

Reinerite, $Zn_3(AsO_3)_2$: an arsenite with a novel type of Zn-tetrahedral double chain¹

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Abstract

Reinerite, $Zn_3(AsO_3)_2$ from Tsumeb, S. W. Africa, is orthorhombic, with cell dimensions $a = 6.092(2)$, $b = 14.407(2)$, $c = 7.811(1)\text{Å}$, space group $Pbam$ and $Z = 4$. The crystal structure has been determined by the symbolic addition method and difference Fourier synthesis and refined by the method of least squares to an R factor of 0.051 based on 1289 reflections, measured on an automatic single-crystal diffractometer. The standard deviation in Zn-O and As-O bond lengths is 0.003 and 0.004 \AA and in O-Zn-O and O-As-O angles 0.02°.

The structure of reinerite contains a new type of Zn-tetrahedral double chain, $[Zn_4O_{10}]_{\infty}$, with two-tetrahedral repeat and four-membered rings; these double chains are cross-linked into a three-dimensional framework through corner-sharing of a new type of edge-sharing Zn-tetrahedral dimers and two types of trigonal pyramidal arsenite groups. The average Zn-O bond distances within the two independent Zn-O tetrahedra are 1.958 and 1.964 \AA . Both the arsenite groups have the point symmetry m , with average As-O bond distances 1.776 and 1.771 \AA and average O-As-O bond angles 98.4 and 96.8°.

Introduction

In the course of our investigation of the stereochemistry of copper and zinc (Ghose and Wan, 1974; Ghose *et al.*, 1974), we have now determined the crystal structure of reinerite, $Zn_3(AsO_3)_2$, from Tsumeb, S.W. Africa. At Tsumeb, it occurs at a depth of 800 m in a second oxidation zone of the lead-zinc-copper deposit, in association with smithsonite, hydrozincite, hemimorphite, willemite, adamite, and olivenite (Geier and Weber, 1958). In addition to the configuration of the arsenite group, the crystal structure of reinerite turned out to be of considerable interest, because it contains a new type of double chain consisting of corner-sharing ZnO_4 tetrahedra, reminiscent of the amphibole-type tetrahedral silicate double chains, and an edge-sharing Zn-tetrahedral dimer.

Experimental

Reinerite was reported to be orthorhombic with possible space group $Pmma$ by Geier and Weber (1958). Precession photographs of a reinerite crystal from Tsumeb revealed extinction conditions as $0kl$, k

$= 2n$ and $h0l$, $h = 2n$ present. Of the two possible space groups, $Pbam$ and $Pba2$, the first proved to be correct on the basis of an $N(z)$ -test of the measured X-ray diffraction intensities.

A single crystal of light blue transparent reinerite was checked for crystal perfection through a transmission Laue photograph and then ground to a sphere of diameter 0.225(2) mm. The single-crystal sphere was mounted on the syntex P1 single-crystal diffractometer, and the unit-cell dimensions were refined by the least-squares method based on 15 reflections with measured 2θ values between 35 and 45°, using $MoK\alpha$ radiation. The cell dimensions (Table 1) are in good agreement with those determined by Geier and Weber. All (hkl) reflections within $2\theta = 65^\circ$ were measured on the diffractometer by the $2\theta-\theta$ scan method, using $MoK\alpha$ radiation monochromatized by reflection from a graphite "single" crystal, and scintillation counter. A variable scan rate was used, the minimum being 1°/min (50 kV, 15 mA). Out of a total of 1289 reflections, 239 were less than $3\sigma(I)$, where $\sigma(I)$ is the standard deviation of the measured intensity as determined by the counting statistics. All the intensities were corrected for Lorentz, polarization, and absorption factors.

¹ Structural chemistry of copper and zinc minerals. Part III.

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	PAGE	
0	0	0	2	47.376	46.050	-46.046	.617	1.325	2.0.1883	1.0000	1	
0	0	0	3	27.395	25.002	-24.953	-1.570	2.393	4.0.7342	1.0000	1	
0	0	0	4	256.381	292.459	291.589	22.537	-36.076	-24.6235	1.0000	*	
0	0	0	5	61.812	59.327	59.143	4.662	2.485	4.0.2272	1.0000	1	
0	0	0	6	202.231	209.324	208.729	15.768	-7.092	-3.0.9130	1.0000	1	
0	0	0	7	88.455	86.737	-86.289	-8.797	1.718	2.0.0852	1.0000	1	
0	0	0	8	37.763	37.535	36.990	6.371	.229	.3310	1.0000	1	
0	0	0	9	83.378	84.553	83.858	10.823	-1.176	-1.0.7840	1.0000	1	
0	0	0	10	131.983	135.951	134.547	19.413	-3.958	-3.0.3026	1.0000	1	
0	0	0	11	63.858	64.632	-63.828	-10.166	-7.774	-1.0.1946	1.0000	1	
0	0	0	12	99.642	99.871	-98.831	-2.818	-2.330	-0.2801	1.0000	1	
0	0	0	13	64.241	67.940	-67.904	-2.227	-3.699	-4.0.9002	1.0000	1	
0	0	0	14	139.338	148.300	148.052	8.568	-8.963	-7.0.8156	1.0000	1	
0	0	0	15	137.158	147.765	147.021	14.802	-10.657	-7.0.8607	1.0000	*	
0	0	0	16	74.682	72.329	-72.162	-2.923	2.353	3.0.4194	1.0000	1	
0	0	0	17	158.955	157.815	-157.362	-11.959	1.140	.6708	1.0000	1	
0	0	0	18	89.851	87.214	86.727	9.201	2.637	3.0.2005	1.0000	1	
0	0	0	19	120.092	120.050	119.297	13.426	.042	.0.0405	1.0000	1	
0	0	0	20	14.681	14.030	-13.922	-1.732	.651	.4312	1.0000	1	
0	0	0	21	48.438	48.152	-48.020	-3.563	.286	.4417	1.0000	1	
0	0	0	22	5.948	*254	.009	.294	5.654	1.0.3307	1.0000	**	
0	0	0	23	10.976	*	13.879	13.619	-2.904	-1.0.6169	1.0000	**	
0	0	0	24	52.493	50.704	50.695	.923	1.789	3.0.2267	1.0000	1	
0	0	0	25	7.393	*	4.864	4.721	1.169	2.529	1.0.7003	1.0000	1
0	0	0	26	81.937	77.845	77.820	1.981	4.092	5.0.2351	1.0000	1	
0	0	0	27	67.554	64.762	-64.240	-8.204	2.793	4.0.5611	1.0000	1	
0	0	0	28	34.728	33.031	32.822	3.706	1.697	2.0.8981	1.0000	1	
0	0	0	29	98.081	97.142	-96.569	-10.539	.938	1.0.1358	1.0000	1	
0	0	0	30	43.374	43.374	-43.150	-4.405	.052	.0.0852	1.0000	1	
0	0	0	31	131.361	130.223	-129.001	-17.794	1.139	1.0.000	1.0000	1	
0	0	0	32	90.309	90.458	89.890	10.123	-.148	-.1.931	1.0000	1	
0	0	0	33	18.506	16.193	-15.712	-3.920	2.313	1.0.6205	1.0000	1	
0	0	0	34	49.079	49.079	-48.575	-7.014	-.538	-.7.325	1.0000	1	
0	0	0	35	116.202	112.146	-111.998	-5.770	4.055	4.0.0927	1.0000	1	
0	0	0	36	152.640	152.361	-152.022	-10.149	.279	1.0.2013	1.0000	1	
0	0	0	37	77.027	75.694	-75.497	-5.459	1.933	1.0.8472	1.0000	1	
0	0	0	38	81.734	80.505	80.475	2.209	.310	.3075	1.0000	1	
0	0	0	39	116.262	115.952	-115.560	-9.532	-.11.517	-6.0.2768	1.0000	1	
0	0	0	40	168.011	179.528	-178.856	-15.521	1.485	.9.822	1.0000	*	
0	0	0	41	12.568	11.083	-11.080	-.259					
0	0	0	42	12.392	10.190	10.181	.423	2.202	1.0.3310	1.0000	1	
0	0	0	43	77.691	76.443	-75.865	-.9.380	1.248	1.0.9659	1.0000	1	
0	0	0	44	33.111	34.055	-33.446	-.6.410	-.943	-1.0.0974	1.0000	1	
0	0	0	45	23.761	25.081	-24.788	-.3.823	-1.320	-1.0.1120	1.0000	1	
0	0	0	46	40.395	41.384	-40.893	-.6.354	-.989	-1.0.1751	1.0000	1	
0	0	0	47	176.709	163.973	183.248	16.320	-.7.264	-4.0.6738	1.0000	1	
0	0	0	48	61.222	59.162	-58.681	-.7.526	2.060	3.0.6137	1.0000	1	
0	0	0	49	27.625	26.701	26.374	4.169	.924	1.0.4556	1.0000	1	
0	0	0	50	18.005	18.320	-18.295	-.948	-.314	-0.3321	1.0000	1	
0	0	0	51	82.302	84.580	84.067	9.301	2.276	-3.0.2167	1.0000	1	
0	0	0	52	64.731	63.960	-63.325	-.8.989	-.771	1.0.5123	1.0000	1	
0	0	0	53	95.560	95.795	95.75	12.129	-.583	-0.7059	1.0000	1	
0	0	0	54	25.685	-25.008	-4.357	-.3253	-.301	.0.3253	1.0000	1	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTR
0	8	8	7.190 *	10.541	10.237	2.516	-3.351	-1.0416	1.0000 **
0	8	9	14.371	10.423	-10.336	-1.341	3.948	2.2221	1.0000
0	8	10	58.002	57.198	56.284	10.184	.804	1.2113	1.0000
0	8	11	35.149	37.691	-36.717	-8.511	-2.542	-2.6857	1.0000
0	10	0	212.294	221.654	221.121	15.354	-9.360	-5.4660	1.0000
0	10	1	76.185	73.013	72.775	5.899	3.172	4.4376	1.0000
0	10	2	36.630	35.306	-35.302	.512	1.324	2.2103	1.0000
0	10	3	120.450	121.348	120.861	10.869	-.898	-8098	1.0000
0	10	4	59.826	61.391	60.864	8.024	-1.566	-3.1959	1.0000
0	10	5	42.043	44.128	43.906	4.424	-2.085	-3.4299	1.0000
0	10	6	96.206	97.744	97.299	9.321	-1.538	-1.9083	1.0000
0	10	7	47.561	46.643	46.308	5.585	1.916	1.4611	1.0000
0	10	8	17.112	15.703	-15.691	.612	1.409	.9646	1.0000
0	10	9	65.566	67.638	66.905	9.934	-2.072	-3.3479	1.0000
0	10	10	46.786	47.568	46.793	8.554	-7.782	-1.6212	1.0000
0	12	0	67.708	66.419	-66.249	-4.759	1.289	2.1515	1.0000
0	12	1	55.757	55.463	55.117	6.189	.294	.5690	1.0000
0	12	2	19.344	19.211	-19.265	.825	.825	.8005	1.0000
0	12	3	151.992	152.413	151.390	17.627	-.421	-.2951	1.0000
0	12	4	73.319	73.789	-73.367	-7.883	-.470	-.7302	1.0000
0	12	5	12.585	11.828	-11.820	-.421	.758	.4448	1.0000
0	12	6	7.150 *	4.747	4.496	1.522	2.403	.7676	1.0000 **
0	12	7	103.374	106.067	105.070	14.656	-2.713	-2.9150	1.0000
0	12	8	48.080	48.799	-48.249	-7.302	-.719	-1.0284	1.0000
0	12	9	22.285	21.105	20.422	5.324	1.180	.9153	1.0000
0	14	0	92.563	90.899	90.489	8.619	1.664	2.0873	1.0000
0	14	1	55.071	54.069	-53.786	-5.519	1.003	1.7868	1.0000
0	14	2	121.680	122.421	-121.488	-15.086	-.741	-.6724	1.0000
0	14	3	25.567	22.965	-.22.402	-5.053	2.603	2.8031	1.0000
0	14	4	18.892	18.831	18.824	-.496	-.061	.0483	1.0000
0	14	5	22.253	23.069	-22.917	-2.645	-.811	-.7270	1.0000
0	14	6	10.230 *	14.720	-14.510	-2.476	-4.491	-1.8830	1.0000 **
0	14	7	68.171	69.359	-68.655	-9.852	-.187	-1.9751	1.0000
0	14	8	41.337	43.918	-43.031	-8.782	-2.581	-3.2018	1.0000
0	14	9	35.997	35.713	35.522	3.688	.285	.3148	1.0000
0	16	0	35.487	35.165	-34.997	-3.428	.323	.4154	1.0000
0	16	1	132.818	137.026	-136.182	-15.188	-4.208	-3.6699	1.0000
0	16	2	43.415	44.362	44.062	5.152	-.948	-1.3598	1.0000 **
0	16	3	10.768 *	10.768	4.450	-1.647	6.023	2.6915	1.0000 **
0	16	4	39.032	37.826	-37.488	-5.046	1.207	1.5660	1.0000
0	16	5	164.814	169.074	-167.678	-21.684	-4.260	-3.1009	1.0000
0	16	6	37.434 *	38.361	37.890	5.993	-9.928	-1.0879	1.0000
0	16	7	6.172 *	8.254	-8.159	-1.248	-2.082	-4.721	1.0000 **
0	16	8	12.813 *	16.039	-15.853	-2.436	-3.226	-1.4094	1.0000 **
0	18	0	111.490	112.910	112.132	13.233	-1.420	-1.5938	1.0000
0	18	1	18.740	16.165	16.104	1.398	2.575	1.7849	1.0000
0	18	2	68.407	67.538	-66.834	-9.73	.869	1.4614	1.0000
0	18	3	8.191 *	7.337	-7.309	.640	.864	.2559	1.0000 **
0	18	4	45.314	44.735	44.414	5.931	.579	.7604	1.0000
0	18	5	36.692	36.265	36.029	4.130	.427	.4791	1.0000
0	18	6	16.602	17.883	17.801	1.705	-1.280	-0.7133	1.0000
0	18	7	9.435 *	4.242	-3.655	-2.154	-5.193	1.7481	1.0000 **
0	20	8	38.756	40.689	40.027	7.913	-1.933	-2.2376	1.0000

