

Guildite, a layer structure with a ferric hydroxy-sulphate chain and its optical absorption spectra¹

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Abstract

Guildite, $\text{Cu}^{2+}\text{Fe}^{3+}(\text{SO}_4)_2(\text{OH}) \cdot 4\text{H}_2\text{O}$, from the United Verde Mine, Jerome, Arizona, is monoclinic, space group $P2_1/m$, with cell dimensions $a = 9.786(2)$, $b = 7.134(1)$, $c = 7.263(1)\text{Å}$, $\beta = 105.28(1)^\circ$, $Z = 2$. The crystal structure has been determined by Patterson and Fourier syntheses and refined by the method of least squares to an R factor of 0.056 for 942 reflections, measured on an automatic single-crystal diffractometer. The crystal structure contains an octahedral-tetrahedral chain, which consists of zig-zag chains of $[\text{FeO}_6(\text{OH})]$ octahedra sharing the (OH) corner; two pairs of octahedral corners on either side of this chain are shared by $\text{S}(1)\text{O}_4$ and $\text{S}(2)\text{O}_4$ tetrahedra. These chains are crosslinked through corner-sharing *trans*- $[\text{CuO}_2(\text{H}_2\text{O})_4]$ octahedra into corrugated sheets parallel to the (001) plane. Adjacent sheets are hydrogen-bonded through water molecules. The average $\text{Fe}^{3+}\text{-O}$ and S-O bond lengths are 2.005 and 1.472Å respectively. Cu^{2+} shows the usual Jahn-Teller distortion with four short $\text{Cu-O}(W)$ bonds (av. 1.985Å) and two long Cu-O bonds (av. 2.264Å).

The pleochroism in guildite is similar to that of other materials containing hydroxobridged Fe^{3+} chains. Intense color and the highest refractive index occur when the vibration direction of the incident light is along the chain direction. An intense absorption band at 430 nm and a band at 874 nm are due to Fe^{3+} , whereas broad absorption bands at 1285 nm and 780 nm have been assigned to Cu^{2+} . Additional bands, including a sharp band at 1953 nm, are due to (OH) ions and water molecules.

Introduction

Guildite is a secondary hydrated basic copper ferric sulphate mineral, formed as a result of a mine fire at the United Verde Mine, Jerome, Arizona, in association with coquimbite, $\text{Fe}_{2-x}\text{Al}_x(\text{SO}_4)_3 \cdot 9\text{H}_2\text{O}$, and ransomite, $\text{CuFe}_2(\text{SO}_4)_4 \cdot 6\text{H}_2\text{O}$ (Lausen, 1928). Lausen (1928) originally proposed a complex chemical formula for guildite, $(\text{Cu,Fe})_3(\text{Fe,Al})_4(\text{SO}_4)_7\text{O}_2 \cdot 17\text{H}_2\text{O}$. The unit-cell dimensions and space group were determined by Laughon (1970), who proposed a simplified chemical formula, $\text{CuFe}(\text{SO}_4)_2(\text{OH}) \cdot 4\text{H}_2\text{O}$, which is consistent with the density, the measured cell volume, and symmetry requirements of the

space group. Our structure determination has confirmed the formula proposed by Laughon (1970). We have also interpreted the optical absorption spectra of guildite in view of its crystal structure.

Experimental

A single-crystal fragment of type guildite (NMNH #95950) from the United Verde Mine measuring $0.20 \times 0.20 \times 0.25$ mm was mounted on the Syntex P1 automatic single-crystal diffractometer, with the long axis parallel to the phi-axis of the diffractometer. The unit-cell dimensions were determined by the least-squares refinement of 15 reflections with 2θ values between 25 and 35° measured on the diffractometer, using $\text{MoK}\alpha$ radiation. Our cell dimensions [$a =$

¹ Structural Chemistry of Copper and Zinc Minerals. Part V.

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
0	0	1	9.095	9.630	9.629	.047	-.535	-2.0628	1.0000	
0	0	2	52.600	53.349	53.317	1.871	-.749	-1.7341	1.0000	
0	0	3	64.356	63.469	63.380	3.352	.887	1.6391	1.0000	
0	0	4	43.056	42.627	-42.617	-.937	.429	1.1499	1.0000	
0	0	5	16.023	16.432	16.163	2.958	-.408	-.9377	1.0000	
0	0	6	14.810	14.398	14.338	1.322	.412	.7793	1.0000	
0	0	7	8.297	8.727	-8.724	.259	-.431	-.4582	1.0000	
0	0	8	58.958	55.140	55.062	2.924	3.819	7.6219	1.0000	
0	1	1	91.040	97.753	97.730	2.109	-6.713	-13.7779	1.0000	
0	1	2	37.316	40.196	-40.123	-2.430	-2.880	-8.5035	1.0000	
0	1	3	44.805	46.905	46.862	2.011	-2.161	-5.3328	1.0000	
0	1	4	2.485	1.606	-1.605	-.054	.879	.4657	1.0000	
0	1	5	25.305	24.751	-24.701	-1.574	.554	1.5409	1.0000	
0	1	6	7.333	6.893	6.674	1.726	.439	.4676	1.0000	
0	1	7	28.121	26.611	-26.571	-1.456	1.511	3.4696	1.0000	
0	1	8	11.341	11.858	-11.858	-.012	-.517	-.5980	1.0000	
0	2	1	88.255	74.193	74.110	3.615	14.056	22.5984	1.0000	
0	2	2	7.575	9.436	9.281	1.706	-1.662	-3.8210	1.0000	
0	2	3	84.284	10.143	10.142	.149	-2.43	-5.4298	1.0000	
0	2	4	30.592	87.812	87.708	4.263	-3.527	-5.4298	1.0000	
0	2	5	11.051	31.463	31.463	.214	-.872	-2.4972	1.0000	
0	2	6	38.412	10.483	10.355	1.607	.567	.8335	1.0000	
0	2	7	17.098	37.302	37.220	2.468	1.110	2.7217	1.0000	
0	2	8	47.562	17.408	-14.403	-.381	2.690	4.3241	1.0000	
0	3	1	81.834	36.454	-36.396	-2.065	11.108	28.7007	1.0000	
0	3	2	47.099	79.937	79.899	2.451	1.897	3.3277	1.0000	
0	3	3	2.733	49.201	-49.158	.2042	-2.10	-5.5292	1.0000	
0	3	4	35.482	.054	.052	.013	2.679	1.3724	1.0000	
0	3	5	13.968	12.963	36.038	1.551	-.589	-1.6723	1.0000	
0	3	6	8.957	9.461	-12.840	-1.780	.645	1.0983	1.0000	
0	3	7	13.211	9.938	9.364	1.354	-.505	-.5196	1.0000	
0	4	1	66.851	56.094	-9.937	.091	3.273	8.3082	1.0000	
0	4	2	57.721	59.669	56.061	1.945	10.757	23.4048	1.0000	
0	4	3	29.676	31.765	9.572	3.395	-1.947	-4.3686	1.0000	
0	4	4	21.953	22.387	-31.753	-.867	-2.088	-5.7557	1.0000	
0	4	5	24.517	25.692	22.185	2.998	-.433	-.9800	1.0000	
0	4	6	6.220	1.076	-1.026	1.396	-1.175	-2.5366	1.0000	
0	5	1	76.910	56.104	56.066	2.072	5.143	3.7971	1.0000	
0	5	2	37.206	29.388	-29.289	-2.410	20.806	29.3709	1.0000	
0	5	3	34.756	33.403	33.346	1.953	7.818	24.3272	1.0000	
0	5	4	2.975	1.046	1.043	-.086	1.353	3.9140	1.0000	
0	5	5	22.050	23.003	-22.947	1.605	1.929	.9076	1.0000	
0	5	6	6.752	7.374	7.187	1.652	-.954	-1.9852	1.0000	
0	6	0	95.003	78.019	-78.011	-1.117	-.621	-.4967	1.0000	
0	6	1	45.043	36.968	36.787	3.648	16.584	21.8445	1.0000	
0	6	2	31.283	26.082	26.017	1.837	8.075	20.4992	1.0000	
0	6	3	18.556	17.316	17.314	.301	5.201	13.6846	1.0000	
0	6	4	59.809	64.708	64.565	4.310	1.240	2.6005	1.0000	
0	6	5	22.365	27.121	27.119	.345	-4.256	-10.1280	1.0000	
0	7	1	60.624	51.386	-51.343	-2.097	9.238	-8.4355	1.0000	
0	7	2	42.196	34.855	34.776	2.339	7.341	18.1862	1.0000	
0	7	3	37.109	33.865	-33.804	-2.035	7.341	18.6342	1.0000	

H	K	L	F(DRS)	F(CALC)	A(CALC)	R(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
0	7	4	3.276 *	1.676	-1.676	-.034	1.600	.6838		1.0000
0	8	0	87.294	84.373	84.224	5.006	2.921	3.7570		1.0000
0	8	1	4.471 *	.897	-.843	.304	3.575	2.1553		1.0000
0	8	2	34.635	33.692	33.627	2.091	.943	2.1319		1.0000
1	0	-3	19.012	17.161	17.156	.411	1.852	3.4570		1.0000
1	0	-7	10.560	10.233	9.890	2.628	.327	.4804		1.0000
1	0	-6	20.865	19.756	-19.756	.002	1.108	2.6293		1.0000
1	0	-5	14.213	14.101	1.987	1.787	.111	.2521		1.0000
1	0	-4	72.501	74.716	74.656	2.997	-2.215	-3.6837		1.0000
1	0	-3	18.491	15.789	-15.789	-.215	2.701	9.8959		1.0000
1	0	-2	111.922	119.997	119.931	3.965	-8.075	-13.9928		1.0000
1	0	-1	38.004	37.167	37.140	1.405	.837	2.5499		1.0000
1	0	0	45.928	53.760	53.757	.544	-7.832	-21.3820		1.0000
1	0	1	57.120	60.852	60.726	3.915	-3.732	-7.4482		1.0000
1	0	2	45.050	45.844	-45.841	-.523	.794	-2.0335		1.0000
1	0	3	5.743	5.301	4.823	2.201	.442	.6728		1.0000
1	0	4	48.530	49.440	49.372	2.601	-.911	-2.1604		1.0000
1	0	5	18.878	19.949	19.949	-.093	-1.072	-2.5631		1.0000
1	0	6	63.914	61.449	61.364	3.235	2.465	4.2208		1.0000
1	0	7	10.363	8.575	8.531	.867	1.788	2.2117		1.0000
1	0	8	29.241	28.019	28.008	.784	1.222	2.4228		1.0000
1	1	-8	5.933 *	1.505	1.281	.790	4.428	3.4447		1.0000
1	1	-7	7.789	6.517	6.514	.192	1.272	1.4161		1.0000
1	1	-6	12.706	14.303	-14.276	.885	-1.597	-2.8889		1.0000
1	1	-5	40.603	41.462	-41.412	-2.035	-.559	-2.4379		1.0000
1	1	-4	24.914	26.435	26.393	1.481	-1.521	-5.1768		1.0000
1	1	-3	17.409	17.302	-17.296	-.476	.107	.3726		1.0000
1	1	-2	31.838	30.356	30.334	-1.136	1.532	5.3422		1.0000
1	1	-1	64.339	64.696	64.646	2.539	-.357	-.6988		1.0000
1	1	0	13.466	12.150	-12.012	-1.825	1.317	6.1452		1.0000
1	1	1	52.531	54.945	54.939	.771	-2.413	-6.0731		1.0000
1	1	2	12.322	11.784	-11.737	1.050	.538	1.6570		1.0000
1	1	3	43.222	43.991	-43.931	-2.310	-.769	-2.0807		1.0000
1	1	4	13.207	14.442	14.348	1.640	-1.235	-2.8356		1.0000
1	1	5	22.661	21.753	-21.739	-.799	.908	2.4112		1.0000
1	1	6	7.457	9.584	9.559	-.688	-2.127	-2.2459		1.0000
1	1	7	30.996	29.915	29.875	1.546	1.081	2.4440		1.0000
1	1	8	17.668	15.903	-15.863	-1.128	1.765	2.6218		1.0000
1	1	-7	18.684	17.203	17.066	2.168	1.481	2.5667		1.0000
1	1	-6	19.652	20.289	20.288	.164	-.637	-1.3260		1.0000
1	1	-5	37.907	36.882	36.764	2.959	1.025	2.9077		1.0000
1	1	-4	29.887	29.888	29.855	1.417	-.001	-.0040		1.0000
1	1	-3	29.897	29.345	29.342	.446	.552	1.8580		1.0000
1	1	-2	78.272	78.028	77.940	3.722	.243	.4316		1.0000
1	1	-1	2.284 *	.736	.664	-.317	1.548	1.0518		1.0000
1	1	0	76.651	69.604	69.566	2.279	7.047	11.1443		1.0000
1	1	1	69.456	59.683	59.601	3.145	9.773	15.8888		1.0000
1	1	2	80.141	71.070	71.070	-.223	9.071	13.8892		1.0000
1	1	3	27.907	34.401	34.169	3.994	-6.494	-26.8481		1.0000
1	1	4	30.485	30.413	30.389	1.206	.072	.2680		1.0000
1	1	5	23.387	23.545	23.535	.717	-.158	-.4629		1.0000
1	1	6	33.643	33.045	32.890	3.203	.598	1.6962		1.0000
1	1	2	22.164	20.302	-20.299	-.335	1.862	4.1768		1.0000

