170	2.370	5.9631	1.0000	
7	3	4	4.051 *	1.312	-1.298	.191	2.739	1.0431	1.0000	**
7	3	5	27.911	27.270	26.986	3.929	.641	1.1067	1.0000	
7	3	6	15.566	15.147	-15.145	-.236	.419	.4219	1.0000	
7	5	-8	54.500	55.639	-55.452	-4.557	-1.140	-2.2745	1.0000	
7	5	-7	5.071 *	1.026	.399	.945	4.045	1.5661	1.0000	**
7	5	-6	54.880	55.568	55.346	4.960	-.688	-1.6257	1.0000	
7	5	-5	3.758 *	1.476	-1.104	-.979	2.282	.8494	1.0000	**
7	5	-4	114.407	117.036	-116.910	-5.424	-2.629	-3.5809	1.0000	
7	5	-3	4.259 *	4.245	4.126	.999	.014	.0071	1.0000	**
7	5	-2	125.300	127.587	127.464	5.585	-2.287	-3.2681	1.0000	
7	5	-1	14.754	14.941	-14.906	-1.018	-.187	-.3135	1.0000	
7	5	0	143.587	147.824	-147.716	-5.634	-4.236	-3.7436	1.0000	
7	5	1	14.426	15.001	14.968	1.001	-.575	-.8995	1.0000	
7	5	2	87.023	86.338	86.172	5.340	.686	1.5871	1.0000	
7	5	3	11.714	11.855	-11.815	-.963	-.141	-.1524	1.0000	
7	5	4	82.479	83.254	-83.101	-5.053	-.775	-1.9934	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
7	5	5	4.976 *	6.457	-6.401	.851	-1.481	-.5513	1.0000	**
7	5	6	55.916	56.396	56.212	4.554	-.480	-.9745	1.0000	
7	7	-7	14.417	16.364	-16.078	-3.042	-1.946	-1.8317	1.0000	
7	7	-6	5.174 *	2.112	-1.109	1.798	3.062	1.2394	1.0000	**
7	7	-5	16.638	18.474	18.201	3.162	-1.836	-2.3356	1.0000	
7	7	-4	32.947	32.486	-32.425	-1.990	.461	1.0260	1.0000	
7	7	-3	14.461	16.435	-16.119	-3.207	-1.974	-2.7208	1.0000	
7	7	-2	32.722	32.663	32.601	2.018	.059	.1450	1.0000	
7	7	-1	16.387	17.976	17.688	3.206	-1.589	-2.5543	1.0000	
7	7	0	47.097	45.099	-45.053	-2.036	1.997	5.5047	1.0000	
7	7	1	29.958	29.428	-29.256	-3.180	.530	1.1794	1.0000	
7	7	2	9.476	9.517	9.331	1.869	-.040	-.0352	1.0000	
7	7	3	19.592	17.798	17.537	3.034	1.794	2.6291	1.0000	
7	7	4	18.072	17.404	-17.312	-1.786	.668	.8400	1.0000	
7	7	5	15.705	12.927	-12.608	-2.853	2.777	2.8708	1.0000	
7	9	-6	13.744	15.217	-15.160	-1.309	-1.473	-1.3323	1.0000	
7	9	-5	4.371 *	4.092	3.384	2.300	.279	.0960	1.0000	**
7	9	-4	14.780	13.523	13.453	1.375	1.257	1.4128	1.0000	
7	9	-3	25.639	25.575	25.481	-2.192	.064	.1136	1.0000	
7	9	-2	31.798	31.444	-31.410	-1.467	.354	.7184	1.0000	
7	9	-1	42.743	42.037	-41.984	2.105	.706	1.6683	1.0000	
7	9	0	21.838	20.336	20.286	1.427	1.502	2.5574	1.0000	
7	9	1	21.389	20.493	20.384	-2.111	.896	1.4210	1.0000	
7	9	2	27.168	24.590	-24.550	-1.399	2.578	4.5906	1.0000	
7	9	3	9.191	8.685	-8.435	2.069	.506	.3445	1.0000	
7	9	4	12.863	10.129	10.050	1.267	2.733	2.3789	1.0000	
7	11	-5	15.186	17.082	17.058	.892	-1.895	-1.7983	1.0000	
7	11	-4	45.006	45.187	45.023	3.847	-.181	-.3608	1.0000	
7	11	-3	24.663	24.720	-24.701	-.977	-.058	-.0878	1.0000	
7	11	-2	67.034	66.955	-66.834	-4.022	.079	.1872	1.0000	
7	11	-1	29.362	28.876	28.858	1.019	.486	.8655	1.0000	
7	11	0	57.022	56.610	56.470	3.975	.412	.9362	1.0000	
7	11	1	36.178	35.172	-35.157	-1.039	1.005	1.9077	1.0000	
7	11	2	44.859	43.819	-43.653	-3.811	1.041	2.0768	1.0000	
7	11	3	22.607	20.971	20.950	.952	1.635	2.1037	1.0000	
7	13	-3	13.804	14.405	14.004	3.374	-.601	-.5113	1.0000	
7	13	-2	35.478	35.254	-35.185	-2.211	.224	.3754	1.0000	
7	13	-1	16.862	18.728	-18.420	-3.386	-1.866	-1.9461	1.0000	
7	13	0	33.577	31.620	31.543	2.195	1.958	3.2379	1.0000	
7	13	1	21.950	19.824	19.543	3.326	2.126	2.6463	1.0000	
8	0	-8	26.269	26.607	26.276	4.182	-.337	-.5008	1.0000	
8	0	-6	6.608 *	5.902	3.903	-4.427	.707	.4283	1.0000	**
8	0	-4	29.647	28.253	27.843	4.798	1.394	3.4326	1.0000	
8	0	-2	67.595	64.385	-64.186	-5.057	3.210	11.6141	1.0000	
8	0	0	118.640	114.180	114.060	5.244	4.460	4.8248	1.0000	
8	0	2	83.317	80.170	-80.005	-5.148	3.147	6.5057	1.0000	
8	0	4	63.890	63.411	63.218	4.951	.478	1.2038	1.0000	
8	0	6	52.349	52.154	-51.947	-4.639	.195	.3894	1.0000	
8	2	-8	4.449 *	.787	-.411	.671	3.662	1.1519	1.0000	**
8	2	-7	73.400	74.032	73.894	4.506	-.631	-1.5220	1.0000	
8	2	-6	18.866	17.821	17.810	-.636	1.045	1.5712	1.0000	
8	2	-5	94.133	95.385	-95.268	-4.727	-1.252	-2.1640	1.0000	
8	2	-4	3.455 *	.921	-.589	.709	2.534	1.0294	1.0000	**

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
8	2	-3	100.724	99.907	99.793	4.768	.817	1.3132	1.0000	
8	2	-2	19.091	17.109	17.095	-.689	1.982	4.1721	1.0000	
8	2	-1	71.975	69.375	-69.221	-4.621	2.600	9.4059	1.0000	
8	2	0	8.984	8.468	-8.436	.726	.516	.5860	1.0000	
8	2	1	70.196	68.577	68.434	4.437	1.618	5.3528	1.0000	
8	2	2	26.598	25.229	25.219	-.689	1.369	3.1076	1.0000	
8	2	3	53.066	52.901	-52.740	-4.127	.165	.4339	1.0000	
8	2	4	9.209	10.630	-10.605	.723	-1.421	-1.0897	1.0000	
8	2	5	37.041	37.739	37.554	3.732	-.698	-1.3244	1.0000	
8	2	6	4.527 *	1.500	-1.300	-.748	3.027	.9369	1.0000	**
8	4	-8	7.567 *	5.553	5.264	-1.766	2.015	1.0274	1.0000	**
8	4	-7	32.817	32.719	32.634	2.368	.098	.1742	1.0000	
8	4	-6	7.654 *	5.546	5.198	1.934	2.107	1.3629	1.0000	**
8	4	-5	39.737	38.226	-38.150	-2.405	1.511	3.5690	1.0000	
8	4	-4	4.924 *	5.057	4.641	-2.008	-.133	-.0697	1.0000	**
8	4	-3	40.886	39.623	39.552	2.365	1.263	3.5652	1.0000	
8	4	-2	18.020	18.481	18.357	2.144	-.462	-.8764	1.0000	
8	4	-1	5.364 *	4.519	-3.955	-2.185	.846	.5725	1.0000	**
8	4	0	5.330 *	3.443	-2.690	-2.150	1.887	1.2624	1.0000	**
8	4	1	16.949	15.699	15.561	2.076	1.249	2.1915	1.0000	
8	4	2	7.101 *	5.761	5.342	2.157	1.340	1.0072	1.0000	**
8	4	3	5.416 *	5.264	-4.917	-1.879	.153	.0775	1.0000	**
8	4	4	6.142 *	5.784	-5.386	-2.108	.358	.1811	1.0000	**
8	4	5	7.783 *	5.705	5.448	1.693	2.078	1.1736	1.0000	**
8	4	6	21.829	19.920	19.813	2.065	1.909	2.3761	1.0000	
8	6	-7	4.423 *	4.001	3.988	-.325	.422	.1334	1.0000	**
8	6	-6	14.677	14.734	-14.432	2.969	-.057	-.0625	1.0000	
8	6	-5	6.980 *	7.319	7.312	.323	-.339	-.2025	1.0000	**
8	6	-4	20.283	18.801	18.538	-3.134	1.482	2.4858	1.0000	
8	6	-3	10.055	9.945	9.943	-.217	.110	.1123	1.0000	
8	6	-2	29.284	28.580	28.379	3.388	.704	1.6299	1.0000	
8	6	-1	3.499 *	1.135	1.119	.192	2.363	.9467	1.0000	**
8	6	0	45.153	43.472	-43.332	-3.487	1.681	4.5243	1.0000	
8	6	1	21.371	19.937	19.937	-.077	1.435	2.6361	1.0000	
8	6	2	43.002	40.961	40.813	3.474	2.041	4.9228	1.0000	
8	6	3	7.878 *	5.739	-5.738	.073	2.139	1.4398	1.0000	**
8	6	4	26.166	24.615	-24.388	-3.335	1.550	2.5638	1.0000	
8	6	5	20.007	18.771	18.771	.014	1.235	1.5050	1.0000	
8	8	-7	55.303	57.648	-57.468	-4.560	-2.345	-4.6015	1.0000	
8	8	-6	25.587	25.586	25.556	1.221	.001	.0020	1.0000	
8	8	-5	84.691	86.631	86.496	4.842	-1.940	-4.7794	1.0000	
8	8	-4	21.760	22.722	-22.686	-1.278	-.962	-1.5048	1.0000	
8	8	-3	65.047	66.542	-66.368	-4.819	-1.495	-3.9343	1.0000	
8	8	-2	27.496	28.980	28.949	1.335	-1.484	-2.9109	1.0000	
8	8	-1	65.263	67.659	67.492	4.748	-2.396	-6.4504	1.0000	
8	8	0	14.901	15.339	-15.284	-1.296	-.438	-.5627	1.0000	
8	8	1	42.613	43.179	-42.945	-4.482	-.565	-1.2834	1.0000	
8	8	2	12.223	11.137	11.067	1.252	1.086	1.0567	1.0000	
8	8	3	55.916	55.616	55.454	4.241	.301	.6691	1.0000	
8	8	4	7.723 *	8.883	-8.804	-1.179	-1.160	-.6305	1.0000	**
8	10	-6	20.222	20.513	-20.222	-3.444	-.291	-.3365	1.0000	
8	10	-5	35.772	36.801	36.741	2.091	-1.029	-1.8326	1.0000	
8	10	-4	29.362	29.372	29.139	3.695	-.010	-.0169	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
8	10	-3	15.515	15.540	-15.408	-2.023	-.026	-.0288	1.0000	
8	10	-2	35.651	35.194	-34.982	-3.862	.457	.9111	1.0000	
8	10	-1	23.643	21.743	21.650	2.007	1.900	3.0136	1.0000	
8	10	0	40.739	38.426	38.223	3.938	2.313	4.7817	1.0000	
8	10	1	8.397 *	4.460	-4.054	-1.859	3.937	2.5318	1.0000	**
8	10	2	32.264	30.362	-30.112	-3.882	1.903	3.2878	1.0000	
8	10	3	23.885	23.791	23.722	1.808	.094	.1299	1.0000	
8	12	-4	17.234	17.164	-17.057	1.915	.070	.0716	1.0000	
8	12	-3	42.440	41.391	41.312	2.558	1.049	1.9283	1.0000	
8	12	-2	5.667 *	3.605	-2.956	-2.062	2.062	.8232	1.0000	**
8	12	-1	23.462	21.011	-20.869	-2.434	2.451	3.4601	1.0000	
8	12	0	18.287	17.009	16.873	2.150	1.278	1.4366	1.0000	
8	12	1	33.413	31.600	31.511	2.366	1.814	2.9993	1.0000	
8	12	2	10.625	12.049	-11.860	-2.127	-1.423	-.9416	1.0000	
9	1	-8	29.872	29.078	28.929	2.931	.794	1.2420	1.0000	
9	1	-7	4.267 *	4.302	-4.136	1.187	-.035	-.0115	1.0000	**
9	1	-6	13.104	12.209	-11.852	-2.929	.896	.9601	1.0000	
9	1	-5	3.732 *	4.327	-4.130	-1.291	-.595	-.2237	1.0000	**
9	1	-4	6.617 *	6.580	5.902	2.911	.037	.0268	1.0000	**
9	1	-4	6.237 *	6.580	5.902	2.911	-.343	-.2339	1.0000	**
9	1	-3	4.604 *	3.344	3.065	1.338	1.260	.6981	1.0000	**
9	1	-2	4.587 *	3.358	1.800	-2.835	1.229	.7006	1.0000	**
9	1	-1	7.991	8.907	-8.801	-1.372	-.917	-.8996	1.0000	
9	1	0	23.488	22.570	22.397	2.792	.917	2.0821	1.0000	
9	1	1	17.164	17.812	17.758	1.379	-.647	-1.1180	1.0000	
9	1	2	7.282 *	8.656	8.264	-2.576	-1.373	-1.0460	1.0000	**
9	1	3	30.779	29.626	-29.594	-1.373	1.153	2.3827	1.0000	
9	1	4	9.304	4.975	-4.348	2.416	4.329	3.2969	1.0000	
9	1	5	20.698	21.476	21.438	1.275	-.779	-1.0014	1.0000	
9	3	-8	8.958 *	9.522	9.520	.150	-.564	-.3295	1.0000	**
9	3	-7	37.162	37.416	37.165	4.325	-.254	-.4738	1.0000	
9	3	-6	9.710	9.987	-9.985	-.210	-.277	-.2213	1.0000	
9	3	-5	91.040	91.015	-90.887	-4.818	.025	.0626	1.0000	
9	3	-4	23.496	22.708	22.706	.302	.789	1.5479	1.0000	
9	3	-3	110.010	108.716	108.598	5.062	1.294	2.1707	1.0000	
9	3	-2	15.083	14.515	-14.511	-.320	.568	.9263	1.0000	
9	3	-1	106.857	105.039	-104.913	-5.134	1.818	4.2094	1.0000	
9	3	0	30.908	29.647	29.645	.386	1.261	3.1735	1.0000	
9	3	1	78.126	75.644	75.477	5.014	2.482	7.5603	1.0000	
9	3	2	13.294	12.961	-12.956	-.349	.334	.4202	1.0000	
9	3	3	78.454	76.756	-76.603	-4.844	1.698	4.4667	1.0000	
9	3	4	24.913	23.971	23.968	.376	.942	1.4944	1.0000	
9	3	5	62.957	61.031	60.865	4.492	1.926	4.1288	1.0000	
9	5	-8	47.312	48.372	-48.175	-4.362	-1.060	-1.9791	1.0000	
9	5	-7	4.423 *	.987	.099	.982	3.436	1.0898	1.0000	**
9	5	-6	43.218	44.535	44.304	4.525	-1.317	-2.7720	1.0000	
9	5	-5	14.176	13.995	-13.952	-1.097	.180	.2087	1.0000	
9	5	-4	28.645	29.288	-28.931	-4.558	-.643	-1.3287	1.0000	
9	5	-3	6.919 *	1.291	-.686	1.094	5.628	4.0976	1.0000	**
9	5	-2	45.231	45.449	45.216	4.591	-.218	-.5873	1.0000	
9	5	-1	15.506	15.523	-15.480	-1.154	-.017	-.0260	1.0000	
9	5	0	40.428	39.093	-38.836	-4.469	1.335	3.4347	1.0000	
9	5	1	10.643	11.477	11.421	1.128	-.834	-.8544	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
9	5	2	37.309	36.015	35.760	4.278	1.295	2.8820	1.0000	
9	5	3	30.191	30.218	-30.196	-1.149	-.026	-.0493	1.0000	
9	5	4	9.787	10.246	-9.463	-3.928	-.458	-.3380	1.0000	
9	5	5	17.363	18.452	18.422	1.042	-1.089	-1.1354	1.0000	
9	7	-7	33.379	34.480	-34.330	-3.217	-1.102	-1.8219	1.0000	
9	7	-6	4.371 *	1.630	.114	1.626	2.741	.8789	1.0000	**
9	7	-5	32.964	32.853	32.671	3.459	.111	.2102	1.0000	
9	7	-4	17.346	16.920	16.850	-1.538	.426	.5667	1.0000	
9	7	-3	59.536	59.006	-58.889	-3.710	.530	1.3630	1.0000	
9	7	-2	7.930 *	6.711	-6.538	1.515	1.219	.9163	1.0000	**
9	7	-1	46.336	46.592	46.441	3.740	-.255	-.6290	1.0000	
9	7	0	7.783 *	8.652	8.532	-1.434	-.868	-.6056	1.0000	**
9	7	1	70.498	68.961	-68.857	-3.782	1.537	3.9535	1.0000	
9	7	2	7.731 *	6.465	-6.322	1.355	1.266	.8010	1.0000	**
9	7	3	61.454	59.817	59.707	3.624	1.637	3.7151	1.0000	
9	7	4	23.168	20.997	20.962	-1.205	2.171	2.9924	1.0000	
9	9	-6	4.552 *	1.126	-.237	-1.101	3.427	1.0550	1.0000	**
9	9	-5	25.397	25.177	25.031	2.702	.220	.3266	1.0000	
9	9	-4	4.233 *	1.614	-1.208	1.070	2.619	.8663	1.0000	**
9	9	-3	52.418	52.361	-52.280	-2.906	.057	.1290	1.0000	
9	9	-2	8.535 *	8.872	8.816	-1.000	-.337	-.2338	1.0000	**
9	9	-1	23.013	22.618	22.438	2.841	.395	.6264	1.0000	
9	9	0	6.030 *	4.695	-4.596	.959	1.335	.6493	1.0000	**
9	9	1	28.844	27.326	-27.180	-2.825	1.517	2.6616	1.0000	
9	9	2	11.757	10.801	10.766	-.873	.956	.7904	1.0000	
9	9	3	17.735	16.301	16.080	2.677	1.434	1.5807	1.0000	
9	11	-5	6.911 *	2.578	2.468	.745	4.332	1.9514	1.0000	**
9	11	-4	6.341 *	7.110	6.361	3.176	-.769	-.3347	1.0000	**
9	11	-3	16.871	16.653	-16.632	-.830	.218	.2424	1.0000	
9	11	-2	7.265 *	7.103	-6.379	-3.124	.162	.0846	1.0000	**
9	11	-2	5.416 *	7.103	-6.379	-3.124	-1.687	-.6688	1.0000	**
9	11	-1	4.354 *	1.186	.894	.779	3.168	1.0188	1.0000	**
9	11	0	14.547	13.393	13.043	3.043	1.154	1.1129	1.0000	
9	11	1	20.404	21.595	-21.579	-.842	-1.192	-1.4369	1.0000	
9	11	2	6.885 *	4.299	-3.216	-2.853	2.585	1.1783	1.0000	**
9	11	0	13.640	13.393	13.043	3.043	.247	.2248	1.0000	
9	11	1	20.585	21.595	-21.579	-.842	-1.010	-1.2310	1.0000	
9	11	2	6.194 *	4.299	-3.216	-2.853	1.894	.7888	1.0000	**
10	0	-8	73.945	75.469	75.302	5.015	-1.524	-3.2671	1.0000	
10	0	-6	105.293	107.249	-107.111	-5.426	-1.955	-4.1919	1.0000	
10	0	-4	77.953	75.427	75.227	5.483	2.526	7.4988	1.0000	
10	0	-2	107.738	104.294	-104.144	-5.580	3.444	6.2300	1.0000	
10	0	0	90.366	84.511	84.338	5.401	5.855	11.2971	1.0000	
10	0	2	104.801	101.676	-101.543	-5.201	3.125	5.0948	1.0000	
10	0	4	50.897	50.402	50.186	4.661	.495	1.0822	1.0000	
10	2	-8	5.451 *	4.387	-4.279	.965	1.064	.3837	1.0000	**
10	2	-7	5.451 *	6.935	5.995	3.487	-1.485	-.5968	1.0000	**
10	2	-6	19.324	18.936	-18.906	-1.071	.388	.5347	1.0000	
10	2	-5	16.931	16.188	-15.758	-3.705	.743	1.0369	1.0000	
10	2	-4	3.706 *	1.033	.261	1.000	2.673	1.0111	1.0000	**
10	2	-3	32.869	32.123	31.889	3.871	.746	1.8001	1.0000	
10	2	-2	37.568	36.531	-36.515	-1.063	1.038	2.7300	1.0000	
10	2	-1	25.578	24.895	-24.587	-3.903	.683	1.4920	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
10	2	0	8.086	9.272	9.225	.929	-1.186	-1.0324	1.0000	
10	2	1	19.462	18.559	18.153	3.863	.903	1.5842	1.0000	
10	2	2	20.922	20.207	-20.187	-.890	.715	1.1832	1.0000	
10	2	3	28.749	28.314	-28.058	-3.793	.435	.7991	1.0000	
10	2	4	18.866	18.898	-18.886	.669	-.032	-.0402	1.0000	
10	2	5	38.976	37.506	37.328	3.649	1.470	2.5786	1.0000	
10	4	-8	31.133	31.759	-31.668	-2.403	-.626	-.9662	1.0000	
10	4	-7	17.372	18.156	-18.081	1.646	-.784	-.8728	1.0000	
10	4	-6	26.019	25.209	25.086	2.495	.809	1.3387	1.0000	
10	4	-5	17.156	16.796	16.710	-1.701	.359	.4728	1.0000	
10	4	-4	53.498	53.755	-53.690	-2.630	-.257	-.6615	1.0000	
10	4	-3	5.321 *	5.384	-5.086	1.765	-.062	-.0345	1.0000	**
10	4	-2	39.011	39.546	39.463	2.558	-.535	-1.3458	1.0000	
10	4	-1	13.726	15.063	14.962	-1.746	-1.337	-1.7787	1.0000	
10	4	0	65.306	64.138	-64.087	-2.540	1.169	3.2997	1.0000	
10	4	1	18.702	18.692	-18.612	1.724	.010	.0162	1.0000	
10	4	2	22.512	22.384	22.269	2.267	.128	.2086	1.0000	
10	4	3	7.274 *	6.652	6.424	-1.728	.621	.3632	1.0000	**
10	4	4	14.417	16.005	-15.873	-2.051	-1.587	-1.5185	1.0000	
10	4	5	8.414 *	6.245	6.006	1.713	2.169	1.1677	1.0000	**
10	6	-7	20.758	20.821	20.820	-.028	-.062	-.0769	1.0000	
10	6	-6	49.714	50.201	50.054	3.837	-.487	-1.0251	1.0000	
10	6	-5	17.717	17.886	-17.886	.013	-.169	-.2124	1.0000	
10	6	-4	53.575	53.558	-53.414	-3.928	.017	.0409	1.0000	
10	6	-3	24.317	24.027	24.027	.025	.290	.5082	1.0000	
10	6	-2	31.651	32.021	31.790	3.834	-.370	-.7782	1.0000	
10	6	-1	19.195	20.383	-20.383	-.017	-1.189	-1.8347	1.0000	
10	6	0	61.739	59.960	-59.840	-3.799	1.778	4.5748	1.0000	
10	6	1	19.583	19.664	19.664	.008	-.081	-.1204	1.0000	
10	6	2	42.656	40.047	39.892	3.523	2.609	5.5937	1.0000	
10	6	3	12.750	14.908	-14.908	.027	-2.157	-1.9064	1.0000	
10	6	4	36.316	35.886	-35.741	-3.224	.430	.7429	1.0000	
10	8	-6	8.509 *	10.193	10.129	1.144	-1.684	-.9604	1.0000	**
10	8	-5	20.758	20.383	20.027	3.789	.375	.4938	1.0000	
10	8	-4	25.621	26.890	-26.860	-1.263	-1.268	-2.0115	1.0000	
10	8	-3	24.680	24.153	-23.832	-3.929	.527	.8465	1.0000	
10	8	-2	22.045	22.307	22.270	1.273	-.262	-.4038	1.0000	
10	8	-1	23.747	23.209	22.865	3.981	.538	.8765	1.0000	
10	8	0	38.130	37.221	-37.198	-1.318	.909	1.8453	1.0000	
10	8	1	16.180	16.927	-16.463	-3.936	-.747	-.8562	1.0000	
10	8	2	18.408	16.924	16.881	1.207	1.484	1.7894	1.0000	
10	8	3	25.621	25.338	25.042	3.862	.283	.4047	1.0000	
10	10	-5	8.293 *	7.673	7.493	1.653	.620	.3450	1.0000	**
10	10	-4	56.124	57.738	57.580	4.271	-1.615	-3.3381	1.0000	
10	10	-3	9.908	8.362	-8.188	-1.699	1.546	1.0781	1.0000	
10	10	-2	71.621	72.017	-71.886	-4.341	-.396	-.8991	1.0000	
10	10	-1	4.544 *	7.201	6.995	1.710	-2.657	-.8839	1.0000	**
10	10	0	67.164	65.479	65.343	4.215	1.684	3.7494	1.0000	
10	10	1	4.406 *	1.684	-.238	-1.667	2.721	.8655	1.0000	**
10	10	2	58.050	56.004	-55.863	-3.970	2.046	4.1557	1.0000	
10	12	-2	9.908	9.876	-9.572	-2.431	.032	.0209	1.0000	
10	12	-1	8.630 *	8.860	-8.631	-2.002	-.230	-.1239	1.0000	**
11	1	-8	21.268	20.964	20.795	2.662	.303	.3621	1.0000	