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	PAGE
1	1	1	1	11.650 *	12.230	11.810	3.176	-0.580	-0.2358	1.0000	**
1	1	1	2	105.591	106.352	104.866	17.717	-0.761	-0.9653	1.0000	
1	1	1	3	33.984	33.170	-32.924	-4.035	.814	.8505	1.0000	
1	1	1	4	89.457	99.173	-99.147	-2.272	-9.717	-10.1717	1.0000	
1	1	1	5	26.687	26.342	-26.284	-1.740	.346	.8868	1.0000	
1	1	1	6	166.435	184.934	184.559	11.773	-18.500	-15.7648	1.0000	*
1	1	1	7	68.828	69.031	-68.573	-7.943	-0.203	-0.3208	1.0000	
1	1	1	8	55.586	51.200	50.989	4.639	4.386	8.5273	1.0000	
1	1	1	9	4.803 *	.391	.390	.027	4.412	1.2857	1.0000	
1	1	1	10	5.934 *	4.058	-3.765	1.514	1.876	.5957	1.0000	**
1	1	1	11	26.295	25.105	-24.911	-3.116	1.190	1.4065	1.0000	
1	1	1	12	87.009	86.012	85.402	10.226	.998	1.3870	1.0000	
1	1	1	13	40.204	39.142	-38.560	-6.724	1.061	1.4758	1.0000	
1	1	1	14	5.961 *	.714	.276	.658	5.247	1.2324	1.0000	**
1	1	1	15	18.760	16.128	15.912	2.633	2.632	1.7666	1.0000	
1	1	1	16	14.652	12.186	12.087	1.547	2.466	3.7796	1.0000	
1	1	1	17	164.117	209.716	209.419	11.153	-45.599	-43.4778	1.0000	*
1	1	1	18	62.001	61.700	61.516	4.767	.301	.4043	1.0000	
1	1	1	19	136.251	134.357	133.806	12.151	1.894	1.3613	1.0000	
1	1	1	20	17.796	15.727	15.599	1.998	2.069	2.4783	1.0000	
1	1	1	21	125.251	120.754	120.396	9.293	4.497	4.3998	1.0000	
1	1	1	22	32.615	29.955	29.773	3.298	2.660	3.9555	1.0000	
1	1	1	23	110.377	106.800	106.201	11.296	3.577	3.7974	1.0000	
1	1	1	24	16.754	18.659	18.458	2.729	-1.905	-1.4068	1.0000	
1	1	1	25	48.026	48.034	47.422	7.645	-0.008	-0.0126	1.0000	
1	1	1	26	6.017 *	8.262	8.106	1.602	-2.246	-0.5226	1.0000	**
1	1	1	27	58.220	58.811	58.172	8.644	-.591	-.8819	1.0000	
1	1	1	28	97.319	101.013	-100.863	-5.504	-3.694	-3.1476	1.0000	
1	1	1	29	125.670	139.676	139.445	8.021	-14.006	-11.9580	1.0000	*
1	1	1	30	88.878	91.903	-91.690	-6.245	-3.925	-3.8025	1.0000	
1	1	1	31	114.418	109.711	-109.613	-4.631	4.708	4.5562	1.0000	
1	1	1	32	111.401	9.778	-9.710	-1.150	1.623	1.2808	1.0000	
1	1	1	33	169.160	171.105	170.543	13.855	-1.945	-1.1226	1.0000	
1	1	1	34	115.035	110.765	-110.286	-10.290	4.270	4.2994	1.0000	
1	1	1	35	30.756	28.332	-28.212	-2.599	2.424	3.2395	1.0000	
1	1	1	36	6.431 *	3.451	3.450	.087	2.980	.8969	1.0000	**
1	1	1	37	26.892	29.117	28.669	5.092	-2.225	-2.2761	1.0000	
1	1	1	38	30.439	30.753	-30.417	-4.533	-.314	-.3283	1.0000	
1	1	1	39	32.125	32.240	31.879	4.806	-.115	-.1163	1.0000	
1	1	1	40	127.549	135.160	134.932	7.982	-7.619	-6.2207	1.0000	
1	1	1	41	69.510	70.160	69.957	5.333	-.650	-.9125	1.0000	
1	1	1	42	41.751	39.581	-39.539	1.812	2.170	5.5063	1.0000	
1	1	1	43	52.989	48.879	48.802	2.751	4.110	7.9907	1.0000	
1	1	1	44	48.135	46.513	46.060	6.474	1.623	3.6991	1.0000	
1	1	1	45	72.480	69.319	68.981	6.832	3.161	5.1249	1.0000	
1	1	1	46	6.258	34.130	33.957	3.462	2.127	3.3878	1.0000	
1	1	1	47	5.337 *	8.731	8.629	1.330	-3.393	-.8995	1.0000	**
1	1	1	48	10.815 *	8.306	7.537	3.491	2.509	1.2466	1.0000	**
1	1	1	49	46.710	46.507	46.141	5.827	-.203	-.2990	1.0000	
1	1	1	50	23.167	21.858	21.376	4.956	1.309	1.1031	1.0000	
1	1	1	51	6.206 *	6.374	6.160	1.635	-.168	-.0379	1.0000	**
1	1	1	52	61.985	61.157	61.041	3.771	-.829	1.2831	1.0000	
1	1	1	53	81.082	86.998	86.796	5.918	-5.916	-7.6345	1.0000	

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	1	5	3	28.438	26.232	26.086	2.760	2.206	3.9470	1.0CCC
1	1	5	4	133.236	129.268	-128.831	-10.610	3.969	3.3190	1.0CCCC
1	1	5	5	13.347	13.964	13.918	1.130	-6.617	-4.4505	1.0CC00
1	1	5	6	44.430	41.251	-40.609	-7.250	3.179	5.5762	1.0CCC
1	1	5	7	80.218	78.819	78.361	8.484	1.399	2.0874	1.0CCC
1	1	5	8	9.123 *	6.606	6.495	1.206	2.517	1.0458	1.0CCC
1	1	5	9	46.481	46.870	-46.516	-5.752	-3.90	-5.644	1.0CCC
1	1	5	10	65.840	66.369	-65.560	-10.460	-5.49	-8.8903	1.0CCC
1	1	5	11	62.829	66.002	65.171	10.438	-3.172	-4.7648	1.0CCC
1	1	6	0	110.501	107.829	-107.742	-4.344	2.672	2.6203	1.0CCC
1	1	6	1	78.559	79.441	-78.939	-8.917	-8.882	-1.2621	1.0CCC
1	1	6	2	76.965	76.196	76.113	3.568	.769	1.0396	1.0CCC
1	1	6	3	46.325	45.997	-45.668	-5.490	.328	.7443	1.0CCC
1	1	6	4	24.701	22.865	-22.705	-2.695	1.837	2.5222	1.0CCC
1	1	6	5	94.260	91.051	-90.414	-10.755	3.209	3.6024	1.0CCC
1	1	6	6	7.840 *	6.287	-6.220	.913	1.553	.6313	1.0CCC
1	1	6	7	13.211	12.653	-12.169	-3.469	.558	.3436	1.0CCC
1	1	6	8	12.020	13.126	13.121	.384	-1.106	-5.758	1.0CCC
1	1	6	9	60.382	58.610	-57.889	-9.166	1.772	2.9481	1.0CC00
1	1	6	10	6.083 *	9.075	-8.946	-1.526	-2.991	-6.6885	1.0CCC
1	1	6	11	11.619 *	11.143	-10.550	-3.587	.476	.1937	1.0CCC
1	1	7	0	103.342	103.492	103.134	8.593	-.149	-1.1640	1.0000
1	1	7	1	4.362 *	2.511	-2.426	-.645	1.852	1.5944	1.0CCC
1	1	7	2	19.134	17.952	-17.932	-.850	1.182	1.4874	1.0CCC
1	1	7	3	198.597	227.501	-226.923	-16.214	-28.904	-17.5412	1.0000
1	1	7	4	123.365	120.889	120.425	10.581	2.477	2.3415	1.0000
1	1	7	5	98.239	95.320	94.958	8.301	2.919	3.2050	1.0CCC
1	1	7	6	37.260	34.962	-34.867	-2.584	2.298	3.5580	1.0CCC
1	1	7	7	126.242	126.818	-125.999	-14.387	-.576	-5.235	1.0000
1	1	7	8	56.835 *	56.593	56.080	7.218	.292	.4919	1.0000
1	1	7	9	5.894 *	1.275	-.1.058	.712	4.619	1.0969	1.0CCC
1	1	7	10	24.913	26.286	25.924	4.350	-1.374	-1.1685	1.0000
1	1	7	11	19.341	22.171	-21.819	-3.935	-2.830	-1.8156	1.0000
1	1	8	0	39.580	36.528	-36.421	-2.791	3.052	6.2874	1.0000
1	1	8	1	94.191	91.553	-91.339	-6.109	2.648	3.0645	1.0000
1	1	8	2	141.048	143.016	-142.580	-11.150	-1.968	-1.6552	1.0000
1	1	8	3	88.573	90.651	90.166	-.9.365	-2.079	-2.4375	1.0000
1	1	8	4	47.913	46.425	-46.243	-4.104	1.487	2.9044	1.0000
1	1	8	5	40.288	38.137	-38.022	-2.952	2.152	3.6463	1.0000
1	1	8	6	73.353	71.592	-71.193	-7.554	1.761	2.8857	1.0000
1	1	8	7	88.357	86.075	-85.526	-9.708	2.281	3.3369	1.0000
1	1	8	8	48.093	48.142	-47.726	-6.319	-.049	-0.0760	1.0000
1	1	8	9	5.970 *	7.666	-7.339	-2.216	-1.696	-3.978	1.0000
1	1	8	10	24.407	24.334	-24.074	-3.547	.073	.0609	1.0000
1	1	9	1	154.522	154.397	-154.038	-10.519	.125	.0740	1.0000
1	1	9	2	47.022	45.246	-45.134	-3.183	1.776	3.6920	1.0000
1	1	9	3	222.254	237.011	236.321	18.072	-14.757	-8.6630	1.0000
1	1	9	4	9.608 *	2.838	-1.632	-2.322	6.771	3.6945	1.0000
1	1	9	5	7.883 *	6.195	-6.126	-.920	1.688	.7274	1.0000
1	1	9	6	72.480	69.723	-69.425	-6.448	2.757	4.6538	1.0000
1	1	9	7	31.562	22.893	-22.672	3.172	8.668	11.1545	1.0000
1	1	9	8	36.777	34.699	-34.447	4.176	2.078	2.8535	1.0000
1	1	9	9	85.239	85.571	84.942	10.361	-.332	-.4618	1.0000

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
1	9	9	71.725	72.416	-71.453	-11.769	.691	-1.1711	1.0000	
1	9	10	16.651	17.443	-17.225	-2.750	.791	-4.621	1.0000	
1	10	0	77.907	77.142	-76.687	-8.370	.765	1.0664	1.0000	
1	10	1	27.195	26.434	26.339	2.239	.761	1.0450	1.0000	
1	10	2	11.269	13.472	13.463	-4.482	-2.203	-1.3313	1.0000	
1	10	3	58.950	56.809	56.548	5.440	2.142	4.4118	1.0000	
1	10	4	52.243	51.550	-51.125	-6.605	.693	1.3026	1.0000	
1	10	5	5.291 *	5.255	-5.238	-4.418	.036	.0096	1.0000	
1	10	6	11.330 *	11.206	-10.862	-2.756	.123	.0649	1.0000	
1	10	7	52.333	50.921	50.546	6.175	1.411	2.2960	1.0000	
1	10	8	15.986	15.611	-15.309	-3.056	.375	.2369	1.0000	
1	10	9	6.063 *	5.011	-4.992	-4.440	1.052	1.2430	1.0000	
1	10	10	22.058	20.071	-19.521	-4.667	1.987	1.5045	1.0000	
1	11	0	6.633 *	5.327	-5.326	-1.02	1.306	.4611	1.0000	
1	11	1	86.885	86.019	85.513	9.318	.866	1.2504	1.0000	
1	11	2	79.084	77.920	-77.556	-7.522	1.164	1.6187	1.0000	
1	11	3	54.668	52.444	-52.219	-4.843	2.225	4.2882	1.0000	
1	11	4	29.520	29.297	29.205	2.321	.223	.2865	1.0000	
1	11	5	137.505	137.269	136.268	16.549	.236	.1908	1.0000	
1	11	6	78.080	79.152	-76.653	-8.876	-1.072	-1.5989	1.0000	
1	11	7	40.803	40.906	-40.696	-4.134	-.103	-.1436	1.0000	
1	11	8	12.038 *	6.825	6.802	.564	5.212	2.5063	1.0000	
1	11	9	52.569	53.092	52.469	8.109	-.523	-.7435	1.0000	
1	11	10	6.262 *	7.360	-7.165	-1.683	-1.098	-2.457	1.0000	
1	12	1	102.759	101.082	100.619	9.665	9.665	1.677	1.9659	1.0000
1	12	2	62.698	59.174	58.708	6.750	3.524	7.0655	1.0000	
1	12	3	27.478	27.036	26.832	3.314	4.442	5.359	1.0000	
1	12	4	5.395 *	6.834	5.588	3.933	-1.438	-.3806	1.0000	
1	12	5	65.985	69.865	69.399	8.055	.275	.4408	1.0000	
1	12	6	35.982	37.368	37.053	6.726	8.236	-1.741	-3.2720	1.0000
1	12	7	7.061 *	6.859	6.429	2.388	.202	-.1387	-.8154	1.0000
1	12	8	30.221	29.870	29.491	4.746	.351	.0586	1.0000	
1	12	9	29.943	29.707	28.895	6.898	.236	.3672	1.0000	
1	13	0	153.482	153.894	-153.107	-15.540	-.612	-.2884	1.0000	
1	13	1	48.545	47.197	47.021	4.073	1.348	2.3742	1.0000	
1	13	2	58.576	56.966	56.737	5.098	1.611	3.0520	1.0000	
1	13	3	10.564 *	9.030	8.732	2.301	1.533	.7729	1.0000	
1	13	4	65.272	63.519	-63.079	-7.466	1.753	3.3217	1.0000	
1	13	5	27.353	27.551	27.446	2.402	-.197	-.2101	1.0000	
1	13	6	41.687	41.281	-40.869	-5.817	.406	.5710	1.0000	
1	13	7	49.180	50.819	50.351	6.880	-1.639	-2.3977	1.0000	
1	13	8	17.947	15.799	15.687	1.873	2.149	1.3905	1.0000	
1	13	9	31.107	29.392	-29.156	-3.716	1.716	1.7313	1.0000	
1	14	0	65.638	65.153	64.904	5.632	.685	1.3263	1.0000	
1	14	1	5.498 *	1.063	-.887	.571	4.434	1.1289	1.0000	
1	14	2	82.039	81.479	80.931	9.433	.560	.8166	1.0000	
1	14	3	24.405	23.426	23.319	2.246	.246	.9874	1.0000	
1	14	4	48.362	48.037	47.659	6.016	.325	.5102	1.0000	
1	14	5	9.305 *	12.825	-12.801	-.786	-3.520	-1.3383	1.0000	
1	14	6	60.246	62.835	62.402	7.369	-2.989	-4.1823	1.0000	
1	14	7	18.814	16.219	16.012	2.581	2.595	1.6349	1.0000	
1	14	8	38.200	37.922	36.952	.678	.678	1.0000	1.0000	

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTR	PAGE
2	1	15	0	22.076	23.216	23.175	1.382	-1.140	-1.0407	1.0000	6
2	1	15	1	12.136	12.116	-11.881	-2.374	.020	.0104	1.0000	
2	1	15	2	13.372	13.541	13.159	3.192	-.170	-.0985	1.0000	
2	1	15	3	97.272	95.899	-95.224	-11.364	1.373	1.7081	1.0000	
2	1	15	4	31.038	30.996	29.991	4.944	.642	.7301	1.0000	
2	1	15	5	26.099	24.564	24.469	2.158	1.536	1.4801	1.0000	
2	1	15	6	7.923 *	3.630	-3.347	-1.405	4.293	1.3213	1.0000	**
2	1	15	7	50.453	51.873	-51.188	-8.400	-1.419	-2.0045	1.0000	
2	1	15	8	28.391	27.569	26.922	5.941	.821	.7621	1.0000	
2	1	16	0	32.031	29.273	-29.181	-2.323	2.758	3.3118	1.0000	
2	1	16	1	17.754	19.925	-19.759	-2.567	-2.172	-1.5630	1.0000	
2	1	16	2	22.087	20.771	-20.444	-3.671	1.316	1.1568	1.0000	
2	1	16	3	27.614	25.757	-25.567	-3.121	1.857	1.9083	1.0000	
2	1	16	4	13.336	12.441	-12.199	-2.441	.895	.4653	1.0000	
2	1	16	5	16.905	12.926	-12.785	-1.901	3.979	2.5277	1.0000	
2	1	16	6	25.696	26.297	-26.139	-2.874	-.600	-.5254	1.0000	
2	1	16	7	17.749	17.421	-17.168	-2.959	.328	.2088	1.0000	
2	1	17	0	27.135	25.845	-25.770	-1.978	1.290	1.2985	1.0000	
2	1	17	1	6.172 *	8.077	-7.875	-1.795	-1.905	-.4811	1.0000	
2	1	17	2	45.853	46.778	46.365	6.198	-.925	-1.3103	1.0000	
2	1	17	3	55.731	55.983	-55.492	-2.399	-.253	-.3928	1.0000	
2	1	17	4	17.444	18.065	17.835	2.874	-.621	-.3975	1.0000	
2	1	17	5	6.181 *	7.131	7.125	.302	-.950	-.2150	1.0000	
2	1	17	6	9.780 *	11.451	-11.433	-6.642	-1.671	-.5787	1.0000	
2	1	17	7	19.306	20.264	-19.867	-3.993	-.958	-.6138	1.0000	
2	1	18	0	59.053	59.007	-58.466	-7.969	-.046	.0734	1.0000	
2	1	18	1	20.677	20.965	-20.799	-2.630	-.287	-.2150	1.0000	
2	1	18	2	62.887	62.279	-61.655	-8.793	.608	.9857	1.0000	
2	1	18	3	6.237 *	11.322	-10.959	-2.845	-.5085	-1.1412	1.0000	
2	1	18	4	52.150	52.102	-51.529	-7.706	.048	.0677	1.0000	
2	1	18	5	15.320	15.266	-15.116	-2.132	.054	.0283	1.0000	
2	1	18	6	46.314	47.088	-46.454	-7.701	-.775	-.9717	1.0000	
2	1	19	0	73.547	73.180	-72.588	-9.286	.367	.6168	1.0000	
2	1	19	1	34.381	34.154	33.725	5.392	.227	.2474	1.0000	
2	1	19	2	21.544	23.637	23.521	2.340	-.2093	-1.5139	1.0000	
2	1	19	3	15.792	17.763	17.696	1.541	-.1.971	-1.0863	1.0000	
2	1	19	4	24.196	22.577	-22.246	-3.850	1.619	1.2958	1.0000	
2	1	19	5	27.988	31.664	31.155	5.657	-3.677	-3.1752	1.0000	
2	20	0	7	12.780 *	12.990	-12.816	-2.118	-.5210	-1.3960	1.0000	
2	20	1	6.230 *	2.014	-1.675	-1.289	4.117	.9249	1.0000		**
2	20	2	6.302 *	2.077	2.087	.623	4.124	.9160	1.0000		**
2	20	3	7.488 *	2.851	2.847	-.148	4.638	1.2390	1.0000		**
2	20	4	10.938 *	9.957	-9.832	-1.575	.980	.3645	1.0000		**
2	21	0	11.742 *	13.335	-13.224	-1.720	-1.594	-.6390	1.0000		**
2	21	1	30.704	31.831	31.308	5.745	-1.126	-1.0518	1.0000		**
2	21	2	20.746	18.439	-18.197	-2.976	2.307	1.5676	1.0000		**
2	22	0	141.132	141.352	138.337	-12.816	-10.280	-23.574	-19.0413	1.0000	
2	22	1	206.155	245.378	-237.867	-11.395	-14.825	-11.3420	1.0000		**
2	22	2	141.457	142.331	-141.975	-10.072	-15.001	-39.223	-29.2604	1.0000	
2	22	3	9.110 *	7.212	7.124	1.126	-.874	-.5790	1.0000		**
2	22	4	74.206	71.090	-70.597	-8.354	1.897	1.0993	1.0000		**
2	22	5	18.533	13.730	-13.688	-1.077	4.605	4.3681	1.0000		**