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F	K	L	F(DBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	2	7	26.898	24.709	24.644	1.802	2.189	4.7621	1.0000
1	3	-7	7.374	6.819	6.818	-.107	.555	.5500	1.0000
1	3	-6	6.343	6.343	8.300	-.845	.030	.0364	1.0000
1	3	-5	15.592	15.777	15.647	2.021	.215	.4524	1.0000
1	3	-4	39.442	39.962	-39.935	-1.460	-.571	-1.5066	1.0000
1	3	-3	25.789	24.480	24.474	.513	1.316	4.3544	1.0000
1	3	-2	11.566	10.027	-9.951	1.154	1.538	3.9398	1.0000
1	3	-1	89.956	78.252	-78.211	-2.548	11.716	15.7703	1.0000
1	3	0	53.264	41.875	41.835	1.837	11.889	25.9514	1.0000
1	3	1	16.275	19.164	10.139	-.720	6.112	20.0979	1.0000
1	3	2	23.691	22.275	22.251	-1.048	1.415	4.9366	1.0000
1	3	3	18.601	20.401	20.278	2.238	-1.800	-5.0075	1.0000
1	3	4	32.423	35.154	-35.112	-1.731	-2.731	-8.2312	1.0000
1	3	5	18.411	17.989	17.973	.745	.422	.9187	1.0000
1	3	6	6.175	7.425	-7.398	.536	-1.250	.9135	1.0000
1	3	7	34.362	34.306	-34.268	-1.611	.056	.1258	1.0000
1	4	-7	13.097	14.074	13.820	2.661	-.977	-1.4072	1.0000
1	4	-6	3.113	2.183	2.185	.103	.931	.4189	1.0000
1	4	-5	20.650	20.578	20.495	1.843	.072	.1623	1.0000
1	4	-4	34.725	35.993	35.869	2.986	-1.269	-3.7846	1.0000
1	4	-3	12.551	10.790	-10.789	-.151	1.760	3.7734	1.0000
1	4	-2	97.388	90.640	90.551	4.000	6.748	7.4533	1.0000
1	4	-1	16.193	13.799	13.724	1.437	2.394	6.9275	1.0000
1	4	0	15.408	12.040	12.026	.580	3.368	9.3729	1.0000
1	4	1	56.543	46.738	46.573	3.932	9.805	21.6592	1.0000
1	4	2	3.490	2.824	2.794	-.407	.665	.4691	1.0000
1	4	3	35.485	37.394	37.324	2.291	-1.909	-6.0718	1.0000
1	4	4	29.704	31.079	30.968	2.615	-1.375	-3.7534	1.0000
1	4	5	7.384	6.974	6.974	-.055	.410	.4331	1.0000
1	4	6	54.777	57.235	57.142	3.268	-2.458	-5.5139	1.0000
1	4	7	6.628	7.516	7.461	.907	-.888	-.6427	1.0000
1	5	-6	8.290	9.885	-9.842	.917	-1.595	-1.6485	1.0000
1	5	-5	32.199	33.262	-33.204	-1.969	-1.064	-2.6533	1.0000
1	5	-4	7.032	8.045	7.910	1.465	-1.013	-1.0980	1.0000
1	5	-3	10.450	11.037	-11.028	-.444	-.587	-.9235	1.0000
1	5	-2	13.957	14.103	14.061	-1.094	-.147	-.3095	1.0000
1	5	-1	39.770	35.607	35.519	2.496	4.163	13.5357	1.0000
1	5	0	4.046	2.138	1.196	-1.773	1.908	1.5254	1.0000
1	5	1	40.343	34.093	34.084	.752	6.251	20.0996	1.0000
1	5	2	6.835	5.506	-5.414	1.001	1.329	1.6028	1.0000
1	5	3	28.339	29.587	-29.497	-2.305	-1.248	-3.3761	1.0000
1	5	4	3.925	4.288	3.998	1.551	-.363	-.2218	1.0000
1	5	5	19.209	19.868	-19.850	-.846	-.659	-1.2964	1.0000
1	5	6	6.624	5.425	5.375	-.734	1.200	.9590	1.0000
1	6	-6	46.557	48.483	48.386	3.071	-1.927	-4.4966	1.0000
1	6	-5	22.900	25.036	24.990	1.515	-2.136	-4.4466	1.0000
1	6	-4	10.989	9.880	9.866	.539	1.108	1.5877	1.0000
1	6	-3	31.273	30.862	30.636	3.724	.411	1.0615	1.0000
1	6	-2	10.816	11.585	-11.583	-.204	-.769	-1.2225	1.0000
1	6	-1	38.588	32.507	32.422	3.349	6.081	17.5966	1.0000
1	6	0	15.816	13.765	13.398	3.159	2.051	4.2392	1.0000
1	6	1	40.250	33.754	33.754	-.076	6.497	18.6143	1.0000
1	6	2	82.954	71.117	70.997	4.135	11.837	17.8406	1.0000

H	K	L	F(FRS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
1	6	3	39.528	39.361	39.332	1.357	.167	.4474		1.0000
1	6	4	18.331	19.331	19.313	.831	-1.000	-1.9032		1.0000
1	6	5	19.907	22.170	21.933	3.238	-2.263	-4.0424		1.0000
1	7	-4	10.211	10.399	-10.312	-1.349	-.198	-.2290		1.0000
1	7	-3	11.633	14.287	14.277	.529	-2.648	-3.8707		1.0000
1	7	-2	4.281	4.434	-4.287	1.133	-.153	-.0949		1.0000
1	7	-1	41.912	39.164	-39.086	-2.747	2.748	7.2967		1.0000
1	7	0	11.006	10.449	10.302	1.749	.557	.8100		1.0000
1	7	1	27.803	26.669	-26.657	-.793	1.134	2.6901		1.0000
1	7	2	3.348	2.112	-1.819	-1.073	1.234	.5808		1.0000
1	7	3	30.606	29.591	29.511	2.183	1.014	2.3115		1.0000
1	7	4	7.651	7.146	-6.950	-1.661	.505	.4803		1.0000
1	8	-2	54.010	56.703	56.555	4.091	-2.693	-6.5480		1.0000
1	8	-1	10.598	12.347	12.243	1.604	-1.749	-2.1093		1.0000
1	8	0	17.914	17.068	17.049	.795	2.846	5.3142		1.0000
1	8	1	26.736	25.969	25.650	3.994	.765	1.6425		1.0000
1	8	2	3.328	.831	.806	-.200	2.497	1.0503		1.0000
1	8	3	20.153	21.356	21.326	1.129	-1.203	-2.2752		1.0000
1	8	4	4.803	4.589	-4.575	.351	.214	.1579		1.0000
1	8	5	50.931	50.849	50.729	3.496	.082	.1899		1.0000
1	8	6	30.678	30.613	30.612	.236	.065	.2078		1.0000
1	8	7	65.227	65.115	65.077	2.214	.112	.2266		1.0000
1	8	8	129.047	128.629	128.590	3.152	.419	.5824		1.0000
1	8	-1	12.340	15.186	-15.172	-.661	-2.847	-9.0522		1.0000
1	8	0	40.862	44.191	44.047	3.569	-3.330	-10.4733		1.0000
1	8	1	31.062	33.860	33.843	1.070	-2.798	-9.7563		1.0000
1	8	2	9.116	8.594	-8.577	.536	.522	1.3729		1.0000
1	8	3	24.655	27.512	27.232	3.912	-2.857	-11.8096		1.0000
1	8	4	13.321	13.173	-13.173	.030	.148	.3905		1.0000
1	8	5	55.043	53.512	53.459	2.395	1.531	3.1426		1.0000
1	8	6	47.673	44.783	44.721	2.347	2.890	6.7998		1.0000
1	8	7	5.802	6.522	6.522	-.038	-.720	-.5905		1.0000
1	8	8	14.859	14.140	13.949	2.316	.719	1.1181		1.0000
1	8	9	10.090	9.603	9.510	1.339	.487	.5704		1.0000
1	8	-7	29.493	29.516	-29.480	-1.461	-.023	-.0574		1.0000
1	8	-6	23.836	23.452	-23.452	.056	.384	.9841		1.0000
1	8	-5	19.005	18.713	18.672	1.236	.292	.7692		1.0000
1	8	-4	41.453	42.646	-42.599	-2.008	-1.194	-3.4541		1.0900
1	8	-3	59.092	58.094	58.055	2.118	1.898	3.4978		1.0000
1	8	-2	60.513	59.207	59.206	-.218	1.307	2.8011		1.0000
1	8	-1	40.019	39.557	39.537	-1.260	.462	1.5180		1.0000
1	8	0	16.552	17.108	16.971	2.159	-.555	-2.3313		1.0000
1	8	1	44.041	49.362	-49.312	-2.219	-5.321	-13.9996		1.0000
1	8	2	34.649	35.635	-35.633	.350	-.986	-3.0359		1.0000
1	8	3	10.830	8.826	-8.785	.852	2.004	4.5659		1.0000
1	8	4	34.379	33.948	-33.903	-1.754	.431	1.4010		1.0000
1	8	5	29.251	27.980	27.929	1.694	1.271	3.4698		1.0000
1	8	6	18.653	18.651	18.648	-.326	.002	.0040		1.0000
1	8	7	3.293	1.152	-1.067	-.434	2.141	.9112		1.0000
1	8	8	13.877	12.954	12.867	1.493	.924	1.3712		1.0000
1	8	9	38.146	36.633	36.549	2.476	1.513	3.9091		1.0000
1	8	-5	15.844	14.416	-14.408	-.461	1.428	2.9102		1.0000
1	8	-6	22.053	22.819	22.622	2.996	-.766	-2.0339		1.0000

