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The forsterite-tephroite series: I. Crystal structure refinements

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Abstract

The crystal structures of the following metamorphic olivines, $M_2^{2+}[SiO_4]$, in the forsterite-tephroite (Fo-Te) series were refined in space group *Pbnm*:

	Cation composition <i>M</i>				Cell parameters (Å)			<i>R</i> factor
	Mg	Mn	Ca	Fe	<i>a</i>	<i>b</i>	<i>c</i>	
Fo ₅₁	1.028	0.964	0.006	0.002	4.794	10.491	6.123	0.029
Te ₉₁	0.181	1.780	0.013	0.026	4.879	10.589	6.234	0.039

Treating minor Fe and Ca as though they were Mn, the refined cation distributions (*esd*'s < 0.01) and mean bond lengths are:

	<i>M</i> (1) site			<i>M</i> (2) site			
	Mg	Mn	(<i>M</i> (1)-O)	Mg	Mn	(<i>M</i> (2)-O)	(Si-O)
Fo ₅₁	0.92	0.08	2.116Å	0.11	0.89	2.185Å	1.637Å
Te ₉₁	0.17	0.83	2.029Å	0.00	1.00	2.227Å	1.640Å

By comparison, a previously refined synthetic Fo₅₃Te₄₇ specimen "heat-treated at 1000°C" is significantly more disordered ($K_D = 0.196$) than the naturally occurring Fo₅₁ ($K_D = 0.011$). As expected, mean *M*(1)-O and *M*(2)-O distances correlate linearly with Mg/(Mg+Mn) occupancy.

Introduction

With the widespread availability of automated X-ray diffractometers and least-squares refinement programs, order-disorder has become a principal theme of contemporary crystal chemical investigations (Burnham, 1973). Both natural and synthetic compounds with the olivine structure have been intensively studied (for a review, see Ganguli, 1977). At least 25 different room-temperature refinements of the geologically-important Mg-Fe olivines have been carried out and 13 additional refinements extend the observational conditions to temperatures of ~1000°C and pressures of ~50 kbar (Basso *et al.*, 1979; Birle *et al.*, 1968; Brown and Prewitt, 1973; Finger, 1970; Finger and Virgo, 1971; Hazen, 1976; Smyth, 1975; Smyth and Hazen, 1973; Wenk and Raymond, 1973).

However, the crystal structures of only two Mg-Mn olivines have previously been refined. One of them contains 11 mole percent of Zn₂SiO₄, thereby complicating the octahedral site refinement (Brown, 1970). The other is synthetic Fo₅₃Te₄₇ which was "heat treated at 1000°C" (Ghose and Weidner, 1974; Ghose *et al.*, 1976) and thus does not represent a naturally equilibrated Mg/Mn distribution. The present refinements were undertaken to examine Mg/Mn ordering in natural olivines uncomplicated by additional substituents.

Experimental procedures and structure refinement

The crystals used for refinement were selected from the suite of specimens described in Part II of this study (in preparation). The manganoan forsterite

REFINE F051E49 FINAL CYCLE

CONTROL PARAMETERS ARE

1 1 1 2 2 0 0 1 1 1 1 1 1 1 1.50 2.50 0 0 1 4 6 1 1 0 1 1 C.C 0 0 0 0 0 0 0 0 0 0 0 0 0

REAL CELL

4.79400 10.49100 6.12300 90.00000 50.00000 50.00000

RECIPROCAL CELL

0.20859 0.05532 0.16332 0.0 0.0 0.0

SYMMETRY CARDS

1/2 X X 1/2 -Y 1/2 -Z
 1/2 -X -Y 1/2 -Z
 -X -Y -Z

SCATTERING CURVES

MG	MN	SI	O	SCALE FACTORS -	A(1)	B(1)	A(2)	B(2)	A(3)	B(3)	A(4)	B(4)	C	DPR	DF1
				8.5120											

EXTINCTION PARAMETERS -

0.88041E-01 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

ATOM LABEL

X Y Z TEMPERATURE FACTOR DATA

ATOM LABEL	TF	SCAT.	SITE	CCUP	DCCA
M1	0.0	0.0	0.0	0.00307	0.00135
M2	0.9870	0.2790	0.2500	0.00612	0.00116
SI	0.4226	0.0916	0.2500	0.00312	0.00096
O1	0.785	0.0867	0.2500	0.00220	0.00169
O2	0.2300	0.4489	0.2500	0.00402	0.00112
O3	0.2582	0.1590	0.0374	0.00394	0.00134

PARAMETER SELECTION INFORMATION

100011111111111000110011100011111100011000111111

DEPENDENT PARAMETER INFORMATION

00.1030E 01 2 1100100--1000E 01

FORMAT FOR STRUCTURE FACTOR INPUT IS
 (I1,I3,214,2F9.4,I3,F11.6,4F7.2,A2,I16)

WAVELENGTH IS 0.7093

REFINE	FOSITE49	H	K	L	FINAL CYCLE	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA
0	4	0	6	7	42.745	42.422	42.572	1.648	0.322	
0	8	0	8	7	31.985	31.821	-1.530	-1.931	0.466	
0	0	0	0	7	6.373	6.399	-26.362	-1.729	-0.444	
0	10	0	31	7	26.347	31.804	31.854	-1.984	-0.051	
0	12	0	31	7	79.48	64.457	65.005	2.646	-0.011	
0	2	0	2	8	5.012	5.165	4.947	-1.484	-0.266	
0	4	0	6	8	22.920	22.758	22.718	-1.662	-0.051	
0	6	0	8	8	23.994	24.540	24.564	0.444	-0.266	
0	8	0	8	8	13.466	13.522	-13.520	0.451	-0.054	
0	0	0	0	9	17.273	17.420	-17.376	-1.411	-0.144	
0	0	0	0	9	29.641	29.283	-29.287	-1.757	-0.358	
1	2	1	4	9	11.565	12.860	-12.908	-0.323	-1.042	
1	4	1	6	9	28.214	28.638	-29.087	-0.200	-0.422	
1	6	1	8	9	83.677	81.038	89.437	1.734	2.632	
1	8	1	3	9	59.145	56.549	58.371	0.113	2.981	
1	5	1	4	9	12.033	10.543	10.467	-1.406	1.981	
1	7	1	6	9	22.197	21.193	21.266	-0.109	0.979	
1	8	1	7	9	86.231	87.022	91.356	2.831	0.276	
1	9	1	8	9	9.744	9.476	-9.477	0.266	-0.042	
1	9	1	9	9	24.754	24.565	-24.543	-2.112	0.182	
1	0	1	0	0	4.057	5.038	5.091	-0.114	-1.022	
1	1	1	1	0	30.839	30.861	30.891	0.127	-0.022	
1	1	1	1	0	4.702	1.574	1.571	-0.104	-3.012	
1	1	1	1	0	13.757	13.457	-13.397	-1.281	-0.330	
1	1	1	1	0	19.098	19.597	-19.616	-1.250	-0.399	
1	1	1	1	0	28.838	29.230	-29.268	-0.190	-0.449	
1	1	1	1	0	17.733	17.279	-17.325	-0.024	-1.440	
1	1	1	1	0	27.732	26.026	-26.477	0.068	-1.440	
1	1	1	1	0	54.403	55.118	-56.809	-2.397	-0.771	
1	1	1	1	0	17.413	17.277	-17.325	-0.225	-0.133	
1	1	1	1	0	34.451	32.727	34.270	2.421	-1.482	
1	1	1	1	0	3.448	4.271	4.270	-0.230	-1.042	
1	1	1	1	0	1.558	3.272	-3.294	-1.468	-1.166	
1	1	1	1	0	5.483	4.033	-4.942	-0.001	-0.433	
1	1	1	1	0	7.922	8.526	-8.689	-0.525	-0.706	
1	1	1	1	0	16.461	16.558	-16.579	0.061	-0.097	
1	1	1	1	0	13.798	14.177	-14.150	-0.032	-0.097	
1	1	1	1	0	11.983	11.077	-11.260	-0.945	-0.377	
1	1	1	1	0	34.958	34.480	34.558	-0.164	-1.679	
1	1	1	1	0	5.032	4.744	4.743	0.155	-1.042	
1	1	1	1	0	11.936	11.494	-11.376	-1.670	-0.444	
1	1	1	1	0	1.043	1.078	-1.077	-0.062	-0.444	
1	1	1	1	0	75.692	73.929	77.230	1.027	3.412	
1	1	1	1	0	49.492	46.073	-46.109	-0.118	1.761	
1	1	1	1	0	6.075	0.225	0.834	0.985	3.095	
1	1	1	1	0	1.573	0.834	0.833	-0.046	0.734	
1	1	1	1	0	46.999	47.563	48.256	2.074	3.412	
1	1	1	1	0	3.999	4.209	-4.207	-0.132	-1.042	

RFINE F05ITE49 FINAL CYCLE

H	K	L	F(09S)
1	7	2	37.877
1	8	2	28.397
1	9	2	68.336
1	0	2	10.476
1	1	2	4.176
1	2	2	11.355
1	3	2	35.270
1	4	2	5.487
1	5	2	4.950
1	6	2	4.864
1	7	2	12.826
1	8	2	26.147
1	9	2	72.749
1	0	3	11.697
1	1	3	22.334
1	2	3	16.712
1	3	3	7.958
1	4	3	4.181
1	5	3	16.109
1	6	3	11.186
1	7	3	11.281
1	8	3	30.481
1	9	3	12.543
1	0	3	5.821
1	1	3	12.339
1	2	3	6.278
1	3	3	8.384
1	4	3	52.266
1	5	3	11.566
1	6	3	11.410
1	7	3	68.805
1	8	3	20.140
1	9	3	21.718
1	0	4	24.666
1	1	4	11.220
1	2	4	12.681
1	3	4	27.133
1	4	4	28.039
1	5	4	57.013
1	6	4	13.009
1	7	4	3.559
1	8	4	9.975
1	9	4	7.061
1	0	5	1.134
1	1	5	12.174

F(CALC)	A(CALC)	B(CALC)
38.633	-38.904	-2.130
29.123	-29.250	-0.342
68.893	-70.271	-2.738
10.476	10.700	-0.154
4.176	4.009	-1.486
11.355	11.501	-0.061
35.270	35.333	-0.061
5.487	-0.324	1.823
4.950	-5.457	-0.635
4.864	-4.748	-0.104
12.826	-11.720	-0.006
26.147	-48.720	-2.334
72.749	-25.086	0.265
11.697	72.086	0.350
22.334	11.134	-2.197
16.712	23.134	-0.423
7.958	17.279	-0.367
4.181	-7.577	-0.492
16.109	16.514	-0.050
11.186	13.425	0.053
11.281	11.245	0.020
30.481	18.515	0.133
12.543	30.545	-0.920
5.821	12.216	-0.166
12.339	6.486	-0.153
6.278	5.266	-0.635
8.384	57.120	-0.087
52.266	57.552	-0.300
11.566	11.024	0.174
11.410	11.560	-0.140
68.805	68.958	-0.106
20.140	21.023	-0.281
21.718	18.194	-0.990
24.666	21.045	-0.270
11.220	24.984	-0.116
12.681	13.084	-0.089
27.133	13.731	-1.224
28.039	12.791	-0.227
57.013	27.811	-0.187
13.009	23.910	-0.220
3.559	56.167	-0.227
9.975	13.180	-0.234
7.061	120.211	-0.180
1.134	12.436	-0.023
12.174	12.485	-0.031

DELTA F	DELTA/SIGMA	EXT. FACTOR
-1.248	-21.011	0.983
0.726	-11.172	0.991
-0.527	-7.935	0.959
-0.224	-2.707	0.999
-0.224	-0.694	0.999
-0.141	-1.551	0.999
0.025	0.312	0.992
0.456	0.710	0.992
0.334	2.401	1.000
1.124	2.203	0.999
0.314	1.184	0.985
0.784	-17.011	0.974
0.630	11.472	0.952
0.803	14.801	0.927
0.122	-14.978	0.989
0.333	1.576	0.997
0.313	1.449	0.996
0.068	1.556	0.999
0.222	-0.833	0.999
0.067	-2.197	0.999
0.455	-0.319	0.999
0.327	3.222	0.999
0.147	-1.065	0.999
0.013	0.175	0.999
0.721	-0.711	0.999
0.542	8.866	0.999
0.420	-6.258	0.999
0.541	6.890	0.964
0.611	-2.488	0.964
0.112	2.929	0.964
0.315	-4.929	0.999
0.273	2.309	1.000
0.089	-4.014	1.000
0.089	1.678	0.999
0.202	0.683	0.999
0.116	-3.044	0.999
0.089	3.998	0.999
0.224	-2.871	0.999
0.187	4.871	0.999
0.220	4.118	0.999
0.227	2.736	0.999
0.234	14.812	0.980
0.344	-2.825	0.997
0.223	-6.173	0.999
0.023	-3.352	0.999
0.486	-3.369	0.999
0.031	-3.615	0.999
0.000	3.549	0.999

STRUCTURE FACTORS

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REFINE FOSITE49 FINAL CYCLE

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	12	5	11.809	11.749	-11.722	-0.861	0.060	0.6510	0.9992
1	13	5	5.745	27.769	-5.888	-0.172	-0.332	-1.0708	0.9998
1	14	5	27.837	28.101	28.115	0.593	-0.078	-3.7393	0.9958
1	1	5	44.623	43.048	43.045	0.140	0.789	-4.1515	0.9995
1	2	5	4.230	43.756	-3.527	0.136	0.867	14.3552	0.9893
1	3	5	1.647	1.118	-0.702	0.870	0.700	6.4276	0.9999
1	4	5	1.837	1.790	-0.791	0.861	0.046	2.0497	1.0000
1	5	5	26.077	25.883	-5.861	-0.060	0.529	0.4976	0.9998
1	6	5	4.912	25.904	-0.903	1.085	0.194	0.949	0.9999
1	7	5	23.793	23.009	-9.034	0.109	0.008	0.008	0.9999
1	8	5	10.218	10.899	-3.864	-1.884	0.106	-1.0477	0.9967
1	9	5	44.540	44.744	2.847	-2.445	0.210	-1.4750	0.9994
1	10	5	2.894	2.284	-0.844	-0.281	0.110	-0.4750	0.9994
1	11	5	15.464	2.023	1.023	-1.303	0.390	-2.4005	1.0000
1	12	5	26.214	26.951	5.912	-0.638	0.744	-1.9894	0.9999
1	13	5	23.454	23.051	-9.955	-0.097	0.150	-8.0289	0.9962
1	14	5	13.875	13.640	-0.645	-0.238	0.440	-1.5893	0.9998
1	15	5	40.570	39.938	-6.445	-0.014	0.235	-1.8938	0.9999
1	16	5	6.306	6.126	-0.049	-0.036	0.040	-0.7441	0.9974
1	17	5	11.946	11.826	6.125	-0.163	0.120	1.1880	0.9999
1	18	5	13.505	13.687	-1.766	-0.229	0.172	-0.4785	0.9998
1	19	5	5.504	5.522	-0.694	-0.047	0.012	-0.8425	0.9999
1	20	5	11.484	10.964	-5.509	-0.415	0.068	-0.016	0.9999
1	21	5	5.489	5.449	-0.967	-0.060	0.543	-0.016	0.9999
1	22	5	3.392	3.336	-0.036	0.801	0.453	0.590	0.9997
1	23	5	3.396	3.336	-0.220	-0.241	0.116	-0.277	0.9999
1	24	5	27.903	27.744	-3.665	-1.388	0.271	-1.6365	0.9999
1	25	5	5.921	6.133	2.739	-0.074	0.674	-1.5717	0.9998
1	26	5	4.038	4.179	0.796	-0.097	0.304	-2.6312	0.9999
1	27	5	4.038	4.077	-0.872	-0.277	0.354	-1.8012	0.9999
1	28	5	15.622	15.177	-0.994	-0.663	0.447	-4.4859	0.9999
1	29	5	14.671	14.305	-0.690	-1.022	0.220	-2.7210	0.9999
1	30	5	30.032	29.794	-2.455	-0.772	0.373	-4.1519	0.9999
1	31	5	11.886	11.351	-0.715	-0.182	0.000	-1.8612	0.9999
1	32	5	11.508	11.311	-0.309	-0.087	0.170	-1.4631	0.9999
1	33	5	39.681	44.914	5.312	-0.009	0.045	0.3260	0.9999
1	34	5	35.561	38.914	3.351	-2.945	0.509	-1.6876	0.9711
1	35	5	19.333	19.916	0.583	-0.943	0.393	-1.7944	0.9603
1	36	5	86.470	84.219	-2.256	-0.125	0.283	-1.9446	0.9837
1	37	5	17.161	17.335	0.174	-0.125	0.283	-1.9446	0.9919
1	38	5	18.853	17.233	-1.624	-0.918	0.245	-1.4150	0.8754
1	39	5	17.665	17.665	-0.000	-0.291	0.071	-0.7147	0.9953