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR		
2	2	0	7	122.973	123.550	-122.684	-14.596	-0.576	-0.5472	1.0000			
2	2	0	8	82.287	79.982	-79.467	-9.057	2.305	3.5088	1.0000			
2	2	0	9	10.760	*	3.004	-2.968	-0.463	7.755	3.5467	1.0000	**	
2	2	0	10	22.025	20.422	20.422	20.127	3.461	1.603	1.2671	1.0000		
2	2	0	11	84.264	85.674	-84.330	-15.116	-1.410	-2.3897	1.0000			
2	2	1	0	54.132	56.076	55.842	5.113	-1.944	-3.2099	1.0000			
2	2	1	1	120.386	135.342	135.092	8.210	-14.956	-11.4811	1.0000	*		
2	2	1	2	94.823	104.938	-104.367	-10.934	-10.115	-12.0812	1.0000	*	**	
2	2	1	3	4.344	*	1.293	-1.107	1.288	0.9838	1.0000			
2	2	1	4	67.347	67.896	62.861	2.104	4.451	7.2952	1.0000			
2	2	1	5	155.201	151.002	150.460	12.789	4.199	3.3255	1.0000			
2	2	1	6	65.506	63.442	-63.227	-5.223	2.064	4.2316	1.0000			
2	2	1	7	16.660	16.319	-16.240	-1.605	.341	.2661	1.0000			
2	2	1	8	13.129	9.543	-8.800	-3.693	3.586	2.0994	1.0000			
2	2	1	9	79.202	79.126	78.361	10.979	.076	.1425	1.0000			
2	2	1	10	19.528	12.368	12.351	.657	7.160	5.1203	1.0000			
2	2	1	11	6.208	*	3.319	3.279	.510	2.889	.6517	1.0000	**	
2	2	2	0	41.836	42.709	-42.506	-4.159	-.873	-1.8066	1.0000			
2	2	2	1	73.731	79.370	-79.124	-6.244	-5.636	-7.6508	1.0000			
2	2	2	2	6.938	*	6.215	6.202	.411	.723	.4106	1.0000		
2	2	2	3	127.756	*	132.542	7.595	-4.786	-4.3864	1.0000			
2	2	2	4	93.730	91.800	-91.519	-7.187	1.929	2.4001	1.0000			
2	2	2	5	144.521	144.637	-144.032	-13.211	-.116	-.0900	1.0000			
2	2	2	6	50.422	47.895	47.757	3.636	2.527	4.7476	1.0000			
2	2	2	7	66.292	63.553	63.275	5.939	.739	5.4426	1.0000			
2	2	2	8	51.315	49.592	-49.247	-5.843	1.723	2.8762	1.0000			
2	2	2	9	29.123	28.467	-28.080	-4.682	.656	.7050	1.0000			
2	2	2	10	13.743	12.825	-12.667	-2.006	.919	.4792	1.0000			
2	2	2	11	10.261	*	11.482	-11.227	-2.403	-1.221	-4.454	1.0000		
2	2	2	12	160.857	-160.564	-9.700	-14.893	-11.2977	-4.4554	1.0000			
2	2	2	13	11.901	10.916	10.512	5.980	-1.705	-1.4422	1.0000			
2	2	2	14	75.286	78.051	77.934	4.263	-2.765	-3.8805	1.0000			
2	2	2	15	150.977	159.835	159.436	11.288	-8.859	-5.7407	1.0000			
2	2	2	16	80.444	80.173	-80.156	-6.790	-.270	-3.8282	1.0000			
2	2	2	17	39.518	36.811	-36.804	.734	2.707	4.7483	1.0000			
2	2	2	18	11.824	4.562	-4.551	-.327	7.262	4.4550	1.0000			
2	2	2	19	95.026	92.881	92.065	12.284	2.145	2.7137	1.0000			
2	2	2	20	5.489	*	4.417	-4.262	1.072	.2735	1.0000			
2	2	2	21	3.006	*	6.511	2.966	3.505	.9291	1.0000			
2	2	2	22	10	31.415	30.127	-29.779	-4.564	1.268	1.3801	1.0000		
2	2	2	23	3	33.621	34.603	33.601	8.270	-.982	-1.0184	1.0000		
2	2	2	24	163.431	184.558	184.037	13.860	-21.127	-15.3528	1.0000			
2	2	2	25	87.061	89.681	89.307	8.176	-2.620	-3.0094	1.0000			
2	2	2	26	102.078	109.143	-106.909	-7.139	-7.065	-7.8732	1.0000			
2	2	2	27	31.101	28.050	27.909	4.575	1.268	1.3801	1.0000			
2	2	2	28	65.624	122.078	127.678	10.697	-6.047	-5.2629	1.0000			
2	2	2	29	78.884	63.338	63.112	5.349	2.286	4.3498	1.0000			
2	2	2	30	34.472	33.079	32.771	4.507	2.597	3.7505	1.0000			
2	2	2	31	95.239	95.068	-94.107	-6.600	1.394	.2408	1.0000			
2	2	2	32	41.451	43.123	-42.615	-1.673	-2.1161	1.0000				
2	2	2	33	14.182	10.268	-10.258	-4.470	3.914	1.9638	1.0000			

* ** *** ****

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR		
2	2	5	0	153.867	165.052	164.748	10.007	-11.185	-7.7277	1.CCCC	*	
2	2	5	1	45.281	45.604	-45.452	-3.716	-0.324	-0.8029	1.0000		
2	2	5	2	8.666	*	7.837	7.834	.197	.5256	1.0000	**	
2	2	5	3	93.353	98.445	-98.143	-7.701	-5.091	-6.5891	1.CCCC		
2	2	5	4	101.944	101.950	101.650	7.811	-0.005	-0.0059	1.0000		
2	2	5	5	7.397	*	1.052	.995	-0.342	6.345	2.5603	1.CCCC	
2	2	5	6	37.859	36.652	36.520	3.109	1.207	1.8815	1.9000	**	
2	2	5	7	75.972	72.646	-72.150	-8.471	3.326	5.8347	1.0000		
2	2	5	8	27.507	29.303	29.103	3.419	-1.797	-1.9348	1.0000		
2	2	5	9	9.185	*	.818	-.791	-0.206	8.368	3.1739	1.0000	**
2	2	5	10	41.731	41.081	40.702	5.567	.650	.8178	1.0000		
2	2	5	11	31.399	33.322	-32.831	-5.696	-1.922	-1.8607	1.0000		
2	2	6	0	95.727	97.498	97.159	8.119	-1.770	-1.8797	1.0000		
2	2	6	1	21.261	19.498	19.300	2.768	1.763	2.4743	1.0000		
2	2	6	2	71.754	72.902	72.708	5.321	-1.148	-1.7716	1.0000		
2	2	6	3	145.637	158.852	158.324	12.942	-13.215	-10.9494	1.0000		
2	2	6	4	40.228	38.058	37.913	3.327	2.170	3.9611	1.0000		
2	2	6	5	38.193	35.935	-35.858	-2.354	2.258	2.7413	1.0000		
2	2	6	6	92.008	90.009	89.446	10.049	1.995	2.5803	1.0000		
2	2	6	7	76.562	75.360	74.772	9.401	1.201	2.1929	1.0000		
2	2	6	8	14.137	6.588	6.555	.659	7.550	4.6256	1.0000		
2	2	6	9	30.070	28.627	28.314	4.219	1.443	1.5394	1.0000		
2	2	6	10	36.859	36.148	35.719	5.553	.711	.8384	1.0000		
2	2	6	11	6.299	*	4.009	1.343	2.071	4.4605	1.0000	**	
2	2	6	12	7.364	*	5.314	5.312	-0.168	2.049	1.0147	1.0000	**
2	2	6	13	70.808	72.985	-72.619	-7.305	-2.177	-3.0750	1.0000		
2	2	6	14	48.095	48.665	48.479	4.250	-.570	-1.2432	1.0000		
2	2	6	15	88.510	91.843	-91.687	-5.348	-3.333	-4.2642	1.0000		
2	2	6	16	9.815	*	2.625	2.542	.654	7.191	3.9143	1.0000	**
2	2	6	17	65.410	64.261	-63.737	-8.193	1.149	2.3032	1.0000		
2	2	6	18	30.108	27.958	27.844	2.525	2.149	2.7896	1.0000		
2	2	6	19	30.491	29.472	-29.210	-3.915	1.019	1.2607	1.0000		
2	2	6	20	17.903	13.891	13.722	2.162	4.012	3.0693	1.0000		
2	2	6	21	57.376	58.238	-57.817	-6.992	-.862	-1.3352	1.0000		
2	2	6	22	6.155	*	3.240	3.156	.732	2.915	.6632	1.0000	
2	2	6	23	120.804	120.037	119.768	8.031	.767	.6208	1.0000		
2	2	6	24	87.245	87.533	-87.256	-6.959	-.288	-.3771	1.0000		
2	2	6	25	39.331	39.075	-38.973	-2.822	.256	.4693	1.0000		
2	2	6	26	5.455	*	3.382	.187	-.334	5.073	1.6192	1.0000	**
2	2	6	27	19.927	19.184	19.098	1.812	.743	.7567	1.0000		
2	2	6	28	85.591	86.034	-85.606	-8.569	-.443	-.5651	1.0000		
2	2	6	29	57.922	55.246	54.998	5.229	-.676	4.9858	1.0000		
2	2	6	30	48.146	46.614	-46.150	-6.557	-.077	-.0874	1.0000		
2	2	6	31	28.317	28.395	-28.173	-3.538	-.077	-.0874	1.0000		
2	2	6	32	28.917	28.270	-28.103	-3.425	1.019	1.102	1.0000		
2	2	6	33	29.157	28.138	-27.928	-3.425	1.019	1.102	1.0000		
2	2	6	34	5.994	*	7.338	-7.245	-1.168	-1.344	-.3138	1.0000	**
2	2	6	35	26.318	28.208	-27.878	-4.303	-1.891	-1.6487	1.0000		
2	2	6	36	44.684	43.390	43.255	3.419	1.293	2.3709	1.0000		
2	2	6	37	65.056	66.946	-66.664	-6.138	-1.890	-3.9666	1.0000		
2	2	6	38	14.186	16.811	-16.620	-2.527	-2.625	-1.8711	1.0000		
2	2	6	39	30.945	28.942	-28.484	-5.427	1.388	2.2179	1.0000		
2	2	6	40	2.003								

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	PAGE	
2	2	9	7	26.543	24.465	24.248	3.251	2.077	2.2265	1.0000	9	
2	2	9	8	44.022	43.688	-43.404	-4.979	.334	.4632	1.0000	9	
2	2	9	9	15.799	15.651	15.510	2.101	.147	.0870	1.0000	9	
2	2	9	10	27.868	27.431	-27.048	-4.573	.436	.3980	1.0000	9	
2	2	10	0	22.205	21.870	21.867	.351	.325	.3667	1.0000	10	
2	2	10	1	82.667	82.520	-82.123	-8.085	.147	.2007	1.0000	10	
2	2	10	2	121.606	122.999	-122.417	-11.950	-1.393	-1.2311	1.0000	10	
2	2	10	3	34.697	34.504	-34.419	-2.433	.192	.2930	1.0000	10	
2	2	10	4	46.131	46.868	-46.538	-5.549	.192	.5694	1.0000	10	
2	2	10	5	73.426	75.036	-74.506	-8.902	-1.610	-1.3130	1.0000	10	
2	2	10	6	14.601	15.104	-14.840	-2.811	-.504	-.3287	1.0000	10	
2	2	10	7	40.123	39.714	-39.324	-5.554	.410	.5694	1.0000	10	
2	2	10	8	68.176	68.197	-67.439	-10.141	-.022	-.0368	1.0000	10	
2	2	10	9	12.407	*	14.061	-13.979	-1.514	-1.653	-7.538	1.0000	10
2	2	10	10	15.714	6.511	-6.511	-1.684	9.203	5.0835	1.0000	10	
2	2	11	0	21.241	22.117	-22.114	.346	-.876	-.8901	1.0000	11	
2	2	11	1	70.986	71.276	71.015	6.101	-.291	-.4923	1.0000	11	
2	2	11	2	43.136	43.295	-42.937	-5.557	-.159	-.2685	1.0000	11	
2	2	11	3	36.786	36.659	36.494	3.475	-.126	.1872	1.0000	11	
2	2	11	4	5.275	*	2.740	2.671	2.535	2.6728	1.0000	11	
2	2	11	5	69.207	70.445	70.036	7.578	-1.238	-2.3869	1.0000	11	
2	2	11	6	43.063	43.308	-43.172	-3.425	-.245	-.3641	1.0000	11	
2	2	11	7	18.123	18.968	18.859	2.035	-.845	-.5996	1.0000	11	
2	2	11	8	11.684	*	7.657	-7.229	-2.523	4.027	1.8157	1.0000	11
2	2	11	9	42.074	43.076	42.582	6.505	-1.002	-1.2392	1.0000	11	
2	2	12	0	31.974	31.445	-31.121	-4.500	.529	.7192	1.0000	12	
2	2	12	1	26.730	25.896	-25.786	-2.385	-.833	1.0059	1.0000	12	
2	2	12	2	48.240	47.303	-46.988	-5.452	.936	1.6428	1.0000	12	
2	2	12	3	76.535	76.418	76.055	7.436	.117	.1841	1.0000	12	
2	2	12	4	66.804	67.458	-66.978	-8.039	-.654	-1.2612	1.0000	12	
2	2	12	5	60.995	61.683	-61.281	-7.029	-.689	-1.2422	1.0000	12	
2	2	12	6	5.674	*	5.649	-.519	.001	.0002	1.0000	12	
2	2	12	7	38.213	37.859	37.513	5.103	.354	.4507	1.0000	12	
2	2	12	8	52.408	53.726	-53.062	-8.421	-1.318	-1.8964	1.0000	12	
2	2	12	9	6.233	*	4.479	-.344	-.333	5.753	1.2925	1.0000	13
2	2	13	0	14.655	12.295	-12.240	1.161	2.364	1.6109	1.0000	13	
2	2	13	1	38.705	37.330	-37.193	-3.200	1.375	2.0512	1.0000	13	
2	2	13	2	69.550	89.709	89.059	10.779	-.159	-.1955	1.0000	13	
2	2	13	3	25.523	26.580	26.566	-.863	-1.057	-1.1388	1.0000	13	
2	2	13	4	16.672	9.728	9.321	2.784	6.944	4.9419	1.0000	13	
2	2	13	5	54.871	55.654	-55.325	-6.046	-.783	-1.3120	1.0000	13	
2	2	13	6	36.823	38.863	38.241	6.921	-.039	-2.5798	1.0000	13	
2	2	13	7	15.111	14.828	14.640	2.351	-.283	.1614	1.0000	13	
2	2	13	8	29.638	30.596	30.071	5.645	-.956	-.9394	1.0000	13	
2	2	13	9	22.499	23.396	-22.792	-5.283	-.698	-.6696	1.0000	13	
2	2	14	0	121.341	123.413	122.526	-2.072	-1.8836	-1.8836	1.0000	14	
2	2	14	1	24.686	24.038	23.799	3.375	.648	.6720	1.0000	14	
2	2	14	2	38.729	38.051	-37.890	-3.498	.678	.9671	1.0000	14	
2	2	14	3	45.639	45.421	45.108	5.326	.218	.3359	1.0000	14	
2	2	14	4	57.047	57.420	56.939	7.422	-.374	-.6242	1.0000	14	
2	2	14	5	25.120	25.790	25.469	4.054	-.670	-.6498	1.0000	14	
2	2	14	6	34.675	34.716	34.163	6.168	-.041	-.0485	1.0000	14	
2	2	14	7	6.032	*	1.918	-1.891	4.115	.9549	1.0000	14	

