

Crystal structures of the humite minerals: V. Magnesian manganhumite

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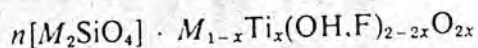
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Abstract

The crystal structure of type manganhumite from the Brattfors mine, Nordmark, Sweden $[(Mn_{0.68}Mg_{0.30}Fe_{0.01}Ca_{0.01})_7(SiO_4)_3(OH)_2]$, *Phmm*, $a = 4.815(1)$, $b = 10.580(2)$, $c = 21.448(5)$ Å has been refined by conventional least-squares methods to $R = 0.051$ ($R_w = 0.081$), using 1562 structure factors with $F_{obs} > 2\sigma(F_{obs})$. Mean Si-O distances for the isolated tetrahedra are $(Si(1)-O) = 1.628$ Å and $(Si(2)-O) = 1.632$ Å. The apical Si-O distances of 1.600 and 1.604 Å are the shortest yet observed in humite-group minerals. Site refinement yielded Mg/(Mg+Mn) ratios of 0.30 in the $M(1)O_6$ octahedron (mean $M-O$ distance = 2.170 Å), 0.0 in the $M(2)O_6$ and $M(2)O_6OH$ octahedra ($(M-O) = 2.222$ and 2.206 Å), and 0.75 in the $M(3)O_4(OH)_2$ octahedron ($(M-O) = 2.117$ Å). The correlation coefficient of Mg/(Mg+Mn) occupancy and mean octahedral bond length is $r = 0.986$, and as expected, octahedral sizes correspond almost exactly to the weighted radii of the larger Mn and smaller Mg cations ($r = 0.989$).

Introduction

The humite minerals are a homologous series of magnesium orthosilicates based on hexagonal closest-packed arrays of anions and structurally related to forsterite. Microprobe analyses of fifty-five humite samples (Jones *et al.*, 1969) led to the establishment of the general formula:



where M is Mg, Fe, Mn, Ca, Zn in decreasing order of abundance, $0 \leq x \leq 1$, and $n = 1$ for norbergite, 2 for chondrodite, 3 for humite, and 4 for clinohumite (see Table 1). Manganese end-members of three of the four homologues are well-known, and unpublished microprobe analyses by C. Richardson (private communication, 1976) indicate extensive, if not complete, solid solution between Mg and Mn end-members.

Ordering of the small concentrations of Fe normally present in Mg humites was initially detected by Ribbe and Gibbs (1969, 1971) in a humite with composition $Mg_{6.6}Fe_{0.4}Si_3O_{12}F(OH)$. Mg/Fe ordering has

been observed in all subsequent refinements of humite group minerals, including several titanian humites (Robinson *et al.*, 1973; Kocman and Rucklidge, 1973). Ribbe and Gibbs (1971) concluded that distortion and ligancy rather than size of the octahedral sites govern the ordering of Fe in Mg humites. Fe preferring those octahedra with no (F,OH) ligands, *i.e.*, $M(1)O_6$ and $M(2)O_6$.

The recent discovery of Mn humites containing considerable Mg provides an opportunity for further investigation of cation ordering in humites. This paper reports the results of a site occupancy refinement of magnesian manganhumite.

Experimental procedures

Crystals of manganhumite from the type specimen from Brattfors Mine, Nordmark, Sweden, were generously donated by Professor P. B. Moore, University of Chicago, and upon completion of this study will be deposited in the Mineralogical Museum of Harvard University. Moore (1978) reports their composition to be $(Mn_{0.68}Mg_{0.30}Fe_{0.01}Ca_{0.01})_7(SiO_4)_3(OH)_2$.

Manganhumite is orthorhombic and was refined in the nonstandard space group *Phmm* to conform with

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FORMAT FOR STRUCTURE FACTOR INPUT IS
(I1,I3,2I4,2F9.0,I3,F11.0,4F7.0)
SIGMA WILL BE COMPUTED BY SIGMA=SQR(T(SIGMA**2+(0.0250*F)**2)
WAVELENGTH IS 0.7093

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
0	0	6	126.183	115.392	-133.672	-2.112	10.790	3.4131	0	7450
0	0	8	149.586	138.655	-162.366	-4.329	10.931	2.9173	0	7287
0	0	1	57.320	99.168	165.894	2.051	-6.848	-4.6297	0	9474
0	0	11	90.329	64.168	104.603	3.364	-9.151	0.0017	0	9004
0	0	12	14.495	3.806	3.339	2.506	10.689	-3.7738	0	9999
0	0	16	25.063	3.339	3.339	2.506	-8.329	-6.9981	0	9927
0	0	18	73.890	75.993	77.275	-0.575	-2.244	-1.1098	0	9670
0	0	22	122.912	121.666	-126.331	-5.463	-0.244	-0.4027	0	9258
0	0	24	39.433	39.377	-39.502	-1.236	0.332	-0.2814	0	9926
0	0	26	82.258	77.889	-75.860	-3.368	-4.368	-2.0558	0	9733
0	0	30	171.234	166.074	-175.669	-9.167	5.160	-1.1991	0	8913
0	0	32	110.852	175.683	-115.112	-2.485	5.169	1.1093	0	9959
0	0	33	51.108	52.726	-17.562	-0.484	6.162	-1.3115	0	9988
0	0	4	80.653	53.960	-53.275	-2.031	-1.878	-1.3245	0	9891
0	0	5	1.054	12.190	-12.066	-1.917	8.563	-7.6732	0	9092
0	0	6	31.690	31.477	-76.340	-2.425	0.213	4.2627	0	8762
0	0	7	165.366	22.253	-31.730	-2.594	3.208	0.8278	0	9970
0	0	8	27.977	173.095	223.877	10.899	-1.782	-1.8680	0	9900
0	0	9	20.845	27.021	-27.069	-2.061	1.095	1.4022	0	9893
0	0	10	30.485	15.246	-10.130	-2.305	5.595	-9.7764	0	9969
0	0	11	30.246	10.499	-25.178	-1.299	-5.014	7.5854	0	9986
0	0	12	104.082	104.118	11.017	0.297	-0.527	-0.7823	0	9929
0	0	13	14.587	63.669	64.633	-0.527	0.041	-0.4015	0	9931
0	0	14	55.695	59.287	57.139	-0.970	3.499	-1.2296	0	9644
0	0	15	15.361	17.110	17.683	-1.321	-2.592	-1.8277	0	9715
0	0	16	38.892	41.318	-41.689	3.011	-2.344	-3.0779	0	9913
0	0	17	30.027	29.750	-29.832	-0.277	0.226	0.4652	0	9881
0	0	18	108.353	109.595	-113.884	-9.775	-0.227	-0.2299	0	9927
0	0	19	10.471	33.322	33.322	-1.429	1.634	0.4559	0	9991
0	0	20	31.980	33.322	33.322	-1.351	-0.909	-1.5012	0	9975
0	0	21	25.066	22.157	22.045	-1.290	2.904	3.7510	0	9999
0	0	22	24.534	22.157	22.045	-1.053	-0.906	-1.1776	0	9999
0	0	23	74.534	71.530	-72.405	-1.463	3.004	-1.5864	0	9974
0	0	24	49.010	50.248	-50.247	-0.426	0.101	0.7584	0	9979
0	0	25	24.344	24.488	-24.278	-0.158	-0.119	-0.1232	0	9984
0	0	26	22.565	22.125	-22.191	-0.385	0.441	0.5475	0	9979
0	0	27	31.508	28.769	-28.395	-2.770	2.086	-2.7865	0	9964
0	0	28	117.070	140.015	-166.107	-1.133	-2.868	-7.0318	0	9975
0	0	29	24.214	21.164	-5.168	1.821	0.619	-0.8262	0	9973
0	0	30	5.030	159.429	-195.874	-6.091	-2.945	0.6194	0	9923
0	0	31	18.235	19.634	-19.625	-1.079	1.804	4.7794	0	9938
0	0	32	64.248	71.897	-74.705	-2.723	-7.649	-2.7613	0	9950
0	0	33						-4.7351	0	9250

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
0	4	6	58.6669	66.7515	-68.8966	-0.6229	-8.082	-5.4794	0.9386
0	4	7	44.7822	52.6550	-53.6111	-1.7579	-7.873	-6.9570	0.9636
0	4	8	28.9776	29.8000	-29.9227	-1.5714	-7.1031	-1.1031	0.9888
0	4	9	31.0330	85.2263	-35.4791	-1.5144	-1.6667	-0.8039	0.9200
0	4	10	205.8000	188.7866	-226.0306	-6.3439	-17.0234	-5.2944	0.9863
0	4	11	336.8180	13.7339	-237.9267	-0.3389	-0.9220	-0.9751	0.9862
0	4	12	113.1840	113.9559	-124.1017	-0.6222	-0.1639	-0.3725	0.9982
0	4	13	11.7790	117.9597	-123.9698	-0.0666	-5.1053	-1.5437	0.9996
0	4	14	5.2294	21.6645	-21.6698	-0.0666	-1.4003	-1.5437	0.9996
0	4	15	21.3390	80.5116	-82.3018	-1.7335	-0.2559	-1.3598	0.9964
0	4	16	77.4670	15.0886	-14.9337	-4.7353	-3.0255	-1.5604	0.9539
0	4	17	14.0661	38.5722	-38.6550	-2.1998	-1.0225	-1.5846	0.9984
0	4	18	35.7339	93.5023	-96.0512	-1.8651	-2.8333	-2.9519	0.9903
0	4	19	94.2339	23.5133	-23.5122	-1.8651	-0.1226	-0.3175	0.9967
0	4	20	23.6339	38.8336	-38.8781	-3.0448	-0.5444	-0.5349	0.9915
0	4	21	48.4662	46.6336	-46.8881	-0.8774	-1.8227	-1.2449	0.9883
0	4	22	19.7322	19.5017	-19.5011	-0.8774	-0.4331	-0.2449	0.9980
0	4	23	18.5115	114.6103	136.3613	5.2229	0.4331	1.3071	0.9334
0	4	24	18.8050	9.9023	9.4403	2.6664	0.0998	0.0998	0.9359
0	4	25	36.8050	53.5600	-53.5442	-0.6777	-0.1335	-0.1234	0.9966
0	4	26	53.5110	8.3550	-10.0912	-6.2438	-0.0337	-0.1234	0.9868
0	4	27	26.9116	17.0889	-17.4498	-0.1037	-1.7339	-0.0267	0.9965
0	4	28	26.9116	27.5113	-27.4981	-0.1037	-1.7339	-1.4849	0.9995
0	4	29	36.7119	38.4221	-38.4221	-3.1119	-1.7033	-1.7335	0.9935
0	4	30	27.3210	22.5209	-22.4432	-2.2954	-2.8338	-3.3673	0.9974
0	4	31	21.3214	58.4446	-59.5885	-2.5444	-0.8888	-1.0673	0.9979
0	4	32	49.5108	82.7999	-86.0446	-2.2226	-0.9332	-1.1098	0.9608
0	4	33	79.1081	4.5885	-4.5556	-0.8220	-3.0337	-0.5139	0.9998
0	4	34	33.6914	39.4461	-39.7770	-1.7709	-5.7667	-6.6139	0.9227
0	4	35	28.9117	211.4411	268.2406	7.7339	17.4750	3.9794	0.6290
0	4	36	22.7885	32.1011	-32.0668	-0.3669	-0.6885	-0.4916	0.9890
0	4	37	18.3317	16.5194	-16.5982	-0.1444	-0.6885	-0.2942	1.0000
0	4	38	171.9310	167.9311	-15.7111	-0.9229	1.1223	0.3223	0.9973
0	4	39	25.3107	28.4770	-28.1811	-0.6937	-4.0119	-0.9335	0.9979
0	4	40	63.4407	66.4770	-67.5998	-1.1444	-2.0662	-0.9335	0.9934
0	4	41	4.7775	2.3044	1.4427	3.4662	3.0662	-1.9085	0.9644
0	4	42	33.7655	36.4441	-36.5571	-1.1984	-2.4771	-1.9085	0.9644
0	4	43	47.3219	45.8663	-46.1977	-1.2033	-2.4771	-3.0065	0.9900
0	4	44	61.6118	59.8791	-60.5777	-1.2033	-1.7336	-2.6133	0.9949
0	4	45	36.8338	38.1111	-38.2264	-1.4224	-1.2733	-1.3097	0.9906
0	4	46	161.3715	153.2110	-164.6665	-7.2689	-8.1665	-2.0191	0.8647
0	4	47	54.7965	55.4770	-55.9244	-0.2689	-0.6774	-0.4803	0.9817
0	4	48	182.3223	171.8916	-186.2229	-0.9666	-1.6027	-1.1104	1.0000
0	4	49	14.4556	16.4446	-16.4442	-0.7111	-2.0115	-2.8405	0.9986
0	4	50	15.8336	81.4671	-82.6773	-4.6557	-0.9990	-1.5418	0.9986
0	4	51	19.6080	18.8771	-18.7773	-2.0667	-3.6337	-1.8410	0.9983

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	0	31	33.038	32.085	32.152	0.0279	0.9533	0.9754	0.9959
1	0	30	3.998	6.937	-6.932	-0.278	-2.939	-1.0360	0.9959
1	0	33	11.341	11.129	-11.132	-0.5939	-2.212	-0.5769	0.9966
1	0	1	12.404	20.185	-20.185	-3.003	-7.747	-0.3966	0.9866
1	0	2	27.182	26.642	-26.778	-5.007	-2.533	0.0762	0.9780
1	0	3	96.618	94.325	-106.955	-5.711	-2.294	0.9477	0.7760
1	0	4	155.167	142.586	-175.722	-4.283	0.072	2.2262	0.6577
1	0	5	101.867	154.910	-105.222	-3.108	12.521	4.4936	0.8120
1	0	6	174.537	155.963	-197.963	-4.718	19.072	4.2759	0.6120
1	0	7	117.712	122.592	-186.829	-3.536	18.685	1.0816	0.7956
1	0	8	28.893	136.635	-139.913	-4.726	6.301	1.0620	0.6966
1	0	9	19.390	114.544	-125.244	-5.016	4.846	0.9523	0.8350
1	0	0	105.232	106.831	-113.124	-2.720	1.599	0.6058	0.8901
1	0	1	67.924	71.212	-72.784	-2.258	-3.997	-0.9180	0.9536
1	0	2	31.316	35.312	-35.477	-1.034	-3.996	-0.8062	0.9870
1	0	3	4.571	10.690	-10.645	-0.034	-2.225	-0.0764	1.0000
1	0	4	11.915	7.239	7.085	1.493	0.851	0.5339	0.9992
1	0	5	8.090	24.239	24.616	4.937	2.935	1.3508	0.9996
1	0	6	21.042	80.870	81.832	3.799	-2.935	-4.0275	0.9950
1	0	7	77.042	96.625	-99.567	-3.329	1.058	0.6138	0.9550
1	0	8	98.142	105.911	-109.107	-2.729	0.058	0.0259	0.9391
1	0	9	106.616	81.491	-83.089	-2.493	0.061	0.2630	0.9411
1	0	0	81.431	48.532	-48.781	-3.226	0.493	0.0294	0.9861
1	0	1	45.029	43.800	-43.451	-1.577	0.061	0.0229	0.9611
1	0	2	45.592	47.565	-42.577	-3.721	0.227	0.7014	0.9959
1	0	3	57.043	56.836	-57.013	4.916	0.209	0.2243	0.9903
1	0	4	14.263	13.806	13.950	1.164	0.220	0.1414	0.9965
1	0	5	19.330	8.945	8.701	0.364	0.385	0.2609	0.9991
1	0	6	3.122	10.473	10.474	0.186	0.348	0.5440	0.9996
1	0	7	7.183	2.183	-2.090	-0.634	0.340	0.7146	0.9995
1	0	8	3.134	5.803	-5.170	-2.953	1.136	0.8387	0.9999
1	0	9	25.267	27.403	-27.283	-2.643	-2.544	0.0664	0.9972
1	0	0	69.676	62.135	-62.578	-4.969	2.205	1.4427	0.9999
1	0	1	44.291	41.902	-42.177	-2.011	-2.544	0.4445	0.9813
1	0	2	13.345	11.948	-11.924	-0.042	1.184	0.3778	0.9963
1	0	3	64.232	62.648	-65.777	-0.447	1.443	0.7958	0.9158
1	0	4	26.031	22.036	-22.177	-0.088	0.284	0.4437	0.9878
1	0	5	44.356	49.375	-50.507	-0.709	0.995	1.0078	0.9555
1	0	6	16.170	14.919	-14.919	0.150	-2.025	0.0078	0.9996
1	0	7	4.889	2.332	-2.993	0.042	-0.832	0.0562	0.9999
1	0	8	25.708	24.054	-24.499	-0.131	-1.029	0.6814	0.9929
1	0	9	76.421	73.072	-75.634	-0.049	3.383	1.9099	0.9929
1	0	0	8.454	5.982	-7.074	-0.049	1.383	0.7529	0.9936
1	0	1	26.687	25.982	-26.063	-0.374	0.805	0.9967	0.9994
1	0	2	11.001	10.104	-10.108	-0.009	0.783	0.4023	0.9997
1	0	3	29.478	30.823	30.932	0.381	0.897	1.7864	0.9928
1	0	4	12.377	11.827	11.831	0.244	0.550	1.0030	0.9989

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	1	1	19.103	18.761	18.783	0.162	0.341	0.5917	0.9977
1	1	1	6.783	17.452	17.429	-0.594	-0.669	-0.8913	0.9997
1	1	1	13.939	13.985	13.991	-0.046	-0.045	-0.0387	0.9988
1	1	1	3.260	19.046	19.046	0.000	0.215	0.13347	0.9997
1	1	1	22.516	19.291	19.310	-0.338	3.131	4.9397	0.9997
1	1	1	15.469	4.600	4.599	-0.077	-3.131	-0.88492	0.9997
1	1	1	15.383	16.554	16.565	0.011	-1.072	-0.88790	0.9987
1	1	1	34.886	5.973	5.982	0.011	-1.072	-0.09440	0.9992
1	1	1	7.169	5.819	5.819	0.000	1.350	1.46668	0.9998
1	1	1	12.370	13.663	13.663	0.000	1.099	0.47333	0.9992
1	1	1	14.879	13.783	13.783	0.000	1.099	0.79338	0.9992
1	1	1	10.744	7.307	7.307	0.000	7.520	1.04480	0.9998
1	1	1	10.288	2.768	2.768	0.000	1.852	1.14801	0.9994
1	1	1	6.018	12.596	12.598	0.006	-0.370	-0.54442	0.9998
1	1	1	3.681	1.311	1.311	0.000	0.617	1.02876	0.9997
1	1	1	9.718	8.834	8.834	0.000	0.883	1.06771	0.9997
1	1	1	3.829	0.276	0.276	0.000	0.555	1.85556	0.9997
1	1	1	170.534	155.283	155.283	-0.012	3.370	1.85556	0.9997
1	1	1	177.127	162.773	162.773	-0.046	1.733	2.79189	0.6331
1	1	1	174.365	166.013	166.013	-0.659	0.535	2.2236	0.8425
1	1	1	96.325	166.662	166.662	-5.675	-0.464	2.2236	0.8425
1	1	1	61.758	161.487	161.487	-4.731	0.464	2.2236	0.8425
1	1	1	18.935	97.615	97.615	3.681	-1.290	-0.5343	0.8591
1	1	1	51.150	66.389	66.389	1.151	-1.290	-0.5343	0.8591
1	1	1	10.150	2.199	2.199	0.022	16.745	-2.97801	0.9999
1	1	1	51.115	9.483	9.483	1.241	0.667	1.67799	0.9988
1	1	1	35.115	5.205	5.205	-0.874	1.011	1.02229	0.9683
1	1	1	105.440	131.623	131.623	-4.424	3.387	1.02229	0.8269
1	1	1	102.026	147.996	147.996	-5.406	3.387	1.02229	0.8269
1	1	1	108.052	139.888	139.888	-4.700	2.244	0.92339	0.9038
1	1	1	88.868	101.816	101.816	-4.402	4.444	0.91338	0.8348
1	1	1	56.307	91.471	91.471	-4.916	0.244	0.91338	0.9369
1	1	1	108.482	107.499	107.499	-0.722	0.398	0.2745	0.9225
1	1	1	81.689	85.466	85.466	-4.145	0.000	0.3766	0.9225
1	1	1	44.742	45.114	45.114	-0.588	0.000	0.3766	0.9225
1	1	1	22.065	22.354	22.354	-1.398	0.000	0.3766	0.9225
1	1	1	18.851	28.839	28.839	-1.057	0.000	0.3766	0.9225
1	1	1	59.765	21.032	21.032	-1.307	0.000	0.3766	0.9225
1	1	1	68.780	71.361	71.361	-3.838	0.000	0.3766	0.9225
1	1	1	72.224	71.304	71.304	-0.840	0.000	0.3766	0.9225
1	1	1	66.837	95.152	95.152	3.943	1.680	0.9848	0.9807
1	1	1	30.671	30.844	30.844	-0.746	0.000	0.1774	0.9959
1	1	1	36.332	30.543	30.543	-3.221	0.000	0.1774	0.9959
1	1	1	49.685	47.985	47.985	-2.077	0.000	0.1774	0.9960
1	1	1	52.240	49.679	49.679	-2.576	0.000	0.1774	0.9960
1	1	1	91.444	164.446	164.446	-0.370	2.697	2.1802	0.9897