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RFINE	F051TE49	H	K	L	FINAL CYCLE	F(DBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
	8	0	0	0	40.024	39.404	39.712	0.597	0.619	0.3237	0.9844	
	9	0	0	0	17.085	16.989	-17.009	-0.199	0.096	0.8873	0.9975	
	10	1	1	1	53.427	51.984	-52.521	1.042	1.443	13.8482	0.9793	
	11	1	1	1	4.611	4.507	-4.519	0.120	0.896	-1.7956	1.0000	
	12	1	1	1	13.010	12.773	-12.779	-0.033	0.023	-1.6449	0.9991	
	13	1	1	1	15.543	15.578	18.541	1.922	0.311	6.7975	0.9956	
	14	1	1	1	32.045	31.558	-31.820	-1.654	0.486	0.0347	0.9988	
	15	1	1	1	18.456	18.259	18.820	0.132	0.197	11.1708	0.9996	
	16	1	1	1	56.216	57.891	-59.422	-1.768	0.397	9.4447	0.9850	
	17	1	1	1	31.292	31.702	-31.883	-0.157	0.410	1.7085	1.0000	
	18	1	1	1	33.881	34.133	-34.280	-0.422	0.251	-3.0242	0.9483	
	19	1	1	1	36.181	36.439	-36.607	-0.218	0.461	-5.3865	0.9875	
	20	1	1	1	33.644	32.209	-31.199	-2.230	0.153	-0.256	0.9873	
	21	1	1	1	20.596	24.476	-24.459	-0.538	0.387	9.2212	1.0000	
	22	1	1	1	17.515	17.238	17.736	0.178	0.149	1.8019	0.9910	
	23	1	1	1	6.110	6.417	-6.191	-0.012	0.574	1.6771	0.9961	
	24	1	1	1	40.172	41.088	-41.405	-0.413	0.215	-1.2881	1.0000	
	25	1	1	1	15.032	15.478	-15.489	-0.512	0.446	19.8394	0.9984	
	26	1	1	1	14.037	14.757	-15.297	-1.527	0.230	-4.7188	0.9975	
	27	1	1	1	11.187	11.701	-11.827	-0.322	0.307	23.4821	0.9980	
	28	1	1	1	16.797	16.529	-17.044	-1.344	0.202	-3.7443	0.9913	
	29	1	1	1	29.925	28.419	-28.539	-1.507	0.528	-8.2387	0.9932	
	30	1	1	1	24.284	25.527	-25.614	-0.074	0.528	-1.1221	0.9968	
	31	1	1	1	20.792	20.323	-20.822	0.210	0.529	4.5834	0.9997	
	32	1	1	1	6.702	6.312	-6.162	-0.144	0.440	5.1269	0.9997	
	33	1	1	1	14.774	14.313	-14.264	-0.376	0.054	-0.4454	0.9988	
	34	1	1	1	9.212	9.824	-10.804	-1.045	0.844	4.5026	0.9995	
	35	1	1	1	11.503	10.808	-10.721	-0.414	0.379	4.1480	0.9994	
	36	1	1	1	40.162	40.066	-41.120	-1.190	0.044	4.0532	0.9915	
	37	1	1	1	21.482	21.201	-21.038	-0.126	0.378	7.0296	0.9992	
	38	1	1	1	8.312	8.591	-8.712	-0.179	0.110	1.7902	0.9995	
	39	1	1	1	34.034	34.591	-34.144	-0.522	0.318	-5.4827	0.9910	
	40	1	1	1	34.087	35.167	-35.385	-1.657	0.209	-5.8144	0.9917	
	41	1	1	1	12.004	13.287	-12.415	-0.407	0.284	-5.7145	0.9887	
	42	1	1	1	43.473	44.723	-45.383	-1.656	0.305	-3.2065	0.9999	
	43	1	1	1	35.111	35.223	-35.634	-0.277	0.446	2.0271	0.9982	
	44	1	1	1	17.958	18.202	-18.230	-0.167	0.265	-3.9395	0.9920	
	45	1	1	1	18.336	18.202	-17.960	0.728	0.333	3.1761	0.9581	

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RFINE F05ITE49 FINAL CYCLE

H K L F(OBS) F(CALC) A(CALC) B(CALC) DELTA F DELTA/SIGMA EXT. FACTOR

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
13	15	3	1.1357	0.5224	0.4993	0.1778	0.6113	1.0781	1.0000
14	15	3	4.0339	7.9166	-7.8660	-0.9499	0.4441	3.6527	0.9997
15	15	3	53.9935	3.6447	-3.6447	-0.0330	0.0330	0.6527	0.9997
1	2	4	23.6665	52.7587	53.2243	0.2802	1.0177	22.0624	0.9991
2	3	4	18.4811	21.9947	-19.0887	-0.5116	0.0118	8.4444	0.9960
3	4	4	14.8112	15.4441	-15.4453	-0.1115	0.6557	1.9086	0.9974
4	4	4	55.3662	4.3888	5.4901	0.9989	0.0630	0.7035	0.9769
5	4	4	4.4445	6.9115	-6.8665	-0.8446	0.0576	0.5444	0.9999
6	4	4	6.9773	15.9777	-15.9985	-0.2816	0.7263	0.7263	0.9996
7	8	4	15.5448	128.9777	-129.0555	-0.4227	0.4227	-6.1330	0.9985
8	9	4	28.5249	14.7189	-14.7226	-0.1993	0.1990	-2.4320	0.9943
9	9	4	14.5228	38.3333	-38.4378	0.9788	0.7118	-2.2721	0.9988
10	11	4	31.0860	0.4535	-0.4375	0.1118	0.6217	-1.1618	0.9919
11	13	4	9.4226	1.1104	-1.0785	0.7922	0.3111	1.7038	1.0000
12	14	4	25.0995	10.1173	-10.1407	0.0332	0.0778	-0.8466	0.9994
13	14	4	18.1022	122.4445	-122.4480	0.1344	0.0717	-0.8284	0.9969
14	14	4	3.5442	45.4044	-45.4408	0.7240	0.1121	-0.8284	0.9980
15	14	4	21.3337	18.7947	-18.4408	0.1344	0.3019	-0.8466	0.9969
16	14	4	45.5441	4.4044	-4.5677	-0.1509	0.1121	-0.8284	0.9980
17	14	4	22.3071	21.2133	-21.2335	-0.6392	0.1335	-0.8284	0.9969
18	14	4	16.6127	21.9814	-21.4588	-0.4824	0.1119	-0.8284	0.9976
19	14	4	3.0417	16.5611	-16.4558	-0.2079	0.1226	-0.8284	0.9990
20	14	4	13.6127	3.2045	-3.1928	-0.9667	0.1226	-0.8284	0.9990
21	14	4	21.2224	21.3337	-21.5328	-0.2272	0.1335	-0.8284	0.9990
22	14	4	15.1225	22.3337	-22.3335	-0.5000	0.1446	-0.8284	0.9993
23	14	4	14.9880	14.4211	-14.4588	-0.1446	0.1446	-0.8284	0.9999
24	14	4	14.1850	14.4211	-14.4588	-0.1446	0.1446	-0.8284	0.9999
25	14	4	14.8550	14.4211	-14.4588	-0.1446	0.1446	-0.8284	0.9999
26	14	4	14.9669	14.4211	-14.4588	-0.1446	0.1446	-0.8284	0.9999
27	14	4	11.3533	11.7118	-11.7118	-0.3466	0.1119	-0.8284	0.9997
28	14	4	2.1844	11.5019	-11.6145	-0.1198	0.2555	-0.8284	0.9993
29	14	4	7.4277	17.0129	-17.0145	-0.1279	0.1655	-0.8284	0.9997
30	14	4	28.5122	24.5236	-24.5522	-0.3832	0.0766	-0.8284	0.9997
31	14	4	14.5122	15.1224	-15.1224	-0.2744	0.1009	-0.8284	0.9999
32	14	4	13.4228	13.1971	-13.2201	-0.0190	0.1009	-0.8284	0.9999
33	14	4	15.5644	15.4811	-15.4447	-0.3327	0.0661	-0.8284	0.9999
34	14	4	2.7332	15.0771	-15.0668	-0.1115	0.2290	-0.8284	0.9999
35	14	4	11.5312	8.2825	-8.2825	-0.1090	0.1211	-0.8284	0.9994
36	14	4	5.3666	5.8250	-5.5055	-0.1590	0.0111	-0.8284	0.9997
37	14	4	18.6588	10.4487	-10.4401	-0.1462	0.1366	-0.8284	0.9985
38	14	4	22.1527	18.8338	-18.8446	-0.8114	0.0222	-0.8284	0.9978
39	14	4	32.0437	21.7252	-21.7766	-0.1631	0.0519	-0.8284	0.9997
40	14	4	2.3327	32.1911	-32.1903	-0.1232	0.1115	-0.8284	0.9950

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	PAGE
2	10	7	24.573	25.262	-25.232	-1.872	0.689	-7.686	0.996
3	11	8	31.609	32.103	-32.099	-2.457	0.495	-4.632	0.993
4	12	8	39.093	38.551	-38.610	0.425	0.262	6.745	0.993
5	13	8	10.553	9.883	9.824	0.517	0.222	2.878	0.999
6	14	8	8.208	14.233	-14.163	-1.088	0.316	-3.293	0.999
7	15	8	23.722	23.752	-23.723	-1.668	0.229	-2.293	0.997
8	16	8	3.547	5.651	-5.654	0.257	0.112	-0.882	0.999
9	17	8	3.114	3.301	-3.302	0.185	0.044	-0.212	0.999
0	18	8	11.181	11.370	-11.372	0.198	0.120	-1.235	0.999
1	19	8	15.072	15.722	-15.725	0.485	0.179	-1.402	0.998
2	20	8	11.574	11.707	-11.703	0.123	0.150	-1.228	0.999
3	21	9	0.695	1.464	-1.462	0.124	0.012	-1.022	0.999
4	22	9	4.517	4.467	-4.462	0.356	0.091	-0.608	0.997
5	23	9	11.725	11.627	-11.623	0.402	0.092	-0.608	0.999
6	24	9	30.476	30.560	-30.488	0.092	0.121	0.335	0.985
7	25	9	44.876	44.791	-44.791	0.452	0.054	0.554	0.984
8	26	9	51.144	50.912	-50.863	0.110	0.104	1.107	0.969
9	27	9	14.705	14.569	-14.563	0.452	0.179	1.269	0.963
0	28	9	17.995	17.797	-17.759	0.452	0.348	2.030	0.999
1	29	9	27.604	27.302	-27.259	0.851	0.299	3.966	0.997
2	30	9	27.247	22.200	-22.850	1.901	0.302	2.195	0.995
3	31	9	27.290	22.734	-22.351	1.530	0.707	1.951	0.994
4	32	9	36.274	34.664	-34.808	2.083	0.327	3.591	0.994
5	33	9	6.742	6.662	-6.659	0.085	0.077	1.701	0.992
6	34	9	15.935	15.221	-15.263	0.488	0.099	3.180	0.999
7	35	9	8.332	8.220	-8.263	0.331	0.056	0.314	0.999
8	36	9	13.376	12.886	-12.891	0.331	0.091	0.760	0.998
9	37	9	49.919	49.918	-49.918	0.000	0.000	0.111	0.998
0	38	9	49.633	50.541	-50.290	0.636	0.000	0.080	0.969
1	39	9	34.142	34.818	-34.690	0.339	0.000	0.871	0.988
2	40	9	34.331	34.818	-34.818	0.000	0.000	0.000	0.988
3	41	9	30.449	30.380	-30.380	0.000	0.000	0.000	0.988
4	42	9	9.197	9.324	-9.324	0.622	0.000	0.394	0.999
5	43	9	1.384	0.307	0.602	0.112	0.065	0.599	0.999
6	44	9	29.029	28.157	-28.234	0.144	0.766	1.778	1.000
7	45	9	12.745	11.502	-11.513	0.881	0.977	3.805	0.994
8	46	9	18.065	17.161	-17.116	0.488	0.270	1.364	0.999
9	47	9	20.236	19.495	-19.443	0.403	0.904	1.451	0.998
0	48	9	5.235	4.495	-4.443	0.403	0.614	0.934	0.999
1	49	9	44.219	43.502	-43.506	0.812	0.919	3.370	0.994
2	50	9	11.283	11.336	-11.305	0.514	0.040	0.569	0.968
3	51	9	19.621	19.336	-19.726	0.901	0.223	0.842	0.999
4	52	9	11.331	11.966	-11.549	0.161	0.052	0.044	0.996
5	53	9	4.433	4.418	-4.398	0.426	0.635	1.476	0.977
6	54	9	4.335	4.418	-4.398	0.011	0.011	0.147	0.999