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
2	2	-4	45.454	45.417	45.399	1.251	.039	.1050	1.0000
2	2	-3	2.291	2.235	2.194	.429	.056	.0341	1.0000
2	2	-2	40.205	41.760	41.548	4.205	-1.555	-4.9993	1.0000
2	2	-1	58.914	52.730	52.730	.089	6.194	12.7826	1.0000
2	2	0	34.856	34.497	34.402	2.552	.359	1.3164	1.0000
2	2	1	56.629	59.323	59.246	3.024	-2.694	-6.4957	1.0000
2	2	2	27.935	27.292	27.289	-4.420	.642	2.4784	1.0000
2	2	3	35.468	38.203	38.061	3.298	-2.735	-9.0984	1.0000
2	2	4	26.898	28.529	28.516	.965	-1.631	-4.7194	1.0000
2	2	5	25.384	25.211	25.200	.727	.174	.4414	1.0000
2	2	6	33.450	31.298	31.169	2.844	2.151	5.3211	1.0000
2	2	7	14.534	14.332	14.329	.259	.202	.3020	1.0000
2	2	8	8.508	9.102	-9.011	-1.242	-5.94	-5.713	1.0000
2	2	-7	31.449	31.543	31.506	1.512	-0.094	-0.2187	1.0000
2	2	-6	14.631	15.040	15.040	-0.28	-0.409	-0.7589	1.0000
2	2	-5	43.979	43.148	-43.130	-1.246	.831	2.4293	1.0000
2	2	-4	28.297	28.008	27.936	2.008	.289	.8805	1.0000
2	2	-3	23.937	22.678	=22.585	-2.048	1.259	4.1400	1.0000
2	2	-2	3.777	4.233	-4.225	.275	-0.457	-0.4375	1.0000
2	2	-1	43.070	38.599	38.578	1.262	4.471	13.6197	1.0000
2	2	0	27.876	24.757	-24.662	-2.164	3.119	12.1983	1.0000
2	2	1	73.700	66.946	66.909	2.218	6.754	11.7741	1.0000
2	2	2	25.830	24.986	24.983	-0.378	.844	2.8750	1.0000
2	2	3	26.231	27.676	-27.660	-0.941	-1.445	-4.4478	1.0000
2	2	4	6.562	5.030	4.751	1.652	1.532	1.6860	1.0000
2	2	5	24.002	23.550	-23.486	-1.731	.452	1.0912	1.0000
2	2	6	5.930	6.863	-6.856	.297	-0.933	-0.7237	1.0000
2	2	7	4.420	1.889	1.851	.378	2.531	1.3268	1.0000
2	2	8	3.217	.758	.637	.411	2.460	1.0704	1.0000
2	2	-7	55.817	57.282	57.172	3.551	-1.465	-3.4467	1.0000
2	2	-6	21.124	20.575	20.575	.286	.548	1.2800	1.0000
2	2	-5	21.096	19.004	18.878	2.193	2.092	5.2180	1.0000
2	2	-4	71.201	68.426	68.354	3.145	2.775	4.8676	1.0000
2	2	-3	2.574	3.171	-3.117	-0.590	-0.596	-0.3243	1.0000
2	2	-2	57.981	53.296	53.173	3.617	4.685	10.2710	1.0000
2	2	-1	33.664	28.300	28.278	1.130	5.364	19.1625	1.0000
2	2	0	3.746	3.797	3.749	.606	-0.051	-0.0419	1.0000
2	2	1	65.082	62.316	62.188	3.928	2.766	5.6366	1.0000
2	2	2	11.680	12.420	12.419	.130	-0.740	-1.3222	1.0000
2	2	3	27.230	28.271	28.169	2.397	-1.041	-2.6904	1.0000
2	2	4	22.620	22.677	22.556	2.341	-0.057	-0.1248	1.0000
2	2	5	4.592	2.565	2.565	.005	2.027	1.1616	1.0000
2	2	6	19.586	20.666	-20.620	-1.381	-1.080	-1.8827	1.0000
2	2	7	20.063	20.212	-20.212	.088	-1.149	-0.2797	1.0000
2	2	8	15.429	16.811	16.764	1.258	-1.382	-2.4307	1.0000
2	2	-3	18.850	19.857	-19.764	-1.924	-1.007	-2.1754	1.0000
2	2	-4	35.623	35.205	35.143	2.098	.418	1.2345	1.0000
2	2	-2	41.211	39.446	39.446	-0.183	1.764	5.5503	1.0000
2	2	-1	23.176	21.355	-21.319	-1.235	1.822	5.1186	1.0000
2	2	0	4.340	3.543	2.863	2.087	.798	.6557	1.0000
2	2	1	29.009	27.429	-27.341	-2.195	1.581	4.5287	1.0000
2	2	2	28.819	25.982	-25.980	.298	2.837	7.8948	1.0000
2	2	3	8.152	9.901	-9.870	.786	-1.749	-2.1819	1.0000

H	K	L	F(DRS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
2	5	4	14.420	17.267	-17.178	-1.752	-2.847	-4.9627	1.0000
2	5	5	19.524	21.260	21.198	1.614	-1.736	-3.2834	1.0000
2	5	6	13.398	15.691	15.687	-.370	-1.793	-2.4706	1.0000
2	6	6	6.116	2.368	-2.347	-.318	2.748	2.6980	1.0000
2	6	6	18.214	16.986	16.711	3.044	1.228	2.2778	1.0000
2	6	6	6.819	7.707	7.598	1.292	-.899	-.8196	1.0000
2	6	6	14.233	14.197	-14.187	.509	.037	.0670	1.0000
2	6	6	57.594	54.950	54.929	4.294	2.644	5.9778	1.0000
2	6	6	42.257	41.005	41.004	.258	2.252	6.5161	1.0000
2	6	6	31.701	29.921	29.805	2.639	1.780	4.8592	1.0000
2	6	6	58.426	51.950	51.856	3.122	6.477	14.6429	1.0000
2	6	6	26.863	25.233	25.231	-.255	1.631	4.0337	1.0000
2	6	6	33.045	32.347	32.173	3.352	.698	1.7425	1.0000
2	6	6	8.121	8.213	8.160	.933	-.092	-.0996	1.0000
2	6	6	3.338	1.304	-1.056	.764	2.035	.8533	1.0000
2	6	6	16.207	18.570	18.464	1.985	-2.364	-3.9315	1.0000
2	7	7	30.426	32.929	-32.867	-2.021	-2.503	-5.7940	1.0000
2	7	7	24.787	24.315	-24.314	.217	.472	1.0502	1.0000
2	7	7	23.086	22.548	-22.514	1.231	.538	1.1395	1.0000
2	7	7	11.310	13.481	-13.315	-2.108	-2.171	-3.1724	1.0000
2	7	7	32.786	32.031	31.960	2.126	.756	1.8377	1.0000
2	7	7	19.773	18.170	18.165	-.383	1.603	3.1346	1.0000
2	7	7	3.663	2.091	-1.880	-.915	1.572	.7698	1.0000
2	7	7	12.433	13.785	13.694	1.583	-1.352	-1.7702	1.0000
2	8	8	5.284	1.653	-1.613	-.361	3.630	2.4777	1.0000
2	8	8	27.434	27.519	27.271	3.686	-.086	-.1819	1.0000
2	8	8	22.814	21.977	21.938	1.313	.837	1.6695	1.0000
2	8	8	4.945	7.251	7.207	.798	-2.306	-1.4111	1.0000
2	8	8	49.087	45.647	45.644	4.079	2.441	5.6960	1.0000
2	8	8	50.914	51.768	51.682	2.980	-.854	-2.0260	1.0000
3	3	3	15.197	16.572	16.391	.854	-1.185	-2.0903	1.0000
3	3	3	4.371	4.475	4.391	.865	-.104	-.0760	1.0000
3	3	3	57.207	57.964	57.854	3.577	-.758	-1.5124	1.0000
3	3	3	35.689	36.612	-36.604	-.779	-.923	-2.9367	1.0000
3	3	3	77.532	78.100	78.055	2.653	-.568	-.7406	1.0000
3	3	3	4.465	2.567	.797	2.440	1.898	2.4515	1.0000
3	3	3	26.901	27.800	-27.794	-.583	-.898	-3.8803	1.0000
3	3	3	162.158	174.234	174.175	4.538	-12.076	-19.6331	1.0000
3	3	3	46.691	48.915	48.908	.806	-2.224	-5.3626	1.0000
3	3	3	30.609	31.240	31.219	1.150	-.631	-2.2825	1.0000
3	3	3	99.692	103.267	103.199	3.752	-3.575	-4.0408	1.0000
3	3	3	30.820	30.942	-30.935	-.664	-.122	-.3667	1.0000
3	3	3	40.022	39.481	39.417	2.253	.541	1.5506	1.0000
3	3	3	19.427	18.308	18.234	1.648	1.119	2.2031	1.0000
3	3	3	17.326	16.195	-16.195	-.139	1.131	1.8383	1.0000
3	3	3	17.720	18.729	-18.718	-.650	-1.009	-1.7598	1.0000
3	3	3	41.660	41.971	41.934	1.778	-.311	-.5267	1.0000
3	3	3	18.822	19.444	-19.368	-1.714	-.622	-1.4052	1.0000
3	3	3	38.792	38.019	38.002	1.157	.773	2.4044	1.0000
3	3	3	37.462	37.433	37.421	.956	.028	.0946	1.0000
3	3	3	16.079	17.274	-17.122	-2.286	-1.195	-3.7590	1.0000
3	3	3	41.778	43.762	43.701	2.296	-1.984	-5.9809	1.0000
3	3	3	56.014	57.386	-57.367	-1.443	-1.371	-2.8964	1.0000