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA / SIGMA	EXT. FACTOR
1	4	1	2.8977	4.6776	4.6777	0.0377	-1.779	-2.1220	0.9997
1	4	2	6.059	3.583	-3.5836	0.0086	-2.4775	-5.5574	0.9999
1	4	3	5.070	2.8988	-2.8988	0.0596	3.8022	8.7514	0.9999
1	4	4	5.070	5.0182	-5.0182	0.0101	0.058	0.1108	0.9996
1	4	5	10.997	1.0181	-1.0181	0.0289	0.815	2.0668	0.9986
1	4	6	5.400	4.4885	4.4885	0.0036	0.015	0.9515	0.9997
1	4	7	5.103	4.6641	4.6642	0.0033	0.462	0.8606	0.9997
1	4	8	10.662	17.776	17.807	0.0133	-1.114	-2.2588	0.9963
1	4	9	16.149	18.251	18.283	0.0211	-1.107	-4.2817	0.9983
1	4	10	11.968	10.651	10.656	0.0530	1.759	-2.3985	0.9983
1	4	11	36.886	35.127	-35.127	0.0307	1.027	-1.8446	0.9983
1	4	12	1.529	1.806	1.806	0.0267	-0.277	-0.1242	0.9966
1	4	13	4.323	2.955	-2.955	0.0234	-1.341	-1.5562	0.9966
1	4	14	74.001	74.981	-74.981	0.0225	-0.549	-0.2945	0.9966
1	4	15	4.001	2.550	-2.550	0.0344	-0.937	-0.3877	0.9993
1	4	16	9.335	10.273	-10.273	0.0122	-0.098	-0.8438	0.9993
1	4	17	26.491	26.285	-26.285	0.0278	-0.207	-0.2440	0.9993
1	4	18	19.402	19.500	-19.500	0.0340	-0.098	-0.1435	0.9998
1	4	19	8.587	8.156	-8.156	0.043	-0.180	-0.2513	0.9973
1	4	20	3.389	1.747	-1.747	0.0185	1.922	1.0474	0.9996
1	4	21	3.667	4.963	-4.963	0.0125	3.744	4.4196	0.9999
1	4	22	8.710	6.885	-6.885	0.0198	-1.608	-2.0301	0.9999
1	4	23	6.433	16.944	-16.944	0.0398	-1.447	-4.3546	0.9998
1	4	24	15.336	3.978	-3.978	0.0017	-0.508	-2.0301	0.9985
1	4	25	4.470	8.695	-8.695	0.0217	-0.438	-1.1457	0.9999
1	4	26	8.250	8.842	-8.842	0.0127	-0.501	-0.4457	0.9998
1	4	27	4.340	7.337	-7.337	0.0069	-1.886	-0.8929	0.9997
1	4	28	7.822	10.416	-10.416	0.0142	-1.886	-0.8929	1.0000
1	4	29	9.225	1.471	-1.471	0.0352	-0.409	0.3365	0.9999
1	4	30	8.052	5.981	-5.981	0.0060	-2.078	-1.6149	0.9995
1	4	31	8.732	3.963	-3.963	0.0292	-1.231	-0.9288	0.9999
1	4	32	31.099	32.760	-32.760	0.0224	-1.661	-1.9982	0.9996
1	4	33	31.589	37.851	-37.851	0.0323	-1.724	-2.4024	0.9868
1	4	34	31.589	86.417	-86.417	0.0566	-6.242	-7.4402	0.9825
1	4	35	81.916	37.970	-37.970	0.0323	-5.381	-7.1752	0.9825
1	4	36	67.219	77.347	-77.347	0.0722	-4.496	-6.2119	0.9148
1	4	37	29.021	31.822	-31.822	0.0519	-1.128	-2.1752	0.9129
1	4	38	105.720	116.021	-116.021	0.0190	-2.766	-3.4954	0.8657
1	4	39	29.021	125.653	-125.653	0.0190	-8.559	-3.9087	0.8497
1	4	40	8.097	101.993	-101.993	0.0200	-1.144	-3.7645	0.9022
1	4	41	35.074	41.436	-41.436	0.0348	-2.361	-3.8322	0.9997
1	4	42	67.743	72.783	-72.783	0.0483	-4.040	-5.7645	0.9845
1	4	43	67.743	71.651	-71.651	0.0220	-5.382	-3.4409	0.9566
1	4	44	63.421	70.769	-70.769	0.0753	-7.348	-4.5267	0.9616
1	4	45	24.252	18.175	-18.175	0.0108	-1.066	-1.5267	0.9957
1	4	46	17.044	18.403	-18.403	0.0658	-0.033	-1.0889	0.9977
1	4	47	6.687	39.776	-39.776	0.0018	-0.716	-1.5244	0.9996
1	4	48	35.564	47.404	-47.404	0.0018	-3.440	-0.5888	0.9996
1	4	49	40.921	44.009	-44.009	0.0356	-3.909	-5.5240	0.9863
1	4	50	40.921	44.009	-44.009	0.0356	-3.909	-5.5240	0.9889

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	5	0	57.818	60.951	-61.355	-5.226	-3.133	-2.1258	0.9798
1	5	0	48.912	50.705	-50.850	-4.524	-1.792	-1.4225	0.9865
1	5	0	46.293	49.381	-49.405	4.992	-3.057	-2.5507	0.9877
1	5	0	12.903	11.981	11.830	2.289	1.922	1.5427	0.9993
1	5	0	24.253	26.571	-26.527	-1.701	-2.318	-1.9562	0.9967
1	5	0	62.358	61.818	-62.239	-3.801	-2.066	-2.7423	0.9828
1	5	0	40.354	45.073	-40.745	-1.692	-1.161	-0.5936	0.9929
1	5	0	22.155	24.218	-24.155	-2.033	-1.244	-0.4715	0.9999
1	5	0	16.483	15.155	-15.130	1.588	0.633	-0.9152	0.9975
1	5	0	13.570	14.677	-14.608	1.470	1.322	-2.9124	0.9990
1	5	0	19.037	17.977	-17.913	0.447	1.105	-1.6124	0.9986
1	5	0	10.324	9.756	-9.759	-0.165	0.561	-1.4584	0.9990
1	5	0	38.601	40.333	-40.673	-0.239	1.730	-1.3089	0.9992
1	5	0	21.443	3.473	-3.472	-0.068	0.537	-1.9433	0.9999
1	5	0	19.222	21.190	-21.176	-0.022	1.056	-1.8333	0.9955
1	5	0	13.723	14.265	-14.278	0.072	0.014	0.0307	0.9980
1	5	0	3.491	3.114	-3.091	0.036	1.755	2.2006	0.9999
1	5	0	6.619	2.762	-2.762	0.021	0.857	0.7223	0.9999
1	5	0	2.408	9.274	-9.300	0.021	0.377	0.0723	0.9999
1	5	0	4.233	46.274	-46.678	-0.160	0.835	0.0723	0.9999
1	5	0	19.927	20.441	-20.441	0.045	0.754	0.3625	0.9999
1	5	0	12.261	29.447	-29.532	0.021	0.314	0.4032	0.9970
1	5	0	14.391	13.008	-13.011	0.016	0.326	0.6253	0.9985
1	5	0	15.840	15.386	-15.385	0.013	0.454	0.8972	0.9989
1	5	0	13.893	13.943	-13.943	0.018	0.655	0.4388	0.9986
1	5	0	13.851	15.944	-15.944	0.029	0.780	1.2188	0.9984
1	5	0	4.449	6.120	-6.121	0.027	0.112	0.0882	0.9991
1	5	0	2.279	8.674	-8.677	0.029	0.672	0.5233	0.9998
1	5	0	5.033	2.986	-2.986	0.010	0.706	0.7626	0.9996
1	5	0	3.503	3.785	-3.780	0.016	0.248	0.3326	0.9990
1	5	0	11.509	3.264	-3.266	0.023	0.085	0.1593	0.9992
1	5	0	1.184	12.441	-12.441	0.077	0.931	1.0166	0.9993
1	5	0	13.822	13.378	-13.380	0.019	0.404	0.6019	0.9992
1	5	0	3.371	0.621	-0.621	0.028	0.101	0.1219	0.9999
1	5	0	7.711	5.947	-5.945	0.015	0.233	0.7210	0.9999
1	5	0	16.435	6.847	-6.844	0.007	0.621	0.7449	0.9998
1	5	0	1.085	18.022	-18.034	-0.087	1.062	2.0628	0.9996
1	5	0	154.016	193.537	-193.533	-7.769	-3.522	-4.4688	0.9891
1	5	0	21.107	163.517	-163.935	-1.158	-2.144	-2.5725	0.9956
1	5	0	14.537	22.553	-22.516	1.358	-2.2280	-4.5728	0.9969
1	5	0	25.478	15.412	-15.899	-1.107	-2.003	-1.9003	0.9998
1	5	0	4.425	25.285	-25.333	-0.996	-0.140	0.2030	0.9947

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STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
1	7	8	52.851	54.681	-55.263	-2.941	-1.829	-1.3619	0.9763	*
1	7	8	57.842	63.697	-63.622	-0.344	-0.855	-3.3111	0.9665	*
1	7	8	39.662	39.346	-39.575	0.421	0.316	-0.2987	0.9883	*
1	7	8	46.502	43.701	-49.127	-0.142	-0.199	-1.8478	0.9827	*
1	7	8	21.240	22.991	-13.898	-2.072	-0.089	-1.7749	0.9986	*
1	7	8	135.436	148.441	-22.556	-1.694	-3.005	-0.9464	0.9985	*
1	7	8	35.833	38.441	-47.021	-2.154	-0.522	-0.8849	0.9965	*
1	7	8	14.137	15.850	-159.410	-6.783	-1.713	-0.1420	0.8687	*
1	7	8	8.588	17.310	-117.428	-1.137	-0.322	-4.1467	0.9221	*
1	7	8	3.855	5.553	-5.027	-1.567	-1.499	-1.7700	0.9997	*
1	7	8	22.241	21.471	-21.383	0.203	0.699	-1.4333	0.9997	*
1	7	8	38.884	39.338	-39.120	0.206	0.454	-0.4427	0.9924	*
1	7	8	35.873	35.272	-35.299	0.759	0.855	-0.6027	0.9924	*
1	7	8	41.716	41.530	-41.284	-0.616	-0.454	-2.1484	0.9942	*
1	7	8	37.771	37.530	-37.258	-0.287	-0.186	-1.6418	0.9942	*
1	7	8	33.037	31.239	-31.111	-0.820	-0.269	-1.4084	0.9925	*
1	7	8	73.830	75.978	-75.978	-0.525	-0.222	-1.4084	0.9925	*
1	7	8	68.107	67.595	-68.111	-0.525	-0.222	-1.4084	0.9925	*
1	7	8	59.663	59.950	-60.242	-0.908	-0.287	-0.2221	0.9925	*
1	7	8	47.155	46.888	-47.262	-0.887	-0.223	-0.2221	0.9925	*
1	7	8	18.199	19.939	-19.614	-0.127	-0.305	-0.2221	0.9925	*
1	7	8	18.281	16.336	-31.530	-0.134	-0.180	-0.2221	0.9925	*
1	7	8	16.130	16.411	-16.327	-0.047	-0.278	-0.2221	0.9925	*
1	7	8	3.246	1.975	-67.619	-0.069	-0.278	-0.2221	0.9925	*
1	7	8	56.555	67.117	-67.311	-0.724	-0.278	-0.2221	0.9925	*
1	7	8	58.068	62.454	-62.580	-0.067	-0.278	-0.2221	0.9925	*
1	7	8	25.773	25.583	-25.925	-0.067	-0.278	-0.2221	0.9925	*
1	7	8	14.158	15.868	-14.965	-0.127	-0.278	-0.2221	0.9925	*
1	7	8	22.283	23.250	-23.288	-0.247	-0.278	-0.2221	0.9925	*
1	7	8	12.173	9.332	-9.332	-0.169	-0.278	-0.2221	0.9925	*
1	7	8	13.101	0.336	-0.336	-0.053	-0.278	-0.2221	0.9925	*
1	7	8	15.173	15.149	-15.157	-0.020	-0.278	-0.2221	0.9925	*
1	7	8	22.507	23.250	-23.250	-0.030	-0.278	-0.2221	0.9925	*
1	7	8	3.771	17.625	-17.630	-0.010	-0.278	-0.2221	0.9925	*
1	7	8	16.855	14.121	-14.437	-0.571	-0.278	-0.2221	0.9925	*
1	7	8	21.271	22.418	-22.418	-0.027	-0.278	-0.2221	0.9925	*
1	7	8	16.012	16.818	-16.273	-0.109	-0.278	-0.2221	0.9925	*
1	7	8	20.683	21.201	-21.201	-0.079	-0.278	-0.2221	0.9925	*
1	7	8	5.122	6.189	-6.189	0.14	-0.278	-0.2221	0.9925	*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	8	28	17.312	15.089	15.089	0.058	1.420	2.185	0.998
1	8	30	3.496	9.078	9.078	-0.013	2.712	1.513	0.000
1	8	0	2.218	9.263	-9.023	-0.183	1.045	-1.165	0.999
1	8	1	5.662	4.067	5.025	-0.137	-0.087	-0.750	0.983
1	8	2	2.134	22.757	12.738	1.065	-0.622	-0.884	0.996
1	8	3	0.768	12.099	12.105	0.000	-0.331	-0.776	0.999
1	8	4	15.977	23.727	-23.749	1.070	-0.428	-2.414	0.996
1	8	5	4.468	15.203	15.490	-0.711	-0.665	-1.024	0.986
1	8	6	41.468	145.267	-155.492	-0.611	-3.799	-1.068	0.870
1	8	7	139.471	145.080	151.452	-7.457	-0.419	-0.744	0.877
1	8	8	125.582	142.001	-135.805	7.032	-0.999	-1.081	0.809
1	8	9	46.462	129.462	135.457	0.537	-0.656	-2.287	0.999
1	8	10	30.874	47.247	47.562	0.975	-0.128	-0.172	0.995
1	8	11	22.876	23.001	-23.808	0.144	-0.059	-0.287	0.996
1	8	12	13.246	23.305	-13.311	-0.056	-0.128	-0.088	0.995
1	8	13	47.781	46.601	46.576	0.075	-0.408	-1.109	0.988
1	8	14	53.549	2.423	2.182	-3.035	-0.052	-0.109	0.984
1	8	15	3.702	4.506	4.366	-1.011	-0.279	-0.695	0.980
1	8	16	18.335	19.533	19.555	-0.118	-0.114	-0.894	0.999
1	8	17	24.391	24.294	24.304	-0.093	-0.097	-0.907	0.999
1	8	18	76.259	98.574	-100.348	-6.246	-0.437	-0.173	0.955
1	8	19	70.827	74.574	70.084	-4.644	-0.097	-0.858	0.977
1	8	20	30.771	28.249	-28.290	-0.706	-0.525	-1.362	0.998
1	8	21	18.019	17.944	17.879	-0.091	-0.139	-0.667	0.999
1	8	22	12.527	12.338	12.339	-0.444	-0.312	-1.058	0.998
1	8	23	14.991	14.333	14.330	-0.421	-0.354	-1.189	0.999
1	8	24	35.020	45.474	45.564	2.091	-0.015	-0.298	0.994
1	8	25	9.923	8.677	8.681	-0.019	-0.012	-0.189	0.991
1	8	26	15.500	18.577	18.596	-0.013	-0.076	-0.668	0.997
1	8	27	5.031	16.685	16.686	-0.207	-0.293	-1.293	0.999
1	8	28	2.904	27.200	27.262	0.051	-0.031	-0.647	0.995
1	8	29	2.940	0.162	0.018	-0.162	-0.778	-0.078	0.999
1	8	30	7.788	3.448	3.320	-0.404	-0.440	-1.399	0.993
1	8	0	0.637	1.443	1.447	0.089	-0.404	-0.485	0.999
1	8	1	2.097	1.438	-3.447	-0.089	-0.661	-0.281	0.999
1	8	2	3.790	4.471	-1.473	-0.115	-0.603	-0.818	0.999
1	8	3	9.439	9.491	4.494	-0.068	-0.621	-0.219	0.999
1	8	4	3.714	0.698	3.695	-0.013	-0.093	-0.060	0.999
1	8	5	10.903	0.059	-0.022	-0.150	-0.093	-0.049	0.999
1	8	6	16.635	1.786	-1.022	-0.260	-0.684	-0.968	0.999
1	8	7	31.829	15.015	-15.026	-0.054	-0.620	-0.808	0.999
1	8	8	9.807	3.765	-3.765	-0.071	-0.936	-0.907	0.999
1	8	9	6.917	8.859	8.860	0.004	-0.602	-1.652	0.995
1	8	10	4.172	6.823	6.822	-0.168	-1.265	-1.271	0.999