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
11	1	-7	8.906	*	9.598	9.505	1.333	-.691	-.4303	1.0000	**
11	1	-6	13.286		13.613	-13.311	-2.849	-.327	-.3155	1.0000	
11	1	-5	7.930	*	7.132	-7.017	-1.274	.798	.5405	1.0000	**
11	1	-4	34.804		33.326	33.184	3.074	1.478	3.2997	1.0000	
11	1	-3	3.706	*	3.217	2.992	1.183	.488	.1842	1.0000	**
11	1	-2	16.439		15.461	-15.144	-3.115	.978	1.5099	1.0000	
11	1	-1	17.985		16.295	16.262	-1.034	1.690	2.7557	1.0000	
11	1	0	53.532		51.323	51.220	3.244	2.209	5.8125	1.0000	
11	1	1	29.008		28.398	-28.383	.893	.610	1.2393	1.0000	
11	1	2	46.889		44.724	-44.611	-3.171	2.166	5.0138	1.0000	
11	1	3	26.313		26.236	26.224	-.792	.076	.1226	1.0000	
11	1	4	46.034		43.620	43.515	3.035	2.414	4.7358	1.0000	
11	3	-7	32.342		33.089	32.802	4.345	-.747	-1.2708	1.0000	
11	3	-6	4.285	*	2.507	-2.502	-.158	1.777	.5812	1.0000	**
11	3	-5	37.456		37.814	-37.551	-4.451	-.358	-.7532	1.0000	
11	3	-4	20.853		21.430	21.429	.235	-.577	-.9152	1.0000	
11	3	-3	63.700		62.425	62.262	4.509	1.274	3.4310	1.0000	
11	3	-2	3.671	*	2.448	-2.441	-.181	1.224	.4675	1.0000	**
11	3	-1	56.340		54.767	-54.592	-4.367	1.573	4.2349	1.0000	
11	3	0	15.843		17.561	17.560	.224	-1.718	-2.3127	1.0000	
11	3	1	34.027		35.256	35.016	4.108	-1.229	-2.5416	1.0000	
11	3	2	4.086	*	1.716	-1.709	-.161	2.370	.8117	1.0000	**
11	3	3	10.314		12.087	-11.489	-3.754	-1.772	-1.3411	1.0000	
11	3	4	11.999		10.638	10.637	.177	1.361	1.1014	1.0000	
11	5	-7	15.532		14.989	14.953	1.048	.542	.5233	1.0000	
11	5	-6	52.400		53.630	53.450	4.385	-1.230	-2.5879	1.0000	
11	5	-5	10.919		11.113	-11.064	-1.046	-.194	-.1616	1.0000	
11	5	-4	42.639		42.801	-42.552	-4.608	-.162	-.3531	1.0000	
11	5	-3	16.093		15.747	15.712	1.051	.346	.4503	1.0000	
11	5	-2	63.008		63.584	63.400	4.831	-.575	-1.4796	1.0000	
11	5	-1	3.913	*	4.471	4.368	-.955	-.558	-.1993	1.0000	**
11	5	0	62.551		66.315	-66.135	-4.875	-3.764	-9.4723	1.0000	
11	5	1	4.034	*	4.505	-4.414	.904	-.471	-.1633	1.0000	**
11	5	2	81.149		84.072	83.932	4.847	-2.923	-7.0492	1.0000	
11	5	3	9.165	*	10.163	10.130	-.816	-.997	-.6450	1.0000	**
11	5	4	60.555		60.682	-60.512	-4.544	-.127	-.2583	1.0000	
11	7	-6	10.193		12.505	12.396	1.650	-2.312	-1.5468	1.0000	
11	7	-5	41.844		43.099	42.968	3.348	-1.254	-2.4609	1.0000	
11	7	-4	4.233	*	3.235	2.767	-1.675	.998	.3301	1.0000	**
11	7	-3	30.856		31.858	-31.688	-3.286	-1.002	-1.8125	1.0000	
11	7	-2	5.269	*	6.687	6.453	1.753	-1.417	-.6121	1.0000	**
11	7	-1	25.907		27.569	27.385	3.180	-1.662	-2.7885	1.0000	
11	7	0	9.295		7.879	-7.680	-1.763	1.415	1.0571	1.0000	
11	7	1	4.259	*	2.930	.135	-2.926	1.329	.4371	1.0000	**
11	7	2	23.021		24.287	24.221	1.789	-1.265	-1.7436	1.0000	
11	7	3	4.725	*	10.055	9.670	2.753	-5.329	-1.6765	1.0000	**
11	9	-5	5.831	*	7.918	7.498	2.545	-2.087	-.8080	1.0000	**
11	9	-4	8.276	*	7.824	7.737	1.166	.452	.2526	1.0000	**
11	9	-3	10.703		10.536	-10.240	-2.480	.167	.1252	1.0000	
11	9	-2	6.315	*	4.179	-4.003	-1.201	2.136	.9889	1.0000	**
11	9	-1	19.065		20.548	20.408	2.395	-1.483	-1.8262	1.0000	
11	9	0	13.977		13.783	13.726	1.257	.194	.1825	1.0000	
11	9	1	11.049		7.491	7.181	-2.134	3.557	2.6915	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
11	9	2	12.327	10.693	-10.622	-1.232	1.634	1.2777	1.0000	
11	11	-3	10.945	12.066	-12.040	-.786	-1.121	-.7725	1.0000	
11	11	-2	16.430	19.792	-19.495	-3.418	-3.362	-3.2981	1.0000	
11	11	-1	17.294	17.719	17.700	.840	-.425	-.4397	1.0000	
11	11	0	32.524	34.323	34.144	3.501	-1.799	-2.8529	1.0000	
12	0	-6	43.036	42.854	-42.636	-4.313	.182	.3706	1.0000	
12	0	-4	39.149	38.228	37.974	4.407	.921	2.0112	1.0000	
12	0	-2	17.570	16.578	-15.992	-4.370	.992	1.4537	1.0000	
12	0	0	13.122	14.194	13.522	4.315	-1.072	-1.1708	1.0000	
12	0	2	22.900	20.400	-19.962	-4.206	2.501	3.7112	1.0000	
12	0	4	35.798	33.590	33.345	4.048	2.208	3.7582	1.0000	
12	2	-7	44.565	45.544	45.354	4.151	-.978	-1.8561	1.0000	
12	2	-6	12.603	13.443	13.425	-.683	-.839	-.7532	1.0000	
12	2	-5	61.505	62.326	-62.169	-4.424	-.821	-1.9385	1.0000	
12	2	-4	24.092	22.966	-22.957	.630	1.127	1.8904	1.0000	
12	2	-3	81.477	79.136	79.004	4.568	2.342	6.3038	1.0000	
12	2	-2	28.481	27.501	27.495	-.591	.979	1.9215	1.0000	
12	2	-1	93.908	93.048	-92.935	-4.580	.860	2.3713	1.0000	
12	2	0	12.690	12.756	-12.741	.613	-.066	-.0691	1.0000	
12	2	1	66.628	67.132	66.991	4.346	-.504	-1.2415	1.0000	
12	2	2	4.198 *	4.112	4.065	-.618	.086	.0288	1.0000	**
12	2	3	45.481	46.646	-46.474	-4.012	-1.165	-2.3259	1.0000	
12	2	4	5.442 *	4.486	4.442	.627	.956	.3481	1.0000	**
12	4	-7	11.584	10.929	10.698	2.236	.655	.4771	1.0000	
12	4	-6	6.056 *	5.852	-5.555	1.841	.203	.0884	1.0000	**
12	4	-5	23.030	23.719	-23.601	-2.363	-.689	-1.0226	1.0000	
12	4	-4	14.996	13.993	13.873	-1.828	1.003	1.1499	1.0000	
12	4	-3	28.602	28.497	28.397	2.390	.105	.1953	1.0000	
12	4	-2	18.253	16.613	-16.514	1.811	1.640	2.3147	1.0000	
12	4	-1	45.110	45.566	-45.503	-2.393	-.457	-1.0366	1.0000	
12	4	0	6.349 *	8.873	8.688	-1.802	-2.524	-1.2984	1.0000	**
12	4	1	19.195	21.056	20.940	2.201	-1.861	-2.4207	1.0000	
12	4	2	11.308	11.256	11.109	1.815	.052	.0420	1.0000	
12	4	3	14.271	13.097	-12.942	-2.009	1.173	1.1042	1.0000	
12	6	-6	16.430	18.181	17.936	2.973	-1.751	-1.7322	1.0000	
12	6	-5	10.504	7.175	-7.166	.345	3.330	2.5028	1.0000	
12	6	-4	14.331	11.804	-11.420	-2.986	2.527	2.6121	1.0000	
12	6	-3	8.958	8.323	-8.314	-.382	.635	.4350	1.0000	
12	6	-2	9.666	7.166	-6.545	2.918	2.501	1.9045	1.0000	
12	6	-1	5.019 *	5.335	-5.326	.303	-.316	-.1283	1.0000	**
12	6	0	13.493	14.698	14.421	-2.841	-1.205	-1.1724	1.0000	
12	6	1	6.332 *	5.204	-5.195	-.303	1.128	.5307	1.0000	**
12	6	2	5.727 *	3.106	1.338	2.804	2.621	1.0571	1.0000	**
12	6	3	6.332 *	8.759	-8.756	.207	-2.427	-.9961	1.0000	**
12	8	-5	42.129	44.657	44.432	4.469	-2.527	-4.5709	1.0000	
12	8	-4	7.308 *	8.361	-8.288	-1.103	-1.053	-.5233	1.0000	**
12	8	-3	74.092	77.482	-77.340	-4.691	-3.391	-7.6963	1.0000	
12	8	-2	9.183	10.804	10.744	1.137	-1.621	-1.0664	1.0000	
12	8	-1	65.643	68.259	68.103	4.624	-2.616	-5.8242	1.0000	
12	8	0	15.359	16.440	-16.399	-1.152	-1.080	-1.0972	1.0000	
12	8	1	61.704	66.860	-66.711	-4.460	-5.156	-10.8524	1.0000	
12	8	2	22.304	25.645	25.619	1.154	-3.341	-4.2040	1.0000	
12	10	-3	30.865	31.121	-31.054	-2.035	-.256	-.3946	1.0000	