H	K	L	F(OBS)	F(CALC)	A(CALC)	R(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	1	0	60.641	61.778	-61.769	-1.004	-1.136	-2.3999	1.0000
3	1	1	36.985	40.774	40.710	2.279	-3.796	-12.1851	1.0000
3	1	1	38.018	40.820	-40.759	-2.232	-2.302	-8.0289	1.0000
3	1	3	29.963	31.019	30.991	1.318	-1.055	-3.5938	1.0000
3	1	4	35.285	34.243	34.235	.763	1.041	3.2405	1.0000
3	1	5	26.507	25.123	-25.068	-1.567	1.384	3.4834	1.0000
3	1	6	26.200	23.739	23.687	1.569	2.461	5.5217	1.0000
3	1	7	16.970	14.900	-14.872	-.916	2.070	3.4422	1.0000
3	2	-3	12.433	11.336	-11.332	-.313	1.097	1.4692	1.0000
3	2	-7	28.891	29.229	29.158	2.025	-.347	-.8170	1.0000
3	2	-6	36.339	35.844	35.777	2.187	.495	1.3899	1.0000
3	2	-5	7.955	6.850	6.842	-.317	1.105	1.5374	1.0000
3	2	-4	104.233	104.632	104.548	4.175	-.399	-.4354	1.0000
3	2	-3	20.236	20.012	19.993	.873	.224	.7366	1.0000
3	2	-2	37.075	34.932	34.915	1.086	2.143	7.3813	1.0000
3	2	-1	9.233	13.773	13.158	4.071	-4.540	-10.9489	1.0000
3	2	0	41.249	40.823	-40.813	-.915	.426	1.3549	1.0000
3	2	1	28.277	30.329	30.207	2.712	-2.052	-8.0250	1.0000
3	2	2	31.172	34.009	33.933	2.261	-2.836	-10.3897	1.0000
3	2	3	21.583	22.600	-22.595	-.436	-1.016	-2.9410	1.0000
3	2	4	87.854	88.118	88.037	3.791	-.264	-.3593	1.0000
3	2	5	22.910	23.088	23.077	.713	-.178	-.4149	1.0000
3	2	6	14.914	13.231	13.189	1.047	1.683	2.7836	1.0000
3	2	7	33.754	30.751	30.644	2.570	3.003	6.4364	1.0000
3	3	-8	9.973	9.693	9.670	.669	.290	.3138	1.0000
3	3	-7	33.177	33.427	-33.383	-1.712	-.250	-.5932	1.0000
3	3	-6	23.346	24.166	24.102	1.756	-.820	-1.8838	1.0000
3	3	-5	45.088	45.346	-45.332	-1.145	-.258	-.6733	1.0000
3	3	-4	26.960	26.985	-26.969	-.919	-.025	-.0728	1.0000
3	3	-3	61.433	59.260	59.213	2.351	-2.173	4.6919	1.0000
3	3	-2	17.609	18.646	-18.509	-2.251	-1.036	-3.0913	1.0000
3	3	-1	40.267	37.657	37.631	1.418	2.610	8.4874	1.0000
3	3	0	10.501	10.470	10.428	.937	.031	.0715	1.0000
3	3	1	58.171	56.230	-56.182	-2.321	1.941	4.4221	1.0000
3	3	2	42.396	43.232	43.176	2.199	-.836	-2.5739	1.0000
3	3	3	41.491	42.977	-42.955	-1.381	-1.486	-4.3893	1.0000
3	3	4	38.077	40.383	-40.375	-.833	-2.307	-6.6754	1.0000
3	3	5	37.683	36.625	36.589	1.639	1.057	2.8069	1.0000
3	3	6	9.043	9.136	-8.998	-1.580	-.093	-.0999	1.0000
3	3	7	9.686	9.807	9.767	.885	-.121	-.1409	1.0000
3	3	8	6.282	6.996	6.936	.918	-.714	-.6152	1.0000
3	3	9	48.699	48.691	48.558	3.600	.008	.0216	1.0000
3	3	10	45.827	44.775	-44.769	-.747	1.052	2.9563	1.0000
3	3	11	47.275	45.513	45.435	2.666	1.762	4.7660	1.0000
3	3	12	47.417	42.981	42.906	2.532	4.436	12.5859	1.0000
3	3	13	19.783	17.181	17.175	-.457	2.602	7.3100	1.0000
3	3	14	125.879	117.544	117.455	4.554	8.335	9.0680	1.0000
3	3	15	26.072	24.691	24.676	.847	1.381	4.2079	1.0000
3	3	16	21.314	20.743	20.708	1.196	.571	1.5297	1.0000
3	3	17	74.291	78.207	78.117	3.768	-3.917	-7.72192	1.0000
3	3	18	34.262	36.348	-36.343	-.628	-2.086	-5.5393	1.0000
3	3	19	16.217	18.862	18.728	2.243	-2.645	-4.6388	1.0000
3	3	20	20.557	19.335	19.261	1.689	1.222	2.2383	1.0000

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	F(FBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT	FACTOR	
4	5	-7	30.357	30.953	30.901	1.786	-.596	-1.2492	1.0000
3	5	-6	15.650	15.100	-15.010	-1.644	.550	.9537	1.0000
3	5	-5	31.369	32.782	32.761	1.185	-1.413	-3.4649	1.0000
3	5	-4	24.426	24.442	24.423	.983	-.181	-.4365	1.0000
3	5	-3	12.212	12.767	-12.572	-2.220	-.556	-.9862	1.0000
3	5	-2	33.170	32.358	32.279	2.267	.811	2.3715	1.0000
3	5	-1	43.364	39.612	-39.586	-1.437	3.752	11.3095	1.0000
3	5	0	36.273	34.913	-34.899	-1.006	1.360	4.1857	1.0000
3	5	1	28.674	25.989	25.893	2.210	2.686	7.4754	1.0000
3	5	2	32.137	31.780	-31.701	-2.236	.357	.9836	1.0000
3	5	3	22.606	22.952	22.917	1.257	-.346	-.8065	1.0000
3	5	4	21.521	23.867	23.857	.706	-2.346	-5.0296	1.0000
3	5	5	18.563	20.112	-20.040	-1.695	-1.549	-2.8010	1.0000
3	6	-6	28.933	25.496	28.407	2.255	.437	.9162	1.0000
3	6	-5	3.193	1.398	-1.382	-.207	1.795	.7871	1.0000
3	6	-4	59.632	61.011	60.867	4.189	-1.379	-2.8305	1.0000
3	6	-3	9.969	9.919	9.871	.976	.050	.0687	1.0000
3	6	-2	41.518	43.024	43.006	1.245	-1.595	-4.1888	1.0000
3	6	-1	59.632	58.405	58.254	4.201	1.227	2.7744	1.0000
3	6	0	23.138	21.154	-21.141	-.764	1.984	4.7060	1.0000
3	6	1	15.809	14.952	14.695	2.761	.857	1.6529	1.0000
3	6	2	30.747	28.673	28.575	2.350	2.075	5.1762	1.0000
3	6	3	14.410	15.242	-15.239	-.311	-.832	-1.4340	1.0000
3	6	4	46.785	51.045	50.903	3.796	-.426	-10.4477	1.0000
3	7	-4	14.738	18.988	-18.968	-1.877	-4.250	-6.6481	1.0000
3	7	-3	20.443	21.787	21.668	2.266	-1.344	-2.6273	1.0000
3	7	-2	35.509	35.297	35.226	-2.243	.212	.5164	1.0000
3	7	-1	38.315	37.228	37.201	1.418	1.087	2.7592	1.0000
3	7	0	27.845	28.426	28.410	.952	-.581	-1.3450	1.0000
3	7	1	35.668	33.372	-33.293	-2.286	2.296	5.6315	1.0000
3	7	2	34.106	31.609	31.539	2.114	2.497	5.8273	1.0000
3	7	3	26.117	25.410	-25.372	-1.389	.707	1.4615	1.0000
3	8	-2	30.906	31.793	31.681	2.664	-.887	-1.8864	1.0000
3	8	-1	8.442	11.070	11.068	-.234	-2.628	-2.5186	1.0000
3	8	0	66.267	70.225	70.073	4.623	-3.958	-8.4223	1.0000
3	8	1	20.533	19.325	19.297	1.035	1.208	2.2415	1.0000
4	0	-8	19.102	17.697	17.695	.285	1.405	2.5579	1.0000
4	0	-7	35.112	35.526	35.417	2.786	-.414	-1.0608	1.0000
4	0	-6	15.287	15.575	-15.571	.348	-.298	-.5741	1.0000
4	0	-5	16.137	16.383	16.344	1.130	-.246	-.5788	1.0000
4	0	-4	28.767	29.355	29.181	3.186	-.587	-1.9762	1.0000
4	0	-3	2.336	1.504	1.475	-.293	.832	.4986	1.0000
4	0	-2	56.263	59.374	59.281	3.329	-3.111	-7.0335	1.0000
4	0	-1	35.672	36.792	36.730	2.139	-1.121	-3.5249	1.0000
4	0	0	21.127	19.801	-19.801	.110	1.326	5.0487	1.0000
4	0	1	122.848	129.849	129.790	3.917	-7.001	-9.0450	1.0000
4	0	2	30.523	30.111	-30.111	-.028	.412	1.4722	1.0000
4	0	3	15.571	15.151	15.090	1.359	.419	.9947	1.0000
4	0	4	26.152	26.265	26.132	2.645	-.114	-.3050	1.0000
4	0	5	13.404	13.261	13.261	-.228	.143	.2474	1.0000
4	0	6	35.126	33.112	33.016	2.513	2.014	4.7387	1.0000
4	0	7	18.245	14.886	14.836	1.220	3.359	5.4920	1.0000
4	0	-8	8.086	6.935	-6.915	-.529	1.150	1.1520	1.0000

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H	K	L	F(DBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
4	1	-7	11.058	12.645	12.645	-.135	-1.598	-2.2203	1.0000
4	1	-6	2.896 *	3.552	-3.273	1.378	-1.656	-.3169	1.0000
4	1	-5	6.707	5.295	-4.949	-1.885	1.412	1.7312	1.0000
4	1	-4	2.561 *	3.890	3.762	.989	-1.330	-.7273	1.0000
4	1	-3	10.163	10.994	-10.994	.063	-.832	-1.8373	1.0000
4	1	-2	5.176	7.230	-7.011	-1.764	-2.053	-2.7507	1.0000
4	1	-1	31.629	32.487	32.405	2.309	-.858	-3.4974	1.0000
4	1	0	49.929	49.926	-49.908	-1.321	.003	.0089	1.0000
4	1	1	19.700	21.103	21.102	.121	-1.403	-4.7203	1.0000
4	1	2	27.727	27.851	27.803	1.635	-.123	-.4247	1.0000
4	1	3	23.829	23.845	-23.758	-2.029	-.015	-.0447	1.0000
4	1	4	22.240	22.198	22.167	1.174	-.045	.1045	1.0000
4	1	5	15.958	16.053	-16.051	-.264	-.095	-.1797	1.0000
4	1	6	3.259 *	4.339	4.206	-1.058	-1.081	-.4646	1.0000
4	2	-8	24.921	23.760	23.637	2.410	1.162	2.3674	1.0000
4	2	-7	18.190	19.638	19.637	.122	-1.448	-2.7202	1.0000
4	2	-6	50.693	51.686	51.617	2.686	-.994	-2.5004	1.0000
4	2	-5	19.589	18.404	18.289	2.053	1.185	2.9072	1.0000
4	2	-4	41.968	41.659	41.655	.187	.308	.9495	1.0000
4	2	-3	37.538	37.437	37.254	3.697	.101	.3564	1.0000
4	2	-2	2.346 *	1.957	-1.951	.154	.390	.2325	1.0000
4	2	-1	11.355	10.368	10.280	1.346	.987	2.5058	1.0000
4	2	0	79.768	78.824	-8.752	3.362	.944	1.6558	1.0000
4	2	1	21.487	21.013	21.09	-.387	.474	1.5711	1.0000
4	2	2	85.190	91.228	91.167	3.344	-6.1039	-9.2466	1.0000
4	2	3	29.044	29.542	29.487	1.797	-.498	-1.4564	1.0000
4	2	4	26.929	27.564	27.561	.373	-.635	-1.6696	1.0000
4	2	5	26.677	23.793	23.601	3.020	2.884	6.8969	1.0000
4	2	6	5.249 *	7.341	-7.340	.055	-2.092	-1.3421	1.0000
4	3	-8	3.673 *	.667	.378	.550	3.006	1.3201	1.0000
4	3	-7	3.234 *	2.802	-2.795	.196	.433	.1874	1.0000
4	3	-6	15.419	17.428	17.380	-1.302	-2.010	-3.7521	1.0000
4	3	-5	13.535	12.883	12.740	1.915	.652	1.2016	1.0000
4	3	-4	10.221	10.128	-10.081	-.976	.093	1.585	1.0000
4	3	-3	24.292	23.799	23.799	-.030	.493	1.4716	1.0000
4	3	-2	22.326	22.695	22.626	1.776	-.369	-1.1366	1.0000
4	3	-1	77.691	70.542	-70.503	-2.366	7.149	11.4928	1.0000
4	3	0	5.328	3.293	3.051	1.238	2.036	2.4961	1.0000
4	3	1	21.518	21.771	-21.770	-.156	-.253	-.7550	1.0000
4	3	2	10.090	11.007	-10.884	-1.640	-.917	-1.6272	1.0000
4	3	3	33.515	34.862	34.805	2.001	-1.347	-3.8976	1.0000
4	3	4	19.099	19.953	-19.916	-1.217	-.855	-1.8457	1.0000
4	3	5	19.202	19.737	19.736	.223	-.535	-1.0460	1.0000
4	3	6	8.162	5.645	5.549	1.033	2.517	2.4202	1.0000
4	4	-7	15.260	16.062	15.823	2.763	-.803	-1.2291	1.0000
4	4	-6	8.822	8.602	-8.592	.408	.220	.2545	1.0000
4	4	-5	24.306	23.558	23.527	1.198	.748	1.8050	1.0000
4	4	-4	22.496	21.484	21.244	3.203	1.012	2.4815	1.0000
4	4	-3	11.307	11.860	11.858	-.208	-.553	-.9589	1.0000
4	4	-2	77.131	73.403	73.323	3.405	3.729	6.5397	1.0000
4	4	-1	56.605	53.931	53.885	2.221	2.674	6.5590	1.0000
4	4	0	12.782	11.960	-11.958	.174	.823	1.6882	1.0000
4	4	1	59.639	60.169	60.044	3.873	-.530	-1.2463	1.0000