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	0	21	7.447	6.860	-6.860	0.270	0.582	0.4917	0.99998
1	0	22	5.481	3.027	-3.860	0.018	1.721	1.2079	0.99999
1	0	23	4.227	5.833	-5.273	0.079	3.902	1.8494	0.00000
1	0	24	8.316	2.834	-2.465	0.048	1.695	2.1765	0.99990
1	0	25	4.161	9.225	-10.541	0.010	0.733	0.8148	0.00000
1	0	26	10.947	17.544	-17.544	0.110	1.342	1.1473	0.99996
1	0	27	88.036	92.266	94.294	0.530	4.223	1.3902	0.99998
1	0	28	63.411	67.593	-67.749	0.900	3.722	2.2742	0.95299
1	1	29	33.210	35.593	-35.705	0.090	2.485	2.0338	0.99248
1	1	30	14.335	16.839	-15.882	1.289	1.755	2.4704	0.99633
1	1	31	13.937	14.826	-14.835	0.105	1.830	2.2514	0.99886
1	1	32	20.632	31.630	-31.711	0.069	1.889	3.5212	0.99888
1	1	33	28.257	23.538	-23.558	0.848	2.999	4.5362	0.99945
1	1	34	20.257	10.328	-10.558	0.069	1.889	2.5212	0.99970
1	1	35	11.885	23.751	-23.829	0.872	3.565	6.1496	0.99994
1	1	36	21.657	20.751	-20.828	1.818	5.725	2.9288	0.99977
1	1	37	21.657	23.115	-23.248	1.566	0.177	1.2168	0.99972
1	1	38	23.281	23.115	-23.248	0.848	0.871	1.1427	0.99979
1	1	39	54.844	55.050	-55.365	0.508	2.142	1.5707	0.98446
1	1	40	51.937	50.791	-50.853	0.544	1.146	0.4064	0.98073
1	1	41	16.237	19.060	-19.071	0.070	0.829	1.5750	0.98299
1	1	42	16.237	19.060	-19.071	0.070	0.829	0.5750	0.98750
1	1	43	18.827	17.383	-17.600	0.544	2.824	3.9960	0.99883
1	1	44	23.928	21.806	-21.877	0.844	2.773	0.9960	0.99882
1	1	45	30.445	39.864	-39.936	0.787	3.805	2.6112	0.99886
1	1	46	30.445	39.864	-39.936	0.787	3.805	2.6112	0.99886
1	1	47	16.928	17.383	-17.600	0.070	0.829	0.5750	0.99929
1	1	48	16.928	17.383	-17.600	0.070	0.829	0.5750	0.99929
1	1	49	31.054	29.940	-29.933	0.424	1.959	3.2447	0.99929
1	1	50	31.054	29.940	-29.933	0.424	1.959	3.2447	0.99929
1	1	51	19.687	19.878	-19.878	0.596	2.844	1.8473	0.99961
1	1	52	19.687	19.878	-19.878	0.596	2.844	1.8473	0.99961
1	1	53	15.846	15.304	-15.320	0.283	1.554	1.4976	0.99983
1	1	54	15.846	15.304	-15.320	0.283	1.554	1.4976	0.99983
1	1	55	7.795	7.371	-7.372	0.029	0.809	1.4976	0.99983
1	1	56	7.795	7.371	-7.372	0.029	0.809	1.4976	0.99983
1	1	57	4.656	1.160	-1.082	0.017	0.497	0.2936	0.99997
1	1	58	4.656	1.160	-1.082	0.017	0.497	0.2936	0.99997
1	1	59	2.553	2.467	-2.044	0.027	0.309	0.9716	0.99996
1	1	60	2.553	2.467	-2.044	0.027	0.309	0.9716	0.99996
1	1	61	14.858	14.444	-14.449	0.103	0.664	0.4058	0.99990
1	1	62	14.858	14.444	-14.449	0.103	0.664	0.4058	0.99990
1	1	63	12.200	13.867	-13.871	0.269	0.449	0.8126	0.99989
1	1	64	12.200	13.867	-13.871	0.269	0.449	0.8126	0.99989
1	1	65	6.574	6.089	-6.090	0.033	0.059	0.3568	0.99990
1	1	66	6.574	6.089	-6.090	0.033	0.059	0.3568	0.99990
1	1	67	7.450	6.410	-6.418	0.187	0.545	1.1951	0.99998
1	1	68	7.450	6.410	-6.418	0.187	0.545	1.1951	0.99998
1	1	69	8.651	3.334	-3.336	0.459	1.726	0.4103	0.99998
1	1	70	8.651	3.334	-3.336	0.459	1.726	0.4103	0.99998

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	2	0	13.590	8.690	-8.688	-0.023	-0.100	-0.086	0.999
1	2	1	12.515	3.852	-10.155	-0.017	-0.213	-0.597	0.999
1	2	2	9.146	1.339	-1.379	-0.067	-1.337	-0.347	0.999
1	2	3	11.602	9.870	-9.869	-0.176	-0.027	-0.022	0.999
1	3	0	14.203	1.180	-10.182	-0.033	-1.422	-0.632	0.999
1	3	1	20.268	5.692	-5.690	-0.065	-1.664	-1.477	0.999
1	3	2	80.236	11.533	-11.518	-0.044	-2.670	-3.374	0.999
1	3	3	49.669	17.863	-17.717	-0.444	-1.607	-1.806	0.998
1	3	4	51.854	48.013	-48.229	-2.223	-1.112	-0.781	0.977
1	3	5	62.672	65.013	-65.505	-4.886	-2.340	-1.331	0.988
1	3	6	95.324	92.783	-91.173	-4.577	-3.541	-1.432	0.979
1	3	7	61.044	52.440	-52.745	-2.122	-2.037	-1.043	0.982
1	3	8	39.589	52.440	-50.781	-2.122	-0.396	-0.235	0.986
1	3	9	61.204	59.198	-59.551	-4.102	-1.085	-0.285	0.982
1	4	0	9.696	10.391	-10.391	-0.103	-0.006	-0.971	0.983
1	4	1	6.808	3.734	-3.715	-0.012	-1.128	-1.249	0.992
1	4	2	31.004	27.924	-27.812	-0.092	-2.080	-0.993	0.999
1	4	3	29.264	3.811	-3.811	-0.084	-3.080	-2.357	0.999
1	4	4	80.432	73.619	-74.902	-1.255	-4.813	-3.212	0.996
1	4	5	47.437	44.766	-44.868	-1.527	-4.813	-3.212	0.996
1	4	6	24.962	20.453	-20.460	-0.541	-2.672	-2.285	0.991
1	4	7	49.948	54.418	-54.319	-3.903	-4.474	-3.016	0.987
1	4	8	59.592	42.410	-42.542	-3.036	-5.271	-3.456	0.987
1	4	9	4.124	4.189	-4.054	-0.016	-0.714	-0.151	0.992
1	5	0	34.822	35.788	-35.894	-0.403	-0.958	-0.934	0.994
1	5	1	17.832	16.738	-16.746	-0.382	-0.523	-0.629	0.998
1	5	2	16.884	6.474	-6.444	-0.036	-0.780	-1.565	0.998
1	5	3	9.527	8.447	-8.442	-0.006	-0.105	-0.629	0.998
1	5	4	9.022	1.035	-1.022	-0.036	-0.992	-1.090	0.999
1	5	5	4.416	1.477	-1.474	-0.016	-0.105	-0.486	0.999
1	5	6	4.979	1.650	-1.645	-0.037	-0.060	-1.998	0.999
1	5	7	4.254	4.382	-4.379	-0.010	-0.701	-0.672	0.999
1	5	8	8.903	8.379	-8.195	-0.031	-0.859	-0.469	0.999
1	5	9	6.522	12.993	-12.379	-0.018	-0.442	-0.859	0.999
1	4	0	12.475	21.115	-21.134	-0.000	-0.360	-0.442	0.998
1	4	1	2.475	21.115	-21.134	-0.000	-0.360	-0.442	0.998
1	4	2	11.649	11.722	-11.722	-0.028	-1.218	-2.412	0.998
1	4	3	18.509	11.722	-11.722	-0.028	-1.218	-2.412	0.998
1	4	4	15.868	14.784	-14.773	-0.030	-1.174	-2.290	0.999
1	4	5	56.368	13.852	-13.857	-0.013	-0.109	-0.290	0.984
1	4	6	27.976	59.109	-59.481	-3.417	-2.133	-1.406	0.984
1	4	7	12.382	26.278	-26.203	-0.418	-1.103	-1.233	0.996
1	4	8	27.917	24.120	-24.888	-2.419	-0.790	-1.410	0.999
1	4	9	27.839	24.203	-24.925	-3.865	-0.635	-0.012	0.997

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H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	1	1	4.1357	4.1669	-4.164	0.032	-0.029	-0.0135	0.9997
1	1	1	4.1353	4.1297	-8.6392	-0.7339	-4.342	-2.0073	0.9997
1	1	1	16.4153	13.160	-13.152	1.263	2.856	3.3755	1.0000
1	1	1	36.818	31.942	-31.772	-0.1892	0.054	0.9327	0.9999
1	1	1	22.5561	19.039	-19.765	-3.934	4.898	4.0228	0.9999
1	1	1	36.889	55.655	19.931	-2.2484	2.2442	5.346	0.9999
1	1	1	54.543	41.030	-41.144	3.366	-0.766	0.5184	0.9982
1	1	1	15.2261	16.030	-15.932	-1.848	0.462	0.9184	0.9989
1	1	1	4.393	0.785	-0.785	0.105	0.767	0.3855	0.9926
1	1	1	2.393	1.765	-0.817	0.082	0.607	0.6422	0.0000
1	1	1	3.507	1.852	-1.852	0.013	0.757	1.6249	0.0000
1	1	1	3.601	4.239	4.238	0.018	1.183	0.7225	1.0000
1	1	1	3.393	2.272	-2.272	0.092	0.361	0.6535	0.9999
1	1	1	8.604	4.401	-4.401	0.016	1.154	0.5457	0.9999
1	1	1	13.911	14.002	-14.000	0.049	0.154	0.1643	0.9999
1	1	1	15.956	14.440	-4.440	0.010	0.169	0.5771	0.9999
1	1	1	15.245	17.481	14.687	0.163	1.127	1.4507	0.9999
1	1	1	34.447	150.779	-51.676	-2.616	-1.169	-3.5771	0.6533
1	1	1	15.407	40.859	-41.261	-2.321	-6.668	-1.2500	0.9631
1	1	1	34.380	113.983	-18.111	-3.679	-2.210	-5.3153	0.9775
1	1	1	115.658	66.645	-122.288	1.928	1.675	0.2100	0.9969
1	1	1	52.487	55.225	56.435	1.320	1.108	0.5767	0.8679
1	1	1	72.095	66.224	67.340	1.120	1.146	0.3482	0.9711
1	1	1	26.034	41.526	41.674	1.396	1.158	0.6463	0.9651
1	1	1	41.841	29.781	-29.020	0.524	0.060	0.5653	0.9918
1	1	1	84.273	83.997	-90.460	-5.033	-1.453	-3.9537	0.9953
1	1	1	32.473	39.714	-33.776	-1.056	-2.241	-2.2064	0.9644
1	1	1	58.798	59.017	-59.776	-3.305	-1.219	-1.3411	0.9953
1	1	1	33.127	98.814	-100.263	-8.389	-0.687	-0.2758	0.9865
1	1	1	33.917	36.705	-36.585	-2.521	-0.787	-0.8179	0.9645
1	1	1	30.187	29.639	-29.585	-2.121	-0.734	-2.7792	0.9962
1	1	1	20.187	110.225	-120.207	-1.392	-0.930	-0.2992	0.8412
1	1	1	27.898	48.141	-49.001	-0.688	-0.301	-0.2004	0.9650
1	1	1	27.404	62.102	-27.253	-0.229	-0.478	0.4240	0.9890
1	1	1	66.098	62.622	-64.444	0.022	0.341	0.9554	0.9442
1	1	1	63.863	25.332	-25.468	0.044	0.017	0.4560	0.9913
1	1	1	28.396	27.319	-27.441	0.027	0.077	1.4560	0.9905
1	1	1	25.371	21.046	-21.079	-0.080	-0.156	-0.9717	0.9946
1	1	1	18.485	21.581	-22.640	-0.352	-0.114	-1.1997	0.9945
1	1	1	21.867	42.353	-42.763	0.021	0.091	0.0788	0.9823
1	1	1	41.091	2.103	-4.463	-0.218	-1.013	0.0788	0.9831
1	1	1	4.116	2.859	2.851	0.209	1.30	1.7583	0.9999

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	1	1	16.677	16.499	-16.509	-0.467	0.178	0.3451	0.9981
14	11	15	65.515	65.476	66.561	1.0218	0.0031	0.0239	0.9673
11	15	6	35.523	37.737	37.942	-0.792	-2.700	-2.2012	0.9849
11	17	3	30.264	32.986	29.942	0.019	0.181	0.8657	0.9948
11	18	9	39.499	38.080	-38.250	-0.202	0.581	1.1709	0.9908
11	19	1	31.105	31.448	-20.471	0.280	-1.344	-2.5963	0.9913
12	20	1	18.083	18.980	-31.864	0.628	0.677	-2.2774	0.9946
12	21	2	11.164	11.547	-11.933	0.021	0.866	-1.1522	0.9982
12	22	3	27.035	27.180	19.560	0.697	-0.677	0.4448	0.9982
12	23	4	8.329	8.500	-18.513	0.297	-1.142	-2.3136	0.9982
12	24	5	22.295	21.677	5.471	0.160	0.849	-0.9308	0.9985
12	25	6	8.220	8.477	1.654	0.278	2.841	4.1398	0.9999
12	26	7	22.209	21.701	1.706	0.027	0.617	0.7416	0.9999
12	27	8	17.928	18.880	-18.328	0.065	0.854	0.7460	0.9981
12	28	9	17.200	17.094	-16.889	0.033	0.048	0.2977	0.9989
12	29	0	14.950	14.570	14.575	0.092	0.047	0.1073	0.9989
12	30	1	10.456	10.214	-10.214	0.023	0.339	0.5169	0.9992
12	31	2	26.273	25.998	-26.059	-0.655	0.024	0.0242	0.9996
12	32	3	11.312	11.508	8.634	-0.973	0.545	0.0245	0.9901
12	33	4	22.338	22.504	-22.243	-0.186	0.627	0.2222	0.9987
12	34	5	7.384	7.914	-7.224	-0.701	0.279	0.4207	0.9997
12	35	6	5.334	5.324	-4.474	-0.546	0.060	0.0139	0.9353
12	36	7	5.678	5.001	-5.002	-0.069	0.067	0.0134	0.9780
12	37	8	14.778	14.730	-14.584	-0.212	0.044	0.0922	0.9996
12	38	9	13.475	13.625	-16.360	-0.216	0.048	0.0927	0.9977
12	39	0	9.253	9.071	-9.953	-0.227	0.687	4.0948	0.9976
12	40	1	24.376	24.046	24.093	-0.099	0.331	0.4044	0.9996
12	41	2	9.892	9.830	-7.812	-0.565	0.299	0.182	0.9961
12	42	3	66.801	70.093	71.028	0.672	2.292	4.1044	0.9999
12	43	4	20.096	23.166	-23.104	-0.624	0.375	1.9512	0.9710
12	44	5	4.541	4.442	-3.868	-0.311	1.151	1.5336	0.9999
12	45	6	50.712	50.688	65.097	2.241	0.030	0.4969	0.9974
12	46	7	4.072	4.771	-5.714	-0.977	0.001	0.0234	0.9747
12	47	8	160.501	160.561	-169.566	-0.637	0.011	0.1309	0.0000
12	48	9	4.538	5.234	15.906	-0.445	0.304	0.0273	0.8937
12	49	0	14.924	15.346	15.072	-0.275	0.599	1.0273	0.0000
12	50	1	18.948	17.616	-13.602	-0.418	0.678	2.2080	0.9986
12	51	2	15.425	13.152	-13.134	-0.769	1.133	1.6832	0.0000
12	52	3	5.785	5.910	-5.989	-0.345	0.769	1.5243	0.9996
12	53	4	5.883	8.003	-9.982	-0.341	0.299	0.9206	0.9996
12	54	5	9.797	10.333	-10.327	-0.411	0.735	2.2065	0.9996
12	55	6	3.973	3.884	-32.894	-1.950	0.089	1.1564	0.9959

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
N	3	30	38.797	37.617	-37.617	-2.748	1.179	1.1287	0.9947
N	3	30	45.795	43.617	-44.179	-0.324	2.178	1.8727	0.9747
N	3	30	27.747	26.313	-26.425	-0.174	1.403	1.9425	0.9915
N	3	30	4.4735	0.844	0.836	-0.119	3.628	6.8037	1.0000
N	3	30	9.8363	10.250	-10.833	-0.465	-0.415	-1.0586	0.9988
N	3	30	2.2281	0.2336	0.070	0.225	2.059	3.2456	0.9993
N	3	30	35.9775	26.790	-25.488	-0.062	0.491	1.9903	0.9993
N	3	30	18.841	18.122	-18.146	-0.151	0.688	1.6855	0.9982
N	3	30	13.0749	13.331	-13.695	-0.278	0.154	0.7441	0.9971
N	3	30	10.6749	9.338	-24.380	-0.495	1.413	1.5393	0.9984
N	3	30	25.2249	24.024	-24.338	-0.271	0.576	1.3573	0.9956
N	3	30	14.6732	15.622	-15.706	-0.020	0.414	1.1579	0.9984
N	3	30	30.432	30.643	-30.732	-0.261	0.344	0.8348	0.9942
N	3	30	13.082	13.497	-13.701	-0.331	0.440	0.6157	0.9986
N	3	30	8.667	10.606	-10.205	-0.051	0.022	0.0037	0.9992
N	3	30	3.427	14.406	-14.022	-0.190	0.893	2.0079	0.9992
N	3	30	14.026	14.024	-14.987	-0.230	0.022	0.5579	0.9990
N	3	30	26.191	27.088	-27.751	-0.244	0.895	1.5579	0.9990
N	3	30	21.477	21.732	-21.751	-0.277	0.920	1.2306	0.9995
N	3	30	7.729	9.964	-9.861	-0.341	0.225	0.4006	0.9997
N	3	30	2.5075	2.864	-2.861	-0.277	0.113	0.2266	0.9997
N	3	30	12.2276	12.172	-12.170	-0.000	0.113	0.9243	0.9997
N	3	30	12.463	12.255	-12.266	-0.000	0.104	2.9243	0.9996
N	3	30	20.256	19.055	-19.070	-0.000	0.159	0.1805	0.9996
N	3	30	13.865	13.802	-13.809	-0.000	0.056	0.8425	0.9993
N	3	30	7.633	7.614	-7.614	-0.000	0.000	0.1753	0.9993
N	3	30	2.2037	2.343	-2.342	-0.000	0.290	0.3561	0.9998
N	3	30	4.437	4.605	-4.584	-0.000	0.056	0.773	0.9998
N	3	30	2.811	3.303	-3.338	-0.000	0.000	0.899	0.9998
N	3	30	3.811	3.708	-3.938	-0.000	0.000	0.773	0.9999
N	3	30	2.811	2.678	-2.922	-0.000	0.000	0.352	0.9999
N	3	30	1.698	1.678	-1.678	-0.000	0.000	0.232	1.0000
N	3	30	3.911	3.884	-3.460	-0.000	0.000	0.338	0.9998
N	3	30	4.824	4.944	-4.633	-0.000	0.000	0.538	0.9998
N	3	30	6.509	6.723	-6.406	-0.000	0.000	0.324	0.9998
N	3	30	85.400	83.717	-86.489	-0.000	0.000	2.260	0.9998
N	3	30	41.408	43.584	-43.982	-0.000	0.000	1.260	0.9998
N	3	30	17.499	16.170	-16.170	-0.000	0.000	0.784	0.9998
N	3	30	39.487	38.422	-38.658	-0.000	0.000	1.217	0.9998
N	3	30	107.361	109.932	-114.744	-0.000	0.000	1.571	0.9998
N	3	30	22.423	22.280	-22.195	-0.000	0.000	0.398	0.9998
N	3	30	209.242	184.641	-209.392	-0.000	0.000	2.153	0.9998
N	3	30	9.180	6.573	-6.573	-0.000	0.000	0.699	0.9998
N	3	30	5.630	4.983	-4.726	-0.000	0.000	0.640	0.9997
N	3	30	117.629	119.590	-124.059	-0.000	0.000	2.667	0.9289
N	3	30	12.003	11.444	-11.254	-0.000	0.000	0.557	0.9992