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	PAGE 1C
2	2	14	8	9.312 *	10.102	-10.051	-1.021	-0.790	-0.2672	1.0000	**
2	2	15	0	89.503	89.787	89.266	9.661	-0.283	-0.3690	1.0000	**
2	2	15	1	5.994	7.306	-6.952	-2.250	-1.312	-0.3398	1.0000	**
2	2	15	2	23.274	20.284	-20.198	-1.866	2.989	2.0087	1.0000	**
2	2	15	3	52.413	51.627	-51.155	-6.963	.786	1.2747	1.0000	**
2	2	15	4	55.731	57.963	57.512	7.221	-2.233	-3.5430	1.0000	**
2	2	15	5	22.416	21.465	21.408	1.560	.951	.7882	1.0000	**
2	2	15	6	9.194 *	13.0638	13.533	1.686	-4.443	-1.5397	1.0000	**
2	2	15	7	43.913	45.642	-44.914	-8.117	-1.728	-2.1988	1.0000	**
2	2	15	8	6.326 *	10.947	10.687	2.370	-4.620	-1.0222	1.0000	**
2	2	16	0	44.083	43.269	42.793	6.402	.814	1.1752	1.0000	**
2	2	16	1	5.743 *	4.279	-4.220	-6.397	.122	.3570	1.0000	**
2	2	16	2	74.442	74.785	74.156	9.676	-.343	-.6183	1.0000	**
2	2	16	3	84.117	83.524	82.941	9.849	.593	.8759	1.0000	**
2	2	16	4	23.481	21.935	21.647	3.540	1.546	1.3536	1.0000	**
2	2	16	5	44.639	44.517	-44.055	-6.397	.122	.1628	1.0000	**
2	2	16	6	68.744	70.089	69.170	11.313	-1.345	-2.1576	1.0000	**
2	2	16	7	50.511	52.597	51.984	8.001	-2.085	-2.8295	1.0000	**
2	2	17	0	85.088	86.640	-85.854	-11.648	-1.553	-2.2711	1.0000	**
2	2	17	1	11.866 *	3.978	3.931	.609	7.888	3.7055	1.0000	**
2	2	17	2	8.811 *	1.167	-1.166	-.061	7.644	2.6529	1.0000	**
2	2	17	3	21.290	21.049	20.377	5.273	.241	.1881	1.0000	**
2	2	17	4	66.702	67.192	-66.576	-9.079	-.491	-.7953	1.0000	**
2	2	17	5	19.101	18.454	-18.198	-3.061	.647	.4329	1.0000	**
2	2	17	6	18.324	17.716	-17.375	-3.463	.608	.3712	1.0000	**
2	2	18	0	65.332	66.098	65.541	8.566	-.766	-1.2506	1.0000	**
2	2	18	1	6.034 *	7.114	-7.037	-1.048	-1.080	-.2506	1.0000	**
2	2	18	2	71.042	71.250	-70.702	-8.822	-.209	-.3488	1.0000	**
2	2	18	3	6.141 *	.792	.775	-.161	5.349	1.2195	1.0000	**
2	2	18	4	8.978 *	10.086	9.882	2.015	-1.107	-.3565	1.0000	**
2	2	18	5	6.324 *	2.485	2.466	.310	3.819	.8481	1.0000	**
2	2	18	6	5.324 *	5.399	5.346	.760	.924	.2046	1.0000	**
2	2	19	0	26.908	24.860	24.833	1.167	2.048	1.8615	1.0000	**
2	2	19	1	20.096	19.155	18.909	3.057	.941	.6615	1.0000	**
2	2	19	2	56.884	56.950	-56.275	-8.744	-.066	-.0969	1.0000	**
2	2	19	3	6.259 *	5.744	-5.626	-1.160	.515	.1153	1.0000	**
2	2	19	4	10.842 *	1.936	1.819	-.662	8.906	3.4069	1.0000	**
2	2	19	5	34.071	34.940	34.415	6.038	-.869	-.8851	1.0000	**
2	2	20	0	43.702	43.712	-43.066	-7.487	-.010	-.0128	1.0000	**
2	2	20	1	27.925	27.762	-27.304	-5.021	.163	.1492	1.0000	**
2	2	20	2	36.115	33.750	-33.246	-5.813	2.365	2.5782	1.0000	**
2	2	20	3	22.479	23.894	23.604	3.708	-1.415	-1.0331	1.0000	**
2	2	21	0	15.518	11.550	-11.547	.232	3.968	2.0918	1.0000	**
2	2	21	1	21.664	23.435	-23.237	-3.044	-1.772	-1.2451	1.0000	**
3	3	1	0	118.823 *	126.868	-126.513	-9.485	-8.045	-7.3737	1.0000	**
3	3	1	1	16.162	14.143	-14.132	-.567	2.018	2.2272	1.0000	**
3	3	1	2	35.739	37.782	37.765	1.152	-2.043	-3.9213	1.0000	**
3	3	1	3	111.198	112.834	-112.607	-7.145	-1.636	-1.6395	1.0000	**
3	3	1	4	25.267	23.175	-22.947	-3.244	2.092	2.6685	1.0000	**
3	3	1	5	19.448	18.292	18.214	1.687	1.157	1.1194	1.0000	**
3	3	1	6	60.694	59.343	-58.977	-6.587	1.350	2.6141	1.0000	**
3	3	1	7	33.877	32.521	-32.377	-3.055	1.356	1.7914	1.0000	**
3	3	1	8	24.739	24.127	24.022	.517	.5061	.5061	1.0000	**

	H	K	L	F(CBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
3	1	9	38.0.594	39.867	-39.597	-4.631	-1.273	-1.5884	1.0.CCCC		
3	1	10	29.733	29.236	-28.757	-5.269	.497	.4866	1.0.CCCC		
3	1	11	15.885	15.495	15.291	2.506	.390	.2110	1.0.CCCC		
3	2	1	21.279	20.519	20.512	.524	.760	1.0560	1.0.CCCC		
3	2	2	108.729	117.811	-117.390	-9.958	-9.083	-9.5079	1.0.CCCC		
3	2	3	13.414	15.149	14.745	3.476	-1.736	-1.3918	1.0.CCCC		
3	2	4	155.844	164.946	-164.238	-15.269	-9.02	-7.1837	1.0.CCCC		
3	2	5	5.195	8.395	-8.206	-1.771	-3.200	-0.8625	1.0.CCCC	**	
3	2	6	85.680	83.419	-82.677	-11.103	2.261	3.3507	1.0.CCCC		
3	2	7	41.105	40.929	40.687	4.442	.177	.2683	1.0.CCCC		
3	2	8	82.338	81.220	-80.515	-10.681	1.117	1.9300	1.0.CCCC		
2	2	9	21.688	20.912	-20.855	-1.544	-1.544	.6280	1.0.CCCC		
2	2	10	66.639	68.108	-67.161	-11.322	-1.469	-2.3559	1.0.CCCC		
2	2	11	23.637	22.715	22.531	2.887	.921	.7361	1.0.CCCC		
3	3	0	6.687	* 6.885	6.597	-1.971	-1.98	-0.0915	1.0.CCCC	**	
3	3	1	36.209	36.249	36.095	3.944	-.041	-.0816	1.0.CCCC		
3	3	2	43.691	44.186	44.058	3.354	-.495	-1.0634	1.0.CCCC		
3	3	3	47.850	49.411	-49.112	-5.431	-1.561	-3.3063	1.0.CCCC		
3	3	4	36.627	35.435	35.324	2.811	1.192	2.0051	1.0.CCCC		
3	3	5	65.740	64.712	64.340	6.934	1.028	1.7750	1.0.CCCC		
6	6	6	14.093	12.957	-12.638	-2.858	1.136	.7695	1.0.CCCC		
7	7	7	23.594	22.559	-22.422	-2.477	1.036	1.0453	1.0.CCCC		
8	8	8	43.593	41.959	41.607	5.421	1.634	2.3980	1.0.CCCC		
9	9	9	11.287	* 4.597	4.592	-.208	6.690	3.0106	1.0.CCCC		
10	10	11	6.121	* 2.071	-1.958	-.673	4.051	.9262	1.0.CCCC	**	
11	11	12	18.052	17.262	16.991	3.571	.690	.4239	1.0.CCCC		
12	12	13	76.633	78.791	78.724	3.251	-2.158	-2.9637	1.0.CCCC		
1	1	14	23.525	23.957	-23.817	-2.582	-.431	-.6112	1.0.CCCC		
1	1	15	125.414	138.457	-138.085	-10.144	-13.064	-10.8677	1.0.CCCC	*	
3	13	16	95.625	99.688	-99.362	-8.053	-4.063	-4.8663	1.0.CCCC		
4	14	17	8.444	* 9.671	9.645	* 718	-1.227	-5.5695	1.0.CCCC	**	
5	15	18	28.905	26.847	26.781	1.887	2.058	2.7672	1.0.CCCC		
6	16	19	35.432	35.251	-34.875	-5.138	-.180	.180	2.586	1.0.CCCC	
7	17	20	78.561	77.234	-76.665	-9.360	1.327	2.1595	1.0.CCCC		
8	18	21	33.737	33.537	-33.310	-3.899	.200	.2457	1.0.CCCC		
9	19	22	16.378	12.952	12.824	1.819	3.425	2.1849	1.0.CCCC		
10	20	23	6.168	* 1.054	1.049	-.108	5.114	1.1610	1.0.CCCC	**	
10	21	24	115.679	117.631	-117.544	-4.515	-1.952	-1.6264	1.0.CCCC		
11	22	25	57.476	59.016	58.836	4.599	-1.539	-2.9924	1.0.CCCC		
12	23	26	117.150	125.905	125.493	10.173	-8.754	-8.6215	1.0.CCCC		
13	24	27	30.047	30.737	-30.737	-.102	-.689	-1.0318	1.0.CCCC		
14	25	28	16.355	13.521	13.340	2.204	2.834	2.4432	1.0.CCCC		
15	26	29	51.413	51.091	50.891	4.969	.322	.6005	1.0.CCCC		
16	27	30	24.897	22.584	-22.582	.269	2.313	2.5217	1.0.CCCC		
17	28	31	29.943	30.127	29.891	3.762	-.164	-.2169	1.0.CCCC		
18	29	32	64.758	64.168	63.635	8.254	.589	1.0217	1.0.CCCC		
19	30	33	22.379	23.175	-23.107	-1.775	-1.796	-6.456	1.0.CCCC		
20	31	34	14.523	-14.483	-14.483	-1.074	-6.671	-.3310	1.0.CCCC		
21	32	35	28.054	-28.022	-28.022	1.345	-.386	.5739	1.0.CCCC		
22	33	36	70.233	71.897	-71.668	-5.735	-1.663	-2.6491	1.0.CCCC		
23	34	37	33.479	34.029	34.255	1.638	-.816	-1.2854	1.0.CCCC		
24	35	38	38.309	39.016	38.771	4.367	-.708	-1.1813	1.0.CCCC		
25	36	39	108.504	110.580	-110.040	-2.076	-2.2150	1.0.CCCC			

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
3	6	6	6	86.397	87.160	86.373	-763	-1.0478	1.0000		
3	6	7	38.894	38.394	38.149	500	.7064	1.0000			
3	6	8	73.299	73.812	73.175	9.678	-9.461	.5511	1.0000		
3	6	9	60.897	60.552	-59.808	-345	-2.447	-1.6931	1.0000		
3	6	10	19.620	22.408	21.992	4.299	-2.789	-1.8691	1.0000		
3	7	0	12.441	6.063	5.995	-905	6.378	4.5179	1.0000		
3	7	1	63.591	63.292	63.150	4.241	-1.760	6.070	1.0000		
3	7	2	8.767 *	6.020	5.893	1.234	2.746	1.3391	1.0000	**	
3	7	3	32.439	33.714	-33.259	-5.524	-1.275	-1.9091	1.0000		
3	7	4	27.119	27.408	27.237	3.059	-2.289	-3.3804	1.0000		
3	7	5	88.067	89.827	89.414	8.603	-1.760	-2.2514	1.0000		
3	7	6	24.527	23.452	-23.178	-3.578	1.075	1.1308	1.0000		
3	7	7	18.798	19.113	-18.855	-3.131	-3.15	-2.522	1.0000		
3	7	8	28.475	28.980	28.640	4.428	-5.505	-5.115	1.0000		
3	7	9	20.896	22.088	22.044	1.391	-1.192	-8.806	1.0000		
3	7	10	6.215 *	3.808	-3.789	-3.388	2.406	.5422	1.0000	**	
3	8	0	156.428	163.282	162.537	15.585	-6.855	-3.7911	1.0000		
3	8	1	78.071	76.362	75.919	8.211	1.710	2.4686	1.0000		
3	8	2	38.963	38.673	-38.537	-3.238	2.90	.4958	1.0000		
3	8	3	9.477 *	10.380	10.376	.285	-903	-4.4501	1.0000	**	
3	8	4	108.123	115.952	115.377	11.527	-7.829	-7.4802	1.0000		
3	8	5	109.221	113.558	112.744	13.570	-4.337	-4.4468	1.0000		
3	8	6	9.461 *	9.753	9.401	2.597	-2.292	-1.297	1.0000		
3	8	7	33.352	32.527	-32.384	-3.047	.825	1.0147	1.0000		
3	8	8	26.289	26.879	26.653	3.477	-5.590	-5.672	1.0000		
3	8	9	80.169	81.079	81.046	11.655	-1.710	-2.9096	1.0000		
3	8	10	46.826	46.416	45.752	7.823	.410	.5337	1.0000		
3	9	1	145.855	151.674	-151.221	-11.704	-5.819	-4.3191	1.0000		
3	9	2	5.142 *	5.513	-5.406	-1.078	-3.71	-1.0111	1.0000	**	
3	9	3	27.015	27.063	26.854	3.516	.032	.0409	1.0000	**	
3	9	4	54.107	54.468	-54.258	-4.779	-3.61	-6.6928	1.0000		
3	9	5	52.996	54.308	-54.100	-4.747	-3.312	-2.4238	1.0000		
3	9	6	5.386 *	1.823	-1.668	-7.735	3.564	.9261	1.0000	**	
3	9	7	58.142	58.246	-57.974	-5.619	-104	-1.1835	1.0000		
3	9	8	7.874 *	.359	-117	-3.340	7.515	2.5279	1.0000	**	
3	9	9	9.083 *	10.111	9.815	2.431	-1.026	-3.6663	1.0000	**	
3	9	10	41.940	42.375	-41.928	-6.135	-4.434	-5.4530	1.0000		
3	10	0	148.514	154.198	-153.442	-15.252	-5.684	-4.0780	1.0000		
3	10	1	40.616	40.934	-39.855	-6.192	.282	.3314	1.0000		
3	10	2	48.244	47.763	47.472	5.269	.481	.8677	1.0000		
3	10	3	30.555	29.997	29.914	2.231	.559	.7555	1.0000		
3	10	4	111.087	113.925	113.245	12.427	-2.838	-3.0132	1.0000		
3	10	5	97.742	102.730	-102.088	-11.466	-4.988	-5.8792	1.0000		
3	10	6	9.762 *	11.082	-11.063	-6.686	-2.120	-9.9580	1.0000	**	
3	10	7	16.384	18.831	-18.557	-3.199	-2.447	-1.6931	1.0000		
3	10	8	99.628	101.154	100.186	-1.526	-1.8176	-1.8176	1.0000		
3	10	9	27.511	25.733	-25.426	-3.966	1.778	1.7209	1.0000	**	
3	10	10	12.641 *	10.637	-10.611	-7.740	2.004	.9318	1.0000	**	
3	11	0	42.076	41.228	-41.011	-8.49	1.3810	1.0000			
3	11	1	15.926	13.738	-13.736	-2.230	2.188	1.6654	1.0000	**	
3	11	2	5.344 *	9.045	-8.885	-1.697	-3.701	-9.9697	1.0000	**	
3	11	3	79.804 *	80.181	-79.664	-9.096	-3.376	-5.578	1.0000		
3	11	4	5.384 *	2.941	-2.932	2.443	1.6353	1.0000	**		