H	X	L	F(DBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
4	4	2	33.992	35.544	-35.544	.002	-1.552	-4.5356		1.0000
4	4	3	19.576	20.830	20.782	1.418	-1.255	-2.8368		1.0000
4	4	4	17.941	18.410	18.217	2.660	-.469	-.9226		1.0000
4	4	5	7.772	8.239	8.237	-.182	-.468	-.4438		1.0000
4	4	6	35.658	36.732	36.643	2.559	-.874	-1.8742		1.0000
4	5	-6	3.321	2.032	1.474	1.398	1.289	-.5436		1.0000
4	5	-5	7.060	6.250	-5.976	-1.829	.810	.7892		1.0000
4	5	-4	2.975	1.021	-.287	.980	1.954	.7892		1.0000
4	5	-3	12.616	12.551	-12.551	.058	.065	.9194		1.0000
4	5	-2	7.924	9.779	-9.624	-1.738	.065	.1097		1.0000
4	5	-1	20.246	18.202	18.063	2.249	-1.856	-2.2660		1.0000
4	5	0	28.695	27.140	-27.109	-1.311	2.044	4.9285		1.0000
4	5	1	18.891	18.915	18.915	.103	1.554	4.2843		1.0000
4	5	2	19.965	20.236	20.175	1.571	-.034	-.0757		1.0000
4	5	3	16.531	16.959	-16.836	-2.037	-.270	-.5918		1.0000
4	5	4	14.168	15.019	14.979	1.097	-.428	-.8086		1.0000
4	5	5	13.183	13.600	-13.597	-.323	-.852	-1.3394		1.0000
4	5	6	24.955	26.713	26.625	2.162	-.417	-.6041		1.0000
4	6	-4	32.282	33.403	33.401	.325	-1.757	-3.5808		1.0000
4	6	-3	26.628	27.624	27.370	3.739	-1.121	-2.6597		1.0000
4	6	-2	10.291	9.220	9.220	.301	-.995	-2.4006		1.0000
4	6	-1	27.862	25.816	25.773	1.483	1.065	1.5111		1.0000
4	6	0	29.790	30.101	29.912	3.371	2.046	5.0182		1.0000
4	6	1	10.166	11.628	-11.623	-.310	-.311	-.7757		1.0000
4	6	2	54.145	56.144	56.042	3.398	-1.461	-1.9761		1.0000
4	6	3	24.227	25.991	25.922	1.890	-1.999	-5.1200		1.0000
4	6	4	22.938	25.503	25.498	.496	-1.764	-3.6999		1.0000
4	6	5	4.893	3.932	-3.824	-.917	-2.565	-4.9816		1.0000
4	7	-4	11.165	12.195	12.195	-.018	.961	.5794		1.0000
4	7	-3	13.815	14.505	14.402	1.725	-1.030	-1.3127		1.0000
4	7	-2	28.477	28.134	-28.041	-2.281	-.690	-1.0567		1.0000
4	7	-1	22.596	22.589	22.556	1.232	.343	.7700		1.0000
4	7	0	14.434	15.970	-15.968	-.198	.007	.0134		1.0000
4	7	1	23.232	23.357	-23.297	-1.682	-1.536	-2.3766		1.0000
4	7	2	19.911	20.979	20.923	1.523	-.126	-.2477		1.0000
5	0	-7	4.230	4.523	-4.522	-.078	-1.068	-1.8878		1.0000
5	0	-6	31.407	30.570	30.395	3.268	-.294	-.1720		1.0000
5	0	-5	15.545	16.314	16.303	.610	.837	2.4224		1.0000
5	0	-4	21.303	21.691	21.638	1.514	-.768	-1.6700		1.0000
5	0	-3	128.474	130.119	130.069	3.635	-.388	-1.1107		1.0000
5	0	-2	3.252	.847	.721	-.444	-1.646	-1.8974		1.0000
5	0	-1	60.873	61.552	61.480	2.972	2.405	1.9494		1.0000
5	0	0	49.967	51.690	51.664	1.659	-.679	-1.4349		1.0000
5	0	1	6.666	5.624	5.624	-.050	-1.723	-4.0211		1.0000
5	0	2	20.754	23.140	22.887	3.412	1.042	1.5381		1.0000
5	0	3	10.387	9.206	9.199	.355	-2.386	-6.7025		1.0000
5	0	4	3.024	4.016	3.701	1.561	1.181	1.9536		1.0000
5	0	5	39.614	35.803	35.717	2.472	-.993	-.4597		1.0000
5	0	6	13.584	12.248	12.248	.076	3.812	9.6758		1.0000
5	1	-8	5.729	5.517	5.341	1.381	1.336	1.8854		1.0000
5	1	-7	5.125	7.144	-7.074	-.001	.212	.1438		1.0000
5	1	-6	17.336	17.071	-17.063	-.538	-2.019	-1.3686		1.0000
5	1	-5	17.509	18.147	18.087	1.473	.265	.5557		1.0000

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	PHI(TA)	DELTA/SIGMA	EXT. FACTOR
5	1	-4	47.400	46.357	-46.311	-2.059	1.043	2.7444	1.0000
5	1	-3	27.555	27.874	27.836	1.450	-0.319	-1.0614	1.0000
5	1	-2	24.679	24.519	24.515	.478	.160	.5590	1.0000
5	1	-1	33.111	33.746	-33.711	-1.522	-1.635	-2.3246	1.0000
5	1	0	16.531	18.640	18.517	2.136	-2.102	-6.2260	1.0000
5	1	1	15.470	17.645	-17.583	-1.476	-2.175	-5.7744	1.0000
5	1	2	17.896	17.351	-17.348	-.288	.545	1.4221	1.0000
5	1	3	3.960	5.436	5.328	1.077	-1.0546	-1.0546	1.0000
5	1	4	17.589	17.200	-17.118	-1.679	.389	.8033	1.0000
5	1	5	4.700	3.657	3.500	1.061	1.042	.6764	1.0000
5	1	6	9.036	9.865	9.865	.078	-.829	-.8505	1.0000
5	1	7	16.518	17.508	17.477	1.138	-.991	-1.5581	1.0000
5	2	-8	48.198	46.251	46.158	2.930	1.947	5.0318	1.0000
5	2	-6	5.681	4.272	4.264	-.265	1.409	1.2278	1.0000
5	2	-5	4.820	2.893	1.465	2.495	1.927	1.2278	1.0000
5	2	-4	26.124	25.087	25.025	1.758	1.037	1.5979	1.0000
5	2	-3	31.933	32.015	-32.014	-.211	-.082	3.0002	1.0000
5	2	-2	43.972	44.194	44.028	3.828	-.222	-.6764	1.0000
5	2	-1	26.162	26.005	26.001	.479	.157	.5207	1.0000
5	2	0	38.820	39.946	39.908	1.760	-1.127	-3.7482	1.0000
5	2	1	67.020	70.340	70.259	3.375	-3.320	-6.1197	1.0000
5	2	2	46.028	47.485	47.485	-.186	-1.457	-3.6355	1.0000
5	2	3	7.640	7.764	7.309	2.620	-.124	-.1511	1.0000
5	2	4	22.717	21.963	21.926	1.272	.754	1.7312	1.0000
5	2	5	3.929	.789	.763	.201	3.139	1.7272	1.0000
5	2	6	15.927	13.989	13.788	2.366	1.938	2.9356	1.0000
5	3	-7	18.301	18.244	18.213	1.062	.056	.1011	1.0000
5	3	-6	32.658	34.107	34.102	.610	-1.449	-3.6141	1.0000
5	3	-5	23.028	22.590	-22.543	-1.457	.438	1.0472	1.0000
5	3	-4	20.830	20.299	20.198	2.020	.531	1.3130	1.0000
5	3	-3	39.307	38.896	-38.868	-1.464	.411	1.3218	1.0000
5	3	-2	23.131	22.519	-22.514	-.486	.612	1.7709	1.0000
5	3	-1	21.625	20.960	20.907	1.487	.665	1.9061	1.0000
5	3	0	36.608	36.360	-36.294	-2.180	.248	.8258	1.0000
5	3	1	29.942	30.487	30.452	1.444	-.545	-1.6426	1.0000
5	3	2	47.116	47.744	47.743	.309	-.628	-1.7138	1.0000
5	3	3	2.982	4.647	4.516	1.096	-1.665	-.7821	1.0000
5	3	4	7.281	8.430	8.277	1.600	-1.150	-1.1838	1.0000
5	3	5	11.137	10.470	-10.409	-1.129	.667	.8778	1.0000
5	4	-7	8.763	9.862	-9.862	-.046	-1.099	-1.0890	1.0000
5	4	-6	36.636	37.199	37.051	3.316	-.564	-1.3710	1.0000
5	4	-5	34.732	35.694	35.687	.714	-.963	-2.4874	1.0000
5	4	-4	25.664	25.130	25.081	1.574	.534	1.3442	1.0000
5	4	-3	89.488	87.581	87.505	3.635	1.908	3.0670	1.0000
5	4	-2	3.169	1.979	-1.942	-.382	1.189	.6531	1.0000
5	4	-1	48.025	45.992	45.895	2.998	2.033	5.3475	1.0000
5	4	0	21.431	20.332	20.263	1.666	1.100	2.7912	1.0000
5	4	1	18.439	19.402	-19.401	-.037	-.963	-2.2112	1.0000
5	4	2	21.113	21.947	21.676	3.433	-.833	-1.9135	1.0000
5	4	3	26.231	26.852	26.848	.454	-.620	-1.4718	1.0000
5	4	4	18.017	18.806	18.734	1.637	-.789	-1.4914	1.0000
5	4	5	33.723	33.593	33.500	2.503	.130	.2863	1.0000
5	5	-6	16.341	16.854	-16.847	-.514	-.513	-.8583	1.0000