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
2	2	2	54.500	57.189	-57.654	-2.804	-2.689	-1.9333	0.9816
2	2	2	60.687	59.818	-30.286	-1.599	-1.869	0.5633	0.9835
2	2	2	229.188	30.522	-30.565	-1.271	-1.344	-1.6826	0.9959
2	2	2	27.013	36.844	-36.844	-2.987	-0.828	-0.8698	0.9933
2	2	2	327.727	27.732	-27.736	-1.463	-0.004	-0.0058	0.9969
2	2	2	5.831	6.276	6.221	0.833	0.444	0.4360	0.9998
2	2	2	49.332	51.993	5.043	4.704	0.661	-0.8290	0.9997
2	2	2	26.433	27.573	-27.536	2.604	0.621	0.8220	0.9972
4	4	4	67.176	66.228	-66.521	-6.167	0.892	0.8934	0.9984
4	4	4	5.936	9.327	4.276	0.060	0.657	0.5221	0.9944
4	4	4	9.079	9.322	9.176	1.688	1.250	1.2347	0.9997
4	4	4	50.852	57.768	-53.987	-2.915	-2.916	-2.2082	0.9999
4	4	4	16.265	17.137	-17.008	0.547	1.269	5.6333	0.9989
4	4	4	18.929	18.564	-18.245	0.224	0.422	2.6068	0.9996
4	4	4	58.816	61.275	-61.231	-1.557	-1.322	-0.8144	0.9996
4	4	4	59.779	60.140	-18.581	0.562	0.442	-0.6805	0.9965
4	4	4	25.546	27.487	-27.409	0.978	1.496	-0.9902	0.9644
4	4	4	49.049	48.964	-49.448	-0.828	0.131	-0.9930	0.9990
5	5	5	23.430	24.671	-24.101	-0.507	-0.899	0.0714	0.9801
5	5	5	34.340	34.045	-34.846	-0.504	-0.331	-0.9575	0.9949
5	5	5	53.267	52.573	-53.167	-0.875	-0.699	-0.3696	0.9898
5	5	5	55.443	56.892	-57.525	-0.998	-1.449	-0.5132	0.9775
5	5	5	18.250	17.932	18.130	0.579	0.158	-0.2362	0.9978
5	5	5	7.779	7.937	7.937	0.176	0.062	-0.0473	0.9999
5	5	5	2.896	2.965	2.925	0.486	0.069	-0.2375	0.9999
5	5	5	2.179	2.333	2.351	0.553	0.472	0.3370	1.0000
5	5	5	21.179	21.062	21.313	-0.275	-0.148	-0.2375	0.9991
5	5	5	40.663	37.635	-40.790	-0.957	-0.036	-0.0337	0.9915
5	5	5	35.369	37.135	-37.274	-0.868	-1.766	-1.8929	0.9920
5	5	5	10.810	12.630	-12.630	0.363	0.827	-3.0915	0.9991
5	5	5	15.966	16.041	-16.038	0.204	0.075	-1.1251	0.9998
5	5	5	19.486	18.721	-18.487	0.598	0.770	1.2617	0.9985
5	5	5	16.262	15.488	-15.495	0.550	0.774	1.3190	0.9988
5	5	5	127.714	124.468	-24.495	-0.550	0.044	1.6949	0.9976
5	5	5	27.630	27.874	-27.914	0.662	0.244	-0.3152	0.9959
5	5	5	31.164	30.434	-30.787	0.794	0.430	-0.5058	0.9994
5	5	5	11.790	12.256	-12.426	0.544	0.644	-0.9981	0.9994
5	5	5	11.718	12.434	-12.259	0.126	0.540	0.7919	0.9999
5	5	5	5.588	4.181	-4.170	0.350	0.490	0.3155	0.9999
5	5	5	5.161	0.671	-0.638	0.208	0.512	0.8824	1.0000
5	5	5	16.834	16.321	-16.321	0.724	0.406	0.5790	0.9982
5	5	5	18.647	22.449	-22.735	-2.057	-4.128	-7.5905	0.9954
5	5	5	11.607	16.607	-16.735	-2.067	-1.599	-3.0512	0.9977
5	5	5	31.237	34.829	-34.316	-2.581	-0.044	-0.0596	0.9914
5	5	5	33.715	31.068	-31.985	1.722	-1.118	-1.2238	0.9891
5	5	5	33.063	32.109	-32.465	1.631	-0.618	-0.2238	0.9913
5	5	5	7.111	6.688	-6.688	0.366	0.422	0.7805	0.9996

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
N	6	7	111.747	118.192	-124.789	-8.405	-6.445	-2.2988	0.8930
N	6	8	15.395	3.623	9.622	0.116	3.772	2.5882	0.9999
N	6	9	13.099	9.783	3.744	0.928	1.310	6.6975	0.9999
N	6	10	184.570	89.515	-92.023	-6.177	4.945	-2.3323	0.9420
N	6	11	18.452	18.611	53.312	1.750	-0.215	-0.3394	0.9827
N	6	12	50.235	52.941	-46.149	3.264	-2.105	-0.1072	0.9825
N	6	13	44.725	44.867	-42.630	-2.049	-0.143	-0.9929	0.9855
N	6	14	23.114	22.668	-47.966	-1.062	-0.445	-0.6783	0.9966
N	6	15	46.761	49.626	49.452	-1.833	-0.915	-0.2761	0.9975
N	6	16	10.891	38.710	-38.836	-1.295	-0.177	-0.2735	0.9924
N	6	17	38.533	39.041	-82.252	-6.704	-0.966	-0.4667	0.9644
N	6	18	82.007	52.624	-52.952	-2.421	-1.035	-0.7819	0.9856
N	6	19	51.588	83.202	13.183	0.807	-1.976	-1.0781	0.9992
N	6	20	81.226	83.785	84.840	6.233	-2.111	-3.3440	0.9992
N	6	21	3.232	12.465	-12.464	-0.033	-0.768	-1.0230	0.9701
N	6	22	12.163	12.976	-12.637	-0.790	-0.494	-0.8085	0.9994
N	6	23	140.970	42.976	-42.978	-4.278	-2.007	-1.8611	0.9920
N	6	24	20.875	21.051	-20.978	-1.970	-0.076	-1.8611	0.9920
N	6	25	41.062	44.335	-43.394	-3.350	-2.292	-2.5251	0.9921
N	6	26	48.074	44.913	-45.050	-1.298	-3.161	-2.5114	0.9918
N	6	27	17.052	17.254	-17.216	-2.297	-2.203	-2.5251	0.9918
N	6	28	26.562	28.849	-28.839	-1.753	-0.287	-2.2898	0.9970
N	6	29	7.219	5.978	-19.839	-1.175	-0.287	-2.2898	0.9970
N	6	30	18.999	19.312	-19.831	-0.699	-1.313	-2.2898	0.9986
N	6	31	30.366	32.185	-32.323	-0.548	-1.819	-2.2662	0.9982
N	6	0	29.890	30.742	-30.132	-0.461	-1.319	-2.2662	0.9986
N	6	1	22.061	22.443	-22.443	-0.228	-0.139	-2.1754	0.9929
N	6	2	22.301	22.443	-22.443	-0.228	-0.139	-2.1754	0.9929
N	6	3	10.742	13.080	-13.094	-0.516	-0.738	-2.2727	0.9991
N	6	4	27.914	27.315	-27.090	-0.313	-0.664	-1.7027	0.9999
N	6	5	30.555	32.158	-32.232	-0.835	-0.894	-1.1947	0.9946
N	6	6	15.183	15.527	-15.532	-0.240	-0.559	-1.0007	0.9572
N	6	7	14.776	21.429	-21.797	-0.474	-0.750	-1.3759	0.9984
N	6	8	21.840	21.429	-21.797	-0.388	-0.071	-1.3759	0.9971
N	6	9	14.094	15.527	-15.532	-0.240	-0.559	-1.0007	0.9985
N	6	10	35.721	35.369	-35.505	-0.437	-0.195	-0.3759	0.9988
N	6	11	12.491	26.127	-26.170	-0.259	-0.353	-0.3759	0.9922
N	6	12	25.437	26.063	-26.079	-0.476	-0.636	-0.9934	0.9964
N	6	13	19.086	20.024	-20.021	-0.154	-1.237	-0.9208	0.9979
N	6	14	16.892	16.784	-16.797	-0.474	-0.108	-0.1189	0.9999
N	6	15	5.052	13.917	-13.032	-0.501	-0.475	-0.1123	0.9994
N	6	16	13.442	13.834	-13.915	-0.013	-0.918	-0.5949	0.9990
N	6	17	17.752	17.790	-17.896	-0.626	-0.475	-0.8345	0.9994
N	6	18	37.685	37.852	-37.896	-0.270	-0.104	-0.5310	0.9994
N	6	19	17.855	18.543	-18.865	-0.025	-0.997	-0.3517	0.9989
N	6	20	15.795	15.056	-15.551	-0.366	-0.207	-0.3517	0.9989
N	6	21	10.260	10.026	-10.022	-0.046	-0.734	-0.3562	0.9996
N	6	22	10.649	10.874	-10.876	-0.179	-0.225	-0.3297	0.9996
N	6	23	27.236	28.314	-28.351	0.463	-1.078	-1.3370	0.9971

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
28	7	0	15.902	15.271	15.274	0.310	0.631	0.9936	0.9992
29	7	0	8.674	9.000	-8.995	-0.332	-0.326	-0.4065	0.9997
30	7	0	3.537	3.670	-3.783	0.133	-0.130	-0.0725	1.0000
1	8	0	147.017	145.827	157.783	5.368	1.193	0.3229	0.8532
2	8	0	3.646	4.652	-4.649	-0.161	1.310	2.0226	0.9998
3	8	0	3.391	5.187	5.172	0.408	-1.541	-0.5264	0.9975
4	8	0	5.336	115.893	-27.802	-1.035	-0.356	-0.4764	0.9998
5	8	0	7.204	66.935	-27.884	-2.636	-0.215	-3.1428	0.9947
6	8	0	7.444	26.771	-67.634	-2.554	-0.806	-3.215	0.9971
7	8	0	2.088	34.442	-26.682	-2.142	-3.590	-5.3711	0.9953
8	8	0	2.275	17.723	-34.501	-2.814	-0.428	-4.3699	0.9928
9	8	0	1.286	17.800	-17.792	-0.948	0.447	-0.5856	0.9951
10	8	0	1.738	143.075	152.157	1.380	4.327	1.2586	0.9980
11	8	0	1.376	22.599	22.038	0.401	0.661	1.2586	0.8822
12	8	0	1.001	93.106	-101.241	-0.530	-1.219	-1.9823	1.0000
13	8	0	3.446	93.918	-101.241	-0.443	-1.536	-1.0456	0.9975
14	8	0	8.647	11.509	-11.243	0.017	-2.863	-1.0456	0.9995
15	8	0	5.688	41.100	-40.985	-0.117	-2.672	-2.6494	0.9999
16	8	0	2.568	24.088	-24.709	0.330	-4.264	-4.3792	0.9925
17	8	0	3.647	4.131	5.985	-0.997	-2.428	-1.7281	0.9998
18	8	0	2.447	11.100	-11.131	0.330	0.817	1.6060	0.9974
19	8	0	2.447	50.032	-50.150	-0.718	-2.817	-2.3035	0.9899
20	8	0	47.215	11.690	-11.579	0.818	2.487	3.8675	0.9995
21	8	0	13.818	16.331	16.287	1.113	3.647	1.5044	1.0000
22	8	0	19.871	16.240	-17.234	0.202	0.850	-1.2201	0.9990
23	8	0	1.626	96.786	-98.488	-1.777	-0.614	0.7844	0.9987
24	8	0	1.345	30.647	-30.636	0.012	-0.287	-1.0045	0.9966
25	8	0	3.495	35.155	-35.153	0.007	-0.067	-1.2609	1.0000
26	8	0	1.061	3.558	-3.659	0.462	-1.757	0.9321	0.9912
27	8	0	3.371	8.655	-8.655	0.327	-1.053	-1.5498	0.9959
28	8	0	4.466	25.235	-25.236	0.005	-0.703	-1.0310	0.9995
29	8	0	9.137	8.461	-8.476	0.407	0.347	-0.6017	0.9995
30	8	0	7.986	35.913	-7.998	-0.577	0.246	0.1302	0.9995
1	9	0	31.861	42.015	-35.140	-0.467	0.087	-0.0948	0.9928
2	9	0	4.928	3.049	-28.114	-0.364	-0.772	-0.7212	0.9893
3	9	0	2.287	2.059	-5.831	0.319	-0.423	-0.0392	0.9953
4	9	0	2.556	1.839	-1.831	0.414	-0.123	-0.1602	0.9998
5	9	0	7.131	15.550	-15.550	0.412	0.719	0.7711	1.0000
6	9	0	1.313	10.817	-10.820	0.086	0.419	-0.3531	0.9986
7	9	0	1.134	29.644	-29.713	-0.086	-0.996	-1.2951	0.9961
8	9	0	4.435	1.302	-1.162	0.307	-0.168	-0.2993	0.9952
9	9	0	3.231	9.066	-9.038	0.307	0.168	-0.2993	0.9989
10	9	0	2.021	13.130	-13.126	0.511	0.599	0.8930	1.0000
11	9	0	9.954	1.130	-1.126	0.000	0.176	0.9288	0.9997

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
2	1	1	25.804	24.366	24.666	0.391	1.168	1.573	0.9976
2	1	1	25.114	23.394	23.418	0.341	1.746	1.042	0.9976
2	1	1	19.931	12.416	-12.416	-0.169	1.515	1.049	0.9994
2	1	1	6.833	8.752	8.752	-0.152	1.638	-1.862	0.9997
2	1	1	8.570	2.202	2.202	-0.384	4.633	5.579	0.0000
2	1	1	8.142	3.985	-8.419	-0.284	0.144	0.192	0.9997
2	1	1	8.614	21.687	-21.687	0.594	0.544	0.640	0.9997
2	1	1	15.854	17.368	-17.368	-0.313	1.844	1.389	0.9981
2	1	1	8.811	35.238	35.238	0.267	1.506	-2.082	0.9992
2	1	1	21.058	19.663	19.663	0.769	1.303	3.082	0.9992
2	1	1	109.880	110.139	-113.825	-7.178	2.227	4.192	0.9998
2	1	1	20.095	119.584	119.584	0.044	0.259	2.227	0.9932
2	1	1	54.711	56.944	-57.584	0.882	1.876	1.746	0.9979
2	1	1	31.644	30.944	33.594	0.656	2.304	1.650	0.9999
2	1	1	31.720	37.398	-39.493	-0.756	1.879	1.746	0.9999
2	1	1	35.356	31.329	39.594	0.947	1.679	1.664	0.9939
2	1	1	13.156	12.949	-12.949	-0.544	1.827	3.311	0.9993
2	1	1	30.428	14.523	-18.388	-2.441	0.932	1.121	0.9938
2	1	1	114.737	114.523	-118.388	-0.471	0.022	0.074	0.9938
2	1	1	31.955	64.966	-65.575	-1.411	0.572	0.659	0.9946
2	1	1	63.478	10.193	10.047	0.192	1.022	1.229	0.9780
2	1	1	33.219	17.081	-16.077	-0.506	0.977	0.917	0.9996
2	1	1	17.769	15.798	-16.366	0.698	0.094	0.502	0.9996
2	1	1	4.714	9.208	-9.208	0.424	0.070	0.216	0.9975
2	1	1	10.744	9.274	-9.274	0.845	1.113	0.531	0.9996
2	1	1	19.556	23.444	-23.444	-0.015	1.213	0.792	0.9981
2	1	1	48.460	23.082	-23.182	-1.853	0.622	0.792	0.9981
2	1	1	44.845	34.837	-34.661	0.853	0.008	0.490	0.9999
2	1	1	35.176	13.655	13.655	0.012	1.265	0.490	0.9999
2	1	1	15.676	21.794	-21.812	-0.673	0.515	0.515	0.9999
2	1	1	20.814	37.369	-37.369	0.333	0.965	1.552	0.9944
2	1	1	36.810	4.510	4.510	-0.996	0.078	0.154	0.9974
2	1	1	7.660	7.660	-7.673	0.044	0.176	0.116	0.9997
2	1	1	22.603	22.836	-22.836	0.418	0.814	0.216	0.9997
2	1	1	11.323	12.133	-12.133	0.351	0.440	0.443	0.9998
2	1	1	6.263	32.633	32.633	0.010	0.340	0.443	0.9998
2	1	1	32.917	16.602	-16.602	-0.966	0.944	0.504	0.9962
2	1	1	14.665	10.155	-10.155	0.595	0.816	0.202	0.9989
2	1	1	12.609	17.855	-17.855	-0.405	1.490	1.501	0.9995
2	1	1	3.222	1.079	-1.079	0.045	0.754	0.904	0.9998
2	1	1	20.630	19.841	-19.841	0.202	1.798	1.817	0.9998
2	1	1	20.011	20.864	-20.864	0.659	1.150	1.221	0.9979

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
2	1	18	28.368	27.749	-27.785	-0.877	0.619	0.7707	0.9965
2	1	19	5.543	5.204	-5.199	-0.235	0.5276	0.9999	0.9999
2	1	20	3.315	0.874	-0.826	-0.372	2.062	1.4849	1.0000
2	1	21	1.315	0.375	-1.037	-0.318	0.944	1.3999	0.9995
2	1	22	9.462	8.420	-8.255	-0.129	1.587	1.7100	0.9997
2	1	23	6.679	5.254	-5.880	-0.806	0.203	1.6830	0.9997
2	1	24	1.113	1.688	-1.988	-0.806	0.203	1.6830	0.9986
2	1	25	1.771	1.626	-1.620	-0.622	1.203	2.5591	0.9999
2	1	0	2.892	5.011	-5.015	-0.127	0.498	1.2244	0.9999
2	1	1	9.046	8.904	-8.895	-0.615	1.988	1.7784	0.9996
2	1	2	3.914	7.300	-7.032	-0.196	0.021	0.7784	0.9996
2	1	3	8.847	6.034	-6.032	-0.196	0.021	0.7784	0.9998
2	1	4	1.799	15.355	-15.324	-0.160	1.220	1.6442	0.9998
2	1	5	17.936	15.222	-15.083	-0.160	1.220	1.6442	0.9983
2	1	6	3.566	3.244	-3.108	-0.488	0.745	0.5984	0.9950
2	1	7	17.936	17.613	-17.622	-0.574	2.234	3.481	0.9987
2	1	8	6.209	6.443	-6.450	-0.310	0.391	0.4146	0.9981
2	1	9	3.699	1.083	-2.083	-0.651	2.616	1.2740	0.9983
2	1	10	3.699	6.074	-6.072	-0.194	0.950	1.8332	0.9980
2	1	11	4.125	5.335	-5.336	-0.450	1.515	1.4816	0.9999
2	1	12	18.445	19.529	-19.492	-0.031	1.081	1.5154	0.9999
2	1	13	4.434	4.432	-4.437	-0.449	1.031	0.9048	0.9982
2	1	14	28.968	27.432	-27.441	-0.477	0.905	1.6605	0.9997
2	1	15	3.531	4.492	-4.479	-0.449	1.031	0.9048	0.9967
2	1	16	4.434	5.990	-5.641	-0.509	1.653	1.6605	0.9865
2	1	17	23.370	25.731	-24.667	-3.184	0.807	0.978	0.9978
2	1	18	4.078	2.999	-2.893	-0.448	1.309	0.4700	0.9980
2	1	19	4.078	13.712	-13.842	-0.161	0.533	1.5066	0.9921
2	1	20	4.078	4.422	-4.095	-0.095	0.101	0.8941	0.9999
2	1	21	4.734	6.702	-6.318	-0.164	0.414	0.886	0.9998
2	1	22	4.815	2.709	-2.699	-0.231	1.062	0.4059	0.9987
2	1	23	4.664	16.821	-16.832	-0.114	1.192	0.3189	0.9986
2	1	24	12.188	12.638	-12.327	-0.088	0.450	0.7027	0.9993
2	1	25	7.728	4.830	-4.769	-0.025	0.057	0.0969	0.9999
2	1	0	4.629	4.312	-4.303	-0.030	0.311	0.3900	0.9999
2	1	1	1.629	6.561	-6.561	-0.069	1.166	0.0199	0.9998
2	1	2	1.337	10.994	-10.996	-0.149	0.382	0.5730	0.9998
2	1	3	4.452	2.930	-2.927	-0.049	0.144	0.1697	0.9997
2	1	4	3.476	8.907	-8.904	-0.158	0.475	0.6416	0.9996
2	1	5	3.826	4.950	-4.476	-0.333	0.915	1.6677	0.9996
2	1	6	4.229	6.941	-6.939	-0.163	0.512	0.7066	0.9999
2	1	7	17.164	17.260	-17.270	-0.102	0.096	0.144	0.9989