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RFINE FOSITE49 FINAL CYCLE

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	7	N	9.408	9.701	-9.534	-1.813	-0.029	-3.426	0.9992
3	8	N	21.534	21.438	-21.459	-2.770	0.096	1.270	0.9965
3	9	N	46.591	46.150	-46.419	-0.441	0.044	5.753	0.9857
3	10	N	13.094	13.500	-13.514	-0.352	-0.735	-4.557	0.9988
3	11	N	6.455	3.554	-3.554	-0.319	0.300	5.820	0.9999
3	12	N	3.854	3.815	-3.540	-0.657	0.084	1.923	0.9938
3	13	N	3.662	3.880	-3.403	-0.542	0.181	1.370	0.9972
3	14	N	3.557	3.377	-2.737	-0.478	0.155	0.999	1.0000
3	15	N	3.548	3.067	-3.033	-0.248	0.488	0.082	0.9934
3	16	N	3.858	3.350	-4.465	-0.637	0.382	3.418	0.9921
3	17	N	39.680	39.420	-39.658	-0.000	0.000	5.744	0.9846
3	18	N	24.342	24.749	-24.658	-0.376	0.000	3.526	0.9878
3	19	N	14.370	14.172	-14.180	-0.035	0.000	2.106	0.9952
3	20	N	12.374	12.666	-12.656	-0.016	0.000	2.830	0.9988
3	21	N	2.036	1.922	-1.461	-0.111	0.452	0.063	0.9988
3	22	N	18.009	17.463	-17.990	-0.121	0.000	2.089	0.9981
3	23	N	16.657	15.889	-15.631	-0.181	0.000	0.414	0.9985
3	24	N	18.008	17.973	-17.490	-0.395	0.000	0.095	0.9948
3	25	N	3.687	3.303	-3.321	-0.084	0.000	0.478	0.9983
3	26	N	18.718	18.469	-18.321	-0.444	0.000	0.229	0.9979
3	27	N	38.890	38.303	-38.323	-0.501	0.000	0.242	0.9941
3	28	N	32.425	32.677	-32.764	-0.112	0.000	0.225	0.9929
3	29	N	9.141	9.045	-9.038	-0.377	0.000	0.196	0.9929
3	30	N	50.022	50.466	-50.961	-0.421	0.000	0.099	0.9993
3	31	N	19.541	19.439	-19.572	-0.393	0.000	0.415	0.9920
3	32	N	4.209	4.312	-4.297	-0.778	0.000	0.281	0.9977
3	33	N	28.804	29.084	-29.082	-0.281	0.000	0.115	0.9949
3	34	N	3.994	3.835	-4.065	-0.283	0.000	0.771	0.9999
3	35	N	4.995	4.471	-1.435	-0.476	0.000	0.037	0.9994
3	36	N	36.843	36.740	-36.811	-0.325	0.000	0.422	1.0000
3	37	N	19.968	19.740	-19.751	-0.146	0.000	0.104	0.9928
3	38	N	33.733	33.057	-33.100	-0.620	0.000	0.228	0.9978
3	39	N	18.706	18.457	-18.466	-0.887	0.000	0.597	0.9943
3	40	N	29.354	29.498	-29.677	-0.258	0.000	0.276	0.9981
3	41	N	2.252	2.214	-4.175	-0.031	0.000	0.240	0.9996
3	42	N	2.257	1.544	-1.534	-0.057	0.000	0.487	0.9999
3	43	N	2.289	1.786	-1.771	-0.104	0.000	0.711	0.9999
3	44	N	13.280	14.599	-14.601	-0.125	0.000	1.171	1.0000
3	45	N	13.280	13.132	-13.071	-0.431	0.000	0.848	0.9989
3	46	N	23.641	23.071	-23.091	-0.727	0.000	1.190	0.9991
3	47	N					0.571		0.9973

STRUCTURE FACTORS

REFINE F05ITE49 FINAL CYCLE

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	3	6	31.963	31.374	31.448	0.442	0.588	8.6596	0.9951
3	3	6	2.526	-1.894	-1.727	-0.776	0.632	3.2863	1.0000
3	3	6	18.867	19.053	-19.070	-0.117	-0.186	-2.5569	0.9982
3	3	6	33.292	33.372	33.405	0.103	-0.080	-1.1012	0.9948
3	3	6	4.685	4.547	4.531	-0.138	0.137	1.0280	0.9999
3	3	6	10.793	10.522	-10.401	-1.612	0.271	-3.0200	0.9974
3	3	6	21.339	21.581	-21.593	-0.716	-0.042	-2.9172	0.9978
3	3	6	5.701	6.122	6.114	0.345	0.437	2.1775	0.9931
3	3	6	5.618	5.181	-5.004	-1.345	0.012	-0.9795	0.9999
3	3	6	21.418	21.318	-21.341	-0.216	0.100	-1.3257	0.9978
3	3	6	18.468	18.098	18.008	-0.936	0.370	4.8303	0.9984
3	3	6	26.684	26.293	26.237	-0.454	0.327	3.3586	0.9997
3	3	6	26.649	26.651	-26.684	-1.034	0.334	0.4453	0.9968
3	3	7	27.199	27.204	-27.174	-0.561	0.356	0.7031	0.9970
3	3	7	5.619	5.838	-5.838	-0.219	0.006	0.0780	0.9987
3	3	7	8.999	9.091	-9.077	-0.088	0.219	-0.9418	0.9998
3	3	7	1.021	1.372	-1.372	-0.354	-0.098	-0.5968	0.9996
3	3	7	3.292	3.705	-3.705	-0.409	-0.513	-1.7632	1.0000
3	3	7	6.698	6.718	-6.718	-0.064	-0.219	-0.7158	0.9995
3	3	7	4.496	4.439	-4.470	-0.409	-0.099	-0.1324	0.9998
3	3	7	25.743	25.695	-25.700	-0.442	-0.023	-0.1176	0.9972
3	3	7	12.708	13.022	-13.013	-0.306	-0.199	-0.4184	0.9999
3	3	7	4.703	4.326	-4.326	-0.409	-0.279	-1.0277	0.9999
3	3	7	28.003	28.821	-28.805	-0.805	0.183	1.0368	0.9999
3	3	8	21.243	20.781	-20.649	-0.562	0.429	1.0368	0.9963
3	3	8	21.210	21.090	-21.073	-0.127	0.110	-0.5440	0.9981
3	3	8	91.480	90.902	-90.572	-0.572	0.429	1.0368	0.9981
4	4	0	16.391	16.057	-16.061	-0.334	0.334	4.0381	0.9981
4	4	0	12.595	12.260	-12.244	-0.316	0.334	4.0381	0.9981
4	4	0	12.522	12.260	-12.244	-0.260	0.334	4.0381	0.9981
4	4	0	29.521	28.542	-28.542	-0.979	0.697	1.5463	0.9982
4	4	0	12.124	11.972	-11.968	-0.154	0.447	1.5463	0.9982
4	4	0	18.535	17.738	-17.738	-0.797	0.697	1.5463	0.9982
4	4	0	10.821	10.422	-10.422	-0.400	0.334	4.0381	0.9982
4	4	0	2.634	2.177	-2.177	-0.457	0.697	1.5463	0.9982
4	4	0	10.449	10.136	-10.136	-0.313	0.447	1.5463	0.9982
4	4	0	29.821	29.974	-29.974	-0.153	0.447	1.5463	0.9982
4	4	0	16.268	16.816	-16.816	-0.548	0.697	1.5463	0.9982
4	4	0	14.508	14.044	-14.044	-0.460	0.447	1.5463	0.9982
4	4	0	14.846	15.570	-15.570	-0.724	0.697	1.5463	0.9982
4	4	0	5.058	5.366	-5.366	-0.308	0.447	1.5463	0.9982
4	4	0	2.244	2.150	-2.150	-0.096	0.447	1.5463	0.9982
4	4	0	1.796	1.194	-1.194	-0.602	0.697	1.5463	0.9982

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RFINE FOSITE49 FINAL CYCLE

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
4	8	1	30.2277	29.373	-29.391	-2.133	0.904	10.7833	0.9935
4	9	1	3.130	2.758	2.697	-0.575	0.372	1.7480	0.9999
4	10	1	28.306	26.688	26.693	1.894	1.617	17.8043	0.9947
4	11	1	25.357	24.041	24.075	0.842	1.956	13.9393	0.9957
4	11	1	19.744	18.788	-18.750	-1.497	0.499	0.4992	0.9997
4	11	1	6.1201	5.906	5.822	0.499	0.744	4.9926	1.0000
4	12	1	10.8715	11.511	-11.383	-1.020	0.646	9.9149	0.9999
4	12	1	35.815	35.412	-35.547	-0.891	0.403	7.1035	0.9992
4	12	1	45.999	45.344	-45.624	-2.400	0.654	11.1220	0.9918
4	12	1	14.819	15.028	-15.028	0.387	0.203	-3.1100	0.9951
4	13	1	15.899	16.089	-16.045	-1.035	0.604	-2.8765	0.9986
4	13	1	17.097	17.201	-17.184	-0.353	-0.104	-1.1197	0.9997
4	14	2	44.432	45.569	45.852	1.256	-1.130	-15.9689	0.9970
4	14	2	17.935	18.174	18.868	0.932	-0.239	-2.8151	0.9979
4	14	2	10.573	10.164	10.192	0.610	-0.409	4.1788	0.9993
4	14	2	6.998	6.803	6.802	0.207	0.192	1.5801	0.9997
4	14	2	3.699	3.884	3.878	0.150	0.186	0.9162	0.9999
4	14	2	3.909	3.771	3.799	-0.214	0.248	-0.9162	0.9929
4	14	2	7.522	6.844	-6.971	-1.468	1.065	-4.9165	0.9998
4	14	2	14.543	14.730	-14.739	-0.221	0.676	-0.9351	0.9988
4	14	2	24.737	24.888	-24.916	-0.872	0.151	-2.4660	0.9966
4	14	2	21.315	21.873	21.866	0.304	0.483	4.6668	0.9998
4	14	2	21.465	22.408	21.866	0.372	0.405	-7.2844	0.9968
4	14	2	29.045	29.476	-29.490	-1.776	0.058	-0.8383	0.9967
4	14	2	18.681	18.542	18.521	0.839	0.431	0.0204	0.9952
4	14	2	18.873	18.765	18.671	0.587	0.109	1.3183	0.9989
4	14	2	4.214	4.197	4.143	-0.516	0.126	1.0846	0.9974
4	14	2	20.422	20.117	20.135	-0.816	0.257	-2.5242	0.9999
4	14	2	21.860	21.384	-21.362	-1.043	0.128	-0.7277	0.9973
4	14	2	65.452	64.403	64.438	0.414	0.052	1.6439	0.9991
4	14	2	17.321	17.253	17.026	0.202	0.135	1.7001	0.9999
4	14	2	10.676	10.993	-10.092	-1.821	0.135	1.7714	0.9984
4	14	2	37.273	37.995	38.080	0.858	0.239	1.3567	0.9996
4	14	2	18.952	19.995	19.080	0.372	0.133	1.1977	0.9994
4	14	2	14.634	15.844	15.825	0.527	0.243	3.3357	0.9928
4	14	2	10.634	10.995	10.909	0.913	0.714	3.3357	0.9982
4	14	2	14.889	15.328	15.330	0.527	0.210	-3.0217	0.9987
4	14	2	13.462	13.776	13.776	0.000	0.437	-5.2724	0.9988
4	14	2	10.303	10.289	10.289	0.000	0.174	1.8323	0.9984
4	14	2	5.924	6.196	6.192	0.244	0.722	3.0662	0.9997
4	14	2	1.360	1.186	1.119	0.067	0.092	5.7976	0.9998
4	14	2	5.562	5.679	5.625	0.053	0.373	1.7552	0.9999
4	14	2	6.362	6.873	6.535	0.168	0.973	10.4886	0.9997
4	14	2	2.208	2.402	2.391	-0.009	0.173	1.9433	0.9998
4	14	2	23.208	23.402	23.421	0.214	0.119	-2.6073	0.9974

STRUCTURE FACTORS DELTA F DELTA/SIGMA EXT. FACTOR PAGE 10

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REFINE FOSITE49 FINAL CYCLE

H	K	L	F(OBS)
4	6	5	28.726
4	7	5	3.690
4	8	5	27.748
4	9	5	5.941
4	10	5	24.361
4	11	5	18.765
4	12	6	14.794
4	13	6	32.834
4	14	6	9.344
4	15	6	7.997
4	16	6	8.805
4	17	6	24.402
4	18	6	13.332
4	19	6	8.586
4	20	6	10.750
4	21	6	18.222
4	22	6	6.446
4	23	6	16.430
4	24	6	15.255
4	25	6	18.733
4	26	6	10.953
4	27	6	32.883
4	28	6	14.369
4	29	6	4.333
4	30	6	6.399
4	31	6	18.594
4	32	6	20.494
4	33	6	16.430
4	34	6	15.255
4	35	6	18.733
4	36	6	10.953
4	37	6	32.883
4	38	6	14.369
4	39	6	4.333
4	40	6	6.399
4	41	6	18.594
4	42	6	20.494
4	43	6	16.430
4	44	6	15.255
4	45	6	18.733
4	46	6	10.953
4	47	6	32.883
4	48	6	14.369
4	49	6	4.333
4	50	6	6.399
4	51	6	18.594
4	52	6	20.494
4	53	6	16.430
4	54	6	15.255
4	55	6	18.733
4	56	6	10.953
4	57	6	32.883
4	58	6	14.369
4	59	6	4.333
4	60	6	6.399
4	61	6	18.594
4	62	6	20.494
4	63	6	16.430
4	64	6	15.255
4	65	6	18.733
4	66	6	10.953
4	67	6	32.883
4	68	6	14.369
4	69	6	4.333
4	70	6	6.399
4	71	6	18.594
4	72	6	20.494
4	73	6	16.430
4	74	6	15.255
4	75	6	18.733
4	76	6	10.953
4	77	6	32.883
4	78	6	14.369
4	79	6	4.333
4	80	6	6.399
4	81	6	18.594
4	82	6	20.494
4	83	6	16.430
4	84	6	15.255
4	85	6	18.733
4	86	6	10.953
4	87	6	32.883
4	88	6	14.369
4	89	6	4.333
4	90	6	6.399
4	91	6	18.594
4	92	6	20.494
4	93	6	16.430
4	94	6	15.255
4	95	6	18.733
4	96	6	10.953
4	97	6	32.883
4	98	6	14.369
4	99	6	4.333
4	100	6	6.399

F(CALC)	A(CALC)	B(CALC)
28.886	28.897	1.757
4.487	-4.462	0.468
28.070	-28.063	-1.969
6.386	6.366	-1.505
24.692	24.672	-1.752
19.240	-19.231	0.782
14.510	-14.444	0.781
18.400	-18.399	-0.781
32.706	-32.778	2.157
9.544	-9.544	0.338
7.006	-7.006	1.180
10.494	-10.494	-1.474
25.425	-25.508	1.106
13.590	13.596	0.198
8.702	8.701	0.198
3.385	3.385	0.198
10.143	-10.141	0.198
16.679	16.675	0.452
15.395	15.363	0.249
18.940	-18.890	0.580
10.591	-10.545	0.580
32.841	32.831	0.774
14.844	-14.811	0.774
4.844	-4.811	0.774
6.844	-6.811	0.774
18.741	-18.774	0.456
26.945	-26.939	0.456
16.015	-16.015	0.456
17.050	-17.066	0.456
27.190	-27.097	0.456
26.244	26.178	0.674
13.113	13.078	0.674
6.698	6.698	0.674
0.066	0.066	0.674
25.066	-25.143	1.450
11.113	-11.078	1.450
4.697	-4.697	0.943
6.863	-6.863	0.943
47.829	-47.829	0.943
5.170	-5.170	0.943
39.654	-39.654	0.943
18.458	-18.458	0.943
14.109	-14.109	0.943
28.544	-28.544	0.943
17.701	-17.701	0.943
15.589	-15.589	0.943
13.416	-13.416	0.943