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
12	10	-2	6.427	*	8.616	-7.958	-3.302	-2.189	-.9281	1.0000	**
12	10	-1	17.709		20.163	20.067	1.967	-2.454	-2.5592	1.0000	
12	10	0	15.938		18.031	17.725	3.307	-2.093	-2.0363	1.0000	
13	1	-7	10.193		11.447	-11.403	1.004	-1.253	-.8106	1.0000	
13	1	-6	47.079		47.651	-47.542	-3.218	-.571	-1.1405	1.0000	
13	1	-5	12.949		11.211	11.161	-1.056	1.738	1.6355	1.0000	
13	1	-4	35.841		34.256	34.112	3.143	1.584	3.1619	1.0000	
13	1	-3	4.060	*	1.963	1.600	1.137	2.097	.7226	1.0000	**
13	1	-2	37.879		36.246	-36.117	-3.049	1.634	3.5023	1.0000	
13	1	-1	12.051		9.640	-9.567	-1.182	2.411	2.3064	1.0000	
13	1	0	4.121	*	2.762	-.086	2.761	1.358	.4624	1.0000	**
13	1	1	7.265	*	6.163	6.051	1.169	1.102	.6132	1.0000	**
13	1	2	14.996		17.757	-17.564	-2.608	-2.760	-2.7787	1.0000	
13	1	3	4.552	*	4.763	4.634	-1.103	-.211	-.0649	1.0000	**
13	3	-7	22.045		22.704	22.397	3.716	-.658	-.7939	1.0000	
13	3	-6	13.675		12.105	-12.105	-.087	1.569	1.4420	1.0000	
13	3	-5	10.729		8.224	-7.239	-3.903	2.505	1.9590	1.0000	
13	3	-4	5.529	*	1.384	-1.381	.084	4.145	1.8384	1.0000	**
13	3	-3	22.114		22.361	21.978	4.122	-.247	-.3666	1.0000	
13	3	-2	18.529		18.574	-18.573	-.197	-.044	-.0582	1.0000	
13	3	-1	44.410		42.710	-42.496	-4.265	1.700	3.7140	1.0000	
13	3	0	4.198	*	2.678	2.672	.176	1.521	.5073	1.0000	**
13	3	1	56.728		56.269	56.106	4.285	.459	1.0227	1.0000	
13	3	2	19.428		19.685	-19.683	-.262	-.257	-.3130	1.0000	
13	3	3	45.075		46.870	-46.689	-4.117	-1.795	-3.3515	1.0000	
13	5	-6	54.983		56.904	56.719	4.595	-1.921	-3.8342	1.0000	
13	5	-5	4.440	*	1.102	-.602	-.922	3.338	1.0530	1.0000	**
13	5	-4	73.901		74.655	-74.506	-4.703	-.753	-1.7439	1.0000	
13	5	-3	16.154		16.474	16.443	1.011	-.320	-.3567	1.0000	
13	5	-2	42.639		44.539	44.309	4.519	-1.900	-3.9273	1.0000	
13	5	-1	14.625		15.193	-15.159	-1.016	-.568	-.5922	1.0000	
13	5	0	36.566		42.495	-42.274	-4.330	-5.929	-11.2520	1.0000	
13	5	1	12.819		13.174	13.136	.997	-.355	-.3157	1.0000	
13	5	2	22.114		25.353	25.037	3.991	-3.238	-4.1196	1.0000	
13	7	-5	19.497		20.331	20.121	2.913	-.834	-.9561	1.0000	
13	7	-4	23.756		23.333	-23.260	-1.842	.423	.5824	1.0000	
13	7	-3	24.455		24.940	-24.751	-3.060	-.484	-.7007	1.0000	
13	7	-2	4.656	*	1.672	-.093	1.669	2.984	1.0282	1.0000	**
13	7	-1	39.495		43.391	43.274	3.190	-3.896	-7.1598	1.0000	
13	7	0	4.812	*	1.619	-.460	-1.553	3.192	1.0966	1.0000	**
13	7	1	32.161		33.838	-33.692	-3.140	-1.677	-2.6962	1.0000	
13	9	-3	12.457		12.777	12.573	-2.275	-.321	-.2458	1.0000	
13	9	-2	12.448		10.891	-10.826	-1.186	1.557	1.2345	1.0000	
13	9	-1	12.975		12.820	12.592	2.410	.155	.1260	1.0000	
14	0	-6	40.816		41.379	-41.115	-4.665	-.562	-1.0172	1.0000	
14	0	-4	93.260		91.718	91.579	5.055	1.542	3.7184	1.0000	
14	0	-2	84.319		81.137	-80.978	-5.083	3.182	7.8381	1.0000	
14	0	0	87.205		85.193	85.045	5.028	2.011	4.7520	1.0000	
14	0	2	54.551		54.481	-54.277	-4.707	.071	.1411	1.0000	
14	2	-6	4.552	*	.957	.055	-.955	3.596	1.1041	1.0000	**
14	2	-5	14.167		14.292	-13.852	-3.518	-.125	-.1166	1.0000	
14	2	-4	20.628		20.109	20.081	1.049	.520	.6915	1.0000	
14	2	-3	7.179	*	8.251	7.479	3.485	-1.073	-.5886	1.0000	**

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
14	2	-2	5.675	*	6.239	6.167	-.945	-.564	-.2435	1.0000	**
14	2	-1	13.096		13.760	-13.326	-3.432	-.665	-.6256	1.0000	
14	2	0	4.518	*	4.347	4.242	.948	.171	.0577	1.0000	**
14	2	1	21.536		21.545	21.287	3.329	-.010	-.0131	1.0000	
14	2	2	8.854	*	7.416	7.368	-.845	1.438	.8283	1.0000	**
14	4	-6	32.938		33.448	33.368	2.310	-.510	-.8082	1.0000	
14	4	-5	11.938		11.075	10.935	-1.757	.863	.6707	1.0000	
14	4	-4	23.833		23.346	-23.227	-2.355	.487	.6967	1.0000	
14	4	-3	17.942		17.269	-17.188	1.675	.673	.7870	1.0000	
14	4	-2	34.994		34.512	34.427	2.415	.482	.8858	1.0000	
14	4	-1	12.578		13.966	13.874	-1.606	-1.389	-1.1910	1.0000	
14	4	0	8.803	*	10.778	-10.535	-2.278	-1.976	-1.2167	1.0000	**
14	4	1	4.492	*	3.704	-3.363	1.552	.788	.2460	1.0000	**
14	4	2	22.106		24.468	24.367	2.219	-2.362	-2.9093	1.0000	
14	6	-5	10.046		11.351	-11.350	.147	-1.305	-.8299	1.0000	
14	6	-4	43.408		43.289	-43.138	-3.607	.119	.2229	1.0000	
14	6	-3	17.380		18.047	18.047	-.069	-.666	-.7276	1.0000	
14	6	-2	60.788		62.359	62.248	3.710	-1.571	-3.3056	1.0000	
14	6	-1	14.046		14.274	-14.274	.041	-.228	-.2092	1.0000	
14	6	0	32.774		38.501	-38.338	-3.549	-5.727	-9.2086	1.0000	
14	6	1	17.398		18.106	18.106	.004	-.708	-.7453	1.0000	
14	8	-3	4.647	*	6.923	-5.949	-3.539	-2.275	-.6859	1.0000	**
14	8	-2	14.253		15.343	15.303	1.106	-1.090	-.9559	1.0000	
14	8	-1	15.368		18.183	17.841	3.511	-2.815	-2.5658	1.0000	
15	1	-5	4.596	*	7.120	-6.976	-1.428	-2.525	-.7691	1.0000	**
15	1	-4	4.501	*	3.491	2.422	2.514	1.010	.3143	1.0000	**
15	1	-3	4.786	*	2.277	1.836	1.347	2.508	.8591	1.0000	**
15	1	-2	17.864		15.905	-15.691	-2.604	1.959	2.3378	1.0000	
15	1	-1	7.386	*	9.150	-9.061	-1.278	-1.765	-.9119	1.0000	**
15	1	0	6.220	*	8.462	8.063	2.569	-2.243	-.9687	1.0000	**
15	1	1	11.757		11.389	11.329	1.166	.368	.2765	1.0000	
15	3	-5	67.950		67.640	-67.490	-4.492	.310	.6521	1.0000	
15	3	-4	7.835	*	9.201	9.200	.173	-1.366	-.7125	1.0000	**
15	3	-3	46.155		46.508	46.301	4.387	-.353	-.6936	1.0000	
15	3	-2	14.366		13.596	-13.595	-.199	.770	.7302	1.0000	
15	3	-1	40.497		43.685	-43.479	-4.237	-3.188	-5.9528	1.0000	
15	3	0	8.284	*	9.502	9.500	.183	-1.218	-.6712	1.0000	**
15	3	1	31.902		35.146	34.922	3.961	-3.244	-5.0754	1.0000	
15	5	-4	28.654		28.252	-27.991	-3.838	.401	.5953	1.0000	

CANISI206, - FINAL STRUCTURE FACTORS LISTING

RESULTS OF STRUCTURE FACTOR CALCULATIONS

ALL REFLECTIONS	NUMERATOR	DENOMINATOR	NUMBER	R
WEIGHTED R	15120.08	8827567.54	1152	.041
UNWEIGHTED R	1699.73	36454.90	1152	.047
RANGES OF F(OBS)				
	1704.19	398886.98	676	.065
	3731.32	2407200.91	270	.039
	2104.82	3021296.33	115	.026
	3428.32	1885313.23	43	.043
	627.53	710921.32	25	.030
	1763.91	319564.79	20	.074
	1626.37	54483.38	2	.173
	133.62	29900.60	1	.067
RANGES OF (SIN(THETA)/LAMBDA)**2				
	3839.25	885040.77	56	.066
	5106.30	1466474.85	96	.059
	1725.50	1623887.98	116	.033
	1178.01	1491982.78	147	.028
	853.62	1240817.05	158	.026
	733.87	985472.89	184	.027
	926.34	674204.44	202	.037
	757.19	459686.76	193	.041

UNREJECTED REFLECTIONS				
WEIGHTED R	15120.08	8827567.54	1152	.041
UNWEIGHTED R	1699.73	36454.90	1152	.047
RANGES OF F(OBS)				
	1704.19	398886.98	676	.065
	3731.32	2407200.91	270	.039
	2104.82	3021296.33	115	.026
	3428.32	1885313.23	43	.043
	627.53	710921.32	25	.030
	1763.91	319564.79	20	.074
	1626.37	54483.38	2	.173
	133.62	29900.60	1	.067
RANGES OF (SIN(THETA)/LAMBDA)**2				
	3839.25	885040.77	56	.066
	5106.30	1466474.85	96	.059
	1725.50	1623887.98	116	.033
	1178.01	1491982.78	147	.028
	853.62	1240817.05	158	.026
	733.87	985472.89	184	.027
	926.34	674204.44	202	.037
	757.19	459686.76	193	.041

SUM FCAL 36351.03

STANDARD DEV OF UNIT WEIGHT OBS 3.70

Crystal structures of $CaNiSi_2O_6$ and $CaCoSi_2O_6$ and some crystal chemical relations in *C2/c* clinopyroxenes

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Table 5 b. $CaCoSi_2O_6$: Observed and Calculated Structure Factors