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
2	14	0	21.821	21.352	-21.266	-2.146	0.469	0.6753	0.9979
2	14	1	27.453	26.236	-77.027	-6.103	0.217	0.1118	0.9735
2	14	2	10.051	11.419	-11.406	0.605	-1.366	-1.9556	0.9994
2	14	3	17.146	15.771	-5.759	0.371	1.375	1.5156	0.9998
2	14	4	60.479	56.051	-56.385	-3.387	0.163	2.8327	0.9856
2	14	5	3.425	8.397	-8.514	-0.128	0.028	0.0361	0.9999
2	14	6	19.450	13.397	13.307	1.623	6.055	9.2281	0.9992
2	14	7	3.425	12.311	-12.307	-0.133	0.054	0.0700	0.9990
2	14	8	14.802	14.749	-14.707	-1.139	0.188	0.0861	0.9990
2	14	9	19.782	17.905	-17.778	-2.215	1.399	2.9638	0.9987
2	14	10	10.219	18.747	-18.743	-0.298	2.038	1.1105	0.9996
2	14	11	71.823	10.406	-10.409	-5.008	-0.188	-0.2586	0.9996
2	14	12	19.575	18.491	-18.360	0.931	0.696	0.3836	0.9804
2	14	13	57.575	56.182	-56.290	-5.062	1.338	1.9587	0.9883
2	14	14	3.575	3.611	-3.546	-0.687	-0.033	0.0287	0.9883
2	14	15	29.847	28.806	-28.851	-0.440	0.033	0.0287	0.9883
2	14	16	7.702	7.777	-7.760	-0.063	0.199	0.4852	0.9999
2	14	17	8.752	22.229	-22.242	-0.717	1.891	1.2061	0.9962
2	14	18	7.310	20.384	-20.407	-0.008	0.467	0.5190	0.9997
2	14	19	9.218	10.251	-10.402	-0.152	0.466	1.1643	0.9997
2	14	20	15.798	14.981	-14.979	-0.002	0.546	0.7758	0.9996
2	14	21	15.543	18.266	-18.266	-0.526	0.000	0.8821	0.9990
2	14	22	8.558	11.858	-11.858	-0.675	0.000	0.8618	0.9997
2	14	23	11.509	10.587	-10.577	-0.443	0.045	0.5099	0.9995
2	14	24	1.226	1.446	-1.453	-0.467	0.024	0.3214	0.9997
2	14	25	4.990	3.643	-3.643	-0.065	0.015	0.2153	0.9997
2	14	26	2.714	19.645	-19.638	-0.134	0.062	0.1950	0.9982
2	14	27	2.835	21.854	-21.866	-0.577	0.150	0.2084	0.9982
2	14	28	3.776	1.854	-1.855	-0.445	0.326	0.8212	0.9982
2	14	29	3.651	1.451	-1.455	-0.445	0.088	0.1293	0.9991
2	14	30	14.346	14.434	-14.425	-0.655	1.088	1.2937	0.9991
2	14	31	12.722	11.837	-11.774	-0.655	0.885	1.3432	0.9994
2	14	32	31.222	15.897	-15.899	-1.251	0.188	0.3452	0.9994
2	14	33	38.251	84.859	-85.021	-0.838	0.333	0.5334	0.9957
2	14	34	4.971	8.846	-8.772	-0.441	0.633	0.3922	0.9933
2	14	35	8.097	7.616	-7.726	-0.122	0.404	0.5514	0.9933
2	14	36	1.622	4.501	-4.183	-0.102	0.661	1.8997	0.9933
2	14	37	8.338	14.574	-14.579	-0.839	0.264	0.5841	0.9933
2	14	38	1.330	1.523	-1.453	-0.479	0.016	0.1319	0.9933
2	14	39	5.990	5.519	-5.521	-0.913	0.074	0.0531	0.9933
2	14	40	1.428	1.169	-1.184	-0.157	0.229	0.8888	0.9933
2	14	41	17.825	18.735	-18.744	-0.533	0.917	1.4173	0.9933
2	14	42	13.242	10.421	-10.402	-0.860	0.179	0.4910	0.9933
2	14	43	11.695	10.131	-10.129	-0.306	1.563	1.1475	0.9996

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
3	0	23	37.976	35.396	35.485	0.059	2.580	2.4685	0.9950	
3	0	25	46.609	44.200	-44.200	0.774	2.565	2.0596	0.9927	
3	0	22	19.137	19.546	-19.546	0.304	0.409	0.5388	0.9986	
3	0	29	6.577	6.892	-6.892	0.062	0.318	0.2431	0.9998	
3	0	31	11.404	13.688	-13.688	0.205	2.284	2.5461	0.9994	
3	0	1	71.441	61.961	-63.086	-0.190	4.603	1.5996	0.9645	
3	0	2	58.963	75.787	-77.831	-0.190	4.363	2.4298	0.9474	
3	0	3	11.888	59.906	60.891	-2.964	0.364	0.6334	0.9655	
3	0	4	102.883	112.880	-119.557	-4.931	0.959	0.3562	0.8899	
3	0	5	64.424	60.541	61.111	-5.305	3.354	1.2991	0.8988	
3	0	6	98.265	106.237	-103.956	-3.087	3.884	0.3891	0.9688	
3	0	7	109.198	99.775	111.458	-2.918	1.502	0.6121	0.9198	
3	0	8	74.528	78.818	-80.620	-2.559	4.290	2.2863	0.9532	
3	0	9	13.258	14.065	13.839	-4.918	0.806	0.9685	0.9539	
3	0	10	58.233	63.894	-64.739	-2.572	5.762	1.7325	0.9984	
3	0	11	80.234	83.774	-85.580	-4.787	3.541	0.9149	0.9553	
3	0	12	71.865	77.452	-74.705	-4.337	1.587	0.8760	0.9635	
3	0	13	64.342	67.345	-68.091	-4.747	1.889	0.8760	0.9553	
3	0	14	31.266	30.958	31.036	-2.421	0.544	0.9737	0.9737	
3	0	15	18.639	19.841	-19.829	-1.553	2.302	0.3735	0.9946	
3	0	16	20.378	21.277	-21.245	-1.153	0.202	0.1547	0.9977	
3	0	17	63.686	67.280	-67.457	-4.966	3.904	2.2277	0.9761	
3	0	18	73.070	76.438	-77.076	-4.489	0.944	0.5684	0.9706	
3	0	19	68.908	70.191	-71.499	-3.312	3.544	1.8855	0.9780	
3	0	20	39.168	38.854	-38.806	-1.979	1.002	0.8855	0.9860	
3	0	21	26.993	24.844	-24.926	-2.586	0.314	0.3070	0.9938	
3	0	22	2.043	2.200	-2.388	-1.329	1.857	0.4817	0.9964	
3	0	23	56.044	57.339	-57.499	-4.489	0.002	0.8855	0.9977	
3	0	24	2.569	2.597	-2.438	-1.586	0.314	0.3070	0.9938	
3	0	25	1.335	1.357	-1.357	-0.435	0.674	0.4817	0.9964	
3	0	26	4.498	4.642	-4.619	-0.674	0.856	0.3269	0.9973	
3	0	27	3.323	3.573	-3.573	-0.223	0.751	0.3127	0.9973	
3	0	28	4.322	4.573	-4.573	-0.223	0.751	0.3127	0.9973	
3	0	29	2.227	2.400	-2.206	-0.684	0.238	0.2958	0.9974	
3	0	30	6.220	6.882	-6.942	-2.703	0.238	0.2958	0.9974	
3	0	31	2.120	2.220	-2.206	-0.684	0.238	0.2958	0.9974	
3	1	0	4.409	4.628	-4.628	-0.100	0.046	0.0278	1.0000	
3	1	1	20.764	20.922	-20.954	-0.766	0.159	0.4065	0.9957	
3	1	2	15.322	16.163	-16.181	-0.138	0.682	0.2548	0.9977	
3	1	3	63.539	62.887	64.059	-0.183	0.852	0.4065	0.9968	
3	1	4	11.449	11.830	-11.859	-0.352	0.158	0.2777	0.9968	
3	1	5	1.577	1.419	205.941	0.091	17.889	3.5737	0.7822	
3	1	6	3.032	3.143	-20.766	0.506	2.511	0.6192	0.9822	
3	1	7	4.279	4.333	-2.833	0.255	1.398	0.8303	0.9999	
3	1	8	34.231	31.672	31.738	-0.548	2.567	1.8191	0.9999	
3	1	9	11.587	13.743	-13.024	-0.725	0.974	0.2155	0.9931	
3	1	10	15.717	8.061	-8.297	-0.218	0.141	0.9453	0.9986	
3	1	11	81.078	81.135	-82.893	-1.068	0.141	0.4099	0.9561	
3	1	12	41.473	42.433	-42.658	-0.879	0.961	0.8985	0.9891	

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
33	2	16	18.604	18.967	18.977	0.142	-0.363	-0.644	0.9979
33	2	17	12.848	12.804	12.808	0.142	-0.044	-0.087	0.9979
33	2	18	52.279	52.656	52.633	-1.681	-0.377	-0.282	0.9876
33	2	19	23.684	22.608	22.633	0.404	-0.077	0.606	0.9974
33	2	20	12.088	11.777	11.780	0.093	0.311	0.575	0.9974
33	2	21	8.393	8.777	8.780	-1.185	0.022	0.461	0.9653
33	2	22	5.562	5.718	5.715	-0.199	0.844	1.107	0.9993
33	2	23	15.679	13.242	13.215	0.156	-0.237	-1.008	0.9993
33	2	24	4.306	4.354	4.319	0.081	0.563	0.937	0.9993
33	2	25	10.249	8.883	8.834	0.948	0.366	0.851	1.0000
33	2	26	3.394	2.075	2.035	0.001	0.335	0.325	0.9997
33	2	27	2.889	2.005	2.019	0.001	0.884	1.967	1.0000
33	2	28	10.399	9.144	9.128	-0.662	-0.017	-1.207	0.9981
33	2	29	8.125	8.414	8.415	-0.107	0.985	2.577	0.9997
33	2	30	10.329	10.737	10.738	0.810	-0.295	-0.484	0.9036
33	2	31	10.444	10.513	10.513	-0.434	-0.975	-0.485	0.9090
3	1	0	106.163	105.137	110.143	-5.434	-1.218	-0.408	0.9829
3	1	1	45.734	46.525	47.323	1.834	-1.190	-0.431	0.8992
3	1	2	116.335	117.525	122.381	5.144	-1.240	-1.744	0.8822
3	1	3	114.721	115.966	122.216	1.275	-1.263	-0.431	0.9785
3	1	4	51.084	53.344	53.845	2.261	-1.522	-0.446	0.9951
3	1	5	22.593	24.117	24.155	1.025	-1.040	-0.744	0.9923
3	1	6	21.078	21.611	21.721	0.985	-0.528	-0.446	0.9951
3	1	7	21.951	21.243	21.282	-0.528	-0.165	-0.277	0.9964
3	1	8	80.254	80.655	81.199	0.445	-0.291	-0.482	0.9964
3	1	9	106.279	108.886	113.819	7.533	-0.636	-0.312	0.9520
3	1	10	70.174	71.088	72.377	1.199	-0.914	-0.514	0.9181
3	1	11	104.052	105.388	108.517	4.465	-0.336	-0.200	0.9651
3	1	12	78.220	78.616	80.621	2.405	-0.029	-0.694	0.9615
3	1	13	58.137	59.162	62.119	4.953	0.099	0.269	0.9792
3	1	14	25.932	25.433	25.371	-0.562	0.068	0.043	0.9969
3	1	15	62.482	62.577	62.856	0.374	0.076	0.694	0.9823
3	1	16	60.674	61.417	62.454	1.780	0.076	0.645	0.9823
3	1	17	36.537	36.200	36.031	-0.535	0.076	0.645	0.9751
3	1	18	13.920	13.880	13.842	-0.118	0.338	0.352	0.9844
3	1	19	25.016	27.518	27.620	2.502	0.047	0.072	0.9991
3	1	20	8.816	8.889	8.842	-0.071	0.573	0.623	0.9991
3	1	21	32.455	34.083	34.511	2.056	1.628	3.072	0.9966
3	1	22	49.039	52.798	52.959	3.919	1.308	2.857	0.9951
3	1	23	41.407	44.883	44.517	3.106	1.628	2.857	0.9951
3	1	24	61.407	62.380	62.372	0.973	0.707	1.961	0.9944
3	1	25	37.295	37.380	37.372	0.085	0.068	0.517	0.9849
3	1	26	28.958	28.542	28.600	-0.414	0.068	0.517	0.9849
3	1	27	20.909	20.542	20.488	-0.421	0.068	0.517	0.9974
3	1	28	29.276	28.220	28.215	-1.056	0.368	1.196	0.9974
3	1	29	155.036	144.498	156.928	11.430	1.817	4.636	0.9974
3	1	30	3.937	4.498	4.215	0.561	0.368	1.196	0.9974
3	1	31	103.550	100.401	104.768	3.267	0.854	2.857	0.9974
3	1	32	24.503	23.269	23.314	-1.234	0.854	2.857	0.9974

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H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
3	4	5	33.362	34.070	-34.224	-0.758	-0.707	-0.8146	0.9905	
3	4	6	90.661	49.453	-49.877	0.3023	1.208	-0.9380	0.9830	
3	4	7	23.701	10.979	-10.979	0.0223	1.373	-2.8182	0.9992	
3	4	8	49.579	122.068	-22.597	-0.5144	-1.633	-1.5129	0.9837	
3	4	9	21.766	51.180	-51.180	0.2292	-2.558	-1.2667	0.9837	
3	4	10	107.788	105.324	109.799	1.7148	2.176	-0.9033	0.9964	
3	4	11	13.770	133.601	13.609	-0.1117	0.008	0.3441	0.9992	
3	4	12	19.419	19.422	19.450	0.0217	0.008	0.0139	0.9992	
3	4	13	12.323	192.084	-14.576	0.1229	2.471	1.0390	0.9480	
3	4	14	16.259	11.590	-11.594	-0.1250	0.818	-0.0392	0.9987	
3	4	15	54.070	53.186	-53.510	-1.293	0.670	-1.5942	0.9874	
3	4	16	11.577	53.400	13.440	0.293	0.819	0.6108	0.9992	
3	4	17	11.577	13.161	13.141	0.0812	0.584	-1.1955	0.9996	
3	4	18	5.259	55.244	52.646	0.0567	0.908	0.8855	0.9996	
3	4	19	11.917	10.244	-10.231	0.0227	0.008	0.6807	0.9855	
3	4	20	11.917	36.810	-36.913	0.5613	1.674	0.9171	1.0000	
3	4	21	33.794	13.365	-14.368	-0.2914	1.003	-1.0651	0.9995	
3	4	22	59.719	159.767	-60.192	-0.378	-1.004	-1.0317	0.9942	
3	4	23	13.680	13.071	-17.476	0.048	0.048	0.047	0.9991	
3	4	24	18.229	17.420	-32.208	-0.168	0.608	-1.0147	0.9854	
3	4	25	30.509	32.153	-17.428	-0.258	0.048	0.0849	0.9993	
3	4	26	16.454	17.071	-17.076	0.005	0.008	-1.0317	0.9993	
3	4	27	9.112	14.095	-17.098	-0.168	0.608	0.0849	0.9993	
3	4	28	2.336	11.657	-17.098	-0.168	0.608	0.0849	0.9993	
3	4	29	16.912	11.657	-17.098	-0.168	0.608	0.0849	0.9993	
3	4	30	2.336	11.657	-17.098	-0.168	0.608	0.0849	0.9993	
3	4	01	4.788	35.037	-4.037	0.524	1.355	-1.9449	0.9992	
3	4	02	34.385	35.037	-35.320	-0.337	1.159	-2.9449	0.9992	
3	4	03	30.389	119.193	-34.129	-0.353	1.299	-1.7235	0.9992	
3	4	04	3.799	118.578	-125.612	-2.392	0.739	-3.4629	0.9992	
3	4	05	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	06	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	07	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	08	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	09	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	10	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	11	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	12	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	13	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	14	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	15	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	16	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	17	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	18	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	19	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	20	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	21	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	22	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	23	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	24	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	
3	4	25	120.263	110.135	-110.094	-0.999	1.156	-0.8102	0.9992	