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H	K	L	F(I)351	F(C)CALC)	A(C)CALC)	B(C)CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
5	5	5	15.049	16.624	16.558	1.477	-1.575	-2.5752	1.0000
5	5	5	27.655	28.195	-28.124	-1.999	-.340	-.8207	1.0000
5	5	5	13.677	13.442	13.369	1.416	.235	.4115	1.0000
5	5	5	25.471	24.170	24.165	.483	1.301	3.2181	1.0000
5	5	5	20.412	20.029	-19.972	-1.505	.393	.9015	1.0000
5	5	5	5.805	6.079	5.722	-2.054	-.274	-.2541	1.0000
5	5	5	7.322	7.530	-7.384	-1.474	-.208	-.2374	1.0000
5	5	5	16.922	16.120	-16.116	-.334	.802	1.5478	1.0000
5	5	5	3.155	1.092	.440	.999	2.063	.9158	1.0000
5	5	5	10.391	10.006	-9.861	-1.694	.385	.4682	1.0000
5	5	5	22.665	22.936	22.786	2.611	-.271	-.5187	1.0000
5	5	5	21.255	23.515	23.442	1.854	-2.260	-4.4497	1.0000
5	5	5	24.403	25.005	-25.004	-.101	-.602	-1.3706	1.0000
5	5	5	36.200	35.668	35.457	3.878	.532	1.3508	1.0000
5	5	5	22.617	20.788	20.779	.605	1.828	4.1016	1.0000
5	5	5	19.152	17.393	17.298	1.824	.759	1.4833	1.0000
5	5	5	34.072	34.641	34.475	3.392	-.570	-1.3968	1.0000
5	5	5	25.046	26.436	26.435	-.075	-1.390	-2.9791	1.0000
5	5	5	19.645	21.626	21.455	2.715	-1.991	-3.6288	1.0000
5	5	5	21.583	24.078	23.995	2.009	-2.495	-4.5414	1.0000
5	5	5	16.549	18.070	-18.016	-1.402	-1.522	-2.4877	1.0000
5	5	5	23.197	21.764	-21.758	-.506	1.433	2.8604	1.0000
5	5	5	19.543	20.227	20.175	1.446	-.696	-1.2916	1.0000
5	5	5	12.243	14.493	-14.337	-2.121	-2.250	-3.0425	1.0000
5	5	5	11.873	12.684	12.610	1.368	-.810	-1.0957	1.0000
5	5	5	17.585	17.143	17.141	.221	.442	.7401	1.0000
5	5	5	34.600	35.542	35.447	2.593	-.942	-2.0647	1.0000
5	5	5	15.792	16.047	15.990	1.357	-.255	-.4480	1.0000
5	5	5	2.996	.885	-.784	.412	2.110	.9851	1.0000
5	5	5	50.928	50.430	50.295	3.695	.497	1.1610	1.0000
5	5	5	18.401	18.413	-18.411	-.246	-.012	-.0306	1.0000
5	5	5	44.691	44.004	43.968	1.795	.686	1.8051	1.0000
5	5	5	62.946	64.602	64.537	2.885	-1.656	-3.0912	1.0000
5	5	5	26.013	26.031	-26.017	-.838	-.017	-.0558	1.0000
5	5	5	73.531	77.742	77.661	3.556	-4.212	-6.4151	1.0000
5	5	5	34.580	34.849	34.822	1.366	-.269	-.8664	1.0000
5	5	5	12.986	14.339	14.329	.4	-1.353	-2.5923	1.0000
5	5	5	56.844	56.677	56.568	3.512	.167	.3257	1.0000
5	5	5	14.931	14.404	-14.403	-.142	.528	.9483	1.0000
5	5	5	27.043	24.484	24.438	1.503	.528	.9483	1.0000
5	5	5	20.398	20.149	-20.117	-1.128	2.559	5.6523	1.0000
5	5	5	31.677	32.571	32.525	1.729	.249	.4562	1.0000
5	5	5	15.996	16.201	-16.138	-1.432	-.894	-2.1034	1.0000
5	5	5	23.304	23.442	23.438	.456	-.206	-.3866	1.0000
5	5	5	47.493	47.548	47.521	1.591	-.055	-.3415	1.0000
5	5	5	39.525	35.1286	-41.227	-2.200	-.055	-.1521	1.0000
5	5	5	36.335	35.306	35.257	1.855	-1.761	-5.3655	1.0000
5	5	5	11.493	12.316	-12.305	-.536	1.029	3.5458	1.0000
5	5	5	49.635	51.142	-51.117	-.536	-.823	-1.7140	1.0000
5	5	5	30.271	31.021	30.953	2.060	-1.507	-3.4612	1.0000
5	5	5	18.546	19.211	-19.132	-1.732	-.751	-2.3357	1.0000
5	5	5	18.954	19.286	19.279	.500	-.665	-1.5767	1.0000
5	5	5	31.262	29.681	29.657	1.177	-.332	-.7504	1.0000
5	5	5					1.582	3.9124	1.0000

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H	K	L	F(OBS)	F(CALC)	A(CALC)	9(CALC)	D(LTA F	D(LTA/SIGMA	EXT. FACTOR
6	1	5	19.873	19.562	-19.506	-1.448	1.310	2.4309	1.0000
6	2	-8	6.749	6.213	-6.218	.015	.531	.4211	1.0000
6	2	-7	21.233	21.742	21.694	1.449	-.504	-.9792	1.0000
6	2	-6	28.387	28.765	28.655	2.521	-.378	-.9117	1.0000
6	2	-5	15.937	15.922	-15.910	-.614	.015	.0303	1.0000
6	2	-4	64.570	63.023	62.928	3.443	1.348	3.2456	1.0000
6	2	-3	46.332	46.101	46.075	1.542	.231	.6556	1.0000
6	2	-2	29.051	28.287	28.283	.484	.764	2.3508	1.0000
6	2	-1	56.056	57.362	57.216	4.093	-1.306	-2.9765	1.0000
6	2	0	3.507	2.276	-2.260	-.269	1.232	.8589	1.0000
6	2	1	13.425	20.010	19.928	1.803	-1.585	-3.8861	1.0000
6	2	2	18.225	16.660	16.472	2.497	1.564	3.6214	1.0000
6	2	3	25.029	25.118	-25.110	-.638	-.089	-.2153	1.0000
6	2	4	36.345	34.870	34.756	2.820	1.475	3.6798	1.0000
6	2	5	15.688	14.483	14.445	1.044	1.205	1.9272	1.0000
6	2	-7	24.109	25.417	-25.362	-1.676	-1.308	-2.6276	1.0000
6	3	-6	24.213	24.045	24.000	1.471	.168	.3649	1.0000
6	3	-5	33.294	32.831	-32.827	-.465	.464	1.2088	1.0000
6	3	-4	67.414	67.719	-67.699	-1.629	-.305	-.6036	1.0000
6	3	-3	30.620	29.978	29.899	2.174	.641	1.6192	1.0000
6	3	-2	19.894	20.700	-20.619	-1.836	-.807	-2.0130	1.0000
6	3	-1	28.494	28.533	28.528	.547	-.039	-.1122	1.0000
6	3	0	49.760	49.588	49.563	1.580	.172	.4484	1.0000
6	3	1	23.888	24.917	-24.830	-2.078	-1.029	-2.6831	1.0000
6	3	2	33.495	35.220	35.178	1.720	-1.725	-4.7099	1.0000
6	3	3	17.216	18.002	-17.993	-.548	-.784	-1.5373	1.0000
6	3	4	44.127	43.699	-43.681	-1.268	.428	1.0861	1.0000
6	3	4	6.870	7.050	6.919	1.354	-.181	-.1401	1.0000
6	3	5	12.654	12.100	12.020	1.387	.554	.7391	1.0000
6	4	-7	7.243	8.412	8.398	.486	-1.169	-1.0882	1.0000
6	4	-6	62.538	62.844	62.731	3.763	-.305	-.6400	1.0000
6	4	-5	17.005	15.915	-15.914	-.190	1.090	2.1460	1.0000
6	4	-4	10.439	11.779	11.643	1.784	-1.339	-1.9477	1.0000
6	4	-3	39.635	38.440	38.332	2.886	1.195	3.4571	1.0000
6	4	-2	21.065	21.167	-21.153	-.771	-.102	-.2456	1.0000
6	4	-1	62.988	63.525	63.424	3.579	-.538	-1.1697	1.0000
6	4	0	24.828	25.987	25.949	1.405	-1.159	-2.8177	1.0000
6	4	1	15.612	16.462	16.452	.575	-.850	-1.5670	1.0000
6	4	2	63.268	65.748	65.650	3.574	-2.480	-5.0899	1.0000
6	4	3	7.326	2.835	-2.834	-.064	4.491	4.2331	1.0000
6	4	4	10.947	13.299	-13.226	-1.386	-2.352	-2.7890	1.0000
6	5	-6	16.943	18.246	18.240	.469	-1.303	-2.2189	1.0000
6	5	-5	32.620	32.198	32.160	1.558	.422	1.0261	1.0000
6	5	-4	26.355	25.864	-25.774	-2.153	.491	1.1848	1.0000
6	5	-3	26.983	26.385	26.323	1.816	.603	1.4654	1.0000
6	5	-2	11.915	10.788	-10.774	-.552	1.127	1.7719	1.0000
6	5	-1	33.629	34.115	-34.077	-1.605	-.485	-1.2425	1.0000
6	5	0	19.710	20.630	20.535	1.982	-.920	-1.9015	1.0000
6	5	1	14.935	16.205	-16.110	-1.751	-1.270	-2.1492	1.0000
6	5	2	14.676	14.647	14.641	.443	.028	.0446	1.0000
6	5	3	18.214	20.365	20.336	1.097	-2.151	-3.5167	1.0000
6	5	4	6.102	3.567	-3.536	-.468	2.535	1.8860	1.0000
6	6	-5	45.655	46.760	46.630	3.492	-1.105	-2.6438	1.0000