DELTA F	DELTA/SIGMA	EXT. FACTOR
-0.160	-2.099	0.995
0.196	-4.633	0.999
-0.196	-3.859	0.995
-0.445	-3.466	0.995
-0.331	-3.680	0.996
-0.334	-3.471	0.997
0.254	-3.236	0.998
0.394	-5.219	0.998
0.067	0.916	0.995
-0.204	-2.277	0.996
0.468	-4.793	0.997
0.217	-2.365	0.999
0.681	-8.475	0.997
0.025	-0.203	0.999
0.116	-1.047	0.999
0.374	0.548	0.997
0.050	0.963	0.995
0.078	0.893	0.998
0.218	0.390	0.998
0.034	-0.390	0.998
0.039	-0.443	0.998
0.109	-0.328	0.999
0.360	-0.427	0.999
0.044	0.951	0.995
0.334	0.460	0.999
0.854	5.442	0.999
0.474	-7.868	0.996
0.353	-3.435	0.997
0.751	-19.433	0.997
0.431	3.222	0.983
0.984	0.216	0.997
0.027	0.218	0.994
0.493	1.305	0.995
0.216	1.154	0.995
0.276	1.282	0.995
0.984	11.182	0.999
0.166	4.960	0.997
0.553	11.343	0.998
0.324	2.672	0.999
0.324	2.672	0.999
0.127	1.116	0.999
0.457	11.911	0.997
0.128	-3.274	0.998
0.387	-1.580	0.998
0.159	-4.876	0.999
0.069	-0.999	0.999
0.324	-2.051	0.999

STRUCTURE FACTORS

RFINE FOSITE49 FINAL CYCLE

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
5	11	1	9.714	9.247	-9.217	-0.772	0.468	3.5991	0.9995
5	12	1	6.226	5.180	-5.157	-0.494	1.044	6.4749	0.9997
5	2	1	6.933	7.001	-6.982	0.052	-0.063	0.7933	0.9996
5	3	1	3.335	1.084	-1.006	0.405	-2.251	17.7853	1.0000
5	4	1	16.698	17.291	-17.292	-0.656	-0.599	8.3475	0.9985
5	5	1	30.011	50.555	-30.280	-0.447	-0.299	-1.8195	0.9999
5	6	1	50.119	4.448	50.961	0.070	0.392	-5.1407	0.9982
5	7	1	8.124	8.168	-8.044	-0.681	0.231	1.1407	0.9999
5	8	1	24.115	24.351	-24.342	-1.427	-0.045	0.4219	0.9996
5	9	1	32.644	33.416	-33.416	-0.977	-0.477	-2.2241	0.9959
5	10	1	11.888	21.611	-11.385	0.711	0.107	-7.7264	0.9923
5	11	1	22.155	21.022	-21.592	-1.496	0.083	0.7633	0.9972
5	12	1	43.782	6.073	-6.012	-0.531	1.009	12.5590	0.9970
5	1	1	20.248	44.078	-20.516	-0.708	0.277	-3.5579	1.0000
5	2	1	18.978	18.828	-18.416	-0.887	-0.296	-4.5469	0.9995
5	3	1	10.002	10.245	-10.192	-0.469	-0.387	-5.6515	0.9980
5	4	1	6.450	16.197	-6.130	-0.224	-0.138	-1.8991	0.9997
5	5	1	4.988	18.840	-18.014	-0.718	0.079	0.7480	0.9998
5	6	1	1.978	10.038	-10.230	-0.648	-0.195	-2.1566	0.9995
5	7	1	1.100	17.045	-17.551	-0.145	0.202	6.7669	0.9995
5	8	1	9.921	4.956	-4.955	-0.148	0.035	-1.7326	0.9995
5	9	1	1.378	1.999	-1.999	-0.033	0.073	-1.2308	0.9995
5	10	1	17.822	17.551	-17.444	-0.733	0.621	1.6671	1.0000
5	11	1	10.512	10.374	-10.386	-0.113	-0.430	-3.6454	0.9980
5	12	1	28.771	22.212	-22.208	-0.425	-0.298	1.9872	0.9986
5	1	1	10.894	20.591	-10.669	-0.317	-0.697	3.3786	0.9956
5	2	1	21.227	22.900	-21.184	-0.457	-0.044	-1.9872	0.9981
5	3	1	22.028	22.900	-22.853	-0.638	0.418	1.1006	1.0000
5	4	1	5.463	11.900	-11.853	-0.933	0.885	-1.1006	0.9970
5	5	1	38.478	5.725	-5.688	-0.658	0.475	5.0701	0.9993
5	6	1	25.918	24.799	-24.810	-1.098	-0.644	-1.9890	1.0000
5	7	1	35.205	38.224	-38.211	-0.983	-0.325	8.2192	0.9998
5	8	1	11.763	21.593	-11.789	-0.637	-0.335	-3.3192	0.9998
5	9	1	14.278	14.593	-14.311	-0.809	0.051	4.8224	0.9999
5	10	1	14.278	14.322	-14.749	-1.071	-0.171	-0.6183	0.9999
5	11	1	26.929	27.722	-27.749	-1.195	-0.344	-0.5255	0.9990
5	12	1	16.875	17.279	-17.642	-0.158	-0.793	8.1442	0.9962
5	1	1	17.098	13.376	-13.614	0.065	-0.404	-4.4034	0.9999
5	2	1	4.930	3.609	-3.589	0.488	-0.563	-2.8793	0.9990
5	3	1	5.759	5.751	-5.721	0.381	-0.571	4.5901	0.9999
5	4	1	6.245	37.914	-37.310	-0.407	0.008	-0.3997	0.9997
5	5	1	6.085	2.352	-2.274	-0.865	-0.078	0.0668	0.9999
5	6	1	2.835	2.352	-2.274	-1.600	0.483	-10.6886	0.9935
5	7	1							1.0000

STRUCTURE FACTORS PAGE 12

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
5	7	6	3.951	3.477	-3.242	-1.239	0.480	2.871	0.999
5	0	7	6.635	6.599	-6.572	-0.608	0.036	0.316	0.999
5	1	7	31.976	32.111	32.131	1.816	-0.136	-1.637	0.995
5	2	7	14.862	14.907	14.894	0.778	-0.045	-0.501	0.998
5	3	7	3.048	3.132	-3.722	-1.257	0.916	-0.501	0.999
5	4	7	3.962	3.488	-3.433	-0.613	0.474	4.936	0.999
5	0	7	4.788	4.581	4.181	1.022	0.208	1.237	0.999
5	1	7	26.053	24.249	24.291	-1.510	0.804	0.604	0.994
5	2	7	19.561	18.844	18.817	0.783	0.171	4.929	0.997
5	3	7	6.976	6.734	-6.689	-1.847	0.242	1.161	0.999
5	4	7	50.248	48.385	48.827	0.847	0.867	13.196	0.999
5	5	7	21.663	20.174	20.207	-0.522	0.058	9.275	0.999
5	6	7	23.136	21.427	-21.451	-0.523	1.339	4.537	0.999
5	7	7	9.771	8.822	-8.821	-0.061	0.950	10.916	0.999
5	8	7	8.431	8.878	8.864	0.550	0.249	3.174	0.999
5	9	7	28.646	28.657	28.658	-0.098	0.049	-0.224	0.999
5	0	1	3.063	3.711	-3.691	-0.484	0.352	-0.022	0.999
5	1	1	6.159	5.249	5.081	-0.032	0.583	-0.352	0.999
5	2	1	14.307	13.725	-13.711	-0.792	0.355	-0.428	0.999
5	3	1	10.337	9.981	9.871	-0.496	0.345	-0.186	0.999
5	4	1	4.671	4.326	-4.326	-0.196	0.355	0.022	0.999
5	5	1	4.152	3.966	-3.966	-0.196	0.355	0.022	0.999
5	6	1	13.187	13.727	-13.707	-0.887	0.773	2.174	0.999
5	7	1	13.645	13.990	13.876	-1.258	0.280	-0.428	0.999
5	8	1	6.558	5.990	5.914	-0.145	0.568	-0.280	0.999
5	9	1	49.921	51.343	51.443	-0.145	0.568	-0.280	0.999
5	0	2	12.865	12.702	-12.330	-0.165	0.829	-0.428	0.999
5	1	2	14.180	14.210	14.128	-0.829	0.029	0.029	0.999
5	2	2	13.864	15.920	15.428	-0.091	0.141	0.014	0.999
5	3	2	8.808	8.838	8.840	0.050	0.091	0.014	0.999
5	4	2	17.987	18.142	18.166	0.050	0.091	0.014	0.999
5	5	2	21.994	21.696	-21.702	-0.857	0.268	-0.098	0.999
5	6	2	12.598	13.807	-13.804	-0.494	0.815	-0.098	0.999
5	7	2	11.388	11.154	-11.591	-0.785	0.103	-0.020	0.999
5	8	2	10.076	10.838	-10.298	-0.785	0.103	-0.020	0.999
5	9	2	39.877	40.827	40.964	-1.092	0.210	-0.305	0.999
5	0	3	6.714	6.504	6.450	0.101	0.950	0.101	0.999
5	1	3	17.425	17.406	17.361	-0.776	0.492	-0.178	0.999
5	2	3	17.238	17.401	-17.361	-1.423	0.130	-0.033	0.999
5	3	3	38.502	40.361	40.576	-1.057	0.132	-0.132	0.999
5	4	3	1.652	1.801	-1.576	-0.557	0.851	-0.132	0.999

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RFINE F051TE49 FINAL CYCLE

STRUCTURE FACTORS DELTA F DELTA/SIGMA EXI. FACTOR

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H	K	L	F(DBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXI. FACTOR
6	7	4	17.655	18.834	18.851	-0.221	-1.179	-13.164	0.9981
6	7	4	5.648	5.818	-5.810	-0.325	-0.171	-1.251	0.9993
6	8	4	16.884	18.248	18.258	-0.498	-1.364	-13.835	0.9981
6	8	4	10.468	10.512	10.514	-0.071	-0.044	-0.488	0.9981
6	6	5	25.363	25.799	25.823	0.842	-0.436	-5.324	0.9971
6	6	5	1.684	1.306	-1.233	0.842	-0.378	-1.172	1.0000
6	6	5	5.290	5.447	-5.364	0.947	-0.378	-1.214	0.9999
6	6	5	7.706	7.657	-9.175	-0.714	-0.089	-0.845	0.9996
6	6	5	7.112	7.657	-7.534	-0.370	0.049	0.443	0.9997
6	6	6	11.523	12.619	12.578	-1.069	-1.096	-1.234	0.9995
6	6	6	9.672	9.322	-9.487	-0.871	-0.118	-1.171	0.9995
6	6	6	36.072	36.915	36.983	-0.871	-0.118	-1.171	0.9995
6	6	6	6.721	6.675	6.640	0.691	0.046	0.388	0.9930
6	6	6	30.497	28.341	28.452	-0.240	0.046	0.388	0.9930
7	3	0	12.851	12.036	11.993	0.317	-0.686	-1.909	0.9998
7	3	0	3.851	3.700	3.725	0.079	-0.899	-1.876	0.9998
7	3	0	12.929	12.036	11.993	0.679	-0.686	-1.876	0.9998
7	3	0	1.827	1.790	-1.153	-0.679	1.127	4.876	0.9999
7	3	0	13.341	11.208	-11.153	-1.164	2.134	11.052	1.0000
7	3	0	27.692	24.674	-24.684	-1.903	3.018	10.591	0.9990
7	3	0	14.745	14.727	14.723	-1.101	0.012	-0.144	0.9984
7	3	0	25.070	25.727	-25.714	-1.720	-0.012	-0.144	0.9984
7	3	0	9.947	9.759	-9.715	-0.944	0.636	-1.777	0.9995
7	3	0	7.951	7.322	7.894	1.156	0.188	1.777	0.9995
7	3	0	10.300	9.920	9.894	0.750	0.629	1.062	0.9996
7	3	0	4.070	4.310	-7.244	-0.989	0.871	-3.210	0.9996
7	3	0	8.181	7.114	-4.081	-0.325	0.044	6.331	0.9996
7	3	0	14.896	14.145	14.144	-0.595	-0.750	-6.056	0.9984
7	3	0	6.191	6.377	6.364	0.419	-0.166	-3.366	0.9998
7	3	0	10.052	10.381	10.378	0.337	-0.329	-1.667	0.9998
7	3	0	5.344	7.363	-7.344	-0.537	0.066	-3.558	0.9997
7	3	0	35.913	4.844	-4.796	-0.684	-0.500	-3.666	0.9997
7	3	0	12.211	11.813	11.785	1.765	-1.044	3.433	0.9997
7	3	0	10.951	10.528	-10.478	0.887	0.398	3.026	0.9995
7	3	0	17.429	16.889	-16.819	-1.051	0.540	4.469	0.9995
7	3	0	8.501	8.246	-8.196	-0.920	0.225	4.213	0.9997
7	3	0	8.026	8.171	-8.095	-1.122	-0.225	4.213	0.9997
7	3	0	10.656	10.953	-10.932	-0.727	-0.297	-1.312	0.9997
7	3	0	14.242	14.623	-14.598	0.994	-0.297	-2.873	0.9994
7	3	0	21.648	22.398	22.421	0.228	-0.381	-3.817	0.9988
7	3	0	5.050	5.323	-5.315	-0.302	-0.273	-8.622	0.9999