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR	
3	3	11	5	47.091	48.827	48.661	4.026	-1.736	-2.7549	1.0000		
3	3	11	6	44.414	46.016	-45.617	-6.049	-1.602	-2.3661	1.0000		
3	3	11	7	40.079	40.059	-39.566	-6.266	.020	.0256	1.0000		
3	3	11	8	16.556	16.269	16.184	1.656	.287	.1749	1.0000		
3	3	11	9	8.918 *	7.983	-7.708	-2.078	.935	.3028	1.0000	**	
3	3	12	0	43.862	43.520	43.443	2.584	.342	.5493	1.0000		
3	3	12	1	24.122	23.112	-22.793	-3.825	1.010	1.0753	1.0000		
3	3	12	2	109.593	109.616	-109.031	-11.315	-1.023	-1.0258	1.0000		
3	3	12	3	95.812	96.872	-96.399	-9.562	-1.060	-1.2144	1.0000	**	
3	3	12	4	7.419 *	.256	.248	-.064	7.164	2.4785	1.0000	**	
3	3	12	5	19.994	21.102	21.081	.928	-1.108	-9.112	1.0000		
3	3	12	6	31.878	34.650	-34.136	-5.947	-2.772	-3.1358	1.0000		
3	3	12	7	69.614	71.080	-70.267	-10.721	-1.466	-2.4565	1.0000		
3	3	12	8	32.495	33.458	-33.111	-4.811	-.964	-.9904	1.0000		
3	3	12	9	6.257 *	2.393	2.203	.935	3.864	.8646	1.0000		
3	3	13	0	48.687	48.488	-48.488	-5.560	-.118	-.1930	1.0000		
3	3	13	1	5.500 *	7.179	6.937	1.848	-1.679	-.4275	1.0000	**	
3	3	13	2	51.689	50.560	50.158	6.367	1.129	1.8984	1.0000		
3	3	13	3	18.589	17.571	-17.409	-2.383	1.018	.8032	1.0000		
3	3	13	4	7.863 *	3.588	-3.584	1.158	4.275	1.4918	1.0000		
3	3	13	5	11.421 *	9.450	9.098	2.553	1.971	.9398	1.0000	**	
3	3	13	6	12.724	10.222	-10.083	-1.684	2.501	1.2851	1.0000		
3	3	13	7	6.003 *	4.070	3.929	1.063	1.933	.4508	1.0000	**	
3	3	13	8	30.415	29.582	29.085	5.399	.833	.8168	1.0000		
3	3	13	9	17.878	-17.722	-2.356	1.125	.9069	1.0000			
3	3	13	10	19.003	17.878	-17.722	-2.356	1.125	.9069	1.0000		
3	3	13	11	86.110	83.999	-83.318	-10.672	2.111	3.1079	1.0000		
3	3	13	12	49.269	48.777	48.361	6.363	.491	.7878	1.0000		
3	3	13	13	47.794	47.707	-47.240	-6.658	.088	.1346	1.0000		
3	3	13	14	7.889 *	10.261	-10.240	-6.658	-2.372	-.7631	1.0000		
3	3	13	15	87.052	89.128	-88.210	-12.757	-2.076	-2.8513	1.0000		
3	3	13	16	24.142	24.752	24.551	3.153	-.610	-.5291	1.0000		
3	3	13	17	23.200	21.996	-21.550	-4.408	1.204	.9851	1.0000		
3	3	13	18	6.279 *	11.491	11.204	2.553	-5.212	-1.1621	1.0000		
3	3	13	19	0	13.098	11.531	-11.518	-5.545	1.567	.8476	1.0000	
3	3	13	20	42.421	40.712	40.392	5.095	1.709	2.4447	1.0000		
3	3	13	21	48.701	47.421	47.190	4.676	1.279	1.9475	1.0000		
3	3	13	22	28.224	26.382	-26.323	-1.774	1.842	1.9144	1.0000		
3	3	13	23	31.611	31.477	31.286	3.461	.133	.1468	1.0000		
3	3	13	24	53.448	53.724	53.191	7.547	-.276	-.4058	1.0000		
3	3	13	25	6.733 *	10.287	-10.252	-.849	-.554	-.2004	1.0000		
3	3	13	26	6.177 *	1.199	1.091	.498	4.978	1.1278	1.0000		
3	3	13	27	16.772	16.680	16.290	3.585	.092	.0593	1.0000		
3	3	13	28	21.047	19.918	19.691	2.995	1.129	.8977	1.0000		
3	3	13	29	5.914 *	6.722	6.712	.975	-.808	-.1913	1.0000		
3	3	13	30	16.351	16.763	16.689	1.571	-.412	-.2525	1.0000		
3	3	13	31	22.940	21.743	21.563	2.788	1.197	.9720	1.0000		
3	3	13	32	23.922	21.974	21.642	3.807	1.947	1.6377	1.0000		
3	3	13	33	10.263 *	1.367	1.000	1.367	8.896	3.3237	1.0000		
3	3	13	34	6.259 *	3.700	3.606	.826	2.559	.9724	1.0000		
3	3	13	35	18.059	-17.683	-3.665	4.246	3.4235	1.0000			
3	3	13	36	16.531	14.466	14.193	2.799	2.065	1.2828	1.0000		
3	3	13	37	28.250	27.051	26.830	3.450	1.199	1.1682	1.0000		
3	3	13	38	19.241	-17.773	-2.496	1.0141	1.0000				

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	17	4	7.569 *	6.131	6.094	.679	1.437	.3977	1.CCCC **
3	17	5	24.552	24.534	24.120	4.487	.018	.0150	1.C000
3	17	6	10.530 *	7.645	-7.266	-2.376	2.885	1.0595	1.0000
3	16	0	6.293 *	2.490	-2.426	.561	3.803	.8905	1.CCCC **
3	18	1	61.912	61.191	60.372	9.976	.721	1.1243	1.CCCC **
3	18	2	6.170 *	7.726	-7.582	-1.485	-1.556	-3.531	1.CCCC **
3	18	3	62.339	62.466	61.809	9.040	-.127	-.1949	1.CCCC
3	18	4	6.302 *	3.023	3.015	.220	3.278	.7281	1.CCCC **
3	18	5	54.579	53.499	52.585	9.847	1.080	1.4928	1.0000
3	19	0	43.702	44.395	-43.916	-6.506	-.694	-.8605	1.CCCC
3	19	1	6.558 *	6.570	-6.516	-.843	-.012	-.028	1.CCCC **
3	19	2	12.499 *	11.106	11.007	1.480	1.392	.6024	1.CCCC
3	19	3	40.115	39.483	-39.138	-5.209	.631	.7268	1.CCCC
3	19	4	14.329	10.312	-10.103	-2.065	4.017	1.9547	1.0000
3	20	0	6.854 *	9.873	-9.685	-1.918	-3.019	-.7007	1.CCCC **
3	20	1	7.998 *	.199	-.056	-.191	7.799	2.1581	1.CCCC
3	20	2	24.641	24.213	23.859	4.125	.428	.3345	1.CCCC
4	0	0	25.483	24.977	24.320	5.694	.505	.6713	1.CCCC
4	0	1	74.698	76.907	76.547	7.432	-2.209	-3.4930	1.CCCC
4	0	3	136.648	145.313	144.623	14.151	-.8.666	-.0241	1.CCCC
4	4	4	5.239 *	1.929	1.865	.493	3.311	.8845	1.CCCC **
4	5	5	29.284	30.123	29.838	4.130	-.839	-.0411	1.CCCC
4	6	6	21.581	22.915	22.355	5.034	-1.334	-1.2198	1.CCCC
4	7	7	78.559	77.022	76.367	10.029	1.537	2.8284	1.CCCC
4	8	8	22.590	20.958	-20.674	-3.442	1.632	1.4041	1.0000
4	9	0	54.530	53.330	52.604	6.773	1.200	1.7968	1.0000
4	10	0	16.749	16.151	15.809	3.305	3.599	.3491	1.0000
4	11	1	54.446	55.846	55.708	3.912	-1.400	-2.5452	1.0000
4	11	3	26.678	27.478	27.217	3.775	-.799	-1.0909	1.0000
4	11	4	42.497	42.080	-41.819	-4.672	.418	.7383	1.0000
4	11	5	6.308 *	.687	.676	.121	5.621	1.8174	1.0000 **
4	11	6	84.689	85.144	84.557	9.980	-.454	-.6713	1.0000
4	11	7	78.550	77.138	-76.666	-8.522	1.412	2.3573	1.CCCC
4	11	8	71.266	70.718	-69.812	-7.536	1.049	1.9707	1.0000
4	11	9	53.691	53.942	-53.509	-6.825	-.251	-.3904	1.0000
4	11	10	65.163	64.752	64.169	8.671	.411	.6707	1.0000
4	11	11	6.193 *	5.087	-5.025	-.701	1.105	-2.499	1.0000 **
4	12	0	101.668	106.728	106.466	7.476	-.5.060	-5.4110	1.0000
4	12	1	4.961 *	4.535	-4.533	-.099	.427	-.1203	1.0000
4	12	2	34.073	34.589	-34.517	-2.231	-.516	-.8246	1.0000
4	12	3	88.769	91.231	91.024	6.145	-2.462	-3.1776	1.0000
4	12	4	18.682	17.619	17.507	1.983	1.063	.9667	1.0000
4	12	5	25.169	26.184	-26.092	-2.0193	-1.015	-1.1370	1.0000
4	12	6	48.881	48.094	47.862	4.725	.787	1.3187	1.0000
4	12	7	19.798	20.950	20.816	2.363	-.1.152	-.9425	1.0000
4	12	8	25.020	22.590	-22.442	-2.575	2.430	2.3416	1.0000
4	12	9	34.327	34.751	34.527	3.935	-.424	-.4697	1.0000
4	12	10	23.875	22.667	22.169	3.652	1.408	1.1268	1.0000
4	12	11	14.529	12.380	-12.203	-2.084	2.150	1.6967	1.0000
4	12	12	29.108	28.349	28.349	.158	.759	1.0714	1.0000
4	12	13	76.873	79.995	79.824	5.231	-.3.122	-4.5821	1.0000
4	12	14	110.382	123.766	-123.304	-6.097	-6.047	-2.0942	1.0000
4	12	15	66.161	-64.693	-7.450	-1.040	2.0942	1.0000	

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTER
4	4	3	6	52.535	51.710	-51.453	-5.145	.825	1.4308	1.0000
4	4	3	7	69.225	69.026	68.608	7.581	.196	.3641	1.0000
4	4	3	8	32.637	29.734	-29.228	-5.461	2.903	3.3256	1.0000
4	4	3	9	34.614	34.842	-34.260	-6.341	-2.277	-2.277	1.0000
4	4	3	10	53.466	53.698	-52.854	-9.483	-2.322	-3.283	1.0000
4	4	4	0	57.162	56.922	56.760	4.297	.240	.4773	1.0000
4	4	4	1	103.242	106.356	-105.868	-10.182	-3.114	-3.2676	1.0000
4	4	4	2	43.555	44.700	-44.591	-3.126	-1.146	-2.0998	1.0000
4	4	4	3	40.117	40.825	-40.695	-3.255	-0.703	-1.1994	1.0000
4	4	4	4	12.209	11.053	-11.023	-1.156	1.156	.7143	1.0000
4	4	4	5	102.193	103.216	-102.510	-12.049	-1.022	-1.1448	1.0000
4	4	4	6	33.432	33.380	33.183	3.621	.052	.0689	1.0000
4	4	4	7	37.267	38.005	-37.631	-5.320	-0.736	-0.9843	1.0000
4	4	4	8	38.999	38.088	-37.824	-4.470	.911	1.1726	1.0000
4	4	4	9	35.035	34.514	-34.175	-4.822	.521	.5854	1.0000
4	4	4	10	16.678	15.194	15.010	2.356	1.485	.8581	1.0000
4	4	5	0	102.877	106.958	106.448	10.429	-4.081	-4.2127	1.0000
4	4	5	1	21.546	21.445	-21.272	-2.723	.100	.1069	1.0000
4	4	5	2	36.427	40.280	-40.242	-1.735	-1.853	-3.0372	1.0000
4	4	5	3	75.956	77.686	-77.295	-7.781	-1.730	-2.4825	1.0000
4	4	5	4	62.273	63.689	63.216	7.747	-1.416	-2.8398	1.0000
4	4	5	5	20.127	20.820	20.774	1.372	-0.692	-0.6346	1.0000
4	4	5	6	5.509 *	8.455	8.182	2.131	-2.946	-7.487	1.0000
4	4	5	7	66.829	67.308	-66.714	-8.923	-4.480	-8.649	1.0000
4	4	5	8	10.659 *	9.564	9.232	2.497	1.096	.4629	1.0000
4	4	5	9	10.483 *	11.738	11.677	1.197	-1.255	-4.4865	1.0000
4	4	5	10	25.040	26.903	26.332	5.515	-1.866	-1.5081	1.0000
4	4	6	0	22.501	24.103	24.094	.659	-1.602	-1.7171	1.0000
4	4	6	1	61.756	61.361	-61.056	-6.305	.375	.7387	1.0000
4	4	6	2	78.782	80.551	-80.150	-8.025	-1.779	-2.4602	1.0000
4	4	6	3	5.680 *	6.010	-6.010	-.002	-.330	-.0993	1.0000
4	4	6	4	32.931	34.745	-34.482	-4.267	-1.84	-2.5538	1.0000
4	4	6	5	63.909	63.702	-63.197	-7.999	-7.208	-4.004	1.0000
4	4	6	6	7.228 *	2.326	2.191	-.781	4.902	1.6139	1.0000
4	4	6	7	17.357	19.236	-19.042	-2.726	-1.879	-1.3353	1.0000
4	4	6	8	50.649	51.454	-50.881	-7.652	-.804	-1.1806	1.0000
4	4	6	9	9.439 *	10.116	-10.041	-1.234	-0.677	-0.2372	1.0000
4	4	6	10	6.270 *	1.738	-1.475	-0.919	4.532	1.0121	1.0000
4	4	6	11	59.759	59.341	59.147	4.787	.418	.8270	1.0000
4	4	6	12	5.199 *	4.605	4.590	-.369	.595	.1601	1.0000
4	4	6	13	85.662	87.903	87.310	10.195	-2.241	-2.9510	1.0000
4	4	6	14	17.992	18.963	18.862	1.950	-0.971	-.8398	1.0000
4	4	6	15	37.948	38.468	38.067	5.539	-.520	-.7888	1.0000
4	4	6	16	17.099	14.106	-13.940	-2.163	2.993	2.3537	1.0000
4	4	6	17	65.161	66.499	66.073	7.518	-1.339	-2.4341	1.0000
4	4	6	18	27.462	25.582	25.447	2.620	1.880	1.9368	1.0000
4	4	6	19	36.086	35.570	34.930	6.715	.517	.6238	1.0000
4	4	6	20	15.456	13.556	-13.420	-1.914	1.900	1.0640	1.0000
4	4	6	21	35.866	35.465	35.407	2.018	.401	.5929	1.0000
4	4	6	22	15.663	15.194	14.897	2.993	.469	.3610	1.0000
4	4	6	23	56.196	57.030	-56.732	-5.827	-.834	-1.6217	1.0000
4	4	6	24	91.425	95.990	9.153	-5.000	-6.3257	1.0000	1.0000
4	4	6	25	23.407	-22.379	-2.836	1.028	1.0888	1.0000	1.0000