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H	K	L	F (GSS)	F (CALC)	A (CALC)	R (CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
4	1	1								
5	6	-3	12.032	11.929	11.824	1.577	.103	.1432		1.0000
6	6	-2	3.950	4.381	4.346	.557	-.421	-.2292		1.0000
6	6	-1	53.910	54.383	54.223	4.142	-.473	-1.2440		1.0000
6	6	0	3.172	1.145	-1.136	-1.145	2.027	.8942		1.0000
6	6	1	11.348	12.840	12.703	1.473	-1.492	-2.0370		1.0000
6	6	2	26.494	27.427	27.103	2.594	-.733	-1.5483		1.0000
6	6	-2	25.795	27.494	27.411	2.136	-1.709	-3.4107		1.0000
5	5	-2	25.149	27.506	-27.545	-1.238	-2.457	-4.8041		1.0000
5	5	-1	12.817	12.867	12.857	.489	-.050	-.0661		1.0000
6	7	0	31.283	34.087	34.053	1.518	-2.804	-6.0101		1.0000
7	7	-2	12.848	11.103	11.101	.264	1.745	2.3273		1.0000
7	7	-2	29.624	30.441	30.330	2.596	-.817	-1.7902		1.0000
7	7	-6	8.210	8.606	8.561	.878	-.395	-.4452		1.0000
7	7	-5	5.242	5.559	5.532	.547	-.317	-.2544		1.0000
7	7	-4	43.440	43.283	43.171	3.100	.157	.4328		1.0000
7	7	-3	6.590	7.724	7.722	-1.175	.866	1.2288		1.0000
7	7	-2	65.718	67.184	67.140	2.437	-1.467	-2.9069		1.0000
7	7	-1	5.442	8.824	8.477	2.451	-.383	-.5481		1.0000
7	7	0	8.929	11.341	-11.341	-.056	-2.412	-3.5979		1.0000
7	7	0	49.163	47.686	47.570	3.324	.478	1.1423		1.0000
7	7	0	10.736	10.343	-10.327	.579	.393	.6051		1.0000
7	7	0	2.999	1.699	-1.555	.686	1.300	.6068		1.0000
7	7	0	32.479	29.602	29.502	2.439	2.976	6.8229		1.0000
7	7	4	3.407	4.504	-4.473	-1.192	1.600	.6577		1.0000
7	7	-7	4.575	1.907	-1.797	-.524	.071	.0417		1.0000
7	7	-6	20.471	20.293	20.228	1.629	.177	.3719		1.0000
7	7	-5	11.410	10.636	-10.535	-1.460	.775	1.2052		1.0000
7	7	-4	2.889	.697	.507	.479	2.191	1.0822		1.0000
7	7	-3	17.139	15.344	-16.335	.556	.795	1.8117		1.0000
7	7	-2	7.792	8.359	-8.130	-1.944	-.567	-7.7740		1.0000
7	7	-1	12.720	13.538	13.430	1.705	-.818	-1.5885		1.0000
7	7	0	20.374	20.288	-20.275	-.723	.086	.2165		1.0000
7	7	1	10.771	11.463	11.454	-.447	-.692	-1.1182		1.0000
7	7	2	22.803	22.454	22.387	1.741	.349	.849		1.0000
7	7	3	13.604	12.386	-12.300	-1.465	1.218	2.0612		1.0000
7	7	4	13.563	11.364	11.345	.670	2.199	3.3666		1.0000
7	7	5	8.096	6.818	-6.815	.206	1.279	1.1784		1.0000
7	7	-7	11.925	11.389	11.388	.170	.536	.7282		1.0000
7	7	-6	30.398	31.247	31.182	2.020	-.849	-2.0302		1.0000
7	7	-5	30.087	30.033	29.932	2.452	.055	.1391		1.0000
7	7	-4	22.592	22.738	22.738	.054	-.146	-.3489		1.0000
7	7	-3	52.203	52.830	52.724	3.359	-.628	-1.5930		1.0000
7	7	-2	3.780	.837	.314	.775	2.944	2.0236		1.0000
7	7	-1	28.249	28.997	28.989	.694	-.748	-2.1224		1.0000
7	7	0	18.076	17.665	17.395	3.079	.411	.9821		1.0000
7	7	1	6.669	9.004	9.000	-.282	-.2.335	-2.3544		1.0000
7	7	2	46.425	45.914	45.856	2.300	.511	1.3214		1.0000
7	7	3	28.837	28.386	28.313	2.029	.451	1.0603		1.0000
7	7	4	9.133	8.986	8.985	.144	.147	.1606		1.0000
7	7	-7	4.603	3.209	-3.166	.523	1.394	.7744		1.0000
7	7	-6	16.991	17.242	-17.168	-1.597	-.252	-.4359		1.0000
7	7	-5	11.051	9.244	9.128	1.462	1.807	2.5631		1.0000
7	7	-4	16.262	14.723	-14.715	-.505	1.539	3.1136		1.0000

H	K	L	F(ORIS)	F(CALC)	A(CALC)	R(CALC)	D ⁺ TA F	DELTA/SIGMA	EXT. FACTOR
7	3	-3	20.671	19.396	19.376	-.547	1.295	3.0230	1.0000
7	3	-2	39.937	39.364	39.314	1.986	-.427	-1.2362	1.0000
7	3	-1	5.487	1.906	.881	-1.690	3.591	3.2388	1.0000
7	3	0	14.669	15.032	15.016	.683	-.363	-.7095	1.0000
7	3	1	19.866	20.023	-20.020	.383	-.157	-.3505	1.0000
7	3	2	24.570	29.078	-29.022	.383	-.508	-1.2554	1.0000
7	3	3	11.103	8.639	8.525	-1.796	-.508	-1.2554	1.0000
7	3	4	11.103	21.345	-21.332	1.399	2.464	3.4113	1.0000
7	4	-5	6.303	6.278	6.211	-.751	1.413	2.6011	1.0000
7	4	-4	9.669	7.080	7.054	.915	.025	.0189	1.0000
7	4	-3	26.922	26.520	26.339	.601	2.589	3.2295	1.0000
7	4	-2	9.430	9.059	-9.057	3.096	.302	.7050	1.0000
7	4	-1	43.505	47.239	47.175	-.153	.372	.4909	1.0000
7	4	0	28.007	27.291	27.174	2.453	1.266	3.5932	1.0000
7	4	1	16.711	17.094	17.094	2.524	.715	1.7857	1.0000
7	4	2	43.122	43.778	43.649	.062	-.383	-.7653	1.0000
7	4	3	8.701	7.493	-7.467	3.351	-.656	-1.7577	1.0000
7	4	4	3.328	4.834	4.777	.626	1.208	1.4323	1.0000
7	5	-5	22.537	22.643	22.510	.744	-1.507	-.6337	1.0000
7	5	-4	6.911	7.769	-7.638	2.447	-.106	-.6337	1.0000
7	5	-3	3.193	1.500	1.423	-1.421	-.858	-.7034	1.0000
7	5	-2	16.300	16.929	-16.921	.476	1.693	.7422	1.0000
7	5	-1	8.542	7.614	-7.366	.524	-.629	-1.1233	1.0000
7	5	0	10.004	9.175	9.026	-.927	.928	1.0744	1.0000
7	5	1	17.412	16.620	-16.603	1.648	.829	1.0904	1.0000
7	5	2	12.589	12.594	12.586	-.743	.792	1.4890	1.0000
7	5	3	17.986	18.024	17.947	-.465	-.038	-.0681	1.0000
7	5	4	11.417	10.195	-10.085	1.669	1.222	1.5116	1.0000
7	6	-4	14.548	15.166	15.165	.167	-.618	-.8982	1.0000
7	6	-3	21.989	23.332	23.089	3.358	-1.344	-2.5927	1.0000
7	6	-2	3.324	6.728	-6.674	.850	-3.403	-1.4336	1.0000
7	6	-1	29.676	30.654	30.643	.823	-.977	-2.1591	1.0000
7	6	0	23.294	25.817	25.623	3.155	-2.523	-5.0702	1.0000
7	6	1	9.689	8.668	8.667	-.160	1.021	1.1772	1.0000
7	6	2	10.526	11.241	-11.237	-.295	-.715	-.8518	1.0000
7	6	3	33.194	32.531	32.417	2.722	.663	1.5861	1.0000
7	6	4	20.077	21.109	21.086	.977	-1.032	-2.1330	1.0000
7	6	5	21.051	23.281	23.266	.846	-2.230	-5.0032	1.0000
7	6	6	71.295	72.966	72.893	3.486	-1.672	-2.9860	1.0000
7	6	7	24.037	23.733	23.733	.009	.304	.7773	1.0000
7	6	8	11.922	12.206	12.014	2.157	-.284	-.5043	1.0000
7	6	9	33.356	33.384	33.323	2.023	-.028	-.0768	1.0000
7	6	10	25.391	26.522	-26.520	-.329	-1.131	-2.7504	1.0000
7	6	11	35.067	34.520	34.416	.547	1.4015	1.4015	1.0000
7	6	12	11.476	12.152	12.136	.618	-.676	-.8970	1.0000
7	6	13	11.580	10.671	10.634	.889	.909	1.1433	1.0000
7	6	14	4.941	1.244	1.179	-.396	3.698	2.2623	1.0000
7	6	15	11.262	10.187	-10.147	-.910	1.074	1.4393	1.0000
7	6	16	3.863	2.487	2.029	1.438	1.376	.7717	1.0000
7	6	17	15.277	14.982	-14.884	-1.711	.295	.5687	1.0000
7	6	18	6.901	6.006	-5.977	.590	.895	.9488	1.0000
7	6	19	22.074	21.939	21.920	.903	.135	.3284	1.0000
7	6	20	14.638	12.647	-12.558	-1.494	1.991	4.0289	1.0000

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTDR
3	1	0	20.129	20.489	20.413	1.762	-.361	-.8287		1.0000
3	1	1	7.246	6.701	-6.668	-.661	.545	.5867		1.0000
3	1	2	16.307	15.795	-15.782	-.640	.511	.9608		1.0000
3	1	3	5.964	5.104	4.990	1.075	.860	.6763		1.0000
3	1	4	13.864	13.621	-13.555	-1.343	.243	.3342		1.0000
3	2	-7	50.696	50.415	50.327	2.981	.281	.6612		1.0000
3	2	-6	15.512	16.884	16.884	1.23	.281	.6612		1.0000
3	2	-5	14.220	13.335	13.195	1.923	.885	1.5239		1.0000
3	2	-4	13.950	11.662	11.466	2.126	2.288	3.9891		1.0000
3	2	-3	12.226	11.082	-11.075	-.411	1.143	1.9127		1.0000
3	2	-2	4.316	5.710	4.863	2.993	-1.394	-.9472		1.0000
3	2	-1	18.007	17.950	17.931	.830	.056	.1209		1.0000
3	2	0	2.892	.989	17.931	.906	1.903	.9211		1.0000
3	2	1	57.573	58.215	58.129	3.163	-.642	-.3865		1.0000
3	2	2	25.225	24.842	24.842	.111	.383	.8664		1.0000
3	2	3	22.993	21.561	21.472	1.957	1.432	2.8793		1.0000
3	2	4	17.070	16.173	16.102	1.506	.898	1.4276		1.0000
3	3	-6	17.153	17.881	17.856	.945	-.728	-1.2041		1.0000
3	3	-5	3.635	4.868	4.660	-1.405	-1.232	-.6257		1.0000
3	3	-4	16.182	16.663	16.575	1.708	-.480	-.8741		1.0000
3	3	-3	7.930	7.034	7.009	-.592	.897	1.0095		1.0000
3	3	-2	11.296	10.291	-10.252	-.894	1.005	1.5310		1.0000
3	3	-1	20.768	20.160	20.106	1.480	.608	1.3735		1.0000
3	3	0	36.850	37.153	-37.108	-1.831	-.303	-.8115		1.0000
3	3	1	10.339	12.182	-12.169	.571	-1.843	-2.4924		1.0000
3	3	2	13.463	13.387	13.374	.589	.075	.1173		1.0000
3	3	3	3.352	2.969	-2.753	-1.111	.383	.1598		1.0000
3	4	-6	17.495	18.990	18.795	2.711	-1.494	-.3894		1.0000
3	4	-5	22.150	21.798	21.774	1.030	.352	.6833		1.0000
3	4	-4	23.449	23.092	23.074	.901	.357	.7549		1.0000
3	4	-3	55.119	55.727	55.617	3.490	-.607	-1.4766		1.0000
3	4	-2	23.588	23.607	23.606	.076	-.019	-.0413		1.0000
3	4	-1	26.165	25.910	25.815	2.225	.255	.5809		1.0000
3	4	0	37.766	38.509	38.453	2.081	-.743	-1.8707		1.0000
3	4	1	23.577	23.685	-23.683	-.280	-.108	-.2255		1.0000
3	4	2	17.417	17.820	17.621	2.659	-.405	-.6886		1.0000
3	4	3	6.416	6.215	6.181	.645	.202	.1451		1.0000
3	5	-5	4.102	5.368	5.174	1.430	-1.266	-.5929		1.0000
3	5	-4	9.275	9.280	-9.127	-1.677	-.005	-.0053		1.0000
3	5	-3	4.872	6.673	-6.649	.563	-1.801	-1.1065		1.0000
3	5	-2	22.105	21.291	21.273	.885	.814	1.6133		1.0000
3	5	-1	10.882	8.449	-8.317	-1.490	2.432	3.3043		1.0000
3	5	0	11.645	9.935	9.791	1.682	1.710	2.3571		1.0000
3	5	1	6.058	3.946	-3.886	-.685	2.111	1.6423		1.0000
3	6	-3	8.739	9.490	-9.485	-.301	-.751	-.7339		1.0000
3	6	-2	10.408	11.336	10.917	3.053	-.928	-1.0529		1.0000
3	6	-1	30.056	31.556	31.540	.976	-1.499	-3.1670		1.0000
3	6	-7	21.984	20.826	20.759	1.675	1.158	2.1346		1.0000
3	6	-6	12.858	12.701	12.701	.111	.157	.2261		1.0000
3	6	-5	47.206	45.913	45.792	3.330	1.293	3.3422		1.0000
3	6	-4	6.096	6.397	-6.385	.396	-.302	-.2531		1.0000
3	6	-3	3.075	1.394	-.960	1.011	1.682	.8030		1.0000
3	6	-2	45.810	45.531	45.439	2.895	.279	.7202		1.0000