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
3	5	27	18.361	16.375	16.375	-0.450	1.988	3.1038	0.9991	*
3	5	28	13.638	13.035	-12.975	-1.822	0.563	0.9105	0.9993	*
3	5	29	23.880	24.035	-23.975	-2.064	0.636	0.8877	0.9980	*
3	5	30	37.205	36.834	-37.011	-0.849	2.195	0.3428	0.9983	*
3	6	1	48.444	49.820	-20.911	-0.416	0.368	0.3795	0.9980	*
3	6	2	78.471	7.088	50.278	-0.935	-1.371	-2.3744	0.9968	*
3	6	3	3.805	3.366	7.001	-0.088	0.384	1.1202	0.9818	*
3	6	4	10.291	9.534	4.386	-0.018	1.587	0.9873	0.9585	*
3	6	5	1.347	1.582	9.113	-0.099	0.755	0.6047	0.9994	*
3	6	6	45.347	1.201	-0.187	-1.024	1.144	1.334	0.9994	*
3	6	7	5.353	4.503	7.142	0.422	1.126	0.8451	1.0000	*
3	6	8	17.814	19.100	-4.912	-0.112	-0.152	0.2777	0.9997	*
3	6	9	10.995	10.459	1.912	0.099	2.229	0.9903	1.0000	*
3	6	10	22.139	21.369	10.438	-0.099	0.539	0.9767	0.9993	*
3	6	11	53.905	52.844	-12.651	-0.311	1.444	0.7438	0.9978	*
3	6	12	67.109	65.013	-6.528	-0.430	0.255	0.9090	0.9849	*
3	6	13	3.587	3.139	-5.595	0.098	0.098	0.9090	0.9991	*
3	6	14	16.954	16.842	-1.638	-0.222	0.210	0.9690	0.9823	*
3	6	15	7.806	7.429	-7.430	-0.054	0.145	0.1458	1.0000	*
3	6	16	23.331	26.428	-1.566	-0.263	0.377	0.3612	0.9988	*
3	6	17	5.745	8.905	-3.330	-0.091	0.897	0.5232	0.9998	*
3	6	18	12.228	12.551	-2.898	-0.263	0.637	0.4652	0.9998	*
3	6	19	7.749	8.905	-8.898	0.079	0.925	0.0978	1.0000	*
3	6	20	15.124	15.661	-5.497	-0.459	2.263	1.0697	0.9997	*
3	6	21	158.233	152.563	-164.694	-7.835	2.206	2.5287	1.0000	*
3	6	22	125.940	127.103	-134.694	-6.999	2.206	2.5287	1.0000	*
3	6	23	27.442	29.044	-29.773	-1.393	0.811	0.4464	0.9999	*
3	6	24	23.498	23.077	-23.077	-0.516	1.811	0.4464	0.9946	*
3	6	25	19.803	19.661	-19.529	-1.152	0.462	0.5191	0.9956	*
3	6	26	23.498	23.077	-23.077	-0.516	1.811	0.4464	0.9946	*
3	6	27	18.079	20.027	-20.320	-1.241	0.140	0.5129	0.9970	*
3	6	28	125.940	127.103	-134.694	-6.999	2.206	2.5287	0.9975	*
3	6	29	107.701	105.487	-108.667	-1.429	0.387	0.8572	0.9945	*
3	6	30	87.660	87.689	-89.351	-1.433	0.215	0.1500	0.9973	*
3	7	1	13.320	13.191	-13.101	-1.531	0.635	0.0128	0.9587	*
3	7	2	19.030	19.151	-19.101	-1.531	0.635	0.0128	0.9587	*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
3	3	3	31.341	29.784	29.3766	2.182	1.5588	1.8248	0	0.9959
3	3	3	16.823	15.378	15.4709	2.0367	1.4778	2.5340	0	0.9989
3	3	3	23.416	24.788	24.709	2.0367	1.4778	1.6550	0	0.9973
3	3	3	12.4173	39.774	38.7771	-1.01536	-1.3581	-1.3605	0	0.9999
3	3	3	13.0965	6.2292	-6.2292	-0.8944	-2.3320	-3.8055	0	0.9999
3	3	3	53.9064	29.463	29.4423	-2.3117	-0.7733	-1.2209	0	0.9999
3	3	3	53.9064	40.267	-40.267	-3.9160	-0.3037	1.1774	0	0.9966
3	3	3	42.6227	42.686	-42.6229	-0.3117	-0.3304	1.1944	0	0.9936
3	3	3	151.6007	42.298	-42.298	-0.4833	-0.4833	2.4487	0	0.8807
3	3	3	151.6007	55.5075	-55.5075	-0.159	-0.159	0.1722	0	0.9999
3	3	3	8.2210	7.2119	-7.2119	-0.0930	-0.1223	0.1092	0	0.9999
3	3	3	6.2224	4.5561	-4.5561	-0.1309	-0.1449	-0.5159	0	0.9999
3	3	3	48.9780	49.5015	-49.5015	-0.522	-1.6663	-1.5580	0	0.9999
3	3	3	37.784	38.456	-38.456	-0.672	-2.6125	-0.4221	0	0.9853
3	3	3	7.4042	5.756	-5.756	-0.220	-0.672	-0.8816	0	0.9999
3	3	3	4.2612	6.493	-6.493	-0.1316	-0.6338	-0.0817	0	0.9999
3	3	3	13.978	12.483	-12.483	-0.510	-0.672	-0.8816	0	0.9999
3	3	3	13.978	12.483	-12.483	-0.510	-0.672	-0.8816	0	0.9999
3	3	3	105.782	100.949	-103.723	-0.0844	-0.4937	-1.1799	0	0.9993
3	3	3	113.4	5.648	-5.648	-0.152	-0.4337	-0.5107	0	0.9999
3	3	3	5.9665	4.48	-4.48	-0.016	-0.4337	-0.5107	0	0.9999
3	3	3	9.8955	1.235	-1.235	-0.016	-0.4337	-0.5107	0	0.9999
3	3	3	3.5524	1.9362	-1.9362	-0.016	-0.4337	-0.5107	0	0.9999
3	3	3	3.5524	1.9362	-1.9362	-0.016	-0.4337	-0.5107	0	0.9999
3	3	3	51.843	3.0627	-3.0627	-0.016	-0.4337	-0.5107	0	0.9999
3	3	3	30.233	29.080	-29.080	-0.146	-1.805	-1.6697	0	0.9999
3	3	3	7.578	4.842	-4.842	-0.146	-1.805	-1.6697	0	0.9999
3	3	3	5.578	3.722	-3.722	-0.146	-1.805	-1.6697	0	0.9999
3	3	3	17.527	3.922	-3.922	-0.146	-1.805	-1.6697	0	0.9999
3	3	3	17.527	3.922	-3.922	-0.146	-1.805	-1.6697	0	0.9999
3	3	3	53.083	6.334	-6.334	-0.175	-1.805	-1.6697	0	0.9999
3	3	3	53.083	6.334	-6.334	-0.175	-1.805	-1.6697	0	0.9999
3	3	3	30.672	4.425	-4.425	-0.227	-2.033	-1.9514	0	0.9999
3	3	3	5.672	7.426	-7.426	-0.456	-2.944	-1.1665	0	0.9999
3	3	3	6.229	7.051	-7.051	-0.125	-0.245	-0.6222	0	0.9999
3	3	3	13.765	4.425	-4.425	-0.125	-0.245	-0.6222	0	0.9999
3	3	3	9.925	13.656	-13.656	-0.386	-0.633	-0.4795	0	0.9499
3	3	3	9.925	13.656	-13.656	-0.386	-0.633	-0.4795	0	0.9499
3	3	3	112.929	100.324	-102.775	-0.644	-0.433	-0.1722	0	0.9999
3	3	3	112.929	100.324	-102.775	-0.644	-0.433	-0.1722	0	0.9999
3	3	3	11.250	15.498	-15.498	-0.260	-0.5996	-0.2709	0	0.9631
3	3	3	14.161	6.607	-6.607	-0.148	-0.5996	-0.2709	0	0.9988
3	3	3	19.250	11.087	-11.087	-0.479	-2.332	-4.6750	0	0.9999
3	3	3	11.087	11.087	-11.087	-0.148	-0.5996	-0.2709	0	0.9999
3	3	3	5.030	11.087	-11.087	-0.148	-0.5996	-0.2709	0	0.9999
3	3	3	5.030	11.087	-11.087	-0.148	-0.5996	-0.2709	0	0.9999
3	3	3	12.080	11.087	-11.087	-0.148	-0.5996	-0.2709	0	0.9999
3	3	3	12.080	11.087	-11.087	-0.148	-0.5996	-0.2709	0	0.9999
3	3	3	38.364	37.698	-37.744	-0.046	-2.475	-2.7039	0	0.9999

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H	K	L	F(0BS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTUR
3	3	15	47.712	49.604	-49.783	-2.698	-1.892	-1.531	0.989
3	3	16	15.202	12.444	-12.403	-1.119	-2.753	4.763	0.999
3	3	17	18.922	16.589	-16.548	-1.283	2.333	3.770	0.998
3	3	18	16.607	6.775	-6.774	-0.122	0.833	1.144	0.999
3	3	19	16.286	17.230	-17.216	-0.903	-0.944	-1.549	0.998
3	3	20	78.986	79.654	-80.135	5.556	-0.999	-0.759	0.976
3	3	21	57.056	56.890	-57.065	-0.068	1.555	0.105	0.983
3	3	22	3.365	1.840	-1.083	-0.333	0.906	0.758	0.986
3	3	23	3.408	1.133	-1.468	-0.068	1.525	0.105	1.000
3	3	24	5.830	4.491	-4.442	-0.333	0.943	0.335	0.999
3	3	25	18.139	16.481	-16.444	-1.127	0.998	0.943	0.999
3	3	26	19.041	19.177	-19.187	-0.127	0.122	0.122	0.999
3	3	27	30.260	29.953	-30.025	-0.173	0.309	0.065	1.000
3	3	28	15.260	15.101	-15.109	-0.173	0.286	0.365	0.995
3	3	29	78.913	77.323	-78.871	-0.486	0.015	0.286	0.970
3	3	30	16.754	16.097	-16.097	-0.651	0.220	0.451	0.998
3	3	31	16.244	16.566	-16.566	-0.323	0.662	0.220	0.998
3	3	32	3.944	3.553	-3.553	-0.225	0.865	0.731	1.000
3	3	33	6.788	7.644	-7.644	-0.353	3.446	1.716	0.994
3	3	34	56.624	54.872	-54.872	-0.256	0.753	1.209	0.986
3	3	35	19.108	12.307	-12.310	-0.165	1.209	0.416	0.999
3	3	36	14.840	13.054	-13.054	-0.148	1.331	0.107	0.999
3	3	37	10.785	12.508	-12.508	-0.476	1.199	0.835	0.999
3	3	38	39.469	37.833	-37.833	-0.156	1.722	0.751	0.999
3	3	39	63.416	61.536	-61.536	-0.130	1.171	0.407	0.999
3	3	40	22.369	23.572	-23.572	-0.707	1.203	0.743	1.000
3	3	41	22.608	21.028	-21.028	-0.707	1.203	0.743	0.998
3	3	42	11.437	10.997	-10.997	-0.001	1.225	1.110	0.999
3	3	43	11.509	10.997	-10.997	-0.001	1.225	1.110	0.999
3	3	44	84.233	83.378	-84.529	0.488	-0.488	-0.735	0.999
3	3	45	68.888	70.957	-71.613	0.141	-0.657	0.444	0.965
3	3	46	20.076	21.836	-21.836	-0.692	0.062	-0.426	0.997
3	3	47	11.359	12.100	-12.100	-0.927	0.675	0.620	0.999
3	3	48	11.007	11.944	-11.944	-0.045	1.158	0.204	0.999
3	3	49	15.773	15.381	-15.375	-0.088	1.722	0.697	0.998
3	3	50	41.041	39.721	-39.757	-0.747	1.947	0.269	0.998
3	3	51	23.651	22.139	-22.656	-0.705	1.766	0.512	0.997
3	3	52	52.723	59.747	-59.812	-0.349	2.416	0.837	0.983
3	3	53	54.426	54.467	-61.980	-4.931	-1.004	0.633	0.985

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	11	16	7.166	6.562	-6.544	-0.486	0.605	0.7135	0.9998
3	11	17	5.177	1.570	-1.426	-0.657	3.604	2.4402	1.0000
3	11	18	9.772	10.355	-10.067	-2.425	-0.581	-2.4424	0.9996
3	11	19	14.931	13.449	-13.441	-0.602	-0.482	-2.4426	0.9996
3	11	20	22.177	23.753	-23.769	-0.127	-1.579	-2.2828	0.9976
3	11	21	23.517	27.562	-27.082	-0.491	-1.150	-0.7174	1.0000
3	11	22	28.976	32.613	-32.692	-0.718	-1.414	-1.7176	0.9968
3	12	0	30.864	4.478	-4.479	-0.026	-0.256	-0.0604	0.9949
3	12	1	4.222	4.647	-4.649	-0.028	-0.187	-0.8543	0.9999
3	12	2	3.462	57.779	-58.232	-1.219	0.046	0.0311	0.9841
3	12	3	57.825	3.116	-3.116	-0.033	3.238	-0.0283	1.0000
3	12	4	6.335	30.635	-30.686	0.030	-0.758	-0.9873	0.9997
3	12	5	29.494	38.225	-38.248	0.036	-0.075	-0.9873	0.9997
3	12	6	27.494	25.233	-25.270	0.030	0.751	-0.9873	0.9997
3	12	7	4.946	46.650	-46.848	-0.952	0.469	1.3333	0.9999
3	12	8	47.481	6.764	-6.764	-0.067	0.619	0.7752	0.9999
3	12	9	7.383	6.875	-6.875	-0.142	0.834	0.6752	0.9999
3	12	10	67.414	6.875	-6.875	-0.078	0.053	0.3322	0.9999
3	12	11	67.528	6.875	-6.875	-0.078	0.053	0.3322	0.9999
3	12	12	11.716	3.996	-3.996	-0.031	0.122	-1.8306	0.9996
3	12	13	11.716	3.996	-3.996	-0.031	0.122	-1.8306	0.9996
3	12	14	22.688	3.081	-3.081	-0.199	0.393	-0.5598	0.9999
3	12	15	6.310	3.322	-3.322	-0.154	0.443	-2.6753	0.9999
3	12	16	0.657	38.226	-38.226	-0.028	-2.644	0.3181	1.0000
3	12	17	36.821	3.996	-3.996	-0.154	0.443	-2.6753	0.9999
3	12	18	4.792	1.989	-1.989	-0.028	0.403	-0.4134	1.0000
3	12	19	6.886	12.887	-12.887	-0.056	0.803	-0.3919	0.9998
3	12	20	14.873	1.686	-1.686	-0.094	0.414	-0.6349	0.9995
3	13	0	2.996	0.774	-0.774	-0.467	0.203	1.2743	1.0000
3	13	1	2.996	0.774	-0.774	-0.467	0.203	1.2743	1.0000
3	13	2	39.208	36.913	-36.838	-0.421	0.296	-1.7477	0.9942
3	13	3	39.208	36.913	-36.838	-0.421	0.296	-1.7477	0.9942
3	13	4	28.203	22.601	-22.601	-0.322	0.398	-1.8222	0.9963
3	13	5	28.203	22.601	-22.601	-0.322	0.398	-1.8222	0.9963
3	13	6	63.027	65.416	-65.416	-0.550	0.675	-1.0960	0.9925
3	13	7	81.480	79.216	-79.229	-0.501	0.799	-1.0960	0.9712
3	13	8	60.031	60.832	-60.832	-0.960	0.264	-0.9600	0.9853
3	13	9	30.904	31.522	-31.522	-0.611	0.799	-1.0960	0.9982
3	13	10	35.790	35.080	-35.078	-0.743	0.114	-0.5188	0.9982
3	13	11	14.472	15.369	-15.369	-0.733	0.624	-1.1858	0.9951
3	13	12	21.608	19.953	-19.953	-0.656	0.927	-0.4128	0.9991
3	13	13	3.374	1.718	-1.718	-0.038	0.892	-0.4165	1.0000
3	13	14	36.095	32.774	-32.774	-0.322	0.655	-1.0960	0.9999
3	13	15	26.666	32.774	-32.774	-0.415	0.311	-0.5711	0.9973
3	13	16	36.095	32.774	-32.774	-0.322	0.655	-1.0960	0.9973
3	13	17	15.179	15.493	-15.484	-0.009	0.224	-0.4086	1.0000
3	13	18	6.259	5.763	-5.763	-0.776	0.112	-1.4718	0.9997
3	13	19	7.377	17.613	-17.613	-0.729	0.313	-1.9151	0.9999
3	13	20	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	0	2.115	0.099	-0.099	-0.000	0.000	0.7814	1.0000
3	14	1	2.115	0.099	-0.099	-0.000	0.000	0.7814	1.0000
3	14	2	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	3	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	4	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	5	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	6	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	7	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	8	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	9	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	10	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	11	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	12	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	13	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	14	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	15	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	16	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	17	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	18	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	19	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987
3	14	20	17.607	17.526	-17.510	-0.975	0.081	-1.2864	0.9987

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	14	6	10.864	10.931	-10.923	-0.482	-0.067	-0.0986	0.9995
3	14	7	7.779	66.533	-67.106	-1.242	1.246	0.7198	0.9827
3	14	8	7.995	5.767	-5.763	-0.336	-1.026	0.2673	0.9999
3	14	9	1.886	16.420	-16.382	-0.976	-1.027	-1.0685	0.9999
3	14	10	5.530	4.618	-4.579	-0.221	-1.251	-1.1978	0.9999
3	14	11	6.778	6.618	-6.579	-0.221	-1.251	-1.0210	0.9999
3	14	12	4.498	2.779	-2.805	0.065	-1.944	-1.4691	0.9998
3	14	13	52.154	3.879	-3.879	-0.657	-1.705	-1.9702	0.9999
3	14	14	52.954	48.697	-48.808	-3.990	-3.397	-1.2277	0.9999
3	15	1	31.193	37.975	-37.888	-2.436	-1.025	-2.5462	0.9898
3	15	2	38.515	30.343	-35.159	-3.706	-0.850	-0.8455	0.9963
3	15	3	4.451	2.025	-10.827	-0.709	-3.226	-0.9706	0.9958
3	15	4	7.783	10.853	-10.827	-0.446	-0.426	-3.1922	0.9950
3	15	5	4.704	10.524	-10.518	-0.791	-1.867	-1.3507	0.0000
3	15	6	4.851	10.248	-10.075	-0.423	-3.229	-3.4533	0.9995
3	15	7	7.708	37.988	-37.906	-3.756	-2.720	-1.8589	0.9995
3	15	8	40.770	269.050	-311.449	-12.274	3.117	-1.4888	0.9944
3	15	9	12.377	11.655	-9.493	-1.250	-2.170	-4.4888	0.6098
3	15	10	300.220	37.065	-34.334	-3.756	-2.720	-1.9573	0.9994
4	0	2	14.377	6.669	-9.493	-1.250	-2.170	-1.1381	0.9994
4	0	4	11.987	6.986	-6.111	-1.094	-5.070	-8.5424	0.9994
4	0	6	9.337	35.956	-35.122	-2.825	-1.292	-5.6451	0.9994
4	0	8	30.071	9.110	-9.923	-1.094	-5.070	-5.7030	0.9994
4	0	10	33.523	32.888	-32.883	-2.444	-3.885	-0.9945	0.9994
4	0	12	12.725	20.453	-23.402	-1.591	-1.684	-0.9275	0.9994
4	0	14	13.035	10.644	-10.437	-2.233	-1.267	-0.9275	0.8181
4	0	16	13.640	10.539	-10.437	-1.233	-1.391	-0.0578	0.9995
4	0	18	53.390	54.802	-54.966	-0.107	-1.102	-0.9357	0.9995
4	0	20	51.823	10.802	-10.003	-4.130	-4.112	-1.0044	0.9996
4	0	22	38.317	34.170	-34.135	-2.733	-1.796	-2.0745	0.9996
4	0	24	36.187	88.055	-88.982	-7.031	-2.147	-2.3231	0.9958
4	0	26	42.111	44.275	-44.541	-2.064	-2.163	-0.0578	0.9860
4	0	28	19.239	19.068	-19.549	-1.061	-0.312	-0.5599	0.9973
4	1	1	9.104	4.755	-4.757	0.302	-0.477	-0.6470	0.9995
4	1	2	8.876	19.189	-8.757	0.053	-0.344	-0.5608	0.9995
4	1	3	18.254	52.951	-19.213	-0.403	-0.412	-0.7609	0.9974
4	1	4	18.527	27.951	-27.446	-1.053	-0.312	-0.5617	0.9949
4	1	5	5.875	55.005	-53.445	-0.403	-1.105	-1.4617	0.9949
4	1	6	5.443	55.005	-55.681	-1.178	-1.430	-0.0854	0.9811
4	1	7	4.470	30.951	-31.032	-0.363	-0.130	-0.3243	0.9762
4	1	8	18.425	47.738	-47.752	-0.220	-0.281	-1.6190	0.9804
4	1	9	5.128	21.826	-21.804	-0.432	-0.389	-0.6956	0.9983
4	1	10	21.067	43.732	-43.745	-0.756	-1.387	-1.7343	0.9977
4	1	11	22.067	21.459	-21.227	-1.152	-1.050	-0.7868	0.9909
4	1	12	6.447	3.859	-4.451	-0.848	-1.029	-1.7868	0.9979
4	1	13	2.856	8.859	-3.857	-0.069	-1.002	-2.9364	0.9999
4	1	14	8.856	3.859	-3.857	-0.069	-1.002	-0.6864	0.9999