IHC2091 IBCOM - PROGRAM INTERRUPT (P) - DIVIDE CHECK OLD PSM IS 078D00GF42093046 * REGISTER CONTAINED 000000052160000

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

TESTS 0015 4209281A 00092E88 00000001 0009260C

INPUT 0122 420A083E 00092448 00000001 0009DB00

RFINE 0007 4208615E 0009D510 00E7D0D8 00000000

MAIN 0000AF58 00085F80 00E7D0D8 00084FF8

ENTRY POINT= 00085F80
STANDARD FIXUP TAKEN , EXECUTION CONTINUING

RESULTS OF STRUCTURE FACTOR CALCULATIONS

REFINE F051TE49 FINAL CYCLE		ALL REFLECTIONS		RANGES OF F(OBS)		RANGES OF (SIN(THETA)/LAMBDA)**2	
WEIGHTED R	UNWEIGHTED R	NUMERATOR	DENOMINATOR	NUMBER	R	WEIGHTED R	UNWEIGHTED R
76529.69	387.10	98295360.00	13372.56	731	0.028	76498.36	374.43
RANGES OF F(OBS)							
12357.42	13784.93	54996976.00	409	0.015	53716336.00	12326.01	13784.93
12102.32	26494.09	25548720.00	190	0.023	26304384.00	12102.32	13784.93
2570.74	3968.74	9412686.00	70	0.036	9691087.00	2570.74	12102.32
56.85	5199.80	5109745.00	38	0.032	5260878.00	2570.74	12102.32
6783.21	4263.11	1210202.00	38	0.018	1245997.00	3968.74	12102.32
18018560.00	154466.94	154463699.00	97	0.015	138444.13	56.85	12102.32
16404966.00	941268.69	16404966.00	122	0.014	138444.13	5199.80	12102.32
5109745.00	7799080.00	18018560.00	154	0.019	969108.88	5199.80	12102.32
RANGES OF (SIN(THETA)/LAMBDA)**2							
43109.16	7815.09	7799080.00	38	0.092	5260878.00	43109.16	7815.09
4999.67	4999.67	10353953.00	77	0.032	7815.09	4999.67	7815.09
3864.24	2769.07	12102026.00	90	0.022	10383311.00	3864.24	2769.07
2932.21	4263.11	130432292.00	97	0.018	12183083.00	2932.21	4263.11
6783.21	154466.94	154463699.00	115	0.015	134229081.00	6783.21	154466.94
18018560.00	941268.69	16404966.00	122	0.014	14931968.00	18018560.00	941268.69
5109745.00	7799080.00	18018560.00	154	0.019	16336411.00	5109745.00	7799080.00
UNREJECTED REFLECTIONS							
WEIGHTED R	UNWEIGHTED R	76498.36	98295360.00	710	0.028	76498.36	98295360.00
RANGES OF F(OBS)							
12326.01	13784.93	53716336.00	388	0.015	53716336.00	12326.01	13784.93
12102.32	26494.09	26304384.00	190	0.023	26304384.00	12102.32	13784.93
2570.74	3968.74	9691087.00	70	0.035	9691087.00	2570.74	12102.32
56.85	5199.80	5260878.00	38	0.071	5260878.00	56.85	12102.32
6783.21	4263.11	1245997.00	9	0.045	1245997.00	6783.21	4263.11
18018560.00	154466.94	138444.13	7	0.064	138444.13	18018560.00	154466.94
5109745.00	7799080.00	138444.13	1	0.020	138444.13	5109745.00	7799080.00
RANGES OF (SIN(THETA)/LAMBDA)**2							
43109.16	7815.09	7815.09	38	0.091	5260878.00	43109.16	7815.09
4999.67	4999.67	7815.09	57	0.031	7815.09	4999.67	7815.09
3864.24	2769.07	10383311.00	75	0.022	10383311.00	3864.24	2769.07
2932.21	4263.11	12183083.00	88	0.022	12183083.00	2932.21	4263.11
6783.21	154466.94	134229081.00	97	0.018	134229081.00	6783.21	154466.94
18018560.00	941268.69	14931968.00	108	0.014	14931968.00	18018560.00	941268.69
5109745.00	7799080.00	16336411.00	118	0.014	16336411.00	5109745.00	7799080.00
5109745.00	7799080.00	17859280.00	129	0.016	17859280.00	5109745.00	7799080.00
6777.21	17859280.00	17859280.00	129	0.019	17859280.00	6777.21	17859280.00

SUM FCAL 13263.44
 STANDARD DEV OF UNIT WEIGHT OBS 10.69

REFINE F051TE49 FINAL CYCLE
 ESTIMATED STD. DEV. FOR OBS. OF UNIT WEIGHT
 EXTINCTION CORRECTION ISOTROPIC

OLD
 10.69

CHANGE

NEW

ERRUM

SHIFT/ERRUM

ATOM 1 M1

EQUIPOINT FRACTION = 0.500
 OCCUPANCY SPECIES 1
 OCCUPANCY SPECIES 2
 TOTAL OCCUPANCY (FIXED) =

0.52050
 0.07950
 1.00000

0.00000

0.52050
 0.07950

0.00000

0.00000

2

ATOM 2 M2

EQUIPOINT FRACTION = 0.500
 OCCUPANCY SPECIES 1
 OCCUPANCY SPECIES 2
 TOTAL OCCUPANCY (FIXED) =

0.10950
 0.89050
 1.00000

0.00000

0.10950
 0.89050

0.00000

0.00000

6

ATOM 3 S1

EQUIPOINT FRACTION = 0.500
 OCCUPANCY SPECIES 1
 OCCUPANCY SPECIES 2
 OCCUPANCY SPECIES 3

1.00000
 0.42262
 0.09099
 0.25000
 0.00312
 0.00096
 0.00252
 0.00000
 0.00000

0.00000

1.00000
 0.42262
 0.09099
 0.25000
 0.00311
 0.00096
 0.00251
 0.00000
 0.00000

0.00000

0.00000

12

ATOM 4 O1

EQUIPOINT FRACTION = 0.500
 OCCUPANCY SPECIES 1
 OCCUPANCY SPECIES 2
 OCCUPANCY SPECIES 3
 OCCUPANCY SPECIES 4

1.00000
 0.75850
 0.08671
 0.25000
 0.00220
 0.00169
 0.00365
 0.00016
 0.00000

0.00000

1.00000
 0.75850
 0.08670
 0.25000
 0.00220
 0.00169
 0.00365
 0.00015
 0.00000

0.00000

0.00000

21

ATOM 5 O2

EQUIPOINT FRACTION = 0.500
 OCCUPANCY SPECIES 1
 OCCUPANCY SPECIES 2
 OCCUPANCY SPECIES 3
 OCCUPANCY SPECIES 4

1.00000
 0.75850
 0.08671
 0.25000
 0.00220
 0.00169
 0.00365
 0.00016
 0.00000

0.00000

1.00000
 0.75850
 0.08670
 0.25000
 0.00220
 0.00169
 0.00365
 0.00015
 0.00000

0.00000

0.00000

26

ATOM 5 02 EQUIPOINT FRACTION = 0.500
OCCUPANCY SPECIES = 4

X	1.000000	0.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y	0.2300500	0.4488900	0.2500000	0.4488921	0.2500000	0.4488921	0.2500000	0.4488921	0.2500000
Z	0.4488900	0.2500000	0.4488921	0.2500000	0.4488921	0.2500000	0.4488921	0.2500000	0.4488921
BETA11	0.00011200	0.00037800	0.000445	0.0011158	0.0037755	0.0044827	0.0011158	0.0037755	0.0044827
BETA22	0.00037800	0.000445	0.0011158	0.0011158	0.0037755	0.0044827	0.0011158	0.0037755	0.0044827
BETA33	0.000445	0.0011158	0.0037755	0.0037755	0.0044827	0.0044827	0.0037755	0.0044827	0.0044827
BETA12	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
BETA13	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
BETA23	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000

ATOM 6 03 EQUIPOINT FRACTION = 1.000
OCCUPANCY SPECIES = 4

X	1.000000	0.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y	0.2781799	0.1589600	0.0374200	0.2781839	0.1589592	0.0374240	0.2781839	0.1589592	0.0374240
Z	0.1589600	0.0374200	0.00039400	0.0374240	0.00039388	0.00039388	0.0374240	0.00039388	0.00039388
BETA11	0.00039400	0.00039400	0.00039400	0.00039388	0.00039388	0.00039388	0.00039388	0.00039388	0.00039388
BETA22	0.00039400	0.00039400	0.00039400	0.00039388	0.00039388	0.00039388	0.00039388	0.00039388	0.00039388
BETA33	0.00039400	0.00039400	0.00039400	0.00039388	0.00039388	0.00039388	0.00039388	0.00039388	0.00039388
BETA12	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
BETA13	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
BETA23	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000

MAXIMUM SHIFT/ERROR = 0.13
AVERAGE SHIFT/ERROR = 0.02

ROW 11	1.0000	12	-0.1682	13	-0.2630	14	0.0229	15	0.0309	16	-0.0007	17	-0.1100	18	0.0185	19	0.0495	20	-0.0000
ROW 21	0.0532	22	-0.0088	23	-0.2684	24	-0.0009	25	0.0059	26	0.0128	27	-0.0150	28	-0.0017	29	-0.0497	30	-0.0000
ROW 31	0.0196	32	0.0177	33	-0.0226	34	0.0090	35	-0.0134	36	-0.0625	37	0.0045	38	0.0015	39	0.0037	40	0.0000
ROW 41	-0.0139																		
ROW 12	1.0000	13	-0.2521	14	0.0088	15	-0.0070	16	0.0278	17	0.0180	18	-0.1199	19	0.0205	20	0.0129	21	-0.0000
ROW 22	0.0048	23	-0.0042	24	0.0129	25	0.0119	26	0.0143	27	-0.0048	28	0.0390	29	-0.0105	30	-0.0284	31	-0.0000
ROW 32	-0.0192	33	0.0133	34	-0.0175	35	-0.0005	36	0.0052	37	0.0258	38	-0.0012	39	-0.0105	40	-0.0118	41	-0.0000
ROW 13	1.0000	14	-0.0007	15	0.0225	16	-0.0013	17	0.0446	18	0.0318	19	-0.1179	20	0.0052	21	0.0013	22	-0.0000
ROW 23	0.0094	24	-0.0157	25	0.0308	26	-0.0054	27	0.0041	28	0.0072	29	-0.0061	30	0.0194	31	-0.0054	32	-0.0000
ROW 33	0.0094	34	-0.0156	35	0.0497	36	0.0041	37	0.0042	38	0.0054	39	-0.0061	40	0.0217	41	-0.0072		
ROW 14	1.0000	15	-0.0042	16	-0.0585	17	-0.0179	18	0.0125	19	0.0125	20	-0.0329	21	0.0017	22	-0.0342	23	-0.0000
ROW 24	0.0022	25	0.0051	26	-0.0056	27	0.0226	28	0.0311	29	0.0050	30	-0.0218	31	-0.0218	32	-0.0000	33	-0.0000
ROW 34	-0.0085	35	0.0041	36	-0.0093	37	-0.0040	38	0.0045	39	0.0264	40	-0.0181	41	0.0060				
ROW 15	1.0000	16	0.0053	17	-0.0694	18	0.0120	19	0.0113	20	0.0329	21	0.0342	22	-0.0028	23	0.0028	24	-0.0000
ROW 25	-0.0203	26	0.0060	27	-0.0001	28	0.0082	29	0.0077	30	0.0050	31	-0.0218	32	-0.0028	33	0.0028	34	-0.0000
ROW 35	0.0232	36	0.0222	37	-0.0052	38	-0.0173	39	0.0264	40	0.0264	41	0.0060						
ROW 16	1.0000	17	0.0153	18	0.0018	19	-0.0059	20	-0.0315	21	-0.0017	22	-0.1912	23	0.0219	24	-0.0674	25	-0.0000
ROW 26	0.0310	27	0.0046	28	0.0033	29	-0.0241	30	-0.0319	31	0.0151	32	0.0221	33	0.0267	34	0.0149	35	-0.0000
ROW 36	-0.0032	37	0.0136	38	0.0019	39	-0.0316	40	0.0081	41	0.0092								
ROW 17	1.0000	18	-0.2000	19	-0.2666	20	-0.0004	21	-0.0535	22	-0.0058	23	-0.1323	24	0.0300	25	0.0017	26	-0.0000
ROW 27	0.0268	28	0.0152	29	-0.0241	30	-0.0099	31	0.0202	32	0.0109	33	0.0300	34	-0.0058	35	0.0018	36	-0.0000
ROW 37	0.0083	38	0.0000	39	0.0038	40	-0.0144	41	0.0031										
ROW 18	1.0000	19	-0.4510	20	0.0059	21	0.0154	22	0.0403	23	0.0566	24	-0.2530	25	-0.0414	26	0.0020	27	-0.0000
ROW 28	-0.0015	29	-0.0031	30	-0.0106	31	0.0134	32	0.0213	33	-0.0003	34	0.0057	35	-0.0091	36	0.0000	37	-0.0000
ROW 38	0.0368	39	0.0106	40	0.0084	41	-0.0003												
ROW 19	1.0000	20	-0.0087	21	0.0164	22	0.0038	23	0.0717	24	0.0395	25	-0.1760	26	0.0024	27	0.0012	28	-0.0000
ROW 29	0.0187	30	0.0149	31	-0.0513	32	-0.0151	33	-0.0112	34	-0.0087	35	0.0363	36	0.0024	37	0.0012	38	-0.0000
ROW 39	-0.0032	40	-0.0305	41	0.0083														
ROW 20	1.0000	21	-0.0011	22	-0.0081	23	-0.0005	24	0.0070	25	0.0110	26	-0.0426	27	-0.0068	28	0.0184	29	-0.0000
ROW 30	-0.0073	31	-0.0005	32	0.0127	33	-0.0033	34	0.0049	35	-0.0160	36	-0.0114	37	-0.0093	38	0.0037	39	-0.0000
ROW 40	-0.0124	41	0.0177																
ROW 21	1.0000	22	-0.0090	23	-0.0113	24	0.0060	25	-0.0072	26	-0.0524	27	-0.0099	28	-0.0086	29	-0.0204	30	-0.0000
ROW 31	-0.0031	32	0.0341	33	-0.0087	34	0.0156	35	0.0019	36	0.0091	37	0.0075	38	0.0056	39	0.0305	40	-0.0000
ROW 41	-0.0165																		
ROW 22	1.0000	23	0.0140	24	0.0202	25	-0.0053	26	0.0056	27	-0.0086	28	0.0054	29	0.0052	30	0.0347	31	0.0000
ROW 32	-0.0180	33	0.0045	34	-0.0160	35	-0.0349	36	0.0069	37	-0.0486	38	0.0117	39	-0.0025	40	-0.0092	41	0.0000
ROW 23	1.0000	24	-0.1947	25	-0.2834	26	-0.0029	27	0.0065	28	-0.0061	29	0.0129	30	0.0327	31	-0.0371	32	-0.0000
ROW 33	-0.0161	34	0.0036	35	-0.0010	36	-0.0139	37	-0.0045	38	-0.0159	39	0.0024	40	0.0280	41	0.0000		
ROW 24	1.0000	25	-0.2405	26	-0.0099	27	0.0039	28	0.0285	29	0.0101	30	-0.0043	31	-0.0043	32	-0.0019	33	0.0000
ROW 34	-0.0080	35	0.0362	36	-0.0007	37	0.0625	38	-0.0145	39	-0.0075	40	0.0003	41	0.0090				
ROW 25	1.0000	26	0.0029	27	0.0085	28	0.0221	29	-0.0365	30	-0.0022	31	0.0586	32	0.0054	33	-0.0086	34	-0.0000
ROW 35	-0.0247	36	-0.0090	37	-0.0165	38	0.0203	39	0.0007	40	0.0216	41	0.0087						