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTR
4	4	8	5	9.332 *	11.114	-11.104	.484	-1.782	-0.7696	1.0000 ***
4	4	8	6	14.663	15.067	15.040	.910	-0.404	-0.2557	1.0000 ***
4	4	8	7	37.710	36.135	35.713	5.505	1.575	-0.011	1.0000 ***
4	4	8	8	41.923	41.933	-41.463	-6.263	-6.263	-0.0139	1.0000 ***
4	4	8	9	34.955	37.423	36.993	5.661	-2.468	-2.6519	1.0000 ***
4	4	9	0	23.220	22.620	-22.510	-2.229	.601	.6303	1.0000 ***
4	4	9	1	63.163	61.658	61.343	6.215	1.506	2.9923	1.0000 ***
4	4	9	2	5.309 *	1.645	-1.441	-1.128	3.664	0.9742	1.0000 ***
4	4	9	3	41.929	43.234	42.742	6.504	-1.305	-2.0485	1.0000 ***
4	4	9	4	10.967 *	13.785	-13.656	-1.911	-2.823	-1.4470	1.0000 ***
4	4	9	5	44.421	45.903	45.589	5.365	-1.482	-2.2955	1.0000 ***
4	4	9	6	55.669 *	8.134	-8.056	-2.465	-2.465	-6.089	1.0000 ***
4	4	9	7	41.355	41.857	41.418	6.045	-5.502	-6.6691	1.0000 ***
4	4	9	8	6.054 *	4.542	-4.364	-1.259	1.512	0.3497	1.0000 ***
4	4	9	9	19.825	18.165	17.633	4.363	1.660	1.1311	1.0000 ***
10	0	6	69.536	68.295	67.658	9.307	1.241	1.9158	1.0000 ***	
10	1	5	21.706	21.688	21.475	3.034	0.018	0.0175	1.0000 ***	
10	2	2	22.416	24.036	23.956	1.960	-1.620	-1.6127	1.0000 ***	
10	3	72.689	73.784	73.237	8.971	-1.095	-1.9279	1.0000 ***		
10	4	4	37.275	38.044	37.795	4.349	-7.69	-1.0721	1.0000 ***	
10	5	9	9.822 *	2.445	-2.388	0.524	7.377	3.2640	1.0000 ***	
10	6	6	40.858	43.808	43.140	7.620	-2.950	-3.9784	1.0000 ***	
10	7	3	33.962	35.118	34.690	5.470	-1.156	-1.3147	1.0000 ***	
10	8	8	8.003 *	5.874	5.873	1.106	2.129	0.6298	1.0000 ***	
10	9	9	29.892	28.171	27.654	5.376	1.720	1.6367	1.0000 ***	
11	0	5	5.509 *	7.374	-7.185	-1.662	-1.865	-1.865	-4.741	1.0000 ***
11	1	10	10.902 *	3.250	2.632	1.907	7.652	3.9095	1.0000 ***	
11	2	75.902	76.401	-75.863	-9.057	-4.499	-0.8146	1.0000 ***		
11	3	5	5.542 *	5.444	-5.313	-1.187	0.98	0.248	0.000	**
11	4	11	17.992	17.374	-17.139	-2.844	.618	.4714	1.0000 ***	
11	5	5	20.648	20.453	20.021	4.180	.196	.1642	1.0000 ***	
11	6	39.362	40.016	-39.557	-6.041	-6.654	-.8509	1.0000 ***		
11	7	25.521	24.603	-24.491	-2.341	.918	.8243	1.0000 ***		
11	8	28.032	27.662	-27.217	-4.941	.370	.3427	1.0000 ***		
12	0	12	98.248	97.160	96.613	10.296	1.087	1.3234	1.0000 ***	
12	1	29.887	26.551	-26.377	-3.037	3.336	3.9950	1.0000 ***		
12	2	11.975	12.380	12.185	2.186	-.405	-.2100	1.0000 ***		
12	3	32.570	31.888	31.785	2.558	.682	.8439	1.0000 ***		
12	4	38.667	38.556	38.182	5.358	.111	.1501	1.0000 ***		
12	5	35.173	36.226	-35.912	-4.756	-1.052	-1.2805	1.0000 ***		
12	6	57.011	58.671	58.148	7.812	-1.660	-2.5883	1.0000 ***		
12	7	6.017 *	1.271	-1.228	-0.330	4.746	1.1042	1.0000 ***		
12	8	6.193 *	1.694	1.388	.972	4.498	1.0172	1.0000 ***		
13	0	13	60.135	58.107	-57.765	-6.297	2.028	3.9300	1.0000 ***	
13	1	70.053	69.271	-68.749	-8.494	.781	1.4267	1.0000 ***		
13	2	63.310	62.507	62.240	5.780	.803	1.4140	1.0000 ***		
13	3	20.386	19.105	-18.810	-3.346	1.280	1.0378	1.0000 ***		
13	4	20.208	18.599	-18.206	-3.803	1.608	1.2693	1.0000 ***		
13	5	82.162	84.347	-83.533	-11.684	-2.105	-3.5166	1.0000 ***		
13	6	9.775 *	9.566	9.425	1.641	.209	.0781	1.0000 ***		
13	7	7.569 *	2.244	-2.062	-0.887	5.324	1.4607	1.0000 ***		
14	0	7.560 *	7.608	7.591	.509	-.048	-.0150	1.0000 ***		
4	1	36.004	33.884	-33.546	-4.774	2.120	2.6821	1.0000 ***		

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTR
5	4	14	2	50.796	50.364	-50.054	-5.583	.432	.6556	1.0000
5	4	14	3	5.908 *	2.274	2.064	.953	3.634	.8612	1.0000
5	4	14	4	29.562	28.428	-28.197	-3.616	1.134	1.1677	1.0000
5	4	14	5	42.023	41.985	-41.460	-6.619	.037	.0486	1.0000
5	4	14	6	11.655 *	3.827	3.813	.318	7.828	3.3323	1.0000
5	4	14	7	6.727 *	4.696	-4.547	-1.172	2.031	.5093	1.0000
5	4	15	0	81.688	80.882	80.220	10.329	.805	1.1233	1.0000
5	4	15	1	14.273	13.921	-13.852	-1.387	.352	.1951	1.0000
5	4	15	2	35.534	35.465	-35.246	-3.940	.069	.0807	1.0000
5	4	15	3	60.950	60.334	-59.884	-7.341	.616	.9882	1.0000
5	4	15	4	48.661	48.509	47.953	7.328	.151	.2096	1.0000
5	4	15	5	24.630	21.790	21.540	3.290	2.840	2.4156	1.0000
5	4	15	6	8.001 *	3.406	3.336	.685	4.595	1.3514	1.0000
5	4	16	0	12.563 *	12.136	-11.873	-2.514	.427	.1986	1.0000
5	4	16	1	6.872 *	10.161	-9.911	-2.239	-3.289	-.8563	1.0000
5	4	16	2	67.739	67.940	-67.210	-9.936	-.201	-.3268	1.0000
5	4	16	3	19.435	19.049	18.866	2.630	.386	.2665	1.0000
5	4	16	4	41.019	39.788	-39.277	-6.358	1.230	1.5096	1.0000
5	4	16	5	13.271	16.854	-16.451	-3.666	-.3.583	-1.6640	1.0000
5	4	16	6	18.883	17.940	-17.547	-3.738	.942	.6002	1.0000
5	4	17	0	44.541	44.056	-43.390	-7.635	.485	.6274	1.0000
5	4	17	1	35.743	35.194	34.872	4.748	.550	.6157	1.0000
5	4	17	2	47.187	45.922	45.434	6.674	1.265	1.6853	1.0000
5	4	17	3	68.806	68.067	67.245	10.548	.739	1.1763	1.0000
5	4	17	4	33.695	31.566	-31.209	-4.735	2.329	2.4724	1.0000
5	4	17	5	1.189	-1.176	-1.175	5.090	1.1351	1.0000	**
5	4	18	0	25.948	22.848	22.554	3.653	3.100	2.6420	1.0000
5	4	18	1	9.867 *	12.510	-12.454	-1.182	-2.643	-.9088	1.0000
5	4	18	2	14.353	14.341	-14.246	-1.648	-.012	.0061	1.0000
5	4	18	3	31.288	31.525	31.287	3.871	-.238	-.2274	1.0000
5	4	18	4	6.357 *	3.699	-3.696	-.132	2.659	-.5856	1.0000
5	4	19	0	34.808	33.790	33.264	5.939	1.019	1.0638	1.0000
5	4	19	1	36.596	36.306	35.851	5.729	.291	.3115	1.0000
5	4	19	2	45.000	44.978	-44.924	-6.372	.022	.0272	1.0000
5	4	19	3	34.236	35.715	-35.493	-3.974	-1.479	-2.1023	1.0000
5	4	19	4	106.188	110.654	110.189	10.133	-.4.465	-.5.3333	1.0000
5	5	1	2	14.694	11.778	11.611	1.976	2.916	2.0788	1.0000
5	5	1	3	19.827	18.410	18.100	3.368	1.416	1.9280	1.0000
5	5	1	4	5.413 *	1.422	-1.359	-.418	3.991	1.0319	1.0000
5	5	1	5	108.589	110.263	109.603	12.043	-.675	-.1.9584	1.0000
5	5	1	6	25.423	25.800	-25.535	-3.690	-.378	-.3820	1.0000
5	5	1	7	37.413	37.253	36.895	5.157	-.160	-.2033	1.0000
5	5	1	8	18.489	18.163	17.840	3.414	.325	.2206	1.0000
5	5	1	9	28.587	26.808	26.307	5.160	1.779	1.6644	1.0000
5	5	1	10	11.390	5.187	-4.884	-1.747	6.202	3.5081	1.0000
5	5	2	1	46.227	45.881	45.496	5.935	.346	.604	1.0000
5	5	2	2	37.694	37.705	37.468	4.220	-.011	-.0165	1.0000
5	5	2	3	74.348	75.689	75.226	8.358	-.1.340	-.2.3154	1.0000
5	5	2	4	12.354	11.421	-11.403	-.635	-.933	-.5543	1.0000
5	5	2	5	17.268	16.141	15.749	3.536	1.128	.8568	1.0000
5	5	2	6	25.846	25.192	25.114	1.982	.653	.6806	1.0000
5	5	2	7	56.842	56.223	53.367	-.163	-.2625	1.0000	
5	5	2	8	6.679	6.485	6.309	-.471	-.4.471	-.1.095	1.0000

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTR
5	5	2	9	10.677 *	13.034	12.701	2.929	-2.357	-0.8948	1.0000
5	3	0	58.890	59.369	-59.232	-4.033	-0.479	-0.9469	1.0000	**
5	1	41.036	41.703	-41.467	-4.433	-0.667	-1.0891	-2.025	-3.1140	1.0000
5	2	78.292	80.317	79.922	7.954	-2.025	-2.5734	-1.433	1.0000	1.0000
5	3	71.954	73.387	-72.910	-8.353	5.020	3.2439	1.373	1.0000	1.0000
5	4	13.445	8.425	8.312	1.373	1.658	1.9494	-3.381	1.0000	1.0000
5	5	28.747	27.089	-26.877	-3.381	-7.354	-1.717	-1.717	-4.263	1.0000
5	6	5.638 *	7.355	.137	.137	-7.354	-0.4263	1.0000	1.0000	**
5	7	29.003	27.343	-27.026	-4.150	1.660	1.7585	1.660	1.0000	1.0000
5	8	41.517	42.307	41.845	6.237	-7.90	-1.0190	-7.90	1.0000	1.0000
5	9	46.256	46.471	-45.787	-7.939	-215	-0.2828	-215	1.0000	1.0000
5	0	88.087	87.658	87.658	8.682	-3.94	-0.4767	-3.94	1.0000	1.0000
5	1	44.332	45.207	45.042	3.862	-8.75	-1.4723	-8.75	1.0000	1.0000
5	2	11.374	11.583	-11.319	-2.456	-2.09	-0.1151	-2.09	1.0000	1.0000
5	3	27.460	29.609	-29.593	-0.978	-2.149	-2.5401	-2.149	1.0000	1.0000
5	4	65.470	67.194	66.902	6.255	-1.723	-3.3217	-1.723	1.0000	1.0000
5	5	67.183	67.712	67.332	7.157	-5.29	-0.9941	-5.29	1.0000	1.0000
5	6	9.165 *	6.830	6.733	1.144	2.335	.9347	2.335	1.0000	**
5	7	18.301	20.250	-20.067	-2.716	-1.948	-1.3651	-1.948	1.0000	1.0000
5	8	20.159	19.532	19.475	1.490	.627	.4591	.627	1.0000	1.0000
5	9	30.241	30.057	29.450	6.014	.184	.1779	.184	1.0000	1.0000
5	0	25.665	24.762	-24.712	-1.567	.903	1.0351	.903	1.0000	1.0000
5	1	59.333	59.813	-59.470	-6.395	-4.79	-.9315	-4.79	1.0000	1.0000
5	2	7.916 *	3.476	3.385	-0.787	4.440	1.7585	4.440	1.0000	**
5	3	114.307	118.294	-117.397	-14.538	-3.987	-4.1065	-3.987	1.0000	1.0000
5	4	23.857	23.983	23.907	1.907	-1.126	-.1287	-1.126	1.0000	1.0000
5	5	14.166	12.889	-12.769	-1.755	1.278	.8025	1.278	1.0000	1.0000
5	6	42.582	42.074	-41.816	-4.652	.508	.7287	.508	1.0000	1.0000
5	7	79.581	80.953	-80.110	-11.650	-1.372	-2.4736	-1.372	1.0000	1.0000
5	8	29.152	29.039	29.039	3.138	-0.055	-.0561	-0.055	1.0000	1.0000
5	9	26.997	26.729	-26.044	-6.014	.268	.2415	.268	1.0000	1.0000
5	0	67.247	65.741	-65.346	-7.196	1.506	2.9031	1.506	1.0000	1.0000
5	1	75.789	76.718	-76.455	-6.346	-0.929	-1.4382	-0.929	1.0000	1.0000
5	2	63.546	63.191	62.780	7.201	.355	.6930	.355	1.0000	1.0000
5	3	11.243 *	11.154	11.154	.001	.069	.0471	.001	1.0000	**
5	4	43.038	43.018	-42.808	-4.250	.020	.0305	.020	1.0000	1.0000
5	5	98.459	99.695	-99.133	-10.564	-1.235	-1.6270	-1.235	1.0000	1.0000
5	6	20.996	21.912	21.805	2.157	-.916	-.7659	-.916	1.0000	1.0000
5	7	8.455 *	11.617	11.371	2.378	-3.162	-1.0575	-1.0575	1.0000	**
5	8	11.572 *	3.601	3.319	1.397	7.971	3.5028	7.971	1.0000	**
5	9	50.253	51.121	-50.344	-8.877	-.868	-1.9218	-.868	1.0000	1.0000
5	0	136.015	137.128	-136.407	-14.040	-1.112	-1.9218	-1.112	1.0000	1.0000
5	1	26.142	26.4970	24.729	3.462	1.172	1.3286	1.172	1.0000	1.0000
5	2	21.604	18.899	18.868	1.090	2.704	2.6344	2.704	1.0000	1.0000
5	3	9.506 *	1.239	-.853	-.899	8.267	3.7768	8.267	1.0000	**
5	4	60.006	62.543	-62.054	-7.809	-2.537	-4.5219	-2.537	1.0000	1.0000
5	5	14.340	16.457	16.209	2.847	-2.117	-1.2777	-2.117	1.0000	1.0000
5	6	50.622	50.137	-49.676	-6.788	-0.685	.7435	-.685	1.0000	1.0000
5	7	27.500	27.427	27.044	4.567	.073	.0708	.073	1.0000	1.0000
5	8	6.121 *	1.014	-.637	-.788	5.108	1.1679	5.108	1.0000	**
5	9	19.920	20.389	-20.223	-2.595	-4.668	-3.3110	-4.668	1.0000	1.0000
5	0	41.638	39.957	39.747	4.090	1.661	2.5847	1.661	1.0000	1.0000
5	1	9.515 *	7.245	-6.972	-1.970	2.0082	1.0082	2.0082	1.0000	**