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
4	1	18	2.936	2.111	-1.185	0.057	0.825	0.5618	1.0000
4	1	19	13.841	13.784	-13.785	0.057	0.057	0.1019	0.9992
4	1	20	23.100	23.367	-23.377	-0.085	-0.267	-0.3964	0.9977
4	1	21	225.313	226.036	-26.036	-1.360	-0.772	-1.0024	0.9972
4	1	22	26.113	26.888	19.894	0.059	-0.774	-1.0462	0.9973
4	1	23	16.556	19.625	30.630	0.026	-3.068	-5.2122	0.9986
4	1	24	29.607	30.802	12.856	0.022	-1.195	-1.4583	0.9964
4	1	25	13.240	12.297	-11.119	0.055	0.343	0.5380	0.9994
4	1	26	12.172	11.842	-11.832	0.050	0.307	-1.2773	0.9995
4	1	27	117.860	118.666	18.897	-1.333	-0.577	-1.8596	0.9987
4	1	28	130.292	131.746	-17.433	-1.115	-2.041	-3.6494	0.9989
4	1	29	119.860	117.678	-18.923	0.076	-0.411	-0.0214	0.9978
4	1	30	12.659	13.783	-13.679	-1.134	-0.477	-3.1745	0.9986
4	1	31	17.310	18.978	-20.679	-1.712	-0.510	-0.8502	0.9969
4	1	32	21.188	20.976	-18.923	-1.815	-0.803	-1.4818	0.9974
4	1	33	43.833	44.534	-44.758	-2.021	-0.701	-0.6232	0.9974
4	1	34	28.489	27.547	-27.522	-1.321	-0.944	-0.4990	0.9947
4	1	35	22.366	23.124	180.121	1.265	0.759	1.2382	0.9999
4	1	36	170.845	165.083	-180.045	0.065	0.318	1.1809	0.8337
4	1	37	2.845	1.017	-17.103	-1.099	0.828	1.4235	1.0000
4	1	38	17.656	19.202	-17.103	-1.099	0.454	0.8350	0.9981
4	1	39	15.138	14.997	-60.554	-2.065	0.796	1.1820	0.9979
4	1	40	15.293	15.976	-14.866	-2.512	0.698	0.5303	0.9977
4	1	41	30.591	31.976	-32.028	-1.012	0.698	-1.3786	0.9988
4	1	42	35.635	33.818	-17.911	0.036	-1.385	-1.6972	0.9949
4	1	43	16.802	17.456	-17.455	0.010	-1.817	-1.9452	0.9945
4	1	44	49.954	53.177	-53.398	-3.472	0.655	-1.5150	0.9986
4	1	45	10.554	10.245	-10.211	-1.021	0.219	-2.5156	0.9874
4	1	46	10.112	10.429	-17.973	-2.540	0.307	-0.5888	0.9995
4	1	47	17.163	18.138	-17.973	-2.540	0.977	-0.5232	0.9985
4	1	48	38.336	37.860	-37.869	-1.722	0.444	-1.7330	0.9944
4	1	49	7.761	9.870	-10.581	-0.559	0.644	0.6163	0.9997
4	1	50	100.513	99.870	-10.581	-0.559	0.644	0.2544	1.0000
4	2	1	3.855	21.486	21.486	0.041	0.677	0.7485	0.9997
4	2	2	20.032	37.425	-37.482	-1.822	0.606	-0.6024	0.9983
4	2	3	38.032	42.544	-19.642	-2.133	1.150	3.1846	0.9986
4	2	4	22.413	24.744	-24.038	-1.338	0.638	0.3749	0.9986
4	2	5	33.287	31.065	-31.114	-0.637	0.222	0.1846	0.9980
4	2	6	13.868	14.456	-13.816	0.047	0.044	0.0708	0.9994
4	2	7	44.488	44.456	-44.908	-3.798	0.968	-0.8443	0.9929
4	2	8	14.767	14.926	-14.908	-0.054	0.329	0.4509	0.9985
4	2	9	27.132	27.917	-27.935	-0.542	0.566	-1.0693	0.9949
4	2	0	31.571	30.359	-30.619	-0.842	0.566	1.0457	0.9938
4	2	1	19.864	19.599	-19.949	0.043	0.266	0.4596	0.9974
4	2	2	19.841	20.515	-20.536	0.088	0.674	1.1651	0.9972
4	2	3	10.680	11.994	-11.795	0.098	0.843	1.7779	0.9886
4	2	4	22.157	22.635	-22.667	0.046	0.478	-2.3544	0.9991
4	2	5	24.609	23.635	-23.890	-0.438	0.757	-1.1425	0.9968
4	2	6	41.649	39.915	-40.076	-0.338	0.735	1.6125	0.9965

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H	K	L	F(DBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
4	3	11	6.224	8.590	-8.552	-0.823	-2.366	-3.457	0.9996
4	3	12	2.445	13.896	-13.167	-0.327	-0.351	-1.100	0.9991
4	3	13	31.808	33.084	-13.017	-0.256	-1.275	-1.509	0.9949
4	3	14	17.519	18.233	-18.173	-0.768	-0.714	-1.282	0.9985
4	3	15	10.020	9.220	9.173	-0.005	0.816	1.278	0.9996
4	3	16	8.924	7.649	7.650	-0.008	1.433	2.272	0.9998
4	3	17	29.974	27.712	-27.542	-0.006	0.597	-1.810	0.9994
4	3	18	2.787	3.588	-3.572	-0.005	0.287	-0.444	0.9998
4	3	19	31.874	32.888	-32.948	-0.000	0.516	-1.790	0.9954
4	3	20	31.307	32.205	-32.216	-0.000	0.916	-1.587	0.9993
4	3	21	12.322	7.759	-7.757	-0.000	0.368	0.511	0.9998
4	3	22	7.917	26.495	-26.530	-0.000	0.422	0.550	0.9973
4	3	23	25.007	2.160	-2.078	-0.000	0.054	0.511	0.9996
4	3	24	17.940	19.786	-19.783	-0.000	0.422	0.600	0.9996
4	3	25	13.583	14.837	-14.837	-0.000	0.254	-3.122	0.9986
4	3	26	13.498	10.801	-10.822	-0.000	0.984	-2.011	0.9992
4	3	27	13.761	14.837	-14.837	-0.000	0.697	-1.709	0.9992
4	3	28	15.944	15.139	-15.470	-1.000	2.586	0.646	0.8568
4	4	0	159.677	157.820	-163.814	-1.000	1.443	0.646	0.9999
4	4	1	22.940	21.126	-21.088	-1.000	0.814	-2.830	0.9971
4	4	2	22.677	57.757	-59.185	-1.000	0.284	-3.706	0.9787
4	4	3	54.445	19.757	-19.706	-1.000	0.489	-2.370	0.9977
4	4	4	20.244	18.686	-18.597	-1.000	0.730	-0.797	0.9980
4	4	5	16.956	7.789	-7.789	-1.000	0.366	-0.075	0.9997
4	4	6	7.789	39.424	-39.014	-1.000	0.848	-0.847	0.9997
4	4	7	38.427	3.275	-3.275	-1.000	0.485	-0.485	0.9988
4	4	8	128.261	14.793	-14.818	-1.000	0.732	-0.933	0.9988
4	4	9	28.561	7.930	-7.930	-1.000	0.322	-0.697	0.9997
4	4	10	17.427	3.063	-3.063	-1.000	0.485	-0.485	0.9997
4	4	11	79.421	12.423	-12.423	-1.000	0.722	-0.349	0.9916
4	4	12	3.421	121.936	-124.013	-1.000	0.711	0.144	0.9999
4	4	13	15.825	16.014	-16.014	-1.000	0.812	-0.702	0.9270
4	4	14	15.333	18.831	-18.961	-1.000	0.680	-1.702	0.9999
4	4	15	15.223	16.885	-16.542	-1.000	0.607	-1.144	0.9988
4	4	16	17.409	18.559	-18.786	-1.000	0.524	-0.928	0.9984
4	4	17	17.371	18.559	-18.429	-1.000	0.188	-0.892	0.9984
4	4	18	30.679	28.448	-28.504	-1.000	0.401	-1.959	0.9987
4	4	19	4.110	2.702	-2.702	-1.000	1.196	-2.622	1.0000
4	4	20	4.458	4.824	-4.824	-1.000	0.944	-1.101	0.9970
4	4	21	20.380	21.039	-21.039	-1.000	0.556	-1.275	0.9923
4	4	22	20.818	21.039	-21.039	-1.000	0.944	-1.275	0.9999
4	4	23	51.378	55.705	-55.705	-1.000	0.191	-0.281	0.9884
4	4	24	3.378	4.039	-4.039	-1.000	0.974	-0.673	0.9938
4	4	25	3.126	6.385	-6.385	-1.000	0.122	0.616	0.9939
4	4	26	3.378	4.987	-4.987	-1.000	0.914	-0.470	0.9851
4	4	27	64.981	63.887	-63.887	-1.000	0.122	0.616	0.9851
4	4	28	50.865	37.339	-37.339	-1.000	0.478	-1.138	0.9814
4	4	29	39.419	39.908	-40.125	-1.000	0.623	-0.521	0.9914
4	4	30	87.419	66.908	-67.140	-1.000	0.033	-0.521	0.9909
4	4	31	45.544	46.987	-47.282	-1.000	0.440	-0.619	0.9750
4	4	32						-1.231	0.9866

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
4	5	5	26.156	26.720	-26.768	-0.735	-0.564	-0.7886	0.9957
4	5	6	7.155	6.891	-6.866	-0.600	-0.264	-0.4584	0.9997
4	5	7	30.802	31.826	-31.886	-0.234	-1.022	-1.2505	0.9948
4	5	8	10.361	10.825	-10.875	-0.822	-0.157	-0.3041	0.9994
4	5	9	38.821	39.645	-39.728	-0.771	-0.176	-0.2080	0.9943
4	5	10	38.004	42.489	-42.644	-1.281	-0.097	-1.1022	0.9914
4	5	11	33.275	32.516	-32.572	-0.963	-0.787	-1.7044	0.9916
4	5	12	29.307	28.543	-28.577	-0.248	-0.575	-1.1422	0.9973
4	5	13	23.162	22.522	-22.544	-0.988	-0.744	-1.0255	0.9965
4	5	14	21.507	22.538	-30.583	-0.541	-0.665	-1.1665	0.9976
4	5	15	28.374	28.580	-30.535	-1.455	-0.106	-1.1224	0.9962
4	5	16	26.977	35.064	-35.135	-1.338	-0.177	-1.4464	0.9842
4	5	17	34.888	38.073	-38.054	-0.455	-1.106	-1.1904	0.9946
4	5	18	10.985	12.704	-12.700	-0.571	-0.719	-1.8257	0.9997
4	5	19	27.510	28.312	-16.703	-0.944	-1.171	-1.0398	0.9994
4	5	20	27.855	28.718	-22.703	-0.525	-0.802	-1.4479	0.9989
4	5	21	22.176	22.521	-16.521	-0.944	-1.034	-1.4779	0.9983
4	5	22	22.596	19.718	-19.698	-0.525	-0.076	-1.1108	0.9983
4	5	23	23.176	22.428	-22.521	-0.944	-1.034	-1.4779	0.9987
4	5	24	23.596	25.428	-15.428	-0.525	-0.076	-1.1108	0.9989
4	5	25	14.805	15.249	-15.428	-0.944	-1.034	-1.4779	0.9983
4	5	26	23.849	23.567	-25.567	-0.067	-0.915	-1.2392	0.9991
4	5	27	29.748	29.958	-43.797	-1.115	-0.797	-2.2392	0.9993
4	5	28	43.348	42.831	-43.958	-1.184	-1.115	-2.6109	0.9963
4	5	29	27.229	22.831	-19.861	-2.158	-0.174	-0.7739	0.9988
4	5	30	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	31	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	32	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	33	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	34	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	35	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	36	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	37	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	38	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	39	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	40	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	41	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	42	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	43	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	44	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	45	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	46	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	47	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	48	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	49	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	50	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	51	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	52	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	53	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	54	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	55	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	56	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	57	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	58	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	59	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	60	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	61	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	62	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	63	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	64	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	65	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	66	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	67	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	68	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	69	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	70	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	71	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	72	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	73	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	74	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	75	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	76	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	77	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	78	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	79	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	80	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	81	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	82	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	83	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	84	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	85	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	86	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	87	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	88	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	89	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	90	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	91	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	92	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	93	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	94	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	95	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	96	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	97	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	98	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	99	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947
4	5	100	4.978	11.310	-11.414	-1.158	-0.611	-0.7739	0.9947

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
4	7	2	12.579	10.477	-10.461	0.523	2.108	4.307	0.9994
4	7	3	22.292	11.278	-11.256	0.768	1.015	1.966	0.9993
4	7	4	7.344	5.087	-5.053	-0.584	1.279	2.120	0.9998
4	7	5	6.347	5.795	-5.795	-0.015	1.830	2.830	0.9998
4	7	6	22.534	21.975	-21.981	0.999	2.221	1.830	0.9998
4	7	7	6.552	4.335	-4.351	0.196	1.555	3.239	0.9997
4	7	8	1.449	1.660	-1.624	0.044	2.166	0.059	0.9999
4	7	9	9.449	8.630	-8.641	1.044	0.528	0.985	0.9989
4	7	10	22.225	23.000	0.225	0.578	0.758	1.380	0.9989
4	7	11	19.605	18.773	-18.778	0.554	2.282	1.567	0.9996
4	7	12	26.738	25.776	-25.801	0.655	0.966	1.184	0.9983
4	7	13	10.883	12.274	-12.277	0.353	0.966	1.346	0.9978
4	7	14	3.366	2.181	-2.008	0.420	0.966	1.808	0.9968
4	7	15	5.045	1.033	-1.000	0.952	0.864	3.295	0.9994
4	7	16	13.290	12.033	-12.000	0.833	0.864	1.808	0.9998
4	7	17	18.218	17.664	-17.665	0.129	0.864	3.295	0.9998
4	7	18	7.743	2.842	-2.842	0.789	1.555	1.744	0.9981
4	7	19	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	20	11.964	10.614	-10.864	0.818	1.071	2.719	0.9999
4	7	21	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	22	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	23	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	24	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	25	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	26	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	27	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	28	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	29	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	30	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	31	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	32	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	33	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	34	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	35	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	36	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	37	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	38	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	39	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	40	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	41	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	42	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	43	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	44	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	45	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	46	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	47	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	48	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	49	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	50	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	51	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	52	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	53	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	54	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	55	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	56	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	57	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	58	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	59	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	60	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	61	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	62	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	63	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	64	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	65	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	66	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	67	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	68	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	69	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	70	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	71	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	72	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	73	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	74	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	75	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	76	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	77	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	78	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	79	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	80	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	81	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	82	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	83	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	84	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	85	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	86	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	87	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	88	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	89	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	90	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	91	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	92	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	93	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	94	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	95	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	96	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	97	11.964	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	98	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999
4	7	99	4.518	10.893	-10.888	0.238	0.871	3.201	0.9999
4	7	100	1.466	10.614	-10.584	0.818	1.071	2.719	0.9999