REFINE F051TE49 FINAL CYCLE
 CORRELATION COEFFICIENTS WITH LARGEST MAGNITUDES

PARAMETERS	VALUE	PARAMETERS	VALUE	PARAMETERS	VALUE	PARAMETERS	VALUE
2	-0.5502	2	-0.5401	2	-0.5066	1	-0.3154
23	-0.2834	29	-0.2725	17	-0.2666	11	-0.2630
36	-0.2613	37	-0.2559	18	-0.2530	12	-0.2521
18	-0.2510	30	-0.2496	24	-0.2405	17	-0.2000
23	-0.1947	16	-0.1912	19	-0.1760	29	-0.1752
5		3		4		2	
25		31		19		13	
38		38		24		13	
19		31		25		18	
24		22		25		30	

REFINE F051TE49 FINAL CYCLE
BOND ANGLES

CENTRAL ATOM . X Y Z
M1 0.0 0.0 0.0

ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
01	01	179.960
01	02	94.649
01	03	85.351
01	03	85.929
01	03	94.071
01	03	85.351
01	02	94.649
01	01	54.071
01	02	85.929
02	03	180.000
02	03	105.389
02	03	74.611
02	03	74.611
02	03	105.389
02	03	179.956

CENTRAL ATOM X Y Z
M2 0.58704 0.27904 0.25000

ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
01	02	175.326
01	03	78.880
01	03	92.529
01	03	92.529
01	03	78.880
02	03	97.302
02	03	90.093
02	03	90.093
02	03	97.302
02	03	90.093
02	03	97.302
03	03	89.131
03	03	157.953
03	03	169.388
03	03	111.690
03	03	157.953
03	03	189.131

CENTRAL ATOM X Y Z
SI 0.42262 0.09099 0.25000

ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
02	03	101.800
02	03	114.552
03	01	101.800
03	01	115.772
03	01	105.267
03	01	115.772

CENTRAL ATOM	X	Y	Z	ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
01	0.75850	0.08671	0.25000			
				8	15	116.904
				8	17	96.077
				15	18	96.077
				15	17	123.836
				17	18	123.836
				17	15	92.228
CENTRAL ATOM	X	Y	Z			
02	0.23005	0.44289	0.25000			
				20	21	95.076
				20	22	123.888
				21	23	92.460
				21	22	123.888
				22	23	92.460
				22	21	120.674
CENTRAL ATOM	X	Y	Z			
03	0.27818	0.15896	0.03742			
				1	15	90.531
				1	22	96.286
				15	22	116.204
				15	24	92.611
				22	24	126.205
				22	15	126.149

REFINE FOSITE49 FINAL CYCLE
 ELLIPSOIDS OF VIBRATION

ELLIPSOID FOR M1

EQUIVALENT ISOTROPIC B = 0.4155

AXIS RMS AMPLITUDE ANGLE WITH A ANGLE WITH B ANGLE WITH C
 1 0.056096 31.14 60.50
 2 0.068756 58.87 143.65
 3 0.088562 90.88 70.75

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM M1

ATOM	X	Y	Z	RAW	LOWER	UPPER	U-C
01	-0.24150	0.08671	0.25000	2.12392	2.12393	2.12431	0.06931
02	0.24150	-0.08671	-0.25000	2.12392	2.12393	2.12431	0.06931
03	0.00000	0.00000	0.00000	2.07496	2.07496	2.07516	0.00000
01	0.26995	-0.05111	0.25000	2.14757	2.14759	2.14807	0.05255
02	-0.26995	0.05111	-0.25000	2.14757	2.14759	2.14807	0.05255
03	0.00000	0.00000	0.00000	2.14757	2.14759	2.14807	0.05255

ELLIPSOID FOR M2

EQUIVALENT ISOTROPIC B = 0.5412

AXIS RMS AMPLITUDE ANGLE WITH A ANGLE WITH B ANGLE WITH C
 1 0.078267 58.70 50.00
 2 0.083376 90.00 180.00
 3 0.086522 31.29 90.00

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM M2

ATOM	X	Y	Z	RAW	LOWER	UPPER	U-C
01	0.75850	0.08671	0.25000	2.29598	2.29600	2.29642	0.08451
02	1.43005	0.44889	0.25000	2.12898	2.12898	2.12900	0.08505
03	1.27818	0.15896	0.03742	2.28676	2.28676	2.28722	0.08229
01	0.717818	0.034104	-0.03742	2.12671	2.12671	2.12686	0.08229
02	0.0717818	0.34104	0.53742	2.12671	2.12671	2.12686	0.08229
03	1.27818	0.15896	0.46258	2.28676	2.28676	2.28722	0.08229

ELLIPSOID FOR S1

EQUIVALENT ISOTROPIC B = 0.3625

AXIS RMS AMPLITUDE ANGLE WITH A ANGLE WITH B ANGLE WITH C
 1 0.060183 3.23 53.23 90.00
 2 0.069116 90.00 180.00
 3 0.075309 86.77 3.23 90.00

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM S1

ATOM	X	Y	Z	RAW	LOWER	UPPER	U-C
02	0.26995	-0.05111	0.25000	1.66074	1.66079	1.66150	0.07147
03	0.27818	0.15896	0.03742	1.63771	1.63783	1.63895	0.06817
01	0.0717818	0.08671	0.25000	1.61083	1.61106	1.61275	0.06019
03	0.27818	0.15896	0.46258	1.63771	1.63783	1.63895	0.06817

ELLIPSOID FOR O1

EQUIVALENT ISOTROPIC B = 0.49884

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.090403	3.35	56.65	90.00
2	0.083315	90.00	50.00	90.00
3	0.097243	93.35	3.35	90.00

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM O1

ATOM	X	Y	Z	RAW	LOWER	DISTANCES RIDING	A1	NON-CORR	UPPER	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
M2	0.98704	0.27904	0.25000	2.29598	2.29600	2.29642	2.30139	1.01906	2.30675	0.08677	0.08677	0.08677
SI	0.42262	0.09099	0.25000	1.61083	1.61106	1.61275	1.61906	1.01906	1.62705	0.05091	0.05091	0.05091
M1	1.00000	0.0	0.0	2.12392	2.12393	2.12431	2.12948	2.12948	2.13503	0.07925	0.07925	0.07925
M1	1.00000	0.0	0.50000	2.12392	2.12393	2.12431	2.12948	2.12948	2.13503	0.07925	0.07925	0.07925

ELLIPSOID FOR O2

EQUIVALENT ISOTROPIC B = 0.4756

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.063236	28.56	91.04	50.00
2	0.083078	118.96	28.96	50.00
3	0.084681	90.00	90.00	0.0

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM O2

ATOM	X	Y	Z	RAW	LOWER	DISTANCES RIDING	A1	NON-CORR	UPPER	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
M1	0.50000	0.50000	0.0	2.07496	2.07496	2.07516	2.08070	2.08070	2.08643	0.07576	0.07576	0.07576
SI	0.50000	0.50000	0.25000	2.07496	2.07496	2.07516	2.08070	2.08070	2.08643	0.07576	0.07576	0.07576
M2	-0.01296	0.27904	0.25000	2.12898	2.12898	2.12900	2.13527	2.13527	2.14155	0.08507	0.08507	0.08507
SI	0.07738	0.39099	0.25000	1.66074	1.66079	1.66150	1.66671	1.66671	1.67264	0.08364	0.08364	0.08364

ELLIPSOID FOR O3

EQUIVALENT ISOTROPIC B = 0.4978

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.067706	1.34	89.69	86.69
2	0.077061	89.17	51.75	141.73
3	0.091604	91.05	36.26	51.76

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM O3

ATOM	X	Y	Z	RAW	LOWER	DISTANCES RIDING	A1	NON-CORR	UPPER	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
M1	0.0	0.09099	0.0	2.14757	2.14759	2.14807	2.15285	2.15285	2.15811	0.08655	0.08655	0.08655
SI	0.42262	0.27904	0.25000	1.63771	1.63783	1.63895	1.64452	1.64452	1.65122	0.07568	0.07568	0.07568
M2	-0.01296	0.27904	0.25000	2.25675	2.25677	2.25723	2.26243	2.26243	2.26809	0.08375	0.08375	0.08375
M2	0.48704	0.22096	-0.25000	2.12670	2.12671	2.12687	2.13302	2.13302	2.13933	0.07651	0.07651	0.07651

PARAMETERS WRITTEN OUT TO UNIT 10.
SUMMARY OF ERRORS FOR THIS JOB

ERROR NUMBER 209
NUMBER OF ERRORS 1

H	K	L	F(0BS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
0	2	0	26.7442	24.9229	25.6777	-0.1444	1.812	30.9051	0.8426
0	4	0	54.7775	58.405	63.093	4.176	-3.633	-42.2599	0.8532
0	6	0	13.351	13.403	13.412	0.872	-0.055	-0.9289	0.9946
0	8	0	31.1255	31.480	31.748	0.257	-0.355	-2.9262	0.9782
0	10	0	54.580	53.983	55.743	2.969	0.597	4.5010	0.9504
0	12	0	27.5937	27.5913	27.743	0.428	0.001	0.0075	0.9884
0	14	0	31.8897	31.913	31.945	0.425	-0.026	-0.1444	0.9867
0	16	0	29.5542	26.6114	26.901	0.855	2.750	-3.9444	0.9910
0	18	0	30.2254	30.0000	-31.668	-0.785	-0.360	-6.8007	0.9340
0	20	0	1.121	58.8004	-63.315	-0.007	1.116	1.9999	1.0000
0	22	0	55.6888	82.250	90.738	2.651	-3.111	-4.9350	0.8617
0	24	0	80.6449	82.250	90.738	2.651	-3.111	-4.9350	0.8617
0	26	0	11.1449	52.0326	53.264	-2.327	-1.602	-21.8544	0.8210
0	28	0	51.967	43.151	-43.659	-2.501	-0.117	-17.1449	0.9981
0	30	0	44.086	11.512	-11.143	-1.970	0.935	8.7221	0.9541
0	32	0	12.444	14.512	-4.509	0.841	1.278	8.7221	0.9731
0	34	0	47.917	50.873	-54.689	-0.181	-0.278	-0.3856	0.9984
0	36	0	47.917	71.704	-80.468	-0.728	-2.957	-49.9570	0.8652
0	38	0	63.7226	0.0000	-0.000	4.844	-7.979	-13.8448	0.7912
0	40	0	21.168	22.934	23.135	0.000	1.127	2.4514	1.0000
0	42	0	21.300	118.908	141.553	0.479	-1.634	-23.1703	0.9823
0	44	0	115.315	38.965	39.497	3.653	-3.393	-45.4932	0.7062
0	46	0	37.289	8.554	-8.512	1.929	1.151	-19.9151	0.9709
0	48	0	8.710	44.793	45.256	0.891	0.156	1.2151	0.9938
0	50	0	44.291	6.276	6.273	-0.233	-0.502	-4.7524	0.9732
0	52	0	6.642	45.035	45.447	0.544	0.279	1.5877	0.9995
0	54	0	47.829	8.244	-8.217	-0.766	2.019	2.0234	0.9760
0	56	0	8.264	0.000	0.000	0.000	0.000	0.9979	1.0000
0	58	0	1.258	71.691	76.418	2.099	-5.293	-7.9996	0.8794
0	60	0	66.398	62.273	-69.610	-0.009	1.248	-5.0484	0.9144
0	62	0	6.684	6.946	-6.561	-2.289	-4.331	-15.5839	0.9992
0	64	0	33.951	35.448	-35.681	-2.774	-1.497	-15.5839	0.9827
0	66	0	42.481	4.138	43.377	-0.015	-0.831	-7.9665	0.9773
0	68	0	4.138	9.945	9.946	0.308	0.641	4.0162	0.9999
0	70	0	10.586	9.828	181.981	0.308	0.641	4.0162	0.9989
0	72	0	136.168	19.748	19.832	0.262	0.641	-3.4225	0.6241
0	74	0	19.489	0.000	-0.000	0.000	0.000	-3.4225	0.9915
0	76	0	47.203	50.354	-0.000	0.872	0.714	0.7036	1.0000
0	78	0	26.241	27.465	-2.334	0.793	-3.054	-4.1515	0.9923
0	80	0	26.241	47.403	27.583	2.099	-0.054	-0.1929	0.9999
0	82	0	45.800	17.870	17.885	2.762	-1.260	-13.3518	0.9894
0	84	0	17.457	28.483	28.430	0.391	-0.413	-9.5751	0.9727
0	86	0	28.219	26.694	-26.848	0.173	-0.418	-9.5751	0.9964
0	88	0	25.219	28.072	-28.000	0.691	-1.475	-18.3293	0.9879
0	90	0	1.773	28.072	-28.183	-0.792	-1.729	-13.8612	1.0000
0	92	0	26.943	52.464	57.219	-2.422	-3.596	-42.0623	0.9882
0	94	0	12.434	13.823	-13.693	-2.004	-1.537	-12.9812	0.9581
0	96	0	42.634	44.171	-44.588	-2.337	-1.537	-15.3545	0.9787
0	98	0	29.258	29.200	-29.283	1.637	0.059	0.5331	0.9912
0	100	0	12.739	12.360	-12.341	0.833	0.379	2.6382	0.9985