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
0	0	2	211.258	211.289	-211.213	-5.641	-.030	-.0528	1.0000	
0	0	4	141.368	139.504	139.403	5.304	1.864	2.1323	1.0000	
0	0	6	58.007	57.083	-56.891	-4.689	.924	2.0528	1.0000	
0	0	8	63.840	62.853	62.715	4.172	.987	2.3042	1.0000	
0	2	0	43.061	44.239	44.233	.725	-1.178	-2.5216	1.0000	
0	2	1	7.101	6.744	5.616	3.734	.357	1.2315	1.0000	
0	2	2	47.007	42.419	42.415	-.626	4.588	12.1871	1.0000	
0	2	3	40.902	41.238	-41.073	-3.677	-.336	-.9247	1.0000	
0	2	4	28.283	29.167	29.159	.694	-.884	-4.3477	1.0000	
0	2	5	38.798	38.877	38.719	3.507	-.079	-.2838	1.0000	
0	2	6	2.834 *	.633	.235	-.588	2.201	1.6464	1.0000	**
0	2	7	22.454	22.607	-22.381	-3.189	-.152	-.4513	1.0000	
0	2	8	18.910	17.442	17.432	.601	1.468	3.6870	1.0000	
0	4	0	32.303	35.311	-35.222	-2.509	-3.008	-10.6944	1.0000	
0	4	1	65.472	64.687	-64.677	1.151	.785	1.1778	1.0000	
0	4	2	88.125	88.860	88.824	2.538	-.735	-.9818	1.0000	
0	4	3	25.821	26.423	26.397	-1.183	-.602	-3.0261	1.0000	
0	4	4	32.411	32.353	-32.270	-2.323	.058	.2683	1.0000	
0	4	5	8.382	8.045	-7.956	1.197	.337	.7481	1.0000	
0	4	6	48.487	48.184	48.133	2.196	.304	.9484	1.0000	
0	4	7	13.116	12.476	12.425	-1.130	.640	1.3816	1.0000	
0	6	0	138.183	139.931	-139.882	-3.711	-1.748	-2.2070	1.0000	
0	6	1	40.304	40.827	40.826	.098	-.522	-1.6092	1.0000	
0	6	2	130.814	131.149	131.098	3.654	-.335	-.3853	1.0000	
0	6	3	27.301	26.803	-26.803	-.059	.498	2.2574	1.0000	
0	6	4	42.728	41.648	-41.517	-3.300	1.080	3.8386	1.0000	
0	6	5	22.407	22.230	22.230	.022	.177	.6101	1.0000	
0	6	6	36.648	36.050	35.923	3.024	.598	2.0622	1.0000	
0	6	7	11.415	12.306	-12.306	.045	-.891	-1.6088	1.0000	
0	8	0	7.019	6.588	-6.498	-1.088	.431	.9053	1.0000	
0	8	1	3.609 *	5.372	-3.907	-3.687	-1.764	-1.9688	1.0000	**
0	8	2	28.599	28.519	28.497	1.119	.080	.3442	1.0000	
0	8	3	25.743	25.377	25.114	3.641	.366	1.4339	1.0000	
0	8	4	16.063	16.117	-16.085	-1.028	-.055	-.1616	1.0000	
0	8	5	28.114	27.701	-27.484	-3.457	.414	1.3656	1.0000	
0	8	6	30.200	29.888	29.871	.987	.313	.9630	1.0000	
0	10	0	98.026	97.241	97.136	4.511	.785	.9915	1.0000	
0	10	1	8.356	8.549	8.461	-1.224	-.193	-.3917	1.0000	
0	10	2	79.168	79.640	-79.519	-4.387	-.472	-.6952	1.0000	
0	10	3	5.245	4.021	3.828	1.229	1.224	1.4807	1.0000	
0	10	4	71.669	72.259	72.139	4.151	-.590	-.9953	1.0000	
0	10	5	4.578 *	5.005	-4.866	-1.172	-.427	-.3666	1.0000	**
0	12	0	53.347	52.737	52.696	2.062	.610	1.5840	1.0000	
0	12	1	9.862	9.324	9.057	2.215	.538	1.0110	1.0000	
0	12	2	35.635	35.618	-35.563	-1.976	.017	.0573	1.0000	
0	12	3	12.540	11.416	-11.210	-2.160	1.124	2.3201	1.0000	
0	12	4	14.414	13.793	13.673	1.810	.622	1.3300	1.0000	
0	14	0	17.703	16.853	-16.841	-.652	.850	2.0037	1.0000	
0	14	1	23.722	21.948	-21.891	1.578	1.774	4.7673	1.0000	
0	14	2	13.332	11.250	11.233	.621	2.082	4.0774	1.0000	
1	1	-8	3.181 *	3.926	-3.446	1.882	-.746	-.4511	1.0000	**
1	1	-7	3.540 *	2.141	1.893	1.001	1.399	1.1264	1.0000	**
1	1	-6	5.487	6.738	-6.377	-2.175	-1.251	-1.7514	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
1	1	-5	7.837	7.269	-7.195	-1.041	.567	1.3109	1.0000	
1	1	-4	28.772	28.734	-28.640	2.325	.038	.1964	1.0000	
1	1	-3	8.577	8.071	8.003	1.041	.506	1.8258	1.0000	
1	1	-2	37.539	35.916	-35.822	-2.610	1.623	5.2084	1.0000	
1	1	-1	19.966	20.488	-20.463	-1.013	-.522	-2.2744	1.0000	
1	1	0	46.886	46.288	46.206	2.742	.598	1.5538	1.0000	
1	1	1	10.892	10.719	10.678	.938	.173	.8872	1.0000	
1	1	2	103.803	101.488	-101.448	-2.860	2.315	3.6893	1.0000	
1	1	3	13.285	13.507	-13.479	-.867	-.222	-.9873	1.0000	
1	1	4	32.005	31.090	30.969	2.742	.914	4.4012	1.0000	
1	1	5	5.656	5.159	-5.104	.752	.496	.8135	1.0000	
1	1	6	31.581	30.966	-30.854	-2.630	.615	2.2907	1.0000	
1	1	7	14.284	13.680	13.666	-.635	.604	1.3959	1.0000	
1	3	-8	6.906	6.414	6.409	.251	.492	.6049	1.0000	
1	3	-7	65.675	66.231	66.105	4.089	-.556	-1.2978	1.0000	
1	3	-6	27.850	27.301	-27.299	-.363	.549	2.0154	1.0000	
1	3	-5	120.848	121.751	-121.666	-4.542	-.902	-.8690	1.0000	
1	3	-4	12.333	12.008	12.003	.349	.325	1.1216	1.0000	
1	3	-3	157.479	156.703	156.631	4.739	.776	.9906	1.0000	
1	3	-2	57.484	55.795	-55.793	-.421	1.689	3.5163	1.0000	
1	3	-1	138.114	137.515	-137.434	-4.716	.599	1.0415	1.0000	
1	3	0	6.378	7.192	7.184	.354	-.814	-2.4749	1.0000	
1	3	1	25.111	29.646	29.305	4.485	-4.535	-21.3860	1.0000	
1	3	2	41.758	40.601	-40.599	-.368	1.157	3.1096	1.0000	
1	3	3	53.221	54.048	-53.880	-4.255	-.826	-1.9484	1.0000	
1	3	4	7.750	7.285	7.280	.277	.465	1.1203	1.0000	
1	3	5	46.739	46.688	46.526	3.894	.051	.1561	1.0000	
1	3	6	15.418	15.445	-15.444	-.247	-.027	-.0753	1.0000	
1	3	7	42.485	41.847	-41.704	-3.455	.638	2.1684	1.0000	
1	5	-7	2.566 *	1.309	1.076	.745	1.257	.6850	1.0000	**
1	5	-6	20.537	19.834	19.474	3.760	.703	2.1965	1.0000	
1	5	-5	10.256	10.172	-10.138	-.831	.084	.2083	1.0000	
1	5	-4	38.370	39.174	-38.948	-4.208	-.804	-3.2605	1.0000	
1	5	-3	2.956 *	4.196	4.109	.850	-1.240	-1.3146	1.0000	**
1	5	-2	50.629	50.753	50.551	4.517	-.124	-.3008	1.0000	
1	5	-1	40.356	39.326	-39.315	-.908	1.030	3.2620	1.0000	
1	5	0	142.446	140.470	-140.388	-4.812	1.975	2.7667	1.0000	
1	5	1	18.841	18.954	18.935	.854	-.113	-.5929	1.0000	
1	5	2	112.501	109.942	109.837	4.809	2.559	3.1123	1.0000	
1	5	3	34.597	35.605	-35.595	-.847	-1.009	-4.9591	1.0000	
1	5	4	86.360	86.824	-86.699	-4.661	-.465	-.6281	1.0000	
1	5	5	4.448 *	4.120	4.058	.713	.328	.3792	1.0000	**
1	5	6	53.213	53.125	52.950	4.304	.088	.2666	1.0000	
1	5	7	6.067	4.663	-4.619	-.634	1.404	1.5752	1.0000	
1	7	-7	43.031	43.313	-43.197	-3.174	-.282	-.9066	1.0000	
1	7	-6	18.850	18.615	-18.596	.841	.234	.6444	1.0000	
1	7	-5	50.798	50.082	49.963	3.445	.716	2.0696	1.0000	
1	7	-4	17.647	17.289	17.263	-.945	.358	1.2168	1.0000	
1	7	-3	84.888	82.831	-82.750	-3.673	2.057	2.8637	1.0000	
1	7	-2	24.817	24.446	-24.425	1.015	.371	1.6501	1.0000	
1	7	-1	69.501	69.063	68.966	3.665	.437	.6831	1.0000	
1	7	0	16.085	16.184	-16.143	-1.164	-.100	-.4051	1.0000	
1	7	1	84.642	86.089	-86.013	-3.617	-1.447	-1.5775	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
1	7	2	7.465	7.407	7.310	1.190	.058	.1273	1.0000	
1	7	3	46.843	46.506	46.385	3.349	.337	1.0379	1.0000	
1	7	4	9.845	9.144	-9.063	-1.210	.701	1.6199	1.0000	
1	7	5	45.480	45.257	-45.152	-3.079	.223	.7565	1.0000	
1	7	6	2.622 *	2.332	-2.027	1.153	.290	.1549	1.0000	**
1	9	-6	2.696 *	1.698	1.380	-.989	.998	.5184	1.0000	**
1	9	-5	37.418	36.814	36.750	2.168	.605	2.0850	1.0000	
1	9	-4	9.265	8.466	-8.397	1.074	.799	1.5782	1.0000	
1	9	-3	56.445	55.719	-55.673	-2.252	.726	1.5123	1.0000	
1	9	-2	4.808	3.694	-3.494	-1.197	1.114	1.5323	1.0000	
1	9	-1	8.469	8.231	7.962	2.088	.238	.5277	1.0000	
1	9	0	6.526	4.569	4.393	1.259	1.956	3.5877	1.0000	
1	9	1	2.969 *	2.847	2.048	-1.978	.121	.1057	1.0000	**
1	9	2	17.668	16.856	-16.805	-1.321	.812	2.7591	1.0000	
1	9	3	20.174	20.646	-20.568	1.785	-.472	-1.5807	1.0000	
1	9	4	9.555	8.567	8.469	1.289	.988	1.9025	1.0000	
1	9	5	11.896	11.393	-11.263	-1.715	.502	1.0557	1.0000	
1	9	6	12.614	12.719	-12.656	-1.258	-.105	-.2014	1.0000	
1	11	-5	3.319 *	1.346	-1.273	.435	1.973	1.2128	1.0000	**
1	11	-4	8.192	6.547	-6.055	2.488	1.645	2.5686	1.0000	
1	11	-3	16.855	17.035	-17.026	-.558	-.180	-.4732	1.0000	
1	11	-2	7.032	8.599	-8.154	-2.730	-1.567	-2.3063	1.0000	
1	11	-1	12.086	10.885	10.869	.575	1.201	2.8922	1.0000	
1	11	0	27.651	28.388	28.238	2.915	-.737	-2.5809	1.0000	
1	11	1	36.319	36.035	-36.029	-.668	.284	1.0414	1.0000	
1	11	2	38.703	39.043	-38.928	-2.991	-.340	-1.2272	1.0000	
1	11	3	17.621	17.562	17.552	.596	.059	.1602	1.0000	
1	11	4	25.064	25.214	25.047	2.899	-.150	-.4396	1.0000	
1	11	5	25.367	25.631	-25.624	-.592	-.264	-.7263	1.0000	
1	13	-3	43.870	43.163	43.013	3.600	.707	2.2683	1.0000	
1	13	-2	16.833	15.793	-15.722	-1.498	1.040	2.4780	1.0000	
1	13	-1	55.800	55.982	-55.861	-3.680	-.182	-.4624	1.0000	
1	13	0	25.488	24.279	24.228	1.575	1.209	3.5820	1.0000	
1	13	1	35.103	35.842	35.668	3.522	-.739	-2.3717	1.0000	
1	13	2	27.046	25.615	-25.567	-1.575	1.430	4.1843	1.0000	
1	13	3	44.961	44.664	-44.537	-3.361	.297	.9527	1.0000	
2	0	-8	55.034	54.634	54.494	3.908	.400	1.0512	1.0000	
2	0	-6	54.463	54.904	-54.738	-4.263	-.441	-.9982	1.0000	
2	0	-4	24.285	24.313	23.902	4.448	-.028	-.1343	1.0000	
2	0	-2	11.143	13.179	-12.355	-4.587	-2.036	-9.8039	1.0000	
2	0	0	62.767	60.478	60.300	4.641	2.289	5.2893	1.0000	
2	0	2	140.325	135.556	-135.476	-4.611	4.769	7.2510	1.0000	
2	0	4	54.680	53.141	52.967	4.295	1.539	3.2035	1.0000	
2	0	6	28.365	28.321	-28.051	-3.901	.044	.1564	1.0000	
2	2	-8	6.158	7.078	-7.065	.425	-.920	-1.0269	1.0000	
2	2	-7	41.646	41.313	41.159	3.572	.332	1.1815	1.0000	
2	2	-6	3.263 *	3.573	3.547	-.423	-.310	-.2743	1.0000	**
2	2	-5	74.892	75.609	-75.499	-4.076	-.716	-1.2171	1.0000	
2	2	-4	9.018	9.037	-9.029	.381	-.019	-.0552	1.0000	
2	2	-3	158.024	160.410	160.347	4.516	-2.386	-3.2063	1.0000	
2	2	-2	4.873	6.004	5.994	-.351	-1.132	-2.7529	1.0000	
2	2	-1	187.835	191.457	-191.399	-4.702	-3.622	-6.8617	1.0000	
2	2	0	50.326	48.457	-48.456	.281	1.870	3.4842	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
2	2	1	156.955	159.716	159.647	4.713	-2.761	-4.7619	1.0000	
2	2	2	32.641	31.438	31.437	-.269	1.202	4.7903	1.0000	
2	2	3	104.595	106.378	-106.282	-4.536	-1.783	-2.1354	1.0000	
2	2	4	48.777	48.705	-48.704	.205	.073	.1930	1.0000	
2	2	5	97.135	96.491	96.396	4.274	.644	.8315	1.0000	
2	2	6	24.683	23.065	23.064	-.247	1.617	5.4171	1.0000	
2	2	7	68.172	67.719	-67.641	-3.825	.453	.9180	1.0000	
2	4	-8	10.680	9.691	-9.543	-1.686	.989	1.8136	1.0000	
2	4	-7	5.807	5.086	4.873	1.457	.721	.8683	1.0000	
2	4	-6	12.965	13.184	13.059	1.812	-.219	-.5565	1.0000	
2	4	-5	12.614	12.797	-12.691	-1.639	-.183	-.5272	1.0000	
2	4	-4	16.149	16.919	-16.814	-1.883	-.770	-2.9659	1.0000	
2	4	-3	66.004	65.794	65.767	1.867	.210	.3521	1.0000	
2	4	-2	2.986 *	3.343	2.770	1.872	-.357	-.4886	1.0000	**
2	4	-1	48.989	48.487	-48.449	-1.911	.503	1.2488	1.0000	
2	4	0	12.251	11.482	-11.330	-1.860	.769	3.7008	1.0000	
2	4	1	51.889	50.579	50.542	1.941	1.309	3.1190	1.0000	
2	4	2	22.437	21.190	-21.117	1.753	1.247	6.5515	1.0000	
2	4	3	22.121	22.248	-22.171	-1.857	-.127	-.5886	1.0000	
2	4	4	16.301	15.761	15.673	-1.661	.540	1.9207	1.0000	
2	4	5	39.192	38.765	38.723	1.816	.427	1.7307	1.0000	
2	4	6	23.181	22.138	-22.087	1.502	1.044	3.2591	1.0000	
2	4	7	22.524	22.582	-22.522	-1.641	-.058	-.1608	1.0000	
2	6	-7	14.457	14.430	14.429	-.159	.028	.0624	1.0000	
2	6	-6	15.669	15.454	15.237	2.585	.215	.5702	1.0000	
2	6	-5	4.834	3.573	3.565	.235	1.261	1.6183	1.0000	
2	6	-4	12.060	12.500	12.221	-2.624	-.440	-1.2865	1.0000	
2	6	-3	11.801	12.107	12.105	-.209	-.306	-.9825	1.0000	
2	6	-2	40.456	40.773	-40.689	2.625	-.317	-1.0333	1.0000	
2	6	-1	17.400	17.917	17.915	.283	-.517	-2.2980	1.0000	
2	6	0	2.540 *	3.104	-1.559	-2.684	-.564	-.5590	1.0000	**
2	6	1	15.245	14.602	14.600	-.236	.643	2.6546	1.0000	
2	6	2	21.113	21.173	21.007	2.643	-.060	-.2603	1.0000	
2	6	3	11.299	11.068	11.064	.294	.230	.6821	1.0000	
2	6	4	16.344	16.064	-15.867	-2.509	.280	.9127	1.0000	
2	6	5	6.344	5.382	5.376	-.254	.962	1.4244	1.0000	
2	6	6	9.983	10.125	-9.875	2.238	-.142	-.2532	1.0000	
2	6	7	4.808 *	4.352	4.343	.285	.456	.3871	1.0000	**
2	8	-7	26.267	26.141	-25.905	-3.507	.125	.3487	1.0000	
2	8	-6	18.746	18.818	18.796	.914	-.073	-.1927	1.0000	
2	8	-5	72.201	71.425	71.308	4.083	.776	1.3691	1.0000	
2	8	-4	31.295	31.407	-31.390	-1.033	-.112	-.4259	1.0000	
2	8	-3	90.172	89.818	-89.708	-4.436	.354	.4627	1.0000	
2	8	-2	32.186	31.460	31.441	1.079	.726	3.1673	1.0000	
2	8	-1	129.451	130.981	130.897	4.707	-1.530	-1.5649	1.0000	
2	8	0	31.762	31.482	-31.463	-1.093	.280	1.2956	1.0000	
2	8	1	86.857	85.808	-85.682	-4.634	1.050	1.4791	1.0000	
2	8	2	12.268	13.412	13.372	1.029	-1.144	-3.3038	1.0000	
2	8	3	91.250	92.486	92.374	4.538	-1.236	-1.5358	1.0000	
2	8	4	10.035	10.573	-10.530	-.961	-.538	-1.1310	1.0000	
2	8	5	66.368	67.090	-66.958	-4.207	-.723	-1.4274	1.0000	
2	8	6	6.361	6.197	6.138	.854	.164	.1930	1.0000	
2	10	-6	39.417	38.175	-38.028	-3.345	1.242	3.8277	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
2	10	-5	26.383	25.749	25.707	1.463	.635	1.9300	1.0000	
2	10	-4	35.839	35.791	35.615	3.545	.047	.1626	1.0000	
2	10	-3	21.372	20.731	-20.673	-1.552	.641	2.0587	1.0000	
2	10	-2	35.596	35.451	-35.262	-3.656	.145	.5587	1.0000	
2	10	-1	46.670	46.417	46.386	1.691	.253	.7036	1.0000	
2	10	0	29.469	29.721	29.497	3.646	-.252	-.9724	1.0000	
2	10	1	16.833	15.436	-15.352	-1.613	1.397	4.3629	1.0000	
2	10	2	25.172	24.974	-24.723	-3.534	.198	.6815	1.0000	
2	10	3	31.857	31.507	31.465	1.625	.350	1.2086	1.0000	
2	10	4	13.791	13.260	12.843	3.297	.531	1.2280	1.0000	
2	10	5	17.071	16.462	-16.394	-1.486	.610	1.4029	1.0000	
2	12	-4	20.710	20.612	-20.572	1.296	.098	.2545	1.0000	
2	12	-3	53.027	51.141	51.071	2.667	1.886	5.8104	1.0000	
2	12	-2	28.876	28.745	28.716	-1.277	.131	.4219	1.0000	
2	12	-1	40.361	38.776	-38.680	-2.733	1.584	5.5466	1.0000	
2	12	0	16.526	16.628	-16.578	1.295	-.103	-.2692	1.0000	
2	12	1	57.488	55.968	55.897	2.811	1.520	3.5854	1.0000	
2	12	2	2.614 *	1.329	.268	-1.302	1.284	.6887	1.0000	**
2	12	3	35.003	33.985	-33.881	-2.660	1.018	3.1795	1.0000	
2	12	4	2.765 *	1.635	-1.078	1.229	1.130	.5729	1.0000	**
2	14	-2	11.437	11.822	-11.816	.362	-.385	-.6839	1.0000	
2	14	-1	23.467	24.430	-24.316	-2.358	-.963	-2.5890	1.0000	
2	14	0	6.119	7.821	7.812	-.366	-1.702	-1.7480	1.0000	
2	14	1	29.196	30.652	30.558	2.408	-1.456	-4.1546	1.0000	
3	1	-8	47.674	48.687	48.614	2.655	-1.013	-3.3445	1.0000	
3	1	-7	18.516	17.843	-17.834	.575	.673	1.9942	1.0000	
3	1	-6	56.523	56.279	-56.205	-2.901	.244	.5927	1.0000	
3	1	-5	29.863	29.706	29.701	-.588	.156	.6941	1.0000	
3	1	-4	102.258	101.641	101.592	3.137	.617	.7097	1.0000	
3	1	-3	50.292	48.370	-48.366	.608	1.921	4.3532	1.0000	
3	1	-2	28.249	31.480	-31.328	-3.092	-3.231	-13.8283	1.0000	
3	1	-1	64.732	62.027	62.023	-.650	2.705	4.8837	1.0000	
3	1	0	122.739	121.385	121.344	3.146	1.355	2.5450	1.0000	
3	1	1	57.099	54.053	-54.049	.690	3.045	6.8992	1.0000	
3	1	2	56.822	54.766	-54.687	-2.944	2.055	3.9250	1.0000	
3	1	3	20.286	18.820	18.805	-.752	1.466	6.9150	1.0000	
3	1	4	70.916	71.101	71.046	2.786	-.185	-.3214	1.0000	
3	1	5	3.077 *	2.322	2.175	.813	.754	.6603	1.0000	**
3	1	6	7.309	7.850	-7.489	-2.353	-.541	-.8509	1.0000	
3	1	7	8.507	8.461	-8.420	-.834	.046	.0707	1.0000	
3	3	-8	12.437	12.158	12.157	.141	.279	.5601	1.0000	
3	3	-7	8.200	8.846	-8.265	3.154	-.646	-1.0740	1.0000	
3	3	-6	3.181 *	4.858	4.857	-.130	-1.678	-1.3947	1.0000	**
3	3	-5	8.802	8.407	-7.614	-3.562	.395	.9715	1.0000	
3	3	-4	24.886	25.939	25.937	.249	-1.052	-4.8637	1.0000	
3	3	-3	63.403	62.274	62.150	3.929	1.129	1.9624	1.0000	
3	3	-2	13.138	11.529	11.527	-.220	1.608	7.7439	1.0000	
3	3	-1	142.575	138.753	-138.690	-4.180	3.822	6.0088	1.0000	
3	3	0	58.964	56.837	56.836	.329	2.127	4.6814	1.0000	
3	3	1	83.023	81.551	81.443	4.186	1.473	2.1137	1.0000	
3	3	2	9.044	8.421	8.418	-.258	.623	2.0264	1.0000	
3	3	3	33.653	32.251	-31.994	-4.064	1.402	5.8905	1.0000	
3	3	4	28.140	28.782	28.780	.331	-.642	-2.6955	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
3	3	5	29.971	30.307	30.058	3.678	-.337	-1.2750	1.0000	
3	3	6	2.648 *	2.844	-2.834	-.238	-.195	-.1183	1.0000	**
3	3	7	40.391	40.293	-40.130	-3.628	.098	.3135	1.0000	
3	5	-7	4.072 *	.868	.635	.592	3.204	2.8152	1.0000	**
3	5	-6	107.183	107.203	107.101	4.678	-.021	-.0236	1.0000	
3	5	-5	2.194 *	2.899	-2.823	-.659	-.705	-.4503	1.0000	**
3	5	-4	106.663	106.669	-106.554	-4.961	-.006	-.0062	1.0000	
3	5	-3	14.739	14.861	-14.846	.669	-.122	-.4715	1.0000	
3	5	-2	140.719	140.993	140.898	5.172	-.274	-.3352	1.0000	
3	5	-1	9.611	8.741	8.712	-.718	.870	2.9558	1.0000	
3	5	0	104.513	106.556	-106.434	-5.101	-2.043	-2.6378	1.0000	
3	5	1	13.172	12.754	-12.733	.724	.419	1.6972	1.0000	
3	5	2	141.693	143.878	143.791	5.004	-2.185	-2.4637	1.0000	
3	5	3	7.253	7.208	-7.169	-.753	.044	.0955	1.0000	
3	5	4	78.099	77.885	-77.751	-4.560	.214	.3346	1.0000	
3	5	5	13.311	14.393	14.373	.751	-1.082	-2.7183	1.0000	
3	5	6	55.523	56.779	56.633	4.068	-1.256	-3.2603	1.0000	
3	5	7	13.891	14.372	-14.354	-.709	-.481	-.9673	1.0000	
3	7	-7	16.959	16.908	-16.716	-2.539	.051	.1242	1.0000	
3	7	-6	32.779	32.423	32.392	1.420	.356	1.1921	1.0000	
3	7	-5	6.837	5.178	4.372	2.774	1.660	2.6449	1.0000	
3	7	-4	18.002	18.124	-18.068	-1.415	-.122	-.4089	1.0000	
3	7	-3	19.711	20.520	-20.295	-3.033	-.809	-3.1168	1.0000	
3	7	-2	27.889	27.710	27.673	1.442	.179	.8124	1.0000	
3	7	-1	17.694	17.187	16.894	3.161	.507	2.0547	1.0000	
3	7	0	4.660	3.590	-3.326	-1.354	1.070	1.6595	1.0000	
3	7	1	30.313	29.460	-29.282	-3.238	.852	3.9386	1.0000	
3	7	2	32.835	33.277	33.249	1.350	-.441	-1.9604	1.0000	
3	7	3	30.053	30.215	30.045	3.196	-.162	-.6453	1.0000	
3	7	4	6.244	6.036	-5.920	-1.181	.208	.3083	1.0000	
3	7	5	41.464	40.712	-40.594	-3.093	.752	2.6736	1.0000	
3	7	6	2.756 *	4.953	4.840	1.054	-2.197	-1.1157	1.0000	**
3	9	-6	18.365	17.324	-17.269	-1.384	1.041	2.6141	1.0000	
3	9	-5	31.438	31.365	-31.333	1.407	.073	.2408	1.0000	
3	9	-4	31.061	30.398	30.362	1.495	.663	2.3570	1.0000	
3	9	-3	4.249 *	1.914	-1.018	-1.621	2.336	2.6853	1.0000	**
3	9	-2	19.140	18.882	-18.824	-1.481	.258	.8897	1.0000	
3	9	-1	8.815	8.024	7.839	1.715	.791	1.8273	1.0000	
3	9	0	29.776	29.679	29.642	1.487	.097	.3930	1.0000	
3	9	1	3.267 *	2.693	-2.049	-1.747	.575	.5290	1.0000	**
3	9	2	15.717	14.123	-14.056	-1.378	1.593	4.7819	1.0000	
3	9	3	19.070	18.790	-18.714	1.692	.280	.8634	1.0000	
3	9	4	18.162	16.979	16.930	1.287	1.183	3.2927	1.0000	
3	9	5	9.092	9.490	9.339	-1.683	-.398	-.6256	1.0000	
3	11	-5	11.961	12.643	12.631	.547	-.682	-1.2512	1.0000	
3	11	-4	52.399	51.776	51.674	3.250	.623	1.8705	1.0000	
3	11	-3	18.378	17.880	-17.869	-.611	.498	1.3872	1.0000	
3	11	-2	39.084	39.655	-39.519	-3.279	-.571	-2.0623	1.0000	
3	11	-1	6.712	7.079	7.054	.596	-.368	-.5446	1.0000	
3	11	0	44.870	44.974	44.855	3.265	-.104	-.3129	1.0000	
3	11	1	16.807	16.085	-16.073	-.618	.722	2.0112	1.0000	
3	11	2	43.615	43.695	-43.583	-3.130	-.081	-.2908	1.0000	
3	11	3	17.153	16.324	16.313	.585	.830	2.1542	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