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
4	9	3	24.258	23.955	23.969	-0.867	0.309	0.444	0.9971	
4	9	4	29.804	28.525	-8.461	-1.052	1.279	2.244	0.9997	
4	9	5	7.643	7.310	7.263	-0.842	0.279	0.504	0.9997	
4	9	6	20.629	21.013	-21.031	-0.477	-0.384	0.044	0.9998	
4	9	7	17.208	17.600	-17.610	-0.315	-0.393	-0.665	0.9978	
4	9	8	14.901	14.809	14.812	0.087	0.099	0.165	0.9986	
4	9	9	13.921	16.465	6.442	0.687	2.399	0.399	0.9990	
4	9	0	13.921	12.198	12.173	0.846	0.555	0.096	0.9998	
4	9	1	10.782	11.198	12.426	0.950	1.177	3.014	0.9993	
4	9	2	10.988	11.794	11.794	0.270	0.807	0.030	1.0000	
4	9	3	29.884	29.911	19.963	-0.272	-0.288	-1.033	0.9957	
4	9	4	12.895	11.744	11.743	-0.295	1.151	0.634	0.9954	
4	9	5	12.676	12.903	-13.125	-0.437	-0.170	-1.170	0.9995	
4	9	6	4.476	28.580	28.616	0.683	0.773	1.129	0.9992	
4	9	7	4.476	1.174	-7.628	0.685	0.355	1.660	0.9978	
4	9	8	8.347	17.611	17.617	0.850	0.677	2.774	0.9969	
4	9	9	15.891	17.373	-17.380	0.457	0.672	0.939	1.0000	
4	9	0	1.590	0.486	-8.527	-0.372	-2.696	-2.795	0.9987	
4	9	1	1.777	20.478	-20.381	-0.425	0.922	-1.071	0.9988	
4	9	2	21.577	16.225	16.147	0.191	1.295	0.773	1.0000	
4	9	3	13.510	13.335	-13.321	-0.566	0.002	-0.973	0.9980	
4	9	4	13.332	18.294	-18.328	-0.357	0.585	0.040	0.9941	
4	9	5	6.769	6.447	-6.447	-0.080	0.002	0.002	0.9991	
4	9	6	4.955	4.727	-4.727	-0.133	0.185	0.170	0.9956	
4	9	7	6.607	28.994	-28.053	-0.021	0.123	0.478	0.9997	
4	9	8	5.222	5.044	-5.044	-0.545	0.611	0.417	1.0000	
4	9	9	22.221	21.061	-21.197	-0.224	0.071	0.926	0.9999	
4	9	0	22.076	21.539	-21.582	-0.161	0.320	0.354	0.9998	
4	9	1	47.310	48.307	-48.234	-0.407	0.620	0.244	0.9998	
4	9	2	15.440	15.638	-15.632	-0.011	0.107	0.973	0.9978	
4	9	3	11.750	11.802	-11.808	-0.096	0.290	0.193	0.9990	
4	9	4	19.337	18.022	-18.093	-0.661	0.527	0.815	0.9995	
4	9	5	82.532	82.335	-78.993	-0.777	0.463	0.709	0.9982	
4	9	6	18.379	17.785	-17.725	-0.597	0.398	0.531	0.9972	
4	9	7	3.032	2.269	-2.262	-0.474	0.595	0.093	1.0000	
4	9	8	3.115	3.340	-3.333	-0.117	0.775	0.497	1.0000	
4	9	9	22.548	22.960	-22.979	-0.623	0.442	0.651	0.9975	
4	9	0	38.522	39.660	-38.452	-1.190	0.291	0.080	0.9954	
4	9	1	46.522	45.630	-45.977	-1.532	0.000	0.282	0.9936	
4	9	2	3.587	3.330	-3.336	-0.598	0.000	0.000	0.9991	
4	9	3	3.187	1.456	-1.456	-0.532	0.131	0.413	0.9991	
4	9	4	3.207	1.141	-1.141	-0.598	0.000	0.000	1.0000	
4	9	5	1.287	1.141	-1.141	-0.532	0.131	0.413	1.0000	
4	9	6	3.399	1.238	-1.238	-0.115	0.066	0.258	0.9990	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
4	1	0	50.048	49.740	-49.957	-1.508	0.308	0.2375	0.9904
4	1	1	33.478	32.895	-32.955	-1.244	0.583	0.6389	0.9950
4	1	1	21.642	21.159	-21.155	-0.977	0.483	0.7080	0.9987
4	1	1	18.995	18.356	-18.356	-0.665	0.633	0.7045	0.9987
4	1	1	7.202	9.351	9.351	0.384	0.609	0.2509	0.9997
4	1	1	2.900	30.276	30.308	1.024	0.447	-1.8133	0.9967
4	1	1	84.7	29.414	-28.947	0.855	0.461	-0.6640	0.9962
4	1	1	95.3	28.928	-28.837	-1.338	0.913	-0.5587	0.9964
4	1	1	78.1	6.848	-6.837	-0.118	0.040	1.1885	0.9964
4	1	1	27.84	25.599	-26.035	-0.105	0.560	-3.5802	0.9969
4	1	1	43.5	17.561	-17.563	-0.591	0.334	-2.1444	0.9969
4	1	1	22.7	1.091	-1.096	-0.597	0.629	-0.5485	0.9986
4	1	1	22.7	60.964	-10.967	0.013	1.627	-1.0275	0.9986
4	1	1	17.8	10.964	-10.967	0.831	1.574	1.6526	0.9995
4	1	1	99.3	82.472	-83.590	-5.443	0.823	0.8038	0.9983
4	1	1	3.300	20.934	-20.566	-2.173	0.205	0.6651	0.9978
4	1	1	79.1	69.934	-70.566	-4.735	0.220	0.1222	0.9983
4	1	1	1.39	7.893	-7.874	0.018	0.205	0.6651	0.9978
4	1	1	5.356	2.893	-2.874	0.022	0.205	0.6651	0.9978
4	1	1	3.72	71.314	-71.911	-0.092	1.521	1.3958	0.9998
4	1	1	4.56	7.877	-7.852	-0.433	0.058	0.9255	0.9998
4	1	1	0.72	10.023	-10.024	-0.009	0.214	1.6836	0.9998
4	1	1	0.53	1.057	-1.056	-0.008	0.049	0.9141	0.9998
4	1	1	3.86	14.077	-14.077	-0.419	1.519	2.4431	0.9996
4	1	1	0.05	21.547	-21.541	-0.052	0.049	0.3536	0.9996
4	1	1	3.25	5.355	-5.355	-0.009	0.061	0.4081	0.9996
4	1	1	4.25	30.544	-30.547	-0.257	0.593	0.8841	0.9980
4	1	1	0.81	5.068	-5.078	-0.010	0.281	-1.1966	0.9999
4	1	1	5.64	2.686	-2.788	-0.490	0.166	0.4050	0.9999
4	1	1	5.44	5.314	-5.267	-0.078	0.061	0.1094	0.9999
4	1	1	3.48	5.437	-5.423	-0.016	0.061	0.0621	0.9999
4	1	1	3.34	2.989	-2.941	-0.044	0.061	0.2337	0.9994
4	1	1	6.60	12.226	-12.221	-0.044	0.566	0.9261	0.9994
4	1	1	4.98	14.522	-14.520	-0.044	0.046	0.0369	0.9994
4	1	1	11.20	19.998	-19.998	-0.041	0.800	1.5213	0.9997
4	1	1	5.72	12.522	-12.520	-0.044	0.060	0.3207	0.9997
4	1	1	2.33	1.001	-1.001	-0.048	0.091	-2.0991	0.9987
4	1	1	3.31	18.433	-18.433	-0.107	0.681	3.3207	0.9987
4	1	1	3.19	19.173	-19.162	-0.041	0.060	0.3207	0.9987
4	1	1	5.37	2.752	-2.755	-0.033	0.612	1.1885	0.9992
4	1	1	3.74	2.329	-2.284	-0.052	0.106	1.4716	0.9992
4	1	1	4.45	13.996	-13.996	-0.021	0.963	1.3214	0.9985
4	1	1	5.05	15.523	-16.022	-0.447	0.104	0.8159	0.9985
4	1	1	0.28	16.220	-16.224	-0.038	0.296	0.4471	0.9998
4	1	1	3.23	10.488	-10.488	-0.028	0.296	0.8364	0.9998
4	1	1	4.84	26.744	-26.744	-0.024	0.673	3.2057	0.9998
4	1	1	4.17	3.344	-3.344	-0.015	0.248	0.2057	0.9999
4	1	1	0.68	1.931	-1.931	-0.028	0.248	0.0480	0.9999
4	1	1	3.15	0.688	-0.676	-0.128	1.267	0.0480	0.9999

IHC2091 IBCOM - PROGRAM INTERRUPT (P) - DIVIDE CHECK OLD PSM IS C78DD00F42083046 . REGISTER CONTAINED 0000000C

TRACEBACK ROUTINE CALLED FROM ISN REG. 14 REG. 15 REG. 0 REG. 1

TESTS 0015 4208281A 00082E88 00000001 0008260C

INPUT 0122 4209083E 00082448 00000001 0008DB00

REFINE 0007 4207615E 0008D510 008DC830 00000000
MAIN 0000C8A0 00075F80 008DC830 00074FF8

ENTRY POINT = 00075F80
STANDARD FIXUP TAKEN , EXECUTION CONTINUING

MANGANHUMITE REFINE 4

RESULTS OF STRUCTURE FACTOR CALCULATIONS

ALL REFLECTIONS

WEIGHTED R	UNWEIGHTED R	NUMERATOR	DENOMINATOR	NUMBER	R
5985.80	3144.57	1470314.00	54525.11	1800	0.082
RANGES OF F(OBS)					
7771.50	1261.26	998179.75	262205.88	1222	0.088
452.00	111.02	111090.31	49010.46	321	0.069
47.78	140.60	17970.50	16336.82	136	0.064
112.85	89.92	8985.25	6534.72	60	0.048
				22	0.052
				20	0.093
				11	0.112
				8	0.117

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

2905.78	1615.47	98020.88	162551.31	120	0.172
923.15	851.88	205843.94	200126.00	199	0.100
791.96	979.73	199309.13	200942.88	252	0.067
830.25	1090.22	194408.06	209111.19	244	0.065
				246	0.063
				238	0.070
				256	0.065
				256	0.072

UNREJECTED REFLECTIONS

WEIGHTED R	UNWEIGHTED R	RANGES OF F(OBS)	WEIGHTED R	UNWEIGHTED R	RANGES OF F(OBS)	NUMBER	R
9545.66	2738.87	1469092.00	53725.94	1562	0.081	1562	0.051
RANGES OF (SIN(THETA))/LAMBDA)**2							
7331.25	1261.26	925471.44	301906.81	984	0.089	321	0.065
452.00	111.02	127910.63	56431.19	136	0.059	160	0.044
47.78	140.60	20691.43	18810.39	22	0.048	22	0.086
112.85	89.92	10345.71	7524.15	20	0.104	11	0.104
				8	0.109		

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

2831.49	1588.85	105338.13	172115.06	112	0.164	183	0.096
879.41	820.20	220081.63	205033.25	234	0.063	218	0.063
731.74	916.65	198449.63	194687.56	211	0.061	207	0.069
755.44	1024.13	183401.25	189984.94	195	0.064	202	0.073
				202			

SUM FCAL 54028.18
 STANDARD DEV OF UNIT WEIGHT OBS 2.51

MANGANHUMITE REINE $\sqrt{4}$ BOND DISTANCES BETWEEN, 1.50 AND 2.50 ANG.

ATOM 1	X	Y	Z	ATOM 2	X	Y	Z	DISTANCE	NUMBER
M(3)5	0.49070	0.86569	0.02703	O(2,4)	0.28033	0.73699	-0.04468	2.02056	1
				O(2,1)	0.78033	0.71301	0.04468	2.16658	2
				O(2,2)	0.25677	0.78498	0.15489	2.15489	3
				F,OH	0.77783	0.92525	0.10311	2.22293	4
				F,OH	0.26313	1.03056	0.03330	2.06316	5
				F,OH	0.73687	0.96944	-0.03330	2.06925	6
M(1)	0.00146	0.37972	0.17580	O(2,3)	-0.28499	0.21775	0.16589	2.20909	7
				O(1,3)	0.28315	0.53312	0.18958	2.17525	8
				O(2,1)	0.24323	0.28498	0.10290	2.17525	9
				O(1,2)	0.27855	0.32930	0.25000	2.19135	10
				O(1,1)	0.27855	0.32930	0.25000	2.14391	11
				O(2,2)	-0.24209	0.46800	0.25000	2.18583	12
				O(2,1)	-0.27783	0.42525	0.10311	2.11432	13
M(2)5	0.00851	0.09743	0.10906	O(2,3)	-0.28499	0.21775	0.16589	2.25850	14
				O(2,1)	0.24323	0.28498	0.10290	2.28598	15
				O(1,3)	0.21685	0.03812	0.18958	2.09295	16
				O(2,2)	-0.28033	0.21301	0.04468	2.30945	17
				F,OH	-0.22217	-0.07475	0.10311	2.13616	18
				F,OH	0.26313	0.03056	0.03330	2.15458	19
M(2)6	0.51405	0.15828	0.25000	O(1,2)	0.27855	0.32930	0.25000	2.13415	20
				O(1,3)	0.21685	0.03812	0.18958	2.31100	21
				O(2,3)	0.71501	0.21775	0.16589	2.14106	22
				O(1,3)	0.21685	0.03812	0.31042	2.31100	23
				O(1,1)	0.74209	-0.03200	0.25000	2.29168	24
SI(1)	0.07496	0.96987	0.25000	O(1,3)	0.21685	1.03812	0.18958	1.63268	25
				O(1,2)	0.21685	1.03812	0.31042	1.63268	26
				O(1,1)	-0.25791	0.82930	0.25000	1.64487	27
				O(1,1)	0.25791	0.96800	0.25000	1.60356	28
SI(2)	0.57533	0.28444	0.10435	O(2,1)	0.24323	0.28498	0.10290	1.60004	29
				O(2,3)	0.71501	0.21775	0.16589	1.64027	30
				O(2,2)	0.72217	0.21301	0.04468	1.64016	31
				O(2,1)	0.24323	0.28498	0.10290	1.60004	32
O(2,3)	0.71501	0.21775	0.16589	M(2)6	0.51405	0.15828	0.25000	2.14106	33
				SI(2)	0.57533	0.28444	0.10435	1.64027	34
				M(1)	1.00146	0.37972	0.17580	2.20909	35
O(1,3)	0.21685	0.03812	0.18958	M(2)5	1.00851	0.09743	0.10906	2.25850	36
				M(2)5	0.00851	0.09743	0.10906	2.09295	37
				M(2)6	0.51405	0.15828	0.25000	2.31100	38
				M(1)	0.49854	-0.12028	0.17580	2.17525	39
				SI(1)	0.07496	0.96987	0.25000	1.63268	40
O(2,4)	0.71967	0.21301	0.04468	SI(2)	0.57533	0.28444	0.10435	1.64016	41
				M(2)5	0.00851	0.09743	0.10906	2.09295	42
				M(3)5	0.49070	0.86569	0.02703	2.02056	43
				M(3)5	0.49070	0.86569	0.02703	2.02056	44
O(2,1)	0.24323	0.28498	0.10290	M(3)5	1.00930	0.36569	0.02703	2.16658	45
				M(1)	0.00146	0.37972	0.17580	2.19135	46
				M(2)5	0.00851	0.09743	0.10906	2.09295	47
				SI(2)	0.57533	0.28444	0.10435	1.64016	48
O(1,2)	0.27855	0.32930	0.25000	M(3)5	0.00930	0.36569	0.02703	2.15489	49

3(1,1)	0.74209	0.56800	0.25000	M(1)	0.00146	0.37972	0.17580	2.14391	8
				M(2)	0.51405	0.15328	0.25000	2.13415	20
				M(1)	0.00146	0.37972	0.32420	2.14391	40
				SI(1)	0.42504	0.46987	0.25000	1.64487	41
3(2,2)	0.77783	0.92525	0.10311	M(1)	0.49854	0.87972	0.17580	2.18583	42
				M(1)	0.49854	0.87972	0.32420	2.18583	43
				M(2)	0.51405	1.15828	0.25000	2.29167	44
				SI(1)	1.07496	0.96987	0.25000	1.60355	45
				M(3)	0.49070	0.86569	0.02703	2.22934	5
				M(1)	0.49854	0.87972	0.17580	2.11433	43
				M(2)	1.00851	1.09743	0.10906	2.13616	47
				SI(2)	0.92467	0.78444	0.10435	1.64810	48
F,OH	0.26313	0.03056	0.03330	M(2)	0.00851	0.09743	0.10906	2.15458	19
				M(3)	0.50930	0.13431	-0.02703	2.06925	37
				M(3)	0.49070	-0.13431	0.02703	2.06316	49

MANGANHUMITE REFINE 4

BGND ANGLES

CENTRAL ATOM	X	Y	Z	ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
M(3)5	0.49070	0.86569	0.02703			
				2	3	98.580
				2	4	98.577
				2	5	169.783
				2	6	97.519
				2	7	91.716
				3	4	84.836
				3	5	71.521
				3	6	163.724
				4	5	97.754
				4	7	83.333
				4	6	90.422
				5	7	168.912
				5	6	92.490
				5	7	87.259
				6	7	84.121

CENTRAL ATOM	X	Y	Z	ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
M(1)	0.00146	0.37972	0.17580			
				9	10	177.767
				9	11	84.790
				9	12	105.521
				9	13	93.761
				9	14	73.026
				10	11	96.724
				10	12	72.674
				10	13	84.685
				10	14	108.774
				11	12	194.664
				11	13	178.062
				11	14	85.207
				12	13	84.273
				12	14	178.536
				13	14	95.612

CENTRAL ATOM	X	Y	Z	ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
M(2)5	0.00851	0.09743	0.10906			
				9	11	81.515
				9	16	91.366
				9	17	69.355
				9	18	100.739
				9	19	161.403
				11	16	94.028
				11	17	78.738
				11	18	173.051
				11	19	87.672
				16	17	160.104

O(1,3)	16	O(2,2)	18	92.493
O(1,3)	16	F,OH	19	104.513
O(2,4)	17	O(2,2)	18	95.832
O(2,4)	18	F,OH	19	93.779
				88.373

CENTRAL ATOM X Y Z
M(2)6 0.51405 0.15828 0.25000

ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
O(1,2)	O(1,3)	97.830
O(1,2)	O(2,3)	89.521
O(1,2)	O(1,3)	89.521
O(1,2)	O(1,3)	97.830
O(1,2)	O(1,1)	176.531
O(1,3)	O(2,3)	88.242
O(1,3)	O(1,3)	156.000
O(1,3)	O(1,1)	79.315
O(2,3)	O(1,3)	68.186
O(2,3)	O(2,3)	114.757
O(2,3)	O(1,3)	156.000
O(2,3)	O(1,1)	92.347
O(2,3)	O(1,1)	88.242
O(2,3)	O(1,1)	92.347
O(1,3)	O(1,1)	79.315

CENTRAL ATOM X Y Z
SI(1) 0.07496 0.96987 0.25000

ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
O(1,3)	O(1,3)	105.013
O(1,3)	O(1,2)	102.682
O(1,3)	O(1,1)	115.090
O(1,3)	O(1,2)	102.682
O(1,3)	O(1,1)	115.090
O(1,2)	O(1,1)	114.698

CENTRAL ATOM X Y Z
SI(2) 0.57533 0.28444 0.10435

ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
O(2,1)	O(2,3)	115.295
O(2,1)	O(2,4)	114.225
O(2,1)	O(2,2)	115.186
O(2,3)	O(2,4)	104.815
O(2,3)	O(2,2)	103.004
O(2,4)	O(2,2)	102.779

CENTRAL ATOM X Y Z
O(2,3) 0.71501 0.21775 0.16589

ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
M(2)6	SI(2)	128.186
M(2)6	M(1)	115.399
M(2)6	M(2)5	124.896
SI(2)	M(1)	90.030
SI(2)	M(2)5	93.716
M(1)	M(2)5	95.583

CENTRAL ATOM X Y Z

O(1,3) 0.21685 0.03812 0.18958

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
M(2)5	15	M(2)6	20	126.497
M(2)5	15	M(1)1	35	114.685
M(2)6	20	M(1)1	35	125.878
M(2)6	20	M(1)1	36	93.292
M(1)1	35	M(1)1	36	91.651

CENTRAL ATOM X Y Z

O(2,4) 0.71967 0.21301 0.04468

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
SI(2)2	30	M(2)5	34	91.875
SI(2)2	30	M(3)5	37	124.780
SI(2)2	34	M(3)5	38	93.803
M(2)5	34	M(3)5	37	122.625
M(2)5	34	M(3)5	38	96.343
M(3)5	37	M(3)5	38	119.783

CENTRAL ATOM X Y Z

O(2,1) 0.24323 0.28498 0.10290

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
M(1)1	8	M(2)5	15	95.292
M(1)1	8	SI(2)2	30	121.273
M(1)1	8	M(3)5	39	94.564
M(2)5	15	SI(2)2	30	119.359
M(2)5	15	M(3)5	39	97.371
SI(2)2	30	M(3)5	39	122.609

CENTRAL ATOM X Y Z

O(1,2) 0.27855 0.32930 0.25000

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
M(1)1	8	M(2)6	20	122.785
M(1)1	8	M(1)1	40	95.809
M(1)1	8	SI(1)1	41	92.438
M(2)6	20	M(1)1	40	122.785
M(2)6	20	SI(1)1	41	122.486
M(1)1	40	SI(1)1	41	92.438

CENTRAL ATOM X Y Z

O(1,1) 0.74209 0.56800 0.25000

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
M(1)1	43	M(1)1	44	93.405
M(1)1	43	M(2)6	45	96.742
M(1)1	43	SI(1)1	46	122.816
M(1)1	44	M(2)6	45	96.742
M(1)1	44	SI(1)1	46	122.816
M(2)6	45	SI(1)1	46	117.935

CENTRAL ATOM X Y Z

O(2,2) 0.77783 0.92525 0.10311

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
M(3)5	1	M(1)5	43	94.604
M(3)5	1	M(2)5	47	127.373
M(1)5	43	M(2)5	48	91.321
M(1)5	43	SI(2)5	47	118.743
M(2)5	47	SI(2)5	48	93.190
				123.037

CENTRAL ATOM	X	Y	Z	ANGLE
F,OH	0.26313	0.03056	0.03330	

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
M(2)5	15	M(3)5	37	128.580
M(2)5	15	M(3)5	49	128.952
M(3)5	37	M(3)5	49	95.879

PARAMETERS WRITTEN OUT TO UNIT 10.