	H	K	L	F(CBSS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
5	8	2		91.200	-92.633	-11.468	-2.140	-2.7774	1.0000	
5	8	3		69.253	71.704	-71.197	-8.511	-8.511	1.0000	
5	8	4		21.018	22.803	22.778	1.074	-2.451	-4.5669	1.0000
5	8	5		34.307	35.946	35.801	3.229	-1.785	-1.5747	1.0000
5	8	6		41.575	42.541	-42.177	-5.555	-1.639	-2.0336	1.0000
5	8	7		64.735	65.364	-64.580	-10.098	-9.66	-1.3069	1.0000
5	8	8		21.933	21.505	-21.024	-6.29	-4.523	-1.0271	1.0000
5	9	0		18.533	15.303	15.301	-2.17	3.230	.3238	1.0000
5	9	1		86.455	87.278	86.722	9.840	-6.23	2.6329	1.0000
5	9	2		8.624 *	10.070	-10.010	-1.100	-1.446	-1.1409	1.0000
5	9	3		5.556 *	6.914	-6.833	1.053	-1.358	-5.594	1.0000
5	9	4		22.764	24.716	24.574	2.643	-1.952	-1.7746	1.0000
5	9	5		102.550	105.902	105.031	13.555	-3.352	3.8305	1.0000
5	9	6		21.305	20.474	-20.018	-4.301	.831	.6760	1.0000
5	9	7		12.274 *	7.758	7.545	1.808	4.515	2.1013	1.0000
5	9	8		20.334	18.690	18.438	3.059	1.644	1.1664	1.0000
10	0			102.951	101.066	-100.507	-10.623	1.884	2.1314	1.0000
10	1			7.564 *	2.740	-2.739	.080	4.824	1.6462	1.0000
10	2			29.901	30.695	30.445	3.910	-7.794	-9.121	1.0000
10	3			47.957	50.020	49.624	6.283	-2.063	-3.1832	1.0000
10	4			64.586	65.887	-65.462	-7.469	-1.300	-2.2725	1.0000
10	5			34.040	37.053	-36.763	-4.625	-3.013	-3.5240	1.0000
10	6			13.133	9.575	-9.530	-9.932	3.558	1.8074	1.0000
10	7			50.718	50.709	50.079	7.970	.009	.0129	1.0000
10	8			10.929 *	10.250	-10.161	-1.347	.679	.2643	1.0000
11	0			5.705 *	2.983	-2.981	-.111	2.722	.6680	1.0000
11	1			5.887 *	3.926	3.886	.563	1.961	.5036	1.0000
11	2			102.550	101.884	101.021	13.234	.666	.7258	1.0000
11	3			27.382	26.020	-25.943	-2.004	1.362	1.4356	1.0000
11	4			31.760	30.503	30.503	4.953	.857	.9573	1.0000
11	5			5.916 *	2.547	2.529	.299	3.370	.7973	1.0000
11	6			32.205	32.985	32.620	4.898	-.780	-.8340	1.0000
11	7			9.279 *	8.813	8.669	1.588	.466	.1570	1.0000
12	0			85.796	86.011	85.458	9.734	-.215	-.3007	1.0000
12	1			40.210	39.534	39.293	4.357	.676	.9123	1.0000
12	2			24.781	24.613	-24.533	1.161	.169	.1543	1.0000
12	3			7.676 *		.967	-6.43	6.514	2.0530	1.0000
12	4			48.714	47.496	46.971	7.042	1.218	1.7700	1.0000
12	5			54.635	56.135	55.597	7.754	-1.500	-2.2534	1.0000
12	6			15.482	15.720	15.608	1.878	-.238	-1.1344	1.0000
12	7			6.288 *	11.416	-11.133	-2.528	-5.128	-1.1418	1.0000
13	0			9.136 *	2.526	2.334	*.966	6.610	2.4195	1.0000
13	1			18.045	16.813	-16.622	-2.531	1.232	.8513	1.0000
13	2			22.127	22.476	22.333	2.526	-.349	-.2828	1.0000
13	3			63.954	61.708	-60.996	-9.345	2.246	3.7087	1.0000
13	4			29.852	29.927	29.663	3.967	-.076	-.0769	1.0000
13	5			12.347 *	8.528	8.471	*.984	3.820	1.7432	1.0000
13	6			10.018 *	12.819	-12.747	-1.354	-2.801	-1.0071	1.0000
13	7			41.994	40.573	-39.955	-7.054	1.421	1.7242	1.0000
14	0			6.072 *	7.400	-7.349	-.868	-1.328	-.3062	1.0000
14	1			2.051	2.028	-.307	4.021	.9270	1.0000	1.0000
14	2			58.158	57.655	57.655	8.144	.503	.7729	1.0000
14	3			12.946	13.683	13.380	2.865	-.3491	1.0000	1.0000

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
5	14	4	6.188 *	9.827	9.576	2.203	-3.638	-0.8232	1.0000
5	14	5	14.585	13.458	-13.181	-2.714	1.127	.5853	1.0000
5	14	6	21.074	22.297	21.720	5.039	-1.223	-0.8519	1.0000
5	15	0	96.103	94.353	-93.544	-12.329	1.750	2.0524	1.0000
5	15	1	10.321 *	2.590	2.497	.685	7.731	2.9650	1.0000
5	15	2	18.161	18.844	-16.493	-3.622	-0.683	-0.4346	1.0000
5	15	3	15.910	13.082	-12.746	-2.943	2.828	1.5978	1.0000
5	15	4	47.434	47.147	-46.520	-7.663	.286	.3738	1.0000
5	15	5	7.876 *	6.836	6.650	1.583	1.040	.2850	1.0000
5	16	0	6.250 *	4.880	4.879	-.104	1.371	.3070	1.0000
5	16	1	10.967 *	7.567	-7.539	-.649	3.400	1.3358	1.0000
5	16	2	20.159	21.284	-21.092	-2.855	-1.126	-0.7569	1.0000
5	16	3	10.708 *	4.427	-4.065	-1.754	6.281	2.3745	1.0000
5	16	4	6.333 *	4.492	-4.438	-.697	1.841	.4068	1.0000
5	17	1	22.563	21.922	21.712	3.028	.641	.4767	1.0000
5	17	2	15.362	11.462	-11.299	-1.926	3.900	2.0511	1.0000
5	17	3	15.115	10.436	-10.321	-1.544	4.679	2.4348	1.0000
5	18	0	24.069	24.653	-24.315	-4.068	-.585	-.4383	1.0000
5	18	1	6.377 *	6.692	-6.588	-1.174	-.315	-.0691	1.0000
6	0	0	95.678	96.398	-95.617	-12.251	-.720	-.9985	1.0000
6	0	1	19.695	15.103	-15.102	-.169	4.593	3.9893	1.0000
6	0	2	28.999	28.888	-28.404	-5.270	.110	.1280	1.0000
6	0	3	111.688	113.026	112.538	10.519	-.340	-1.4397	1.0000
6	0	4	95.268	96.777	-95.857	-13.312	-1.508	-2.0465	1.0000
6	0	5	65.047	63.822	-63.514	-6.268	1.225	2.1741	1.0000
6	0	6	3.585 *	11.824	-11.296	-3.494	-.239	-3.2175	1.0000
6	0	7	14.810	11.824	-11.296	-3.494	2.986	1.7279	1.0000
6	1	0	62.845	62.199	61.471	9.488	.646	1.0326	1.0000
6	1	1	54.959	54.959	-.54.011	-10.165	1.457	2.1249	1.0000
6	1	2	94.649	95.373	94.917	9.313	-.723	-.8899	1.0000
6	1	3	30.972	29.700	29.475	3.651	1.271	1.5514	1.0000
6	1	4	25.489	25.534	-25.477	-1.702	-.045	-.0472	1.0000
6	1	5	9.305	9.305	-9.230	-1.177	5.156	3.2842	1.0000
6	1	6	52.856	53.446	53.020	6.732	6.955	-.9744	1.0000
6	1	7	50.981	52.441	51.978	-.356	-.356	.2394	1.0000
6	1	8	17.685	17.329	17.214	1.987	-.538	.4547	1.0000
6	1	9	24.180	23.642	-23.469	-2.860	1.803	.764	.1726
6	1	10	6.199 *	5.435	5.127	1.0000	1.0000	1.0000	**
6	2	0	80.202	79.433	78.870	9.440	.770	1.1715	1.0000
6	2	1	19.958	18.057	-18.009	-1.317	1.901	1.6548	1.0000
6	2	2	83.834	84.409	-83.861	-9.600	-.574	-.8376	1.0000
6	2	3	26.293	24.892	-24.858	-1.314	1.401	1.5015	1.0000
6	2	4	28.424	29.083	28.928	2.996	-.659	-.7253	1.0000
6	2	5	5.747 *	3.726	3.621	.876	2.021	.4923	1.0000
6	2	6	13.151	8.073	-8.073	.003	5.078	2.6861	1.0000
6	2	7	43.112	42.938	-42.591	-5.452	.174	.2246	1.0000
6	2	8	26.959	26.854	-26.439	-4.701	.105	.0936	1.0000
6	3	0	7.822 *	3.511	-3.492	.367	4.911	1.5330	1.0000
6	3	1	24.042	26.651	26.476	3.051	-.2609	-2.5927	1.0000
6	3	2	83.429	85.427	84.720	9.717	-.1846	-2.9610	1.0000
6	3	3	33.377	53.021	52.554	7.019	-.356	-.5983	1.0000
6	3	4	13.979	15.573	15.423	2.157	-.594	-.9445	1.0000
6	3	5	7.112 *	1.435	-1.410	-.265	5.678	1.7345	1.0000

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTER
6	6	3	6	39.756	38.357	37.928	5.719	1.399	1.8316	1.0000
6	6	3	7	48.440	50.304	49.712	7.700	-1.864	-2.5760	1.0000
6	6	3	8	31.715	30.467	30.015	5.228	1.248	1.2710	1.0000
6	6	4	0	74.068	73.166	72.834	6.961	0.902	1.6530	1.0000
6	6	4	1	46.893	47.378	-46.979	-6.133	-0.485	-0.7806	1.0000
6	6	4	2	82.614	82.217	81.590	10.136	0.397	0.7103	1.0000
6	6	4	3	28.647	29.191	29.034	3.025	-0.544	-0.6144	1.0000
6	6	4	4	29.542	28.996	28.663	4.384	0.544	0.6129	1.0000
6	6	4	5	75.384	75.877	-75.122	-10.675	-0.493	-0.8971	1.0000
6	6	4	6	88.060	90.441	89.712	11.455	-2.380	-3.7637	1.0000
6	6	4	7	22.067	21.207	21.088	2.242	0.860	0.6738	1.0000
6	6	4	8	17.776	18.407	17.981	3.938	-0.631	-0.3867	1.0000
6	6	5	0	27.222	28.779	28.616	3.058	-1.558	-1.7060	1.0000
6	6	5	1	15.458	11.193	11.110	1.361	4.264	2.9061	1.0000
6	6	5	2	28.812	29.835	-29.628	-3.514	-1.024	-1.1700	1.0000
6	6	5	3	10.929 *	14.715	-14.631	-1.571	-3.786	-1.8031	1.0000
6	6	5	4	14.941	14.447	14.353	1.646	0.495	0.3116	1.0000
6	6	5	5	25.385	26.036	25.808	3.440	-0.651	-0.6132	1.0000
6	6	5	6	5.935 *	7.377	-7.300	-1.062	-1.392	-0.3255	1.0000
6	6	5	7	18.025	17.877	-17.708	-2.447	1.169	0.959	1.0000
6	6	6	8	6.224 *	4.851	-4.751	-0.979	1.373	0.3088	1.0000
6	6	6	9	88.766	87.318	86.812	9.381	1.449	2.0853	1.0000
6	6	6	0	15.229	17.968	17.862	1.951	-2.739	-1.7907	1.0000
6	6	6	1	38.660	39.424	-39.314	-2.941	-0.764	-1.0518	1.0000
6	6	6	2	32.700	32.168	31.866	4.398	2.169	2.7734	1.0000
6	6	6	3	34.336	23.816	23.464	4.078	0.741	0.7048	1.0000
6	6	6	4	24.956	14.394	14.274	1.852	-0.350	-0.1918	1.0000
6	6	6	5	14.044	14.044	14.040	2.557	2.8421	1.0000	**
6	6	6	6	32.700	30.143	29.871	0.979	0.104	0.0237	1.0000
6	6	6	7	6.128 *	6.024	5.971	-1.543	-3.523	-1.9175	1.0000
6	6	6	8	15.669	19.192	-19.130	-1.020	1.3972	1.0000	**
6	6	6	9	38.291	37.270	-37.025	-4.268	-4.268	-4.268	1.0000
6	6	6	0	53.593	53.169	-52.737	-6.769	0.423	0.7042	1.0000
6	6	6	1	27.685	26.267	-26.013	-3.641	1.418	1.5382	1.0000
6	6	6	2	16.338	15.481	-15.223	-2.816	0.857	0.5750	1.0000
6	6	6	3	43.132	42.735	-42.338	-5.811	0.396	0.5545	1.0000
6	6	6	4	39.135	39.935	-39.628	-4.938	-0.800	-1.0178	1.0000
6	6	6	5	25.523	25.580	-25.216	-4.296	-0.057	-0.0511	1.0000
6	6	6	6	10.336 *	9.927	-9.730	-1.965	0.410	0.1552	1.0000
6	6	6	7	22.408	20.198	-19.833	-3.822	2.209	1.7018	1.0000
6	6	6	8	37.442	36.237	-36.105	-3.088	1.206	1.5834	1.0000
6	6	6	9	32.174	31.241	31.041	3.533	0.933	1.1138	1.0000
6	6	6	0	25.582	-57.831	-7.835	-0.693	1.1795	1.0000	**
6	6	6	1	59.053	58.359	-69.035	8.809	-0.035	-0.0626	1.0000
6	6	6	2	69.000	68.471	-68.471	-0.655	0.667	0.667	1.0000
6	6	6	3	45.411	-44.966	-6.342	-0.202	-0.2849	1.0000	**
6	6	6	4	22.860	22.746	-22.502	-3.324	0.113	0.1001	1.0000
6	6	6	5	9.608 *	9.808	-9.602	-1.999	-0.200	-0.0787	1.0000
6	6	6	6	26.387	25.083	-24.902	-3.007	1.304	1.2923	1.0000
6	6	6	7	12.109 *	15.403	-15.196	-2.516	-3.294	-1.5364	1.0000
6	6	6	8	19.196	-19.015	-3.282	-3.282	-0.149	-0.1049	1.0000

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	PAGE
7	6	9	6	18.551	15.160	-15.023	-2.035	3.391	2.02833	1.0000	22
7	6	9	7	12.087 *	13.099	-12.863	-2.474	-1.012	-4.345	1.0000	**
7	6	10	0	5.936 *	4.420	-4.378	-6.604	1.517	0.3578	1.0000	**
7	6	10	1	39.115	38.265	-37.969	-4.748	0.850	1.1096	1.0000	**
7	6	10	2	28.540	27.090	-26.863	-3.499	1.450	1.4870	1.0000	**
7	6	10	3	31.804	30.883	-30.857	1.269	0.921	1.0116	1.0000	**
7	6	10	4	26.897	25.939	-25.683	-3.637	0.957	0.9188	1.0000	**
7	6	10	5	52.876	51.779	-51.297	-7.045	1.097	1.6049	1.0000	**
7	6	10	6	9.898 *	4.689	4.639	0.685	5.208	1.9048	1.0000	**
7	6	10	7	6.204 *	0.700	0.631	-0.303	5.503	1.2420	1.0000	**
7	6	11	0	45.033	43.971	43.657	5.243	1.063	1.4464	1.0000	**
7	6	11	1	13.104	15.130	14.945	2.361	-2.026	-1.0233	1.0000	**
7	6	11	2	5.948 *	2.443	2.145	1.169	3.505	0.8249	1.0000	**
7	6	11	3	5.985 *	4.050	4.013	0.547	1.935	0.4527	1.0000	**
7	6	11	4	27.208	26.740	26.401	4.240	4.240	0.4376	1.0000	**
7	6	11	5	21.174	22.025	21.744	3.506	-0.851	-0.6371	1.0000	**
7	6	11	6	17.847	16.371	16.209	2.292	1.477	0.9249	1.0000	**
7	6	12	0	69.104	67.918	67.103	1.187	1.0489	1.9813	1.0000	**
7	6	12	1	49.943	48.700	-48.172	-7.154	1.243	1.7894	1.0000	**
7	6	12	2	16.841	16.812	-16.710	-1.844	0.029	0.0178	1.0000	**
7	6	12	3	38.963	39.385	-39.037	-5.222	-0.421	-0.5033	1.0000	**
7	6	12	4	35.523	35.697	35.265	5.535	-0.174	-0.1937	1.0000	**
7	6	12	5	36.006	36.429	-35.897	-6.203	-0.422	-0.4649	1.0000	**
7	6	12	6	18.811	20.370	19.834	4.641	-1.559	-0.9804	1.0000	**
7	6	12	7	7.192 *	1.531	-1.504	-0.289	5.661	1.5053	1.0000	**
7	6	13	1	27.778	25.968	25.699	3.730	1.810	1.6900	1.0000	**
7	6	13	2	47.198	45.415	44.906	6.776	1.783	2.3692	1.0000	**
7	6	13	3	38.765	39.510	38.994	6.362	-0.745	-0.8513	1.0000	**
7	6	13	4	12.806 *	8.651	8.518	1.515	4.155	1.8827	1.0000	**
7	6	13	5	9.982 *	8.519	8.411	1.348	1.464	0.5172	1.0000	**
7	6	14	0	7.693 *	11.848	11.848	-0.068	-4.155	-1.1364	1.0000	**
7	6	14	1	9.962 *	8.833	-0.767	-0.325	9.130	3.2722	1.0000	**
7	6	14	2	25.434	22.844	22.608	3.276	2.590	2.1943	1.0000	**
7	6	14	3	47.414	46.404	45.805	7.432	1.010	1.3187	1.0000	**
7	6	14	4	14.743	12.077	-11.931	-1.875	2.663	1.3606	1.0000	**
7	6	15	0	23.928	22.641	22.343	3.665	1.287	1.0000	1.0000	**
7	6	15	1	10.724 *	11.257	11.130	1.685	-1.533	-0.1972	1.0000	**
7	6	15	2	28.217	26.576	-26.272	-4.004	1.641	1.4509	1.0000	**
7	6	15	3	10.252 *	11.160	-11.023	-1.742	-0.908	-0.3133	1.0000	**
7	6	16	0	47.556	45.958	45.194	5.976	1.969	2.4834	1.0000	**
7	6	16	1	37.284	33.968	33.310	6.656	3.316	3.6591	1.0000	**
7	6	16	2	59.808	58.476	-57.820	-8.738	1.331	1.9102	1.0000	**
7	6	17	1	64.417	62.157	-61.525	-8.738	2.261	3.9348	1.0000	**
7	6	17	2	5.825 *	9.079	9.057	-0.628	-3.253	-0.7817	1.0000	**
7	6	17	3	48.091	47.234	-46.862	-5.919	-0.856	1.2820	1.0000	**
7	6	17	4	37.362	37.598	-37.284	-4.852	-0.236	-0.2940	1.0000	**
7	6	17	5	25.080	24.805	-24.614	-3.077	0.275	0.2390	1.0000	**
7	6	17	6	51.896	51.885	-51.120	-8.879	0.011	0.0152	1.0000	**
7	6	17	7	9.840 *	15.422	-15.150	-2.885	-5.583	-1.9153	1.0000	**
7	6	17	8	9.321 *	4.709	-4.654	-0.722	4.612	1.7596	1.0000	**
7	6	17	9	39.442	38.332	-37.963	-5.449	1.110	1.4791	1.0000	**
2	2	1	20.911	20.997	20.872	2.286	-1.085	-0.8404	1.0000	**	