3	11	4	37.448	38.009	37.899	2.891	-.560	-1.7500	1.0000	
3	13	-3	8.672	9.157	8.664	2.966	-.486	-.7014	1.0000	
3	13	-2	23.908	23.141	-22.083	-1.635	.767	2.1368	1.0000	
3	13	-1	20.092	19.553	-19.298	-3.146	.539	1.4473	1.0000	
3	13	0	26.323	24.395	24.339	1.647	1.928	5.7125	1.0000	
3	13	1	15.825	15.938	15.617	3.182	-.113	-.2656	1.0000	
3	13	2	27.681	27.110	-27.063	-1.608	.770	2.2253	1.0000	
4	0	-8	30.092	30.167	29.936	3.722	-.075	-.2276	1.0000	
4	0	-6	96.239	95.584	-95.481	-4.446	.655	.8089	1.0000	
4	0	-4	106.746	107.416	107.305	4.864	-.670	-.7554	1.0000	
4	0	-2	158.297	157.035	-156.948	-5.220	1.261	1.9178	1.0000	
4	0	0	59.708	65.476	65.264	5.269	-5.768	-9.2569	1.0000	
4	0	2	150.373	151.410	-151.315	-5.360	-1.037	-1.3388	1.0000	
4	0	4	118.793	118.632	118.521	5.131	.161	.1580	1.0000	
4	0	6	105.170	104.589	-104.480	-4.771	.581	.6336	1.0000	
4	2	-8	22.714	22.456	-22.454	.359	.258	.7085	1.0000	
4	2	-7	41.836	42.098	41.949	3.535	-.262	-.9312	1.0000	
4	2	-6	2.229 *	1.560	1.482	-.487	.669	.4199	1.0000	**
4	2	-5	42.637	42.985	-42.819	-3.770	-.348	-1.1651	1.0000	
4	2	-4	25.466	25.719	-25.714	.481	-.253	-1.1927	1.0000	
4	2	-3	57.890	60.304	60.177	3.925	-2.414	-4.2261	1.0000	
4	2	-2	33.861	33.117	-33.111	-.621	.744	2.8192	1.0000	
4	2	-1	108.187	106.332	-106.258	-3.984	1.854	2.8954	1.0000	
4	2	0	8.330	6.343	-6.314	.602	1.987	7.4060	1.0000	
4	2	1	68.579	67.653	67.544	3.841	.926	1.2964	1.0000	
4	2	2	49.997	50.610	-50.605	-.706	-.612	-1.4588	1.0000	
4	2	3	21.944	22.338	-22.050	-3.578	-.395	-1.7533	1.0000	
4	2	4	6.461	6.529	6.499	.629	-.069	-.1279	1.0000	
4	2	5	4.552 *	3.862	2.106	3.237	.691	.8141	1.0000	**
4	2	6	9.286	8.824	-8.801	-.624	.463	.8488	1.0000	
4	2	7	14.159	14.243	-13.941	-2.917	-.084	-.1784	1.0000	
4	4	-8	6.244	7.257	-7.071	-1.633	-1.012	-1.1248	1.0000	
4	4	-7	6.634	3.674	3.375	1.452	2.959	4.0228	1.0000	
4	4	-6	2.311 *	2.195	-1.206	1.834	.115	.0699	1.0000	**
4	4	-5	4.630	5.148	4.939	-1.454	-.518	-.7168	1.0000	
4	4	-4	40.746	41.367	-41.312	-2.134	-.621	-2.2092	1.0000	
4	4	-3	11.273	11.149	-11.057	1.431	.123	.4260	1.0000	
4	4	-2	25.985	26.685	26.591	2.242	-.700	-3.7622	1.0000	
4	4	-1	13.999	14.178	-14.107	-1.418	-.179	-.8125	1.0000	
4	4	0	88.255	89.956	-89.924	-2.417	-1.701	-2.2468	1.0000	
4	4	1	16.374	15.976	-15.924	1.293	.398	1.8036	1.0000	
4	4	2	56.636	57.542	57.493	2.380	-.907	-2.0147	1.0000	
4	4	3	25.579	25.697	25.670	-1.174	-.118	-.5065	1.0000	
4	4	4	62.430	63.623	-63.580	-2.346	-1.193	-2.3768	1.0000	
4	4	5	34.757	34.640	-34.625	1.029	.117	.4283	1.0000	
4	4	6	23.160	23.193	23.098	2.095	-.033	-.0980	1.0000	
4	4	7	13.190	12.063	12.023	-.982	1.126	2.2433	1.0000	
4	6	-7	5.344 *	5.240	5.235	-.209	.105	.1099	1.0000	**
4	6	-6	34.082	33.227	33.114	2.733	.855	2.9930	1.0000	
4	6	-5	15.669	15.573	-15.573	.130	.096	.2918	1.0000	
4	6	-4	69.609	68.345	-68.275	-3.088	1.264	2.3743	1.0000	
4	6	-3	13.185	12.888	12.888	-.089	.297	.9959	1.0000	
4	6	-2	32.970	31.605	31.444	3.189	1.364	6.1824	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
4	6	-1	29.239	29.601	-29.601	.009	-.361	-1.7753	1.0000	
4	6	0	45.540	44.851	-44.728	-3.322	.689	1.9668	1.0000	
4	6	1	16.578	17.115	17.115	.003	-.537	-2.1044	1.0000	
4	6	2	44.645	44.857	44.734	3.320	-.212	-.7113	1.0000	
4	6	3	31.723	33.096	-33.096	-.068	-1.373	-5.6648	1.0000	
4	6	4	73.105	76.283	-76.211	-3.313	-3.178	-5.9222	1.0000	
4	6	5	16.522	16.688	16.608	.031	-.166	-.4519	1.0000	
4	6	6	49.508	50.344	50.252	3.042	-.836	-2.7591	1.0000	
4	8	-7	39.153	37.938	-37.775	-3.513	1.215	3.7440	1.0000	
4	8	-6	4.760 *	4.670	4.591	.853	.090	.0868	1.0000	**
4	8	-5	30.369	30.056	29.825	3.722	.313	1.0781	1.0000	
4	8	-4	22.697	22.817	-22.795	-1.004	-.120	-.4146	1.0000	
4	8	-3	47.769	48.038	-47.878	-3.907	-.269	-.7759	1.0000	
4	8	-2	21.559	20.792	20.765	1.055	.766	2.9031	1.0000	
4	8	-1	48.500	48.610	48.451	3.920	-.109	-.3080	1.0000	
4	8	0	44.177	45.087	-45.073	-1.139	-.910	-3.1376	1.0000	
4	8	1	47.219	48.778	-48.627	-3.827	-1.558	-4.8666	1.0000	
4	8	2	27.599	29.760	29.740	1.087	-2.161	-8.3214	1.0000	
4	8	3	6.063	7.541	6.674	3.509	-1.478	-2.1218	1.0000	
4	8	4	25.289	29.590	-29.571	-1.039	-4.301	-13.6155	1.0000	
4	8	5	10.065	11.267	-10.794	-3.228	-1.201	-2.0717	1.0000	
4	10	-6	36.336	36.009	-35.849	-3.387	.328	.9959	1.0000	
4	10	-5	2.778 *	2.227	1.819	1.284	.552	.2999	1.0000	**
4	10	-4	48.963	48.077	47.929	3.778	.886	3.0557	1.0000	
4	10	-3	13.341	12.636	-12.563	-1.356	.705	1.7714	1.0000	
4	10	-2	68.142	69.778	-69.658	-4.089	-1.636	-3.0002	1.0000	
4	10	-1	7.763	7.364	7.242	1.334	.399	.7375	1.0000	
4	10	0	72.166	75.246	75.128	4.220	-3.080	-5.7870	1.0000	
4	10	1	13.782	14.944	-14.886	-1.318	-1.162	-3.0173	1.0000	
4	10	2	71.686	86.696	-86.592	-4.239	-15.010	-28.6667	1.0000	
4	10	3	6.902	8.882	-8.805	1.165	-1.980	-2.7729	1.0000	
4	10	4	56.298	69.306	69.189	4.027	-13.008	-41.1779	1.0000	
4	12	-4	18.391	18.483	18.411	1.639	-.092	-.2225	1.0000	
4	12	-3	18.824	17.479	17.328	2.298	1.344	3.5301	1.0000	
4	12	-2	8.607	7.772	-7.582	-1.709	.835	1.3210	1.0000	
4	12	-1	26.219	26.913	-26.810	-2.344	-.694	-2.1371	1.0000	
4	12	0	5.336 *	1.999	-.982	1.741	3.337	3.7429	1.0000	**
4	12	1	11.312	11.706	11.492	2.232	-.395	-.7798	1.0000	
4	12	2	10.256	12.960	-12.834	-1.799	-2.704	-4.8065	1.0000	
4	12	3	12.575	16.574	-16.436	-2.129	-3.999	-7.8979	1.0000	
5	1	-8	4.275 *	5.341	-4.990	1.905	-1.066	-.8732	1.0000	**
5	1	-7	19.230	19.426	19.395	1.099	-.195	-.5713	1.0000	
5	1	-6	6.915	7.302	6.999	-2.080	-.387	-.6768	1.0000	
5	1	-5	28.292	28.219	-28.195	-1.172	.072	.3096	1.0000	
5	1	-4	12.181	11.881	11.665	2.254	.301	1.0372	1.0000	
5	1	-3	42.810	43.504	43.487	1.220	-.694	-1.9796	1.0000	
5	1	-2	4.366	4.941	4.371	-2.304	-.575	-1.1068	1.0000	
5	1	-1	36.003	37.003	-36.983	-1.198	-1.000	-3.5538	1.0000	
5	1	0	29.923	29.119	-29.027	2.310	.804	3.5738	1.0000	
5	1	1	23.458	23.851	23.824	1.138	-.393	-2.1616	1.0000	
5	1	2	14.284	14.171	13.981	-2.311	.114	.4536	1.0000	
5	1	3	3.267 *	1.985	1.707	-1.012	1.283	1.3785	1.0000	**
5	1	4	7.638	7.875	7.536	2.286	-.238	-.4819	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
5	1	5	2.419 *	3.679	-3.565	.909	-1.260	-.7297	1.0000	**
5	1	6	18.296	18.190	-18.057	-2.196	.106	.2803	1.0000	
5	1	7	3.155 *	1.322	1.046	-.808	1.833	1.0695	1.0000	**
5	3	-8	15.942	16.043	16.041	.248	-.101	-.2407	1.0000	
5	3	-7	71.288	72.392	72.278	4.067	-1.105	-2.0423	1.0000	
5	3	-6	14.920	15.354	-15.351	-.298	-.434	-1.2526	1.0000	
5	3	-5	67.934	68.826	-68.685	-4.415	-.892	-1.6636	1.0000	
5	3	-4	26.678	26.579	26.576	.370	.099	.4483	1.0000	
5	3	-3	102.630	104.610	104.502	4.737	-1.979	-2.2986	1.0000	
5	3	-2	29.140	28.629	-28.626	-.399	.511	2.7455	1.0000	
5	3	-1	143.649	150.436	-150.356	-4.898	-6.787	-8.9625	1.0000	
5	3	0	33.394	34.970	34.967	.417	-1.576	-7.2839	1.0000	
5	3	1	173.606	189.642	189.579	4.905	-16.036	-19.5036	1.0000	
5	3	2	26.881	27.931	-27.928	-.399	-1.050	-4.9503	1.0000	
5	3	3	106.174	112.349	-112.256	-4.572	-6.175	-6.1245	1.0000	
5	3	4	17.093	16.874	16.870	.345	.219	.7327	1.0000	
5	3	5	63.256	64.052	63.921	4.110	-.796	-1.7864	1.0000	
5	3	6	14.631	14.641	-14.638	-.292	-.011	-.0255	1.0000	
5	5	-7	21.247	21.185	21.169	.817	.062	.1779	1.0000	
5	5	-6	27.292	27.797	27.555	3.658	-.504	-1.7140	1.0000	
5	5	-5	17.751	17.950	-17.929	-.866	-.199	-.6665	1.0000	
5	5	-4	40.084	40.590	-40.395	-3.971	-.506	-1.9833	1.0000	
5	5	-3	42.650	43.493	43.482	.962	-.843	-2.5309	1.0000	
5	5	-2	44.021	43.237	43.038	4.150	.784	2.5528	1.0000	
5	5	-1	16.842	17.235	-17.210	-.918	-.393	-1.6823	1.0000	
5	5	0	23.484	22.542	-22.151	-4.182	.942	4.5353	1.0000	
5	5	1	26.721	26.931	26.915	.923	-.210	-.9884	1.0000	
5	5	2	27.128	26.730	26.407	4.146	.397	1.7062	1.0000	
5	5	3	5.431	5.419	5.360	-.801	.011	.0175	1.0000	
5	5	4	43.792	43.490	-43.303	-4.031	.302	1.0127	1.0000	
5	5	5	7.850	8.071	8.034	.770	-.221	-.3479	1.0000	
5	5	6	42.948	42.451	42.285	3.758	.497	1.6173	1.0000	
5	7	-7	46.025	46.102	-45.994	-3.149	-.077	-.2506	1.0000	
5	7	-6	12.800	12.853	-12.825	.851	-.053	-.1207	1.0000	
5	7	-5	77.800	79.097	79.018	3.545	-1.297	-2.1108	1.0000	
5	7	-4	12.913	12.662	12.631	-.889	.251	.7153	1.0000	
5	7	-3	77.091	77.621	-77.532	-3.718	-.531	-.8636	1.0000	
5	7	-2	20.611	19.887	-19.867	.892	.724	2.8860	1.0000	
5	7	-1	112.081	111.212	111.144	3.866	.869	.8889	1.0000	
5	7	0	33.199	33.260	33.248	-.871	-.061	-.2760	1.0000	
5	7	1	71.249	71.058	-70.960	-3.719	.191	.3179	1.0000	
5	7	2	25.414	25.230	-25.214	.886	.184	.7104	1.0000	
5	7	3	64.446	63.523	63.424	3.533	.924	1.7351	1.0000	
5	7	4	8.282	7.717	7.662	-.920	.565	.9601	1.0000	
5	7	5	27.582	28.145	-27.969	-3.142	-.563	-1.7113	1.0000	
5	9	-6	7.140	5.360	5.274	-.953	1.780	2.3242	1.0000	
5	9	-5	24.228	23.813	23.711	2.203	.415	1.2622	1.0000	
5	9	-4	6.603	5.928	-5.841	1.011	.676	.9761	1.0000	
5	9	-3	10.563	10.703	-10.464	-2.248	-.140	-.3145	1.0000	
5	9	-2	7.980	8.650	8.587	-1.042	-.671	-1.2500	1.0000	
5	9	-1	58.825	58.675	58.625	2.407	.150	.3218	1.0000	
5	9	0	9.325	10.031	-9.975	1.055	-.705	-1.5374	1.0000	
5	9	1	48.924	48.356	-48.300	-2.324	.568	1.7054	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
5	9	2	8.343	6.882	6.800	-1.058	1.461	2.7233	1.0000	
5	9	3	48.872	48.503	48.452	2.215	.370	1.2379	1.0000	
5	9	4	2.653 *	1.135	-.434	1.049	1.517	.8006	1.0000	**
5	9	5	3.674 *	5.781	-5.464	-1.887	-2.107	-1.3412	1.0000	**
5	11	-5	25.531	25.338	25.334	.491	.193	.5300	1.0000	
5	11	-4	6.288	5.734	5.222	2.368	.553	.6490	1.0000	
5	11	-3	9.897	9.693	-9.681	-.478	.204	.3711	1.0000	
5	11	-2	3.786 *	3.401	2.368	-2.441	.385	.3125	1.0000	**
5	11	-1	25.778	25.254	25.248	.560	.523	1.7028	1.0000	
5	11	0	14.496	13.515	-13.292	2.446	.981	2.4128	1.0000	
5	11	1	3.856 *	1.891	1.829	-.477	1.965	1.5989	1.0000	**
5	11	2	8.962	8.178	7.806	-2.440	.783	1.2931	1.0000	
5	11	3	13.146	12.806	12.795	.516	.341	.6964	1.0000	
5	13	-3	66.497	66.320	66.214	3.750	.177	.3758	1.0000	
5	13	-2	16.227	15.422	-15.359	-1.390	.805	1.8244	1.0000	
5	13	-1	54.481	54.168	-54.036	-3.776	.313	.8710	1.0000	
5	13	0	12.566	10.767	10.676	1.397	1.799	3.4937	1.0000	
5	13	1	65.113	63.672	63.561	3.757	1.441	3.0834	1.0000	
6	0	-8	51.754	50.792	50.627	4.095	.962	3.2215	1.0000	
6	0	-6	65.364	64.314	-64.157	-4.499	1.049	1.9717	1.0000	
6	0	-4	138.439	139.888	139.802	4.901	-1.449	-1.5432	1.0000	
6	0	-2	141.113	140.508	-140.421	-4.950	.605	.7811	1.0000	
6	0	0	131.454	127.547	127.454	4.863	3.908	5.1311	1.0000	
6	0	2	22.584	21.656	-21.188	-4.476	.928	4.1252	1.0000	
6	0	4	37.509	37.356	37.121	4.182	.153	.6195	1.0000	
6	0	6	19.789	20.092	-19.749	-3.696	-.304	-.8159	1.0000	
6	2	-8	10.706	11.346	11.328	.644	-.640	-1.1649	1.0000	
6	2	-7	27.245	27.451	27.271	3.144	-.207	-.6821	1.0000	
6	2	-6	5.902	5.997	5.969	-.579	-.095	-.1386	1.0000	
6	2	-5	36.544	37.011	-36.842	-3.536	-.467	-2.0004	1.0000	
6	2	-4	6.296	7.132	7.108	.588	-.836	-1.7693	1.0000	
6	2	-3	38.188	37.539	37.344	3.824	.649	2.1128	1.0000	
6	2	-2	41.118	39.537	39.534	-.463	1.581	4.5679	1.0000	
6	2	-1	78.744	81.332	-81.229	-4.088	-2.588	-3.3041	1.0000	
6	2	0	6.513	7.052	-7.037	.464	-.539	-1.3263	1.0000	
6	2	1	102.808	105.113	105.029	4.202	-2.305	-2.7175	1.0000	
6	2	2	33.225	32.453	32.451	-.353	.772	3.4974	1.0000	
6	2	3	92.331	92.981	-92.889	-4.135	-.649	-.8828	1.0000	
6	2	4	6.227	6.209	6.196	.397	.018	.0287	1.0000	
6	2	5	58.938	58.836	58.710	3.857	.101	.2465	1.0000	
6	2	6	12.341	11.477	11.473	-.293	.865	1.7525	1.0000	
6	4	-8	19.633	19.648	-19.554	-1.919	-.015	-.0395	1.0000	
6	4	-7	6.266	7.101	-6.998	1.202	-.835	-1.0716	1.0000	
6	4	-6	32.489	33.234	33.169	2.083	-.745	-2.7334	1.0000	
6	4	-5	4.358 *	3.914	3.675	-1.347	.444	.5636	1.0000	**
6	4	-4	17.694	17.347	-17.220	-2.094	.348	1.3393	1.0000	
6	4	-3	20.650	21.501	-21.454	1.420	-.851	-3.7110	1.0000	
6	4	-2	33.714	34.390	34.324	2.126	-.676	-2.7398	1.0000	
6	4	-1	10.546	10.557	-10.439	-1.572	-.011	-.0374	1.0000	
6	4	0	10.736	10.200	10.007	-1.975	.536	1.7443	1.0000	
6	4	1	25.016	24.938	24.884	1.648	.078	.3595	1.0000	
6	4	2	16.881	17.794	17.691	1.915	-.913	-3.4041	1.0000	
6	4	3	31.728	31.558	-31.513	-1.676	.170	.7015	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EX . FACTOR	
6	4	4	2.319 *	1.774	-.462	-1.713	.545	.3289	1.0000	**
6	4	5	12.441	11.759	11.653	1.579	.682	1.5296	1.0000	
6	4	6	16.894	16.559	16.483	1.582	.335	.8149	1.0000	
6	6	-7	6.954	6.578	6.577	-.121	.376	.4906	1.0000	
6	6	-6	39.188	38.540	38.428	2.930	.648	2.3041	1.0000	
6	6	-5	21.450	21.520	-21.520	.080	-.070	-.2346	1.0000	
6	6	-4	55.619	55.067	-54.982	-3.070	.551	1.3002	1.0000	
6	6	-3	9.421	8.645	8.644	-.130	.775	1.9693	1.0000	
6	6	-2	80.721	81.979	81.920	3.131	-1.258	-1.7948	1.0000	
6	6	-1	20.152	20.653	-20.653	.119	-.501	-2.0666	1.0000	
6	6	0	23.480	23.018	-22.833	-2.911	.462	1.9773	1.0000	
6	6	1	2.086 *	.194	.045	-.189	1.892	1.2709	1.0000	**
6	6	2	6.114	5.425	4.701	2.706	.690	1.1552	1.0000	
6	6	3	6.443	7.658	-7.655	.191	-1.214	-1.8586	1.0000	
6	6	4	14.942	14.666	14.466	-2.417	.276	.7085	1.0000	
6	6	5	2.769 *	1.618	1.601	-.231	1.152	.6249	1.0000	**
6	8	-6	20.286	20.017	19.997	.888	.269	.7322	1.0000	
6	8	-5	20.308	20.270	19.971	3.468	.038	.1112	1.0000	
6	8	-4	8.421	8.833	-8.784	-.928	-.412	-.7623	1.0000	
6	8	-3	38.695	38.665	-38.476	-3.818	.030	.1183	1.0000	
6	8	-2	18.040	18.157	18.129	1.006	-.117	-.3853	1.0000	
6	8	-1	45.878	45.730	45.553	4.022	.148	.4495	1.0000	
6	8	0	8.797	8.204	-8.144	-.991	.593	1.3059	1.0000	
6	8	1	82.292	82.109	-82.002	-4.189	.183	.2766	1.0000	
6	8	2	26.717	26.760	26.741	1.023	-.044	-.1550	1.0000	
6	8	3	68.817	67.154	67.030	4.082	1.663	2.8894	1.0000	
6	8	4	21.178	20.607	-20.586	-.948	.570	1.6072	1.0000	
6	8	5	53.580	53.395	-53.257	-3.841	.186	.5794	1.0000	
6	10	-5	3.250 *	1.586	-1.047	1.192	1.664	1.0768	1.0000	**
6	10	-4	53.953	54.058	53.927	3.764	-.105	-.2618	1.0000	
6	10	-3	11.788	10.907	-10.825	-1.336	.880	1.9194	1.0000	
6	10	-2	45.060	45.001	-44.840	-3.807	.059	.2183	1.0000	
6	10	-1	4.596 *	5.117	4.927	1.382	-.522	-.5356	1.0000	**
6	10	0	41.516	41.111	40.940	3.749	.405	1.5078	1.0000	
6	10	1	28.712	27.751	-27.711	-1.481	.961	3.2652	1.0000	
6	10	2	30.287	29.770	-29.558	-3.549	.517	1.6815	1.0000	
6	10	3	17.378	16.842	16.782	1.425	.536	1.3185	1.0000	
6	10	4	36.046	35.347	35.192	3.306	.699	2.1257	1.0000	
6	12	-4	24.341	24.116	24.056	1.690	.225	.6129	1.0000	
6	12	-3	14.695	14.373	14.196	2.248	.323	.6906	1.0000	
6	12	-2	23.255	22.834	-22.773	-1.661	.421	1.1870	1.0000	
6	12	-1	33.736	33.081	-32.992	-2.430	.654	2.0996	1.0000	
6	12	0	7.235	5.570	5.356	1.531	1.665	2.2498	1.0000	
6	12	1	28.712	27.981	27.873	2.448	.731	2.1651	1.0000	
6	12	2	14.198	14.334	14.270	-1.353	-.136	-.2838	1.0000	
7	1	-8	12.869	13.066	12.854	2.341	-.196	-.3943	1.0000	
7	1	-7	15.968	15.794	-15.779	.686	.174	.4513	1.0000	
7	1	-6	46.631	46.362	-46.282	-2.724	.269	.8070	1.0000	
7	1	-5	22.545	22.627	22.618	-.666	-.082	-.3115	1.0000	
7	1	-4	49.193	49.111	49.024	2.925	.081	.1953	1.0000	
7	1	-3	29.309	28.713	-28.706	.639	.596	2.8699	1.0000	
7	1	-2	126.859	126.565	-126.525	-3.189	.293	.3460	1.0000	
7	1	-1	22.519	22.180	22.171	-.628	.339	1.6674	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
7	1	0	71.201	71.413	71.345	3.108	-.212	-.3468	1.0000	
7	1	1	15.197	14.843	-14.830	.617	.355	1.3658	1.0000	
7	1	2	76.294	75.922	-75.861	-3.047	.372	.5278	1.0000	
7	1	3	16.855	16.776	16.766	-.591	.079	.2600	1.0000	
7	1	4	29.910	29.816	29.688	2.760	.095	.3469	1.0000	
7	1	5	24.505	24.170	-2 .164	.537	.336	1.0488	1.0000	
7	1	6	42.814	42.305	-42.227	-2.562	.509	1.6342	1.0000	
7	3	-8	2.821 *	1.723	-1.722	.075	1.098	.6056	1.0000	**
7	3	-7	40.819	40.932	4 .795	3.336	-.112	-.3870	1.0000	
7	3	-6	18.499	19.076	-19.075	-.177	-.577	-1.7549	1.0000	
7	3	-5	34.926	35.266	-35.087	-3.549	-.341	-1.3820	1.0000	
7	3	-4	8.741	7.992	-7.991	.129	.749	1.8619	1.0000	
7	3	-3	5.868	3.986	1.676	3.617	1.881	3.5636	1.0000	
7	3	-2	26.673	26.850	-26.849	-.228	-.176	-.8487	1.0000	
7	3	-1	16.132	16.627	16.223	-3.643	-.495	-2.0426	1.0000	
7	3	0	10.931	11.291	-11.290	.164	-.360	-1.1560	1.0000	
7	3	1	7.785	6.931	5.895	3.644	.854	2.0142	1.0000	
7	3	2	22.870	23.043	-23.042	-.245	-.173	-.6900	1.0000	
7	3	3	32.589	32.572	-32.375	-3.577	.016	.0655	1.0000	
7	3	4	2.415 *	1.961	-1.954	.166	.453	.2632	1.0000	**
7	3	5	25.938	25.938	25.723	3.333	-.001	-.0022	1.0000	
7	3	6	14.310	14.087	-14.086	-.204	.223	.4648	1.0000	
7	5	-7	2.635 *	2.628	-2.560	.594	.007	.0039	1.0000	**
7	5	-6	52.287	52.994	52.826	4.225	-.708	-1.9244	1.0000	
7	5	-5	2.441 *	2.404	2.319	-.637	.036	.0228	1.0000	**
7	5	-4	111.133	112.733	-112.633	-4.750	-1.599	-1.4784	1.0000	
7	5	-3	2.086 *	1.093	.864	.670	.992	.6666	1.0000	**
7	5	-2	122.687	124.489	124.389	4.977	-1.801	-1.8502	1.0000	
7	5	-1	13.324	12.848	-12.829	-.703	.476	1.6173	1.0000	
7	5	0	144.951	146.448	-146.359	-5.082	-1.496	-1.5439	1.0000	
7	5	1	9.624	9.898	9.874	.689	-.274	-.7031	1.0000	
7	5	2	84.482	85.011	84.874	4.825	-.529	-.6874	1.0000	
7	5	3	7.188	7.606	-7.577	-.661	-.418	-.7156	1.0000	
7	5	4	79.678	79.871	-79.742	-4.548	-.193	-.2975	1.0000	
7	5	5	9.066	7.835	-7.814	.567	1.231	2.0170	1.0000	
7	7	-7	14.267	14.288	-14.061	-2.537	-.021	-.0435	1.0000	
7	7	-6	2.592 *	1.287	.304	1.251	1.305	.7044	1.0000	**
7	7	-5	14.323	14.611	14.354	2.732	-.288	-.7316	1.0000	
7	7	-4	29.694	29.505	-29.470	-1.429	.189	.6927	1.0000	
7	7	-3	14.267	15.026	-14.752	-2.858	-.759	-2.2772	1.0000	
7	7	-2	27.660	27.357	27.318	1.461	.303	1.2086	1.0000	
7	7	-1	15.976	16.489	16.231	2.910	-.513	-1.6940	1.0000	
7	7	0	41.490	41.261	-41.233	-1.500	.229	.7909	1.0000	
7	7	1	28.123	28.574	-28.425	-2.914	-.451	-1.7352	1.0000	
7	7	2	10.515	8.899	8.793	1.367	1.617	3.6988	1.0000	
7	7	3	17.720	17.411	17.188	2.773	.310	.8728	1.0000	
7	7	4	16.227	16.415	-16.363	-1.313	-.188	-.4626	1.0000	
7	7	5	14.090	13.592	-13.346	-2.578	.497	1.0450	1.0000	
7	9	-6	17.911	17.180	-17.129	-1.312	.731	1.7781	1.0000	
7	9	-5	2.904 *	2.870	-2.418	1.546	.034	.0197	1.0000	**
7	9	-4	16.898	16.171	16.110	1.404	.727	1.9533	1.0000	
7	9	-3	28.746	28.032	27.993	-1.483	.714	2.4271	1.0000	
7	9	-2	33.000	32.995	-32.960	-1.512	.005	.0194	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