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STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
0	0	6	40.185	39.495	-39.913	-0.641	0.690	7.8526	0.9789
0	0	6	48.888	50.602	31.328	4.156	-1.734	-20.4083	0.9656
0	0	6	1.0777	22.000	-0.000	-0.000	-1.099	1.4490	1.0000
0	2	6	21.777	22.376	-22.441	0.443	-0.599	-6.6028	0.9938
0	3	6	62.115	65.264	66.808	3.099	-3.144	-34.7927	0.9523
0	4	6	26.443	27.038	27.092	0.669	-0.495	-6.0089	0.9922
0	6	6	26.109	26.035	25.983	0.791	0.074	0.0775	1.0000
0	10	6	3.894	0.451	-3.397	2.672	0.074	0.6224	0.9934
0	12	6	1.4774	0.000	-3.000	0.612	0.442	2.4791	0.9999
0	23	6	4.4774	4.000	0.109	1.771	0.612	2.5652	0.0000
0	34	6	4.253	4.878	-35.035	1.771	0.612	-0.5862	1.0000
0	40	6	5.281	34.864	-19.463	1.961	0.612	-2.3454	0.9878
0	48	6	5.733	19.427	-30.501	1.769	0.417	-2.3454	0.9998
0	59	6	19.453	30.420	-19.381	-1.769	0.033	2.6837	0.9965
0	72	6	14.651	68.930	70.417	1.412	0.033	8.8672	0.9914
0	88	6	14.273	13.321	13.000	0.000	0.785	3.8188	0.9549
0	102	6	0.785	31.000	1.000	1.255	0.000	0.6611	0.9983
0	122	6	0.461	31.129	3.119	0.609	0.204	3.3311	1.0000
0	140	6	0.993	19.789	-9.774	0.080	0.092	1.3156	0.9909
0	158	6	19.662	18.570	-18.522	0.541	0.092	9.3156	0.9969
0	176	6	34.727	32.955	-3.974	2.217	0.929	1.7118	0.9980
0	194	6	10.914	29.984	-14.909	1.326	1.771	14.2117	0.9903
0	212	6	31.624	29.953	-29.954	0.882	0.611	17.7518	0.9984
0	230	6	31.624	14.691	-27.754	1.441	1.933	17.0204	0.9980
0	248	6	16.572	24.298	-24.298	0.448	1.383	11.9380	0.9950
0	266	6	28.278	17.998	-18.721	3.043	1.489	13.3691	0.9928
0	284	6	32.212	26.965	-27.729	0.203	1.186	15.1025	0.9708
0	302	6	19.186	16.548	-12.869	3.139	1.794	11.8445	0.9458
0	320	6	112.760	97.620	-97.620	0.139	1.186	5.0942	0.5749
0	338	6	112.760	30.911	-87.458	0.139	0.534	16.2268	0.8654
0	356	6	61.065	16.548	-11.458	0.117	0.003	5.2233	0.9659
0	374	6	31.445	98.391	11.122	4.089	0.003	2.0942	0.7825
0	392	6	101.044	97.449	-11.122	0.895	0.649	2.0942	0.9988
0	410	6	13.314	13.391	-13.400	0.274	0.184	0.5412	0.9965
0	428	6	43.497	43.566	-8.570	0.633	0.034	0.5412	0.9987
0	446	6	5.150	4.089	-4.089	0.180	0.450	-0.1432	0.0000
0	464	6	15.819	2.827	-2.816	0.078	0.017	-0.1432	0.9985
0	482	6	15.819	16.227	-16.304	0.236	0.544	2.0942	0.9987
0	500	6	38.926	37.221	-37.221	0.201	1.706	7.2327	0.9965
0	518	6	25.144	25.012	-25.012	0.042	0.105	0.8153	0.9999
0	536	6	56.587	54.130	-60.936	0.089	0.089	0.3963	0.9888
0	554	6	17.935	16.777	-16.033	0.235	1.157	2.8344	0.8088
0	572	6	87.840	79.116	-93.433	0.621	1.815	16.8344	0.9812
0	590	6	38.409	37.191	-38.389	0.235	0.913	12.5495	0.9999
0	608	6	7.771	9.540	-9.540	0.801	0.763	6.5744	0.9982
0	626	6	10.341	7.856	-7.856	0.428	0.801	1.7400	0.9977
0	644	6	11.172	11.101	-11.113	0.189	0.071	-1.7964	0.9987
0	662	6						0.6022	0.9976

H	K	L	F(UBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	10	1	8.661	8.465	8.470	-0.003	0.196	1.4006	0.9988
1	11	1	12.427	12.141	-12.105	-1.098	0.286	2.2632	0.9977
1	12	1	1.797	1.924	-10.912	-0.152	0.872	1.5785	1.0000
1	13	1	39.411	37.695	38.011	1.791	0.872	1.6937	0.9807
1	14	1	17.585	16.162	-16.327	-0.202	0.423	2.1898	0.9993
1	15	1	17.527	16.407	-1.189	-0.073	1.120	1.8540	0.9965
1	16	1	2.280	1.312	110.172	3.107	0.722	1.0335	1.0000
1	1	2	92.035	43.045	-45.012	0.125	0.125	11.0335	0.9145
1	2	3	48.145	28.033	28.755	0.798	2.152	29.0772	0.9145
1	3	4	30.451	68.586	73.315	0.068	0.598	29.7178	0.9677
1	4	5	1.806	6.945	-6.948	-0.129	0.270	7.0710	0.9999
1	5	6	6.476	20.265	-20.352	-0.129	0.270	7.0710	0.9999
1	6	7	19.458	27.769	-27.975	-0.339	0.807	16.7967	0.9988
1	7	8	26.228	84.470	89.887	0.629	1.540	18.9466	0.9952
1	8	9	10.638	11.601	-89.887	-0.048	0.131	1.4186	0.8835
1	9	0	12.293	11.214	12.227	0.058	0.301	2.5718	0.9980
1	0	1	6.562	12.654	16.669	0.180	0.580	4.3718	0.9976
1	1	2	38.006	37.711	-37.938	-0.053	0.245	1.3551	0.9994
1	2	3	3.479	2.427	-1.441	0.048	0.059	0.0801	0.9817
1	3	4	5.086	2.341	2.241	0.069	0.073	0.0801	1.0000
1	4	5	6.613	6.627	6.662	0.008	0.025	1.8741	0.9999
1	5	6	14.245	13.667	-13.364	-0.112	0.618	11.343	0.9995
1	6	7	27.041	50.965	52.668	0.008	0.252	18.4005	0.9995
1	7	8	69.524	26.650	-52.968	-2.568	0.618	13.4005	0.9946
1	8	9	12.641	68.938	-74.967	-0.112	0.252	8.3411	0.9765
1	9	0	26.082	127.237	127.403	0.275	0.874	113.3411	0.9236
1	0	1	13.178	15.822	-15.862	-0.190	0.404	8.3874	0.8665
1	1	2	11.403	13.537	-13.551	-0.054	0.355	4.5469	0.9826
1	2	3	11.222	12.211	-12.225	-0.083	0.489	10.7470	0.9967
1	3	4	11.544	10.019	9.947	0.038	0.501	4.3331	1.0000
1	4	5	19.381	10.019	10.722	0.125	1.525	0.7663	0.9977
1	5	6	17.752	14.351	-14.480	-0.180	0.143	1.2276	0.9987
1	6	7	14.614	17.258	-17.479	-0.179	0.143	1.2276	0.9987
1	7	8	14.280	14.351	-14.355	-0.098	0.071	0.8301	0.9998
1	8	9	74.216	76.023	-80.982	-0.544	0.764	6.1047	0.9955
1	9	0	20.226	21.792	-21.899	-0.111	1.565	2.2079	0.9988
1	0	1	24.416	25.118	-25.683	-0.266	0.702	3.2271	0.9982
1	1	2	76.412	79.575	-83.341	-0.530	1.819	10.6142	0.9882
1	2	3	11.686	12.297	-12.297	-0.061	0.401	2.2262	0.9990
1	3	4	11.446	12.508	-12.505	-0.063	0.611	3.2534	0.9980
1	4	5	34.910	35.873	-35.145	-0.132	0.963	10.8927	0.9999
1	5	6	4.498	3.088	-3.076	0.068	0.650	1.5477	1.0000
1	6	7	4.091	3.088	-3.076	0.022	1.007	3.9981	0.9999

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	15	4	9.996	10.091	-10.095	-0.112	-0.095	-0.6164	0.9989
1	14	4	31.291	31.202	-31.293	2.116	-0.088	-0.7031	0.9897
1	15	4	24.868	26.245	-26.391	0.061	-1.088	-17.0161	0.9889
1	1	4	28.728	28.166	-28.281	-2.332	0.122	1.4310	0.9852
1	2	4	57.632	52.622	-22.014	-0.198	0.122	0.4309	0.9999
1	3	4	10.260	11.081	56.363	-2.336	-0.387	-16.4348	0.9512
1	4	4	23.729	23.503	11.089	-1.022	-0.820	-2.5319	0.9981
1	5	4	11.424	11.742	-32.559	-0.336	-0.226	-3.0528	0.9921
1	6	4	7.645	7.440	-11.753	-0.020	0.317	-0.9846	0.9997
1	7	4	7.400	6.688	-7.414	-0.487	0.170	-0.9846	0.9993
1	8	4	6.400	6.374	-6.371	0.257	-0.233	-1.7322	0.9997
1	9	4	10.476	10.804	-10.811	0.023	0.325	-0.1645	0.9995
1	10	4	9.912	9.929	-9.255	-0.877	-0.270	-2.5555	0.9981
1	11	4	4.912	5.312	-5.317	-0.148	-0.478	-1.8951	0.9997
1	12	4	31.605	31.126	31.223	0.877	0.478	-4.0899	0.9997
1	13	4	6.975	6.548	6.546	1.878	0.478	2.3422	0.9992
1	14	4	56.946	56.870	58.107	0.192	0.427	0.8688	0.9996
1	1	4	3.018	10.487	-10.818	0.137	0.195	0.5872	0.9559
1	2	4	10.523	10.487	-10.442	0.688	0.036	0.8688	0.9999
1	3	4	6.620	39.557	10.544	0.137	0.079	0.3391	0.9986
1	4	4	8.029	39.557	39.786	0.080	0.036	0.5872	0.9995
1	5	4	10.344	10.944	-39.087	-0.435	-0.079	-1.7863	0.9995
1	6	4	8.294	8.776	-5.087	0.106	-0.058	-5.4060	0.9997
1	7	4	54.199	55.253	-19.944	-0.435	-0.601	-3.6804	0.9997
1	8	4	3.581	8.803	8.805	0.266	0.482	-3.5270	0.9992
1	9	4	3.056	1.551	1.545	0.956	-0.054	7.9385	0.9992
1	10	4	29.001	28.751	3.009	-0.019	0.178	1.2300	0.9992
1	11	4	6.027	6.109	-28.747	-0.049	0.047	0.1509	0.9995
1	12	4	24.671	24.144	24.109	-2.627	0.250	4.1509	0.9920
1	13	4	13.218	13.330	13.341	-1.122	0.526	-5.4912	0.9996
1	14	4	37.816	37.608	-37.846	0.203	0.112	1.0750	0.9980
1	1	4	35.595	15.495	5.495	-2.003	-0.112	-2.0633	0.9984
1	2	4	14.360	14.144	-14.168	-0.140	0.438	3.3472	0.9992
1	3	4	11.296	11.057	-11.058	0.017	0.109	-3.3538	0.9999
1	4	4	1.280	0.346	0.346	-0.016	0.438	1.3353	0.9992
1	5	4	8.408	8.278	8.281	0.016	0.130	1.0894	0.9994
1	6	4	3.209	3.199	3.199	0.051	0.017	0.8948	0.9999
1	7	4	7.507	7.337	7.337	0.033	0.017	0.0360	0.9999
1	8	4	7.710	7.921	-8.924	0.106	0.444	1.2937	0.9993
1	9	4	4.763	4.070	-4.401	0.123	0.270	1.9327	0.9995
1	10	4	38.326	36.991	37.024	-0.109	0.693	3.8419	0.9998
1	11	4	14.219	14.005	14.016	-0.059	0.335	3.8419	0.9870
1	12	4	14.671	14.005	14.016	-0.059	0.335	3.8419	0.9992
1	13	4	3.686	3.633	4.032	-0.068	0.053	5.8304	0.9999
1	14	4	9.367	9.084	-8.084	0.244	0.323	2.4773	0.9806
1	1	4	9.077	9.476	-8.084	0.445	0.284	12.0660	0.9992
1	2	4	3.609	3.656	-3.654	-0.121	0.604	4.2310	0.9993

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	0	9	10.423	10.313	-10.318	0.058	0.110	0.8968	0.9991
1	1	9	15.956	13.954	-13.858	-0.143	1.030	0.9141	0.9982
1	2	9	22.114	27.084	27.713	-0.149	0.079	0.0719	0.9980
1	3	9	29.596	5.054	5.051	0.181	0.917	17.6410	0.9933
1	4	9	5.270	1.316	-11.281	-0.019	0.216	1.1174	0.9998
1	5	9	12.710	1.311	-14.332	0.003	0.889	7.0416	0.9998
1	6	9	4.700	1.058	-1.242	0.421	0.179	0.8829	0.9998
1	7	9	2.200	4.038	42.054	0.567	0.889	0.8829	0.0000
1	8	9	69.585	40.546	42.054	0.567	0.889	0.8829	0.7831
1	9	9	43.805	14.885	14.951	-0.154	0.039	2.2531	0.9294
1	0	0	14.999	14.684	11.512	0.154	3.421	0.3989	0.0000
1	1	0	103.799	17.181	11.971	0.154	3.421	0.3989	0.9910
1	2	0	8.881	1.811	-1.971	0.254	0.627	4.5768	0.9999
1	3	0	2.806	17.992	1.971	0.254	0.627	4.5768	0.9999
1	4	0	18.809	53.803	-18.061	-0.279	0.080	1.4684	0.9921
1	5	0	56.865	15.704	-15.740	-0.156	0.080	1.4684	0.9990
1	6	0	15.783	62.702	64.898	2.080	2.347	22.1524	0.9353
1	7	0	65.142	2.452	1.689	0.211	0.684	15.6355	0.9344
1	8	0	5.466	13.944	13.959	0.067	3.014	9.5154	0.9999
1	9	0	14.689	41.454	41.779	0.338	0.719	3.7077	0.9999
1	1	1	11.561	11.141	11.143	0.067	0.422	12.9957	0.9773
1	2	1	33.183	33.088	-33.846	-0.338	0.930	-1.0630	0.9984
1	3	1	32.547	20.269	20.194	0.067	0.422	12.9957	0.9952
1	4	1	62.877	59.003	-62.443	-0.197	1.608	4.3702	0.9852
1	5	1	30.512	38.920	-39.368	-0.539	1.608	4.3702	0.9852
1	6	1	40.838	4.946	-4.759	0.290	0.536	6.1898	0.9607
1	7	1	4.946	38.675	-39.675	-0.290	0.536	6.1898	0.9607
1	8	1	40.773	30.916	-39.225	-0.290	0.536	6.1898	0.9994
1	9	1	32.298	17.089	31.079	0.383	0.741	20.8505	0.9839
1	0	1	17.769	25.311	-17.121	-0.340	0.680	12.5646	0.9839
1	1	1	25.704	15.440	-22.491	-0.209	0.397	3.1453	0.9935
1	2	1	3.037	16.891	-16.891	-0.209	0.397	3.1453	0.9999
1	3	1	9.860	18.901	-8.905	0.037	0.989	13.1888	0.9970
1	4	1	3.794	18.597	-2.585	0.043	0.989	13.1888	0.9970
1	5	1	17.434	12.406	-19.585	-0.153	0.204	3.4400	0.9999
1	6	1	11.542	11.403	-12.426	0.524	0.342	20.6339	0.9982
1	7	1	33.352	12.168	-14.000	-0.822	0.920	-10.8619	0.9952
1	8	1	12.151	32.288	-32.751	-0.455	0.137	10.0317	0.9917
1	9	1	59.061	48.061	-49.308	0.455	0.137	10.0317	0.9962
1	0	2	29.602	29.169	-29.434	0.304	0.434	24.5123	0.9499
1	1	2	31.160	17.613	-30.132	0.182	0.000	12.0116	0.9832
1	2	2	14.555	13.737	-13.721	0.000	0.224	0.3703	0.9947
1	3	2	11.326	11.177	-11.185	0.231	0.149	6.6197	0.9970