	H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	STRUCTURE FACTORS	PAGE 23		
1	7	7	2	3	25.737	25.247	-24.831	-4.565	.490	.4651	1.0000		
1	7	7	2	4	11.096	*	7.400	7.323	1.066	1.6081	1.0000		
1	7	7	5	36.545	36.364	-35.930	-5.597	.695	.181	.2089	1.0000		
1	7	7	6	8.185	*	3.180	2.804	1.499	5.006	1.5159	1.0000		
1	7	7	7	19.838	17.953	-17.543	-3.811	1.885	1.2694	1.0000	**		
1	7	7	0	42.016	40.617	-40.508	-2.969	1.399	1.9458	1.0000	**		
1	7	7	1	12.053	*	6.661	-6.562	-1.145	5.392	2.6612	1.0000	**	
1	7	7	2	84.106	84.292	83.649	10.388	-186	-3486	1.0000	**		
1	7	7	3	20.314	22.409	-22.297	-2.240	-2.094	-2.0855	1.0000	**		
1	7	7	3	20.980	22.469	-22.297	-2.240	-1.425	-1.1456	1.0000	**		
1	7	7	4	12.873	11.770	11.620	1.872	1.103	.5589	1.0000	**		
1	7	7	3	5.2	9.706	*	10.500	-10.313	-1.974	-2.2954	1.0000	**	
1	7	7	6	9.595	*	7.907	7.416	2.743	1.688	.6012	1.0000	**	
1	7	7	3	6.206	*	7.839	7.752	1.162	-1.633	-3.3684	1.0000	**	
1	7	7	0	6.598	*	2.662	-2.656	.184	3.926	1.0979	1.0000	**	
1	7	7	4	10.154	*	8.562	-8.505	-0.987	1.592	.6612	1.0000	**	
1	7	7	4	1	26.151	26.454	-26.318	-2.675	-303	-2.2986	1.0000	**	
1	7	7	4	3	12.485	9.810	-9.546	-2.261	2.675	1.3408	1.0000	**	
1	7	7	4	4	11.038	*	8.476	-8.463	-469	2.562	1.1260	1.0000	**
1	7	7	4	5	6.095	*	1.283	1.060	4.811	1.1468	1.0000	**	
1	7	7	4	6	10.764	*	12.270	-12.276	-1.506	-1.5940	1.0000	**	
1	7	7	4	2	15.449	14.488	-14.282	-2.433	.961	.5303	1.0000	**	
1	7	7	5	0	85.742	85.623	84.976	10.502	1.119	.1735	1.0000	**	
1	7	7	5	1	29.444	29.673	29.327	4.520	-229	-2.2460	1.0000	**	
1	7	7	5	2	27.079	27.534	27.205	4.246	-455	-4.4500	1.0000	**	
1	7	7	5	3	25.692	23.319	-22.868	-4.562	3.373	2.2970	1.0000	**	
1	7	7	5	4	77.296	79.908	79.117	11.216	-2.611	-4.5991	1.0000	**	
1	7	7	5	5	56.519	59.619	58.872	9.409	-3.100	-4.6407	1.0000	**	
1	7	7	5	6	20.965	18.895	18.659	2.980	2.069	1.5184	1.0000	**	
1	7	7	5	7	32.610	31.252	-30.947	-4.354	1.359	1.3931	1.0000	**	
1	7	7	6	0	32.891	32.629	-32.327	-4.425	.262	.2972	1.0000	**	
1	7	7	6	1	35.621	34.746	34.550	3.678	.875	1.0484	1.0000	**	
1	7	7	6	2	5.916	*	3.731	-3.662	2.185	.5171	1.0000	**	
1	7	7	6	3	35.069	35.887	35.489	5.328	-.818	-9.9493	1.0000	**	
1	7	7	6	4	23.412	22.067	-21.802	-3.410	1.345	1.1141	1.0000	**	
1	7	7	6	5	22.904	21.002	20.893	2.141	1.902	1.5305	1.0000	**	
1	7	7	6	6	12.256	*	11.176	-10.995	-2.007	1.080	.4768	1.0000	**
1	7	7	6	7	102.015	99.811	-99.111	-11.794	2.205	2.6193	1.0000	**	
1	7	7	7	1	26.545	28.351	28.026	4.282	-1.807	-1.7117	1.0000	**	
1	7	7	7	2	58.875	59.974	59.535	7.243	-1.099	-1.7195	1.0000	**	
1	7	7	3	29.789	30.236	29.705	5.642	-447	-4532	1.0000	**		
1	7	7	4	36.496	37.693	-37.267	-5.652	-1.197	-1.3745	1.0000	**		
1	7	7	5	8.671	*	4.349	4.193	1.153	4.322	1.4014	1.0000	**	
1	7	7	6	21	16.302	15.907	-15.818	-1.680	.394	.2231	1.0000	**	
1	7	7	7	2	33.617	32.641	32.387	4.064	.976	1.0845	1.0000	**	
1	7	7	8	1	17.767	14.873	14.677	2.404	2.894	1.9058	1.0000	**	
1	7	7	8	2	12.864	9.474	-9.474	-0.52	3.390	1.6495	1.0000	**	
1	7	7	8	3	7.186	*	2.658	-2.617	4.527	1.2496	1.0000	**	
1	7	7	8	4	11.419	*	14.257	13.956	-2.839	-1.1739	1.0000	**	
1	7	7	8	5	24.147	22.835	22.550	3.597	1.312	1.0730	1.0000	**	
1	7	7	8	6	12.679	*	10.143	10.034	1.482	2.5312	1.1435	1.0000	**
1	7	7	9	7	10.043	*	2.151	-0.784	-2.003	7.891	2.9781	1.0000	**
1	7	7	9	8	17.613	15.709	15.612	1.737	1.905	1.2361	1.0000	**	

	H	K	L	F(CBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
6	7	9	2	73.204	71.281	-70.516	-10.414	1.923	3.2337	1.0000
5	7	9	3	58.383	57.236	-56.681	-7.953	1.146	1.7572	1.0000
4	7	9	4	6.190	* 4.258	-4.078	-1.226	1.932	1.4371	1.0000 **
3	7	9	5	52.912	52.190	51.653	7.462	.722	1.0132	1.0000
2	7	10	0	8.898	*	11.811	11.695	1.648	-2.913	-0.9384
1	7	10	1	17.453	18.935	-18.693	-3.015	-1.482	-0.9102	1.0000 **
0	7	10	2	41.845	40.620	40.270	5.324	1.224	1.5361	1.0000
6	7	10	3	6.170	*	4.207	-4.051	-1.135	1.963	* 4455
5	7	10	4	15.215	18.085	17.926	2.394	-2.870	-1.5111	1.0000
4	7	10	5	33.250	24.874	-24.531	-4.115	8.376	10.6860	1.0000
3	7	13	0	27.527	24.052	23.536	4.954	3.475	3.0656	1.0000
2	7	13	1	6.444	*	9.669	9.628	-3.225	-7.195	1.0000 **
1	7	13	2	9.390	*	8.900	8.817	1.211	.490	1.0000 **
0	7	13	3	41.163	41.261	-40.767	-6.364	-0.988	-0.1129	1.0000
7	7	14	0	29.415	26.653	-26.134	-5.236	2.762	2.5005	1.0000
6	7	14	1	6.393	*	3.447	3.299	1.000	2.946	.6450
5	7	14	2	40.705	40.944	-40.614	-5.194	-2.240	-0.2912	1.0000
4	7	14	3	3.465	-3.465	-3.465	-.022	4.497	1.3072	1.0000
3	8	14	2	23.084	25.516	25.201	3.998	-2.432	-1.8701	1.0000
2	8	14	3	70.293	68.068	67.415	9.410	2.225	3.6208	1.0000
1	8	14	4	39.678	37.488	-37.122	-5.226	2.190	2.6152	1.0000
0	8	14	5	41.894	40.714	-40.299	-5.797	1.180	1.4095	1.0000
9	8	14	6	9.862	*	2.890	-2.874	-3.05	6.972	2.5149
8	8	14	7	32.310	32.487	-31.932	-5.977	-1.77	-0.1828	1.0000
7	8	14	8	15.872	16.155	16.090	1.447	-2.83	-0.1607	1.0000
6	8	14	9	44.310	42.032	-41.683	-5.405	2.278	2.9397	1.0000 **
5	8	14	10	6.224	*	3.449	3.446	-1.148	2.775	0.6243
4	8	14	11	28.420	27.495	-26.835	-5.987	0.925	0.8409	1.0000 **
3	8	14	12	75.700	72.491	71.797	10.007	3.209	5.4794	1.0000 **
2	8	14	13	10.693	*	8.357	8.324	0.744	2.336	0.9275
1	8	14	14	55.708	54.211	-53.690	-7.496	1.497	2.2046	1.0000
0	8	14	15	6.332	-6.236	-1.103	1.103	6.767	3.2025	1.0000
7	2	22	1	13.100	32.145	30.816	30.493	4.452	1.329	1.3562
6	2	22	2	19.332	30.816	30.493	4.452	1.329	1.3562	1.0000
5	2	22	3	54.882	53.030	-52.480	-7.625	1.852	2.6653	1.0000
4	2	22	4	6.244	*	5.562	-5.544	-4.452	0.682	1.1529
3	2	22	5	55.183	52.651	-52.131	-7.387	2.531	3.6909	1.0000 **
2	2	22	6	19.332	18.347	-18.252	-1.866	.985	0.6652	1.0000
1	2	22	7	31.856	31.274	-30.950	-4.494	.581	0.5891	1.0000
0	2	22	8	25.351	25.030	25.036	3.846	.022	.0185	1.0000
6	3	21	9	24.398	24.340	24.099	3.414	.058	.0483	1.0000
5	3	21	10	41.662	39.986	-39.463	-6.448	1.676	1.9912	1.0000
4	3	21	11	16.471	13.484	-13.381	-1.666	2.987	1.7377	1.0000
3	3	21	12	25.008	22.101	-21.766	-3.837	2.907	2.4915	1.0000
2	3	21	13	19.564	18.407	18.164	2.981	1.157	.7849	1.0000
1	3	21	14	13.848	12.872	-12.872	-2.748	-1.686	.3347	1.0000
0	3	21	15	17.923	19.775	19.517	3.180	-1.852	-1.1392	1.0000
5	4	20	16	19.666	17.766	-17.402	-3.578	1.901	1.2835	1.0000
4	4	20	17	15.745	12.882	12.635	2.512	2.863	1.5288	1.0000
3	4	20	18	40.428	38.931	38.032	4.773	2.098	2.5327	1.0000

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
8	6	1	6.188 *	7.577	-7.486	-1.167	-1.388	-0.3141	1.0000 **
8	6	2	41.586	38.512	-38.078	-5.762	3.074	3.8036	1.0000
8	6	3	6.262 *	1.114	-1.090	- .229	5.148	1.1513	1.0000 **
8	6	4	10.559 *	6.231	6.185	.754	4.328	1.6012	1.0000 **
8	7	0	6.248 *	1.720	-1.177	1.254	4.528	1.0148	1.0000 **
8	7	1	45.448	42.277	41.676	7.102	3.171	4.0919	1.0000
8	7	2	13.536	10.768	10.732	.873	2.768	1.3115	1.0000
8	7	3	40.640	40.314	39.739	.783	.326	.3876	1.0000
8	7	4	12.071 *	9.505	9.428	1.205	2.566	1.0913	1.0000 **
8	8	0	6.295 *	2.506	2.496	.224	3.789	.8428	1.0000 **
8	8	1	6.313 *	1.161	-1.140	.219	5.152	1.1426	1.0000 **
8	8	2	20.586	15.183	-14.937	-2.726	5.403	3.8269	1.0000
8	8	3	24.242	23.876	23.502	4.207	.366	.2877	1.0000
8	9	0	39.536	36.781	36.330	5.741	2.754	3.1715	1.0000
8	9	1	6.277 *	5.394	-5.382	-3.60	.883	.1970	1.0000 **
8	9	2	28.297	28.685	28.147	5.528	-.388	-.3408	1.0000
3	9	*	6.362 *	5.513	5.499	-.391	1.1867	1.0000 **	

ZN3AS

RESULTS OF STRUCTURE FACTOR CALCULATIONS

ALL REFLECTIONS

NUMERATOR

DENOMINATOR

NUMBER

P

WEIGHTED R	11489.72	5878523.43	1289	.044
UNWEIGHTED R	2707.85	53458.11	1289	.051

RANGES OF F(OBS)	1817.4C 1556.32 1445.28 1288.99 1044.64 2446.67 1284.10 606.32	276324.10 2057941.81 2207373.54 723143.40 336159.36 103842.72 83019.88 30618.62	715 319 158 56 28 7 5 1	.081 .027 .025 .042 .056 .153 .124 .141
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RANGES OF (SIN(THETA)/LAMBDA)**2

6121.47 1706.17 955.03 852.89 517.81 651.29 546.61 138.45	724356.10 982162.49 1187172.39 1093779.54 792645.03 707155.48 298373.85 92878.08	78 119 167 183 209 240 219 74	.092 .042 .028 .028 .026 .030 .043 .039
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UNREJECTED REFLECTIONS

WEIGHTED R	5831.41	5611434.91	1271	.032
UNWEIGHTED R	2351.72	50599.17	1271	.046

RANGES OF F(OBS)

1817.40 1556.32 1299.32 767.43 313.03 32.72 45.19 .00	276324.10 2057941.81 2254546.78 683242.31 274709.52 36851.45 27818.94 .00	715 319 157 52 23 3 2 0	.081 .027 .024 .034 .034 .030 .040 .000
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RANGES OF (SIN(THETA)/LAMBDA)**2

1123.30 1046.04 955.03 852.89 517.81 651.29 546.61 138.45	522682.16 916747.90 1187172.89 1093779.54 792645.00 707155.48 298373.85 92878.08	65 114 167 183 205 240 219 74	.046 .034 .028 .028 .026 .030 .043 .039
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SUM FCAL	53142.83
STANDARD DEV OF UNIT WEIGHT OBS	2.19