7	9	-1	46.640	45.740	-45.718	1.422	.099	3.1011	1.0000	
7	9	0	23.034	22.038	21.988	1.484	.997	3.3378	1.0000	
7	9	1	24.843	24.786	24.744	-1.450	.057	.1855	1.0000	
7	9	2	26.379	25.864	-25.822	-1.458	.516	1.6320	1.0000	
7	9	3	11.679	11.403	-11.313	1.431	.276	.5460	1.0000	
7	9	4	12.921	12.101	12.029	1.325	.820	1.5789	1.0000	
7	11	-4	41.879	42.269	42.156	3.095	-.390	-1.2683	1.0000	
7	11	-3	21.191	20.922	-20.914	-.567	.269	.7399	1.0000	
7	11	-2	64.074	63.340	-63.255	-3.297	.734	1.5139	1.0000	
7	11	-1	25.440	24.371	24.363	.609	1.069	3.2517	1.0000	
7	11	0	54.519	54.508	54.408	3.289	.012	.0336	1.0000	
7	11	1	29.456	29.134	-29.127	-.632	.322	.9908	1.0000	
7	11	2	41.711	41.184	-41.063	-3.158	.526	1.6894	1.0000	
8	0	-8	21.701	21.078	20.821	3.284	.623	1.6554	1.0000	
8	0	-6	5.275	5.207	3.733	-3.630	.068	.0823	1.0000	
8	0	-4	25.358	25.120	24.788	4.071	.237	.9977	1.0000	
8	0	-2	62.213	61.759	-61.602	-4.398	.455	.9820	1.0000	
8	0	0	109.355	111.000	110.903	4.627	-1.645	-1.7932	1.0000	
8	0	2	77.099	77.335	-77.200	-4.554	-.235	-.3857	1.0000	
8	0	4	57.211	56.868	56.702	4.347	.343	.8004	1.0000	
8	2	-8	5.344 *	3.379	-3.359	.370	1.965	2.0092	1.0000	**
8	2	-7	66.294	67.076	66.974	3.700	-.782	-1.6280	1.0000	
8	2	-6	16.543	16.465	16.462	-.353	.078	.2220	1.0000	
8	2	-5	86.485	85.144	-86.052	-3.995	.341	.4235	1.0000	
8	2	-4	2.990 *	1.891	-1.844	.418	1.099	1.0201	1.0000	**
8	2	-3	91.271	92.221	92.129	4.125	-.950	-1.3841	1.0000	
8	2	-2	18.395	17.891	17.886	-.400	.505	2.0465	1.0000	
8	2	-1	64.273	63.789	-63.660	-4.061	.484	.8944	1.0000	
8	2	0	12.082	11.114	-11.105	.435	.968	3.1062	1.0000	
8	2	1	64.446	63.922	63.800	3.937	.525	1.0363	1.0000	
8	2	2	25.808	25.367	25.364	-.410	.441	1.7556	1.0000	
8	2	3	51.408	51.388	-51.256	-3.673	.021	.0545	1.0000	
8	2	4	11.242	10.661	-10.652	.454	.581	1.2429	1.0000	
8	2	5	40.629	40.299	40.163	3.308	.330	1.0881	1.0000	
8	4	-7	27.924	28.362	28.309	1.724	-.438	-1.3314	1.0000	
8	4	-6	5.007 *	4.711	4.431	1.602	.295	.3346	1.0000	**
8	4	-5	30.499	30.813	-30.762	-1.775	-.314	-1.1712	1.0000	
8	4	-4	2.207 *	2.265	1.469	-1.724	-.058	-.0369	1.0000	**
8	4	-3	34.432	33.960	33.914	1.772	.472	2.0964	1.0000	
8	4	-2	18.625	18.984	18.891	1.878	-.359	-1.4068	1.0000	
8	4	-1	4.076 *	1.815	-.789	-1.635	2.261	2.9033	1.0000	**
8	4	0	2.683 *	4.937	-4.555	-1.903	-2.254	-1.8802	1.0000	**
8	4	1	13.904	12.428	12.329	1.562	1.476	4.8031	1.0000	
8	4	2	6.006	7.072	6.808	1.914	-1.065	-1.6636	1.0000	
8	4	3	4.600 *	3.020	-2.675	-1.403	1.580	1.7896	1.0000	**
8	4	4	3.734 *	5.362	-5.030	-1.857	-1.627	-1.2878	1.0000	**
8	4	5	6.911	6.566	6.444	1.260	.345	.4288	1.0000	
8	6	-7	2.661 *	3.279	3.262	-.342	-.618	-.3254	1.0000	**
8	6	-6	15.557	15.965	-15.811	2.211	-.408	-1.0254	1.0000	
8	6	-5	9.148	7.997	7.990	.352	1.151	2.2158	1.0000	
8	6	-4	18.421	18.879	18.724	-2.417	-.458	-1.4703	1.0000	
8	6	-3	9.351	9.372	9.369	-.256	-.021	-.0489	1.0000	
8	6	-2	23.783	23.703	23.550	2.690	.080	.3069	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
8	6	-1	2.203 *	2.404	2.391	.242	-.201	-.1276	1.0000	**
8	6	0	39.763	39.710	-39.610	-2.816	.054	.2140	1.0000	
8	6	1	17.764	17.886	17.886	-.137	-.123	-.3936	1.0000	
8	6	2	37.011	37.224	37.117	2.821	-.213	-.8071	1.0000	
8	6	3	5.500	2.947	-2.943	.140	2.553	3.1220	1.0000	
8	6	4	18.408	17.983	-17.782	-2.684	.425	1.1167	1.0000	
8	6	5	17.019	16.206	16.206	-.055	.813	1.8793	1.0000	
8	8	-6	20.966	20.928	20.912	.823	.038	.0996	1.0000	
8	8	-5	78.198	78.515	78.413	3.997	-.316	-.5220	1.0000	
8	8	-4	19.983	20.023	-20.003	-.895	-.040	-.1169	1.0000	
8	8	-3	58.899	58.921	-58.781	-4.056	-.022	-.0552	1.0000	
8	8	-2	23.636	23.301	23.281	.956	.335	1.1546	1.0000	
8	8	-1	60.275	60.972	60.836	4.064	-.697	-1.6271	1.0000	
8	8	0	10.996	10.751	-10.710	-.936	.245	.5656	1.0000	
8	8	1	37.626	37.183	-36.982	-3.863	.443	1.6239	1.0000	
8	8	2	9.174	9.511	9.467	.916	-.337	-.5991	1.0000	
8	8	3	53.680	52.704	52.576	3.675	.976	2.8551	1.0000	
8	8	4	7.893	7.968	-7.922	-.860	-.075	-.0998	1.0000	
8	10	-5	31.156	30.692	30.657	1.467	.465	1.3764	1.0000	
8	10	-4	28.296	28.425	28.242	3.222	-.129	-.3862	1.0000	
8	10	-3	13.125	12.200	-12.115	-1.435	.925	2.0544	1.0000	
8	10	-2	35.497	35.408	-35.241	-3.444	.088	.2958	1.0000	
8	10	-1	21.745	21.276	21.226	1.457	.468	1.3701	1.0000	
8	10	0	39.041	38.519	38.355	3.552	.522	1.7744	1.0000	
8	10	1	4.959 *	3.509	-3.243	-1.340	1.450	1.4020	1.0000	**
8	10	2	31.048	30.139	-29.934	-3.506	.909	2.8013	1.0000	
8	10	3	22.156	21.418	21.377	1.313	.738	1.9168	1.0000	
8	12	-3	41.507	40.229	40.155	2.445	1.278	3.9908	1.0000	
8	12	-2	4.258 *	1.404	-.234	-1.385	2.854	2.2585	1.0000	**
8	12	-1	23.385	21.671	-21.540	-2.377	1.714	4.6602	1.0000	
8	12	0	13.821	13.944	13.865	1.484	-.123	-.2485	1.0000	
9	1	-7	4.098 *	.978	-.373	.904	3.120	2.7103	1.0000	**
9	1	-6	2.458 *	4.298	-3.684	-2.213	-1.840	-1.0472	1.0000	**
9	1	-5	6.794	6.213	-6.131	-1.005	.581	1.0024	1.0000	
9	1	-4	3.661 *	2.812	1.653	2.274	.849	.9001	1.0000	**
9	1	-3	3.302 *	3.942	3.799	1.055	-.641	-.6580	1.0000	**
9	1	-2	8.590	8.322	8.011	-2.255	.268	.6048	1.0000	
9	1	-1	9.317	9.157	-9.091	-1.096	.160	.4195	1.0000	
9	1	0	20.243	19.337	19.204	2.267	.906	3.6096	1.0000	
9	1	1	16.340	16.608	16.571	1.111	-.268	-.9104	1.0000	
9	1	2	9.118	8.957	8.710	-2.092	.160	.3558	1.0000	
9	1	3	27.322	27.053	-27.030	-1.115	.270	.9443	1.0000	
9	1	4	6.413	5.370	-5.003	1.951	1.043	1.3849	1.0000	
9	1	5	21.083	19.996	19.969	1.037	1.086	2.8858	1.0000	
9	3	-7	36.548	36.031	35.862	3.484	.517	1.7084	1.0000	
9	3	-6	8.252	8.083	-8.081	-.175	.169	.3006	1.0000	
9	3	-5	85.074	85.958	-85.864	-4.019	-.883	-1.2756	1.0000	
9	3	-4	21.831	22.503	22.501	.272	-.672	-2.4632	1.0000	
9	3	-3	101.484	103.642	103.552	4.322	-2.158	-2.8830	1.0000	
9	3	-2	12.064	12.427	-12.423	-.286	-.362	-1.0874	1.0000	
9	3	-1	100.324	100.364	-100.265	-4.452	-.040	-.0557	1.0000	
9	3	0	28.149	28.666	28.664	.355	-.517	-2.1714	1.0000	
9	3	1	69.765	69.601	69.464	4.375	.163	.2970	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
9	3	2	12.039	11.989	-11.984	-.319	.050	.1297	1.0000	
9	3	3	71.660	71.405	-71.279	-4.240	.255	.4958	1.0000	
9	3	4	22.943	23.332	23.329	.347	-.388	-1.1215	1.0000	
9	3	5	61.214	60.715	60.587	3.930	.499	1.3109	1.0000	
9	5	-7	2.683 *	1.084	.865	.654	1.599	.8339	1.0000	**
9	5	-6	35.566	35.382	35.192	3.661	.184	.6169	1.0000	
9	5	-5	11.597	12.030	-12.006	-.763	-.433	-.9810	1.0000	
9	5	-4	20.853	20.705	-20.353	-3.804	.148	.4948	1.0000	
9	5	-3	3.566 *	2.460	-2.337	.770	1.105	1.0961	1.0000	**
9	5	-2	39.114	39.760	39.564	3.942	-.646	-2.7134	1.0000	
9	5	-1	14.336	14.637	-14.613	-.845	-.301	-.9667	1.0000	
9	5	0	36.103	36.286	-36.076	-3.902	-.183	-.7566	1.0000	
9	5	1	10.303	10.746	10.713	.833	-.442	-1.0023	1.0000	
9	5	2	36.752	36.906	36.713	3.766	-.154	-.5756	1.0000	
9	5	3	27.426	27.361	-27.347	-.863	.066	.2140	1.0000	
9	5	4	9.092	10.253	-9.662	-3.430	-1.161	-1.8378	1.0000	
9	7	-6	2.644 *	2.601	-2.394	1.017	.043	.0227	1.0000	**
9	7	-5	34.168	34.624	34.490	3.042	-.456	-1.5256	1.0000	
9	7	-4	18.218	18.798	18.773	-.957	-.580	-1.6958	1.0000	
9	7	-3	57.614	58.757	-58.662	-3.336	-1.143	-3.0364	1.0000	
9	7	-2	9.204	9.542	-9.493	.959	-.338	-.6968	1.0000	
9	7	-1	46.125	46.736	46.612	3.410	-.612	-2.2087	1.0000	
9	7	0	12.618	12.953	12.921	-.901	-.334	-.8216	1.0000	
9	7	1	67.817	67.192	-67.102	-3.476	.626	1.2253	1.0000	
9	7	2	9.429	8.660	-8.618	.853	.769	1.4442	1.0000	
9	7	3	58.219	57.802	57.706	3.335	.417	1.1089	1.0000	
9	7	4	21.797	21.591	21.579	-.732	.205	.5393	1.0000	
9	9	-5	23.051	22.802	22.717	1.975	.249	.6939	1.0000	
9	9	-4	2.618 *	1.279	.701	1.070	1.339	.7165	1.0000	**
9	9	-3	48.405	47.934	-47.885	-2.185	.471	1.6734	1.0000	
9	9	-2	4.578 *	6.220	6.133	-1.039	-1.642	-1.5363	1.0000	**
9	9	-1	20.295	20.045	19.930	2.150	.250	.7299	1.0000	
9	9	0	2.575 *	1.729	-1.395	1.023	.845	.4597	1.0000	**
9	9	1	23.095	22.785	-22.683	-2.156	.309	.9050	1.0000	
9	9	2	6.777	7.912	7.855	-.945	-1.135	-1.4031	1.0000	
9	9	3	12.757	12.201	12.028	2.045	.556	1.0982	1.0000	
9	11	-3	11.515	11.203	-11.195	-.424	.311	.5758	1.0000	
9	11	-2	3.860 *	2.767	-1.393	-2.391	1.093	.8072	1.0000	**
9	11	-1	2.744 *	1.149	-1.078	.398	1.595	.8136	1.0000	**
9	11	0	10.433	10.595	10.326	2.370	-.162	-.2830	1.0000	
9	11	1	19.291	19.090	-19.084	-.475	.201	.4952	1.0000	
10	0	-6	95.088	96.814	-96.710	-4.472	-1.726	-2.2920	1.0000	
10	0	-4	67.817	67.257	67.098	4.633	.560	1.0964	1.0000	
10	0	-2	95.213	96.314	-96.193	-4.828	-1.100	-1.4700	1.0000	
10	0	0	80.072	79.148	79.006	4.742	.924	1.4730	1.0000	
10	0	2	102.462	102.266	-102.161	-4.626	.196	.2320	1.0000	
10	0	4	53.130	53.184	53.022	4.142	-.053	-.1579	1.0000	
10	2	-7	3.792 *	4.463	3.540	2.718	-.681	-.5012	1.0000	**
10	2	-6	16.145	16.305	-16.289	-.741	-.160	-.4163	1.0000	
10	2	-5	15.228	14.394	-14.073	-3.020	.834	2.3793	1.0000	
10	2	-4	4.072 *	1.849	-1.719	.681	2.223	2.4463	1.0000	**
10	2	-3	29.780	30.127	29.950	3.258	-.346	-1.4034	1.0000	
10	2	-2	33.697	33.650	-33.642	-.755	.046	.1940	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
10	2	-1	24.086	24.660	-24.431	-3.353	-.574	-2.2479	1.0000	
10	2	0	6.205	5.924	5.890	.638	.281	.4776	1.0000	
10	2	1	16.136	15.887	15.531	3.344	.250	.7697	1.0000	
10	2	2	18.729	18.849	-18.839	-.625	-.121	-.3721	1.0000	
10	2	3	22.532	22.640	-22.401	-3.281	-.108	-.3272	1.0000	
10	2	4	17.802	17.433	-17.428	.437	.369	.9273	1.0000	
10	4	-7	17.677	18.078	-18.047	1.045	-.401	-1.0065	1.0000	
10	4	-6	21.874	21.984	21.886	2.072	-.109	-.3197	1.0000	
10	4	-5	16.881	17.547	17.512	-1.122	-.667	-1.8340	1.0000	
10	4	-4	48.643	49.569	-49.517	-2.250	-.926	-2.7777	1.0000	
10	4	-3	9.009	8.755	-8.672	1.201	.255	.5554	1.0000	
10	4	-2	35.224	36.031	35.962	2.226	-.807	-3.2716	1.0000	
10	4	-1	16.868	16.564	16.519	-1.209	.304	.9901	1.0000	
10	4	0	60.257	61.470	-61.429	-2.252	-1.213	-2.7474	1.0000	
10	4	1	21.706	21.320	-21.286	1.202	.386	1.2922	1.0000	
10	4	2	22.762	22.795	22.765	2.023	-.033	-.1038	1.0000	
10	4	3	11.376	11.040	10.973	-1.216	.336	.6097	1.0000	
10	4	4	19.347	18.650	-18.559	-1.840	.698	1.7717	1.0000	
10	6	-6	42.507	43.224	43.123	2.962	-.717	-2.3679	1.0000	
10	6	-5	14.804	15.021	-15.021	.076	-.217	-.5288	1.0000	
10	6	-4	47.276	47.290	-47.188	-3.110	-.015	-.0541	1.0000	
10	6	-3	20.105	19.809	19.809	-.051	.295	.9350	1.0000	
10	6	-2	26.388	26.119	25.937	3.080	.269	.9563	1.0000	
10	6	-1	18.690	18.097	-18.097	.052	.593	1.8514	1.0000	
10	6	0	54.619	54.750	-54.661	-3.110	-.131	-.3434	1.0000	
10	6	1	17.863	17.375	17.375	-.058	.488	1.3935	1.0000	
10	6	2	39.647	39.609	39.502	2.908	.038	.1294	1.0000	
10	6	3	12.943	13.376	-13.376	.083	-.433	-.9106	1.0000	
10	8	-5	16.504	17.090	16.825	3.000	-.586	-1.3539	1.0000	
10	8	-4	24.492	24.157	-24.141	-.890	.335	.9933	1.0000	
10	8	-3	22.705	23.152	-22.927	-3.217	-.447	-1.3401	1.0000	
10	8	-2	20.031	20.093	20.072	.919	-.062	-.1827	1.0000	
10	8	-1	21.805	21.552	21.294	3.322	.253	.7808	1.0000	
10	8	0	33.039	33.181	-33.167	-.977	-.142	-.4698	1.0000	
10	8	1	13.999	13.861	-13.460	-3.310	.138	.3181	1.0000	
10	8	2	14.419	13.976	13.948	.890	.442	.9823	1.0000	
10	8	3	19.568	18.560	18.275	3.243	1.008	2.5310	1.0000	
10	10	-4	52.057	51.846	51.716	3.672	.211	.6777	1.0000	
10	10	-3	3.977 *	3.948	-3.789	-1.109	.029	.0214	1.0000	**
10	10	-2	66.268	66.386	-66.276	-3.818	-.118	-.2453	1.0000	
10	10	-1	5.902	3.365	3.165	1.142	2.538	2.8059	1.0000	
10	10	0	62.824	62.040	61.925	3.768	.784	1.7929	1.0000	
10	10	1	2.969 *	1.618	1.157	-1.130	1.351	.7346	1.0000	**
11	1	-7	4.808 *	6.233	6.161	.944	-1.425	-1.2475	1.0000	**
11	1	-6	13.843	13.761	-13.582	-2.211	.082	.1897	1.0000	
11	1	-5	5.310	4.277	-4.177	-.919	1.032	1.2847	1.0000	
11	1	-4	31.503	31.148	31.051	2.463	.354	1.2993	1.0000	
11	1	-3	2.272 *	1.197	.828	.864	1.075	.6626	1.0000	**
11	1	-2	14.362	14.136	-13.905	-2.543	.226	.6700	1.0000	
11	1	-1	16.630	16.490	16.473	-.750	.140	.4422	1.0000	
11	1	0	45.631	46.143	46.064	2.694	-.512	-1.7649	1.0000	
11	1	1	26.539	26.667	-26.659	.642	-.128	-.4411	1.0000	
11	1	2	42.286	41.388	-41.303	-2.658	.898	3.2947	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
11	1	3	26.055	25.348	25.342	-.559	.706	2.1479	1.0000	
11	1	4	44.372	43.485	43.409	2.562	.887	2.8087	1.0000	
11	3	-7	25.985	24.800	24.577	3.322	1.185	3.3805	1.0000	
11	3	-6	2.562 *	1.359	-1.355	-.108	1.202	.6569	1.0000	**
11	3	-5	28.963	28.778	-28.562	-3.527	.184	.6254	1.0000	
11	3	-4	17.893	18.185	18.184	.184	-.291	-.8629	1.0000	
11	3	-3	54.294	54.146	54.026	3.691	.148	.4032	1.0000	
11	3	-2	2.354 *	1.638	-1.631	-.145	.716	.4510	1.0000	**
11	3	-1	50.962	50.204	-50.070	-3.655	.759	2.0875	1.0000	
11	3	0	15.743	15.762	15.761	.191	-.020	-.0577	1.0000	
11	3	1	33.472	33.348	33.166	3.479	.124	.4475	1.0000	
11	3	2	2.527 *	.763	-.750	-.136	1.764	.9778	1.0000	**
11	3	3	7.391	7.888	-7.224	-3.167	-.497	-.6637	1.0000	
11	3	4	11.463	10.013	10.012	.154	1.450	2.6803	1.0000	
11	5	-6	49.699	50.081	49.953	3.586	-.382	-1.2625	1.0000	
11	5	-5	9.109	8.395	-8.366	-.694	.714	1.2410	1.0000	
11	5	-4	40.413	41.205	-41.022	-3.885	-.793	-2.8179	1.0000	
11	5	-3	12.164	12.967	12.947	.717	-.803	-1.8925	1.0000	
11	5	-2	57.293	58.685	58.537	4.163	-1.392	-3.5343	1.0000	
11	5	-1	7.374	6.323	6.290	-.644	1.051	1.7986	1.0000	
11	5	0	60.167	60.733	-60.583	-4.260	-.566	-1.3223	1.0000	
11	5	1	4.236 *	3.716	-3.664	.621	.520	.4787	1.0000	**
11	5	2	79.890	80.245	80.131	4.280	-.355	-.5814	1.0000	
11	5	3	9.659	9.811	9.796	-.550	-.153	-.2500	1.0000	
11	7	-5	37.652	38.217	38.114	2.809	-.566	-1.7908	1.0000	
11	7	-4	4.691 *	2.883	2.658	-1.118	1.808	1.7700	1.0000	**
11	7	-3	28.443	28.522	-28.380	-2.840	-.078	-.2512	1.0000	
11	7	-2	5.331	5.541	5.409	1.206	-.210	-.2369	1.0000	
11	7	-1	27.465	27.620	27.476	2.820	-.155	-.5051	1.0000	
11	7	0	4.743 *	5.250	-5.103	-1.231	-.507	-.4923	1.0000	**
11	7	1	2.640 *	2.935	-1.310	-2.627	-.296	-.1571	1.0000	**
11	7	2	21.070	20.943	20.904	1.279	.126	.3275	1.0000	
11	9	-4	10.667	10.312	10.245	1.176	.355	.6211	1.0000	
11	9	-3	5.331 *	5.200	-4.905	-1.726	.131	.1282	1.0000	**
11	9	-2	8.607	7.407	-7.304	-1.231	1.200	1.8731	1.0000	
11	9	-1	17.383	17.695	17.613	1.705	-.313	-.7768	1.0000	
11	9	0	17.582	16.501	16.450	1.294	1.081	2.6576	1.0000	
11	9	1	8.901	8.604	8.472	-1.500	.297	.4317	1.0000	
12	0	-6	34.116	33.610	-33.442	-3.354	.507	1.6258	1.0000	
12	0	-4	33.472	33.713	33.523	3.570	-.241	-.8440	1.0000	
12	0	-2	12.774	12.041	-11.481	-3.628	.733	1.8827	1.0000	
12	0	0	10.351	9.592	8.873	3.645	.758	1.6079	1.0000	
12	0	2	15.409	15.251	-14.824	-3.582	.159	.3865	1.0000	
12	2	-6	14.124	14.606	14.601	-.363	-.481	-1.0495	1.0000	
12	2	-5	56.060	56.433	-56.315	-3.642	-.373	-1.0503	1.0000	
12	2	-4	21.896	21.614	-21.611	.333	.282	.8579	1.0000	
12	2	-3	71.933	72.664	72.561	3.863	-.732	-1.3208	1.0000	
12	2	-2	28.041	27.770	27.768	-.302	.271	.9493	1.0000	
12	2	-1	89.008	88.932	-88.844	-3.960	.076	.1075	1.0000	
12	2	0	12.657	13.395	-13.391	.334	-.738	-1.7056	1.0000	
12	2	1	66.818	67.077	66.968	3.810	-.259	-.5205	1.0000	
12	2	2	8.295	7.229	7.220	-.342	1.067	1.7002	1.0000	
12	2	3	46.661	46.653	-46.519	-3.534	.008	.0268	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
12	4	-6	2.735 *	4.314	-4.068	1.438	-1.580	-.8094	1.0000	**
12	4	-5	21.217	21.592	-21.522	-1.736	-.375	-1.0828	1.0000	
12	4	-4	13.977	13.827	13.748	-1.475	.151	.3588	1.0000	
12	4	-3	25.003	24.497	24.432	1.787	.506	1.6465	1.0000	
12	4	-2	15.353	14.703	-14.626	1.509	.650	1.7262	1.0000	
12	4	-1	41.486	41.527	-41.486	-1.829	-.041	-.1496	1.0000	
12	4	0	9.364	9.593	9.471	-1.524	-.229	-.4102	1.0000	
12	4	1	21.130	20.304	20.233	1.692	.826	2.3874	1.0000	
12	4	2	10.411	9.600	9.474	1.553	.811	1.4051	1.0000	
12	4	3	13.280	12.930	-12.837	-1.549	.350	.7099	1.0000	
12	6	-5	4.288 *	4.970	-4.956	.372	-.681	-.5583	1.0000	**
12	6	-4	7.101	6.974	-6.620	-2.194	.127	.1735	1.0000	
12	6	-3	9.897	9.628	-9.619	-.411	.268	.4961	1.0000	
12	6	-2	9.321	9.002	-8.731	2.195	.319	.5665	1.0000	
12	6	-1	3.116 *	3.747	-3.732	.339	-.632	-.4159	1.0000	**
12	6	0	19.261	19.177	19.055	-2.158	.084	.2298	1.0000	
12	6	1	6.820	5.876	-5.867	-.340	.943	1.2112	1.0000	
12	6	2	5.033 *	4.057	-3.436	2.158	.975	.9087	1.0000	**
12	8	-4	5.799	4.605	-4.549	-.716	1.193	1.2652	1.0000	
12	8	-3	70.215	70.034	-69.927	-3.874	.180	.3751	1.0000	
12	8	-2	10.013	9.041	9.008	.772	.972	1.6761	1.0000	
12	8	-1	64.909	64.323	64.205	3.897	.587	1.3554	1.0000	
12	8	0	13.627	13.675	-13.651	-.802	-.048	-.0972	1.0000	
12	8	1	66.887	65.870	-65.760	-3.818	1.016	2.2585	1.0000	
13	1	-6	40.464	40.584	-40.511	-2.431	-.119	-.3776	1.0000	
13	1	-5	10.147	9.636	9.606	-.758	.512	.9172	1.0000	
13	1	-4	27.833	27.537	27.429	2.432	.296	.9372	1.0000	
13	1	-3	5.799	1.569	1.322	.845	4.230	5.3708	1.0000	
13	1	-2	32.688	32.898	-32.809	-2.426	-.210	-.7245	1.0000	
13	1	-1	7.876	8.347	-8.299	-.898	-.472	-.7568	1.0000	
13	1	0	3.934 *	3.438	-2.633	2.211	.495	.4001	1.0000	**
13	1	1	6.391	5.547	5.474	.900	.844	1.0602	1.0000	
13	1	2	13.583	14.711	-14.558	-2.114	-1.127	-2.2852	1.0000	
13	3	-6	10.965	11.551	-11.551	-.067	-.586	-1.0410	1.0000	
13	3	-5	7.512	7.343	-6.674	-3.062	.169	.2351	1.0000	
13	3	-4	3.873 *	1.947	-1.946	.063	1.926	1.5671	1.0000	**
13	3	-3	19.274	19.164	18.870	3.340	.110	.3107	1.0000	
13	3	-2	17.928	18.288	-18.287	-.175	-.360	-1.0011	1.0000	
13	3	-1	38.798	39.222	-39.062	-3.543	-.424	-1.4833	1.0000	
13	3	0	2.592 *	2.178	2.173	.152	.414	.2235	1.0000	**
13	3	1	54.857	54.432	54.311	3.622	.425	1.4673	1.0000	
13	3	2	19.287	18.809	-18.807	-.235	.478	1.2279	1.0000	
13	5	-5	3.371 *	.587	.055	-.585	2.784	1.8432	1.0000	**
13	5	-4	66.255	66.959	-66.848	-3.845	-.704	-1.5641	1.0000	
13	5	-3	13.674	13.382	13.364	.676	.293	.6503	1.0000	
13	5	-2	40.175	39.997	39.818	3.784	.178	.6034	1.0000	
13	5	-1	12.026	11.926	-11.905	-.695	.100	.2061	1.0000	
13	5	0	37.920	38.537	-38.359	-3.695	-.617	-2.0067	1.0000	
13	5	1	10.697	10.333	10.309	.694	.364	.6477	1.0000	
13	7	-4	18.685	18.433	-18.392	-1.230	.252	.6190	1.0000	
13	7	-3	25.241	24.551	-24.408	-2.640	.690	1.9937	1.0000	
13	7	-2	3.743 *	2.262	-1.971	1.110	1.481	1.0464	1.0000	**
13	7	-1	42.035	41.579	41.484	2.811	.456	1.4636	1.0000	