H	K	L	F(EFMS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
9	0	-1	39.811	40.046	-40.040	-0.735	-0.235	-0.6358	1.0000	
9	0	0	31.546	31.685	31.595	2.392	-0.120	-0.3937	1.0000	
9	0	1	32.679	31.336	31.293	1.630	1.343	3.2668	1.0000	
9	0	2	16.037	18.378	18.378	.120	-2.341	-3.7022	1.0000	
9	0	3	47.579	44.277	44.143	2.877	3.302	7.4982	1.0000	
9	1	-6	11.849	10.764	-10.719	-0.983	1.085	1.4600	1.0000	
9	1	-5	12.195	13.061	13.058	-0.237	-0.866	-1.2529	1.0000	
9	1	-4	43.820	43.133	43.097	1.768	-0.866	1.8073	1.0000	
9	1	-3	31.508	31.335	-31.285	-1.767	.172	.4338	1.0000	
9	1	-2	27.776	26.824	26.795	1.242	.952	2.3346	1.0000	
9	1	-1	2.989	.869	-.831	.253	2.120	.9927	1.0000	
9	1	0	41.415	41.656	-41.621	-1.703	-0.241	-6.406	1.0000	
9	1	1	15.142	13.901	13.812	1.566	1.242	2.1388	1.0000	
9	1	2	11.894	11.947	-11.895	-1.117	-0.053	-0.736	1.0000	
9	1	3	3.376	2.887	2.881	-0.185	.480	.2029	1.0000	
9	2	-6	25.509	24.229	24.090	2.595	1.270	.26075	1.0000	
9	2	-5	16.030	15.412	-15.403	-0.547	.618	1.0398	1.0000	
9	2	-4	24.355	23.962	23.840	2.410	.393	.8554	1.0000	
9	2	-3	30.488	31.147	31.091	1.449	-0.659	-1.6429	1.0000	
9	2	-2	5.339	5.216	5.216	.022	.122	.0909	1.0000	
9	2	-1	60.365	59.895	59.790	3.539	.470	.9997	1.0000	
9	2	0	10.830	11.185	11.177	.404	-0.355	-0.4845	1.0000	
9	2	1	17.834	17.120	17.085	1.085	.715	1.3427	1.0000	
9	2	2	23.097	21.132	20.990	2.450	1.965	3.9213	1.0000	
9	2	3	10.854	8.923	-8.912	-0.455	1.930	2.2990	1.0000	
9	3	-6	22.337	21.885	21.861	1.025	.451	.8268	1.0000	
9	3	-5	4.368	1.417	1.390	.276	2.951	1.6391	1.0000	
9	3	-4	42.389	41.713	-41.676	-1.769	.676	1.6716	1.0000	
9	3	-3	22.053	21.995	21.927	1.726	.058	.1209	1.0000	
9	3	-2	30.896	29.973	-29.946	-1.270	.023	2.2250	1.0000	
9	3	-1	3.189	3.257	-3.244	-0.290	-0.067	-0.0295	1.0000	
9	3	0	30.160	29.569	29.524	1.636	.591	1.3904	1.0000	
9	3	1	23.525	24.598	-24.544	-1.630	-1.073	-2.2341	1.0000	
9	3	2	18.294	16.501	16.466	1.081	1.793	3.1251	1.0000	
9	4	-5	49.632	50.552	50.439	3.378	-0.920	-2.1652	1.0000	
9	4	-4	7.854	8.175	8.160	.482	-0.320	-0.2924	1.0000	
9	4	-3	7.125	6.029	5.933	1.069	1.097	.9677	1.0000	
9	4	-2	39.683	39.835	39.728	2.917	-0.151	-0.3643	1.0000	
9	4	-1	30.277	30.628	-30.621	-0.669	-0.351	-0.7865	1.0000	
9	4	0	29.662	29.425	29.325	2.422	.238	.5247	1.0000	
9	4	1	16.618	17.270	17.193	-1.632	-0.653	-1.0673	1.0000	
9	5	-3	21.594	22.324	-22.256	-1.742	-0.731	-1.3298	1.0000	
9	5	-2	18.691	19.189	19.152	1.196	-0.498	-0.8474	1.0000	
9	5	-1	3.418	1.382	-1.364	.217	2.036	.8334	1.0000	
9	5	0	31.124	32.045	-31.999	-1.711	-0.921	-1.9456	1.0000	
10	0	-6	13.594	14.378	14.318	1.306	-0.784	-1.0696	1.0000	
10	0	-5	2.310	4.187	4.181	.232	-0.877	-0.3709	1.0000	
10	0	-4	18.269	18.239	18.045	2.647	.031	.0570	1.0000	
10	0	-3	3.217	4.898	-4.898	.063	-1.681	-0.7315	1.0000	
10	0	-2	29.493	28.810	28.774	1.447	.683	1.5939	1.0000	
10	0	-1	25.920	24.812	24.697	2.392	1.108	2.4665	1.0000	
10	0	0	4.717	4.507	4.507	-0.035	.210	.1287	1.0000	
10	0	1	38.923	36.634	36.545	2.541	2.290	5.4313	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
10	0	2	5.460 *	5.116	5.011	1.029	.344	.2209	1.0000 **
10	1	-6	19.907	19.297	19.240	1.482	.611	1.0841	1.0000 **
10	1	-5	3.321 *	1.979	-1.780	-.867	1.341	.5651	1.0000 **
10	1	-4	3.431 *	.960	-.958	.060	2.471	1.1552	1.0000 **
10	1	-3	7.958	6.785	-6.726	.894	1.173	1.1994	1.0000
10	1	-2	25.122	24.755	-24.694	-1.734	.367	.7976	1.0000
10	1	-1	3.183 *	1.033	-.276	.996	2.149	.9452	1.0000 **
10	1	0	10.470	8.985	-8.982	-.242	1.485	1.9191	1.0000
10	1	1	3.670 *	4.033	3.955	-.791	-.363	-.1671	1.0000 **
10	1	2	21.158	18.745	18.688	1.455	2.414	4.4206	1.0000
10	2	-5	14.890	14.362	14.162	2.387	.528	.8003	1.0000
10	2	-4	6.251 *	8.504	8.504	.050	-2.253	-1.7250	1.0000
10	2	-3	33.651	33.841	33.737	2.654	.009	.0216	1.0000
10	2	-2	16.321	17.354	17.305	1.305	-1.034	-1.8019	1.0000
10	2	-1	22.046	23.474	23.472	.327	-1.428	-2.8495	1.0000
10	2	0	17.309	17.775	17.583	2.606	-.466	-.8079	1.0000
10	2	1	3.348 *	3.322	3.322	-.013	.026	.0109	1.0000 **
10	3	-5	9.409	8.715	8.670	.881	.695	.6957	1.0000
10	3	-4	9.679	7.814	-7.813	-.095	1.865	2.1084	1.0000
10	3	-3	10.353	8.283	-8.229	-.945	2.070	2.4552	1.0000
10	3	-2	21.324	20.431	20.361	1.694	.893	1.7114	1.0000
10	3	-1	3.255 *	1.743	1.416	-.1016	1.512	.6502	1.0000 **
10	3	0	11.341	11.386	11.384	.214	-.045	-.0560	1.0000
10	3	1	3.400 *	1.817	-1.655	.750	1.583	.6517	1.0000 **
10	3	2	3.407 *	3.685	-3.684	.111	-.278	-.1144	1.0000 **
10	4	-2	15.664	15.251	15.182	1.451	.413	.6391	1.0000
10	4	-1	16.597	16.834	16.662	2.398	-.237	-.3708	1.0000
10	4	0	3.390 *	1.619	-1.596	.270	1.771	.7312	1.0000
10	4	1	48.481	48.017	47.930	2.893	.464	1.1188	1.0000
10	4	2	27.447	27.748	27.745	.423	-.301	-.6175	1.0000
10	4	3	26.466	26.576	26.534	1.485	-.110	-.2249	1.0000
10	4	4	22.831	21.904	21.807	2.060	.927	1.7649	1.0000
10	0	0	15.623	15.161	-15.115	-1.189	.461	.7135	1.0000
10	1	-3	18.574	19.671	-19.671	-.117	-1.097	-1.8682	1.0000
10	1	-2	6.044 *	4.039	3.928	.940	2.005	1.5392	1.0000 **
10	1	-1	3.514 *	3.708	3.494	-1.241	-.194	-.0847	1.0000 **
10	1	0	15.833	14.602	14.555	1.170	1.232	1.9162	1.0000
10	1	-4	23.695	22.794	22.682	2.259	.900	1.6701	1.0000
10	1	-3	5.083 *	3.596	-3.585	-.283	1.487	.9137	1.0000
10	1	-2	9.316	8.837	8.575	2.137	.479	.5211	1.0000
10	2	-1	9.292	8.968	8.908	1.030	.324	.3304	1.0000

ALL REFLECTIONS

WEIGHTED R	NUMERATOR	DENOMINATOR	NUMBER	R
21066.88	4952614.49		942	.065
UNWEIGHTED R	1358.98	24117.41	642	.056

RANGES OF F(OBS)

2831.17	374885.58	499	.087
7224.76	2166330.36	298	.059
5640.88	1491266.31	97	.062
2665.43	505993.61	31	.073
1955.20	205944.02	12	.097
195.99	50571.55	2	.062
167.98	98119.75	4	.041
385.46	69503.32	1	.074

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

4699.63	715770.19	51	.081
4982.08	811910.31	84	.078
3220.98	884781.95	98	.060
2146.10	724426.79	113	.054
2365.33	550450.95	132	.066
1598.24	611714.78	147	.051
1017.74	356364.69	154	.053
1035.78	297194.94	163	.059

UNREJECTED REFLECTIONS

WEIGHTED R	8744.06	4326048.67	905	.045
UNWEIGHTED R	1040.31	21659.13	905	.048

RANGES OF F(OBS)

2412.83	371999.81	497	.081
3950.32	2064305.86	288	.044
1892.61	1347088.04	88	.037
414.72	398437.43	24	.032
69.46	77084.72	5	.030
.19	12956.45	1	.004
3.94	54176.36	2	.009
.00	.00	0	.000

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

1310.90	453817.83	40	.054
1643.39	677182.45	75	.049
1183.27	787668.19	92	.039
1077.10	696092.46	111	.039
570.02	471751.52	126	.035
920.27	585997.67	145	.040
1017.74	356364.69	154	.053
1021.36	297173.85	162	.059

SUM FCAL 23820.38
 STANDARD DEV OF UNIT WEIGHT OBS 3.28