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
13	7	0	2.709	*	1.082	.292	-1.042	1.627	.8410	1.0000	**
14	0	-4	84.793		83.936	83.834	4.146	.857	1.3947	1.0000	
14	0	-2	76.628		76.632	-76.512	-4.275	-.004	-.0077	1.0000	
14	0	0	80.622		80.553	80.438	4.307	.068	.1197	1.0000	
14	2	-5	9.343		9.173	-8.763	-2.712	.170	.2702	1.0000	
14	2	-4	17.984		18.080	18.065	.729	-.096	-.2426	1.0000	
14	2	-3	5.552		4.528	3.573	2.782	1.024	1.1483	1.0000	
14	2	-2	4.847	*	5.650	5.613	-.649	-.804	-.7771	1.0000	**
14	2	-1	9.170		9.414	-8.985	-2.812	-.245	-.4132	1.0000	
14	2	0	6.314		4.798	4.751	.671	1.515	1.8428	1.0000	
14	2	1	20.157		19.802	19.606	2.783	.354	.9093	1.0000	
14	4	-5	13.055		13.081	13.033	-1.125	-.026	-.0526	1.0000	
14	4	-4	23.714		23.244	-23.161	-1.960	.469	1.3066	1.0000	
14	4	-3	17.768		18.034	-18.000	1.094	-.266	-.6604	1.0000	
14	4	-2	33.770		33.938	33.876	2.058	-.168	-.5327	1.0000	
14	4	-1	16.885		16.734	16.700	-1.062	.151	.3759	1.0000	
14	4	0	12.047		11.643	-11.475	-1.968	.404	.7987	1.0000	
14	4	1	5.007	*	5.144	-5.036	1.049	-.138	-.1211	1.0000	**
14	6	-3	16.331		16.189	16.189	-.106	.142	.3216	1.0000	
14	6	-2	58.349		57.691	57.616	2.934	.659	2.0291	1.0000	
14	6	-1	10.602		11.125	-11.124	.093	-.523	-.8821	1.0000	
15	1	-4	2.852	*	2.880	2.185	1.876	-.028	-.0149	1.0000	**
15	1	-3	2.679	*	1.280	.793	1.004	1.399	.7314	1.0000	**
15	1	-2	12.497		13.802	-13.655	-2.008	-1.305	-2.5988	1.0000	
15	1	-1	7.919		7.306	-7.242	-.970	.613	.8686	1.0000	
15	1	0	9.710		8.515	8.271	2.023	1.196	1.9594	1.0000	
15	3	-4	8.581		7.941	7.940	.129	.640	.9604	1.0000	
15	3	-3	39.227		39.353	39.198	3.496	-.127	-.4007	1.0000	
15	3	-2	11.333		10.938	-10.937	-.154	.395	.7305	1.0000	
15	3	-1	37.652		37.196	-37.035	-3.455	.456	1.4226	1.0000	

CACOSI206,ANISOTROPIC,1-3

RESULTS OF STRUCTURE FACTOR CALCULATIONS

ALL REFLECTIONS	NUMERATOR	DENOMINATOR	NUMBER	R
WEIGHTED R	8064.03	8872159.89	984	.030
UNWEIGHTED R	754.23	30769.67	984	.025
RANGES OF F(OBS)				
	2629.06	1489531.47	604	.042
	1517.97	3859236.25	214	.020
	3055.96	1696910.18	95	.042
	130.88	544690.41	36	.016
	64.56	303366.38	15	.015
	238.13	672510.94	17	.019
	380.39	44585.43	1	.092
	47.09	261328.81	2	.013
RANGES OF (SIN(THETA)/LAMBDA)**2				
	1728.92	1069748.03	47	.040
	997.82	1199659.28	82	.029
	504.49	1139785.75	106	.021
	356.05	1065877.72	116	.018
	444.82	1161669.73	142	.020
	1374.04	1247250.57	149	.033
	2095.13	947761.54	160	.047
	562.75	1040407.26	182	.023

UNREJECTED REFLECTIONS				
WEIGHTED R	8064.03	8872159.89	984	.030
UNWEIGHTED R	754.23	30769.67	984	.025
RANGES OF F(OBS)				
	2629.06	1489531.47	604	.042
	1517.97	3859236.25	214	.020
	3055.96	1696910.18	95	.042
	130.88	544690.41	36	.016
	64.56	303366.38	15	.015
	238.13	672510.94	17	.019
	380.39	44585.43	1	.092
	47.09	261328.81	2	.013
RANGES OF (SIN(THETA)/LAMBDA)**2				
	1728.92	1069748.03	47	.040
	997.82	1199659.28	82	.029
	504.49	1139785.75	106	.021
	356.05	1065877.72	116	.018
	444.82	1161669.73	142	.020
	1374.04	1247250.57	149	.033
	2095.13	947761.54	160	.047
	562.75	1040407.26	182	.023

SUM FCAL	30657.89
STANDARD DEV OF UNIT WEIGHT OBS	2.93