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
N	3	6	9.126	9.076	-9.080	0.129	0.050	0.4160	0.9990
N	4	6	13.626	13.102	13.110	0.386	0.524	4.8647	0.9980
N	5	6	2.705	2.944	-4.094	-0.229	-0.236	-0.8225	0.9999
N	6	6	41.016	40.653	40.943	2.889	0.363	3.6285	0.9819
N	7	6	15.004	14.885	14.885	0.253	0.135	1.1394	0.9917
N	8	6	17.348	16.851	16.799	1.610	0.496	1.4337	0.9971
N	9	6	11.028	10.859	10.864	0.170	0.169	1.4423	0.9988
N	10	6	5.842	5.029	4.956	0.857	0.813	1.4423	0.9987
N	11	6	5.083	5.765	-4.762	-0.185	0.319	1.5199	0.9998
N	12	6	26.135	25.363	-25.307	0.334	0.772	1.6349	0.9997
N	13	6	10.266	6.936	-6.937	0.068	0.330	1.6794	0.9995
N	14	6	10.154	9.844	-6.846	-0.045	0.313	1.7945	0.9995
N	15	6	7.143	6.684	-5.130	-0.618	0.459	1.8343	0.9997
N	16	7	5.113	5.113	-5.130	0.120	0.418	2.0880	0.9995
N	17	7	19.103	18.866	-18.832	0.471	0.237	2.1081	0.9997
N	18	7	18.275	17.758	-17.779	0.821	0.517	2.2113	0.9964
N	19	7	21.146	20.891	-20.855	0.474	0.255	2.3226	0.9958
N	20	7	6.403	6.277	-6.275	-0.174	0.127	2.3228	0.9996
N	21	7	32.309	31.447	-31.532	2.049	0.036	2.7654	0.9996
N	22	7	4.342	4.306	-4.300	-0.048	0.033	2.7922	0.9998
N	23	7	22.910	22.581	-22.570	1.698	0.249	2.7440	0.9998
N	24	7	8.388	8.142	-8.137	0.361	0.224	2.7407	0.9953
N	25	7	52.194	49.495	-49.904	0.884	0.663	2.5139	0.9978
N	26	8	8.651	7.980	-7.980	0.397	0.105	2.2296	0.9994
N	27	8	4.432	4.270	-4.269	-0.106	0.166	2.3488	0.9996
N	28	8	6.882	6.226	-6.203	0.040	0.156	1.7426	0.9999
N	29	8	3.069	3.220	3.203	0.209	0.631	1.8780	0.9999
N	30	8	4.106	3.473	-3.467	0.209	0.129	1.8717	0.9987
N	31	8	13.023	11.894	-11.878	0.740	0.188	1.9071	0.9988
N	32	8	12.637	11.736	-11.763	0.219	0.442	2.0717	0.9987
N	33	8	21.736	20.993	-20.970	1.650	0.744	2.8259	0.9988
N	34	8	8.136	7.724	-7.746	0.146	0.419	2.5472	0.9995
N	35	8	11.590	10.744	-10.746	0.639	0.844	2.8622	0.9990
N	36	9	9.090	8.258	-8.258	0.000	0.000	2.0222	0.9994
N	37	9	1.963	1.557	-1.542	0.415	0.414	1.0144	1.0000
N	38	9	23.506	22.057	-22.066	1.267	0.450	1.2725	0.9998
N	39	9	17.029	15.263	-15.260	0.328	0.028	1.7451	0.9992
N	40	9	17.029	15.455	-15.511	1.744	1.181	1.3116	0.9980
N	41	9	54.051	32.324	-32.810	1.773	0.473	1.4062	0.9227
N	42	9	69.517	65.685	-69.748	3.674	0.000	1.1170	0.9705
N	43	9	44.544	44.049	-45.137	0.180	0.496	1.1170	0.8845
N	44	9	18.618	17.914	-17.917	0.000	0.706	3.9448	0.9523
N	45	9	5.306	6.213	-6.199	0.443	0.906	3.9448	0.9928
N	46	9	83.083	80.329	-85.105	0.523	0.706	3.2101	0.9992
N	47	9	45.913	45.474	-46.262	0.857	0.439	2.0832	0.8884
N	48	9	19.045	19.300	-19.350	-0.446	0.255	1.5841	0.9943
N	49	9	6.581	6.300	-6.285	0.465	0.281	1.5841	0.9943
N	50	9	45.046	44.469	-44.908	3.689	0.000	3.6065	0.9740
N	51	9	11.016	10.254	-10.259	0.293	0.000	3.5793	0.9987
N	52	9	6.464	7.252	-7.253	0.394	0.000	4.1223	0.9985
N	53	9	8.496	7.252	-7.253	0.394	0.000	4.1223	0.9994
N	54	9	19.964	19.527	-19.466	2.009	1.437	2.1175	0.9957

H	K	L	F(DBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	0	1	13.766	14.028	-14.061	0.374	-0.263	-2.8157	0.9947
3	1	1	50.467	50.245	-51.945	-2.556	0.222	-2.7397	0.9333
3	2	1	21.726	21.493	-21.619	-0.663	0.233	2.5781	0.9874
3	3	1	57.577	55.125	-57.474	2.066	2.446	27.6419	0.9185
3	4	1	38.377	37.397	-38.043	0.665	0.980	10.7639	0.9660
3	5	1	16.745	16.449	-16.435	-1.446	0.297	2.7053	0.9940
3	6	1	29.564	29.204	-29.454	0.001	0.361	3.3705	0.9831
3	7	1	8.149	7.980	-7.964	0.578	0.168	1.1670	0.9995
3	8	1	5.853	5.852	-5.547	0.026	0.341	1.1676	0.9995
3	9	1	27.458	27.372	-27.835	0.311	0.601	2.1148	0.9995
3	10	1	11.831	11.640	-11.602	-0.090	0.216	1.8874	0.9894
3	11	1	19.897	19.393	-19.434	-0.466	0.191	1.3254	0.9982
3	12	1	19.817	19.552	-19.525	0.691	0.504	1.9446	0.9953
3	13	1	9.716	9.166	-9.156	0.512	0.264	1.9467	0.9954
3	14	1	22.032	21.365	-21.343	-1.819	0.667	4.1456	0.9994
3	15	1	60.965	62.228	-62.138	0.522	-0.377	-1.1224	0.9143
3	16	1	59.457	60.222	-62.847	0.802	-0.406	-0.9346	0.9183
3	17	1	14.847	14.442	-14.978	0.222	0.405	0.9232	0.9060
3	18	1	14.539	14.945	-14.881	0.150	0.652	0.9207	0.9953
3	19	1	72.037	71.259	-74.881	4.128	0.357	7.2075	0.9928
3	20	1	1.617	3.144	1.131	-0.318	0.822	0.7172	1.0000
3	21	1	3.971	3.393	-3.184	-0.428	0.357	0.7172	0.9998
3	22	1	22.206	22.377	-22.465	-0.780	-0.187	-1.7514	0.9994
3	23	1	59.437	59.720	-61.097	0.425	-0.223	-2.7271	0.9509
3	24	1	8.416	8.998	-8.000	-0.422	-0.079	-2.4224	0.9997
3	25	1	5.619	5.083	5.079	-0.110	0.535	2.4224	0.9997
3	26	1	19.051	40.095	40.618	2.891	-0.294	-2.4014	0.9916
3	27	1	4.431	19.451	19.128	0.439	0.310	2.2635	0.9960
3	28	1	28.687	29.504	30.014	0.790	0.922	3.8247	0.9998
3	29	1	31.422	32.738	32.738	0.288	-1.079	-1.4212	0.9834
3	30	1	11.955	12.316	-12.317	0.663	-0.082	-1.2421	0.9803
3	31	1	47.396	47.452	-48.431	-2.142	-0.362	-3.5050	0.9971
3	32	1	38.363	39.387	-39.918	-0.618	-0.024	-0.6130	0.9581
3	33	1	24.180	24.985	-25.069	1.469	-0.804	-1.2471	0.9899
3	34	1	11.214	11.532	-13.171	0.469	-0.024	-8.3770	0.9899
3	35	1	11.684	12.412	-12.416	0.496	-0.728	-6.1242	0.9978
3	36	1	22.550	22.132	-22.132	0.001	0.118	-0.2982	0.9999
3	37	1	19.038	19.621	-19.612	-0.211	0.931	3.5954	0.9999
3	38	1	17.602	17.783	-17.780	0.101	0.217	1.8775	0.9956
3	39	1	3.032	3.255	-3.297	-0.137	-0.144	-1.5101	0.9935
3	40	1	20.466	20.613	-20.689	0.500	-0.183	-1.2124	0.9935
3	41	1	29.134	29.176	-29.168	-1.527	0.316	-0.6333	0.9991
3	42	1	33.809	34.523	-34.878	0.659	-0.785	-1.9415	0.9991
3	43	1	25.068	25.644	-26.826	-3.411	-0.945	-1.0111	0.9816
3	44	1	56.660	55.505	-56.647	0.178	-0.504	-5.5219	0.9857
3	45	1	11.447	11.382	-11.391	-0.165	-0.846	-8.8793	0.9893
3	46	1	3.418	3.376	-3.352	-0.405	0.042	0.5761	0.9982
3	47	1	60.591	62.310	-63.684	4.177	-1.719	-17.6023	0.9992

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H	K	L	F(0BS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	8	4	31.376	31.993	32.175	0.781	-0.617	-6.0089	0.9881
3	9	4	11.677	12.058	-12.101	-0.417	-0.422	-3.3372	0.9984
3	10	4	2.367	36.444	-2.412	-0.418	-0.081	-0.2021	0.9999
3	11	4	35.742	36.628	36.726	3.411	-0.086	-7.8247	0.9862
3	12	4	7.564	37.470	-7.469	0.215	0.094	0.5381	0.9994
3	13	4	4.913	3.969	-3.448	0.274	0.213	0.8017	0.9998
3	14	4	8.191	1.845	-8.448	-0.373	0.460	3.7224	0.9993
3	1	5	2.744	37.815	-1.806	-2.270	0.786	-8.6505	1.0007
3	2	5	37.029	17.573	-38.099	0.388	0.260	-2.6440	0.9817
3	3	5	36.833	13.423	-17.599	-0.562	0.409	4.2472	0.9819
3	4	5	36.833	21.090	21.138	2.041	0.308	-0.9815	0.9994
3	5	5	21.045	27.677	-21.547	-0.614	-0.345	-1.9665	0.9996
3	6	5	26.744	27.198	27.312	-1.213	0.307	-1.9665	0.9996
3	7	5	3.037	22.573	-2.509	0.057	-0.457	-4.5225	0.9919
3	8	5	2.172	22.298	-2.268	0.049	-0.109	-0.5634	0.9997
3	9	5	2.574	23.296	-2.423	0.358	-0.277	-0.7781	0.9999
3	10	5	3.834	23.366	-2.423	0.064	-0.527	-0.5634	0.9999
3	11	5	10.991	10.106	-10.422	-0.827	-0.169	-0.6325	0.9998
3	12	5	14.698	14.486	-14.077	-0.370	-0.456	-1.1590	0.9990
3	13	5	34.750	134.294	-14.413	1.393	0.417	1.5752	0.9869
3	14	5	8.801	22.859	34.438	4.227	0.712	0.5894	0.9911
3	1	6	15.254	8.188	15.207	0.168	-0.074	0.4414	0.9992
3	2	6	2.924	43.192	43.672	1.443	-0.468	-0.8774	0.9992
3	3	6	2.554	2.525	-1.480	-3.567	-0.235	-3.1481	0.9807
3	4	6	2.643	20.361	-20.390	0.267	-0.120	3.3715	0.9807
3	5	6	2.630	46.220	-46.538	-0.684	-0.269	-0.5856	0.9961
3	6	6	4.950	4.408	-4.385	0.379	0.012	0.5202	0.9800
3	7	6	4.936	4.282	-4.279	-0.188	0.065	0.1856	0.9998
3	8	6	17.862	18.960	18.992	0.190	0.090	0.9711	0.9998
3	9	6	17.505	17.041	-16.947	2.007	0.464	0.3061	0.9975
3	10	6	6.851	6.722	6.706	-1.573	0.122	0.8061	0.9930
3	11	6	27.432	26.506	-26.603	-1.725	0.000	0.1785	0.9947
3	12	6	23.972	23.091	-23.154	-0.481	0.087	0.4422	0.9973
3	13	6	15.593	17.051	-17.057	1.256	0.000	0.9425	0.9940
3	14	6	8.062	11.857	-4.857	0.088	0.000	0.1022	0.9994
3	1	7	8.299	1.122	-1.129	-0.346	0.000	0.0000	0.9994
3	2	7	2.154	1.423	-1.419	0.028	0.163	0.0000	0.9994
3	3	7	1.103	10.625	-10.630	-0.107	0.732	0.4778	1.0000
3	4	7	1.609	15.814	-15.485	0.312	0.000	0.0000	0.9990
3	5	7	3.586	11.264	-11.859	-0.378	0.104	0.5639	0.9956
3	6	7	5.076	4.148	-4.146	0.159	0.198	0.4610	0.9881
3	7	7	0.387	1.399	-1.365	-0.310	0.928	0.9957	0.9999
3	8	7	0.507	34.944	-13.972	0.329	-0.012	0.4489	0.9899
3	9	7	1.175	13.997	13.093	0.201	0.078	0.8256	0.9886
3	10	7	2.957	0.779	-0.713	0.313	-1.178	-0.0390	1.0000

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H	K	L	FI(OBS)	FI(CALC)	AI(CALC)	BI(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	1	9	21.109	19.511	-19.468	-1.703	1.598	13.886	0.996
3	2	9	9.016	8.137	-8.137	-0.396	0.876	6.151	0.999
3	3	9	21.630	19.874	-19.874	-1.568	1.754	15.083	0.996
3	4	9	11.584	11.402	-11.398	-0.497	1.181	9.159	0.998
4	1	0	100.033	100.513	111.678	4.693	-0.480	-3.694	0.808
4	2	0	15.228	15.631	15.631	-0.410	-0.331	-2.168	0.994
4	3	0	15.382	14.431	14.997	-0.415	-0.412	-2.323	0.999
4	4	0	63.745	60.013	62.128	-0.415	-0.412	-2.323	0.999
4	5	0	28.632	28.843	29.050	0.210	0.211	1.421	0.989
4	6	0	22.922	22.561	-22.643	-0.403	-0.306	-1.055	0.989
4	7	0	22.254	23.912	-22.922	-0.403	-0.306	-1.055	0.989
4	8	0	23.700	23.266	-23.380	-0.244	-0.237	-1.178	0.992
4	9	0	12.136	12.809	-13.387	-0.412	-0.327	-1.178	0.992
4	10	0	14.840	15.098	15.113	0.269	0.251	1.347	0.997
4	11	0	8.991	8.670	8.669	-0.321	-0.321	-1.347	0.997
4	12	0	33.813	31.016	-33.183	-0.300	-0.379	-1.079	0.991
4	13	0	6.732	7.134	7.092	0.144	0.098	0.879	0.988
4	14	0	14.449	14.018	14.013	-0.050	-0.357	-0.523	0.990
4	1	1	22.085	21.422	-21.655	-0.961	0.431	-3.234	0.990
4	2	1	22.035	21.614	-21.372	-0.597	0.431	-3.234	0.990
4	3	1	31.748	31.326	-31.582	-0.839	0.422	-3.818	0.990
4	4	1	37.569	37.668	-38.041	-0.477	0.422	-3.792	0.990
4	5	1	28.534	28.319	-28.485	-0.162	0.156	-0.947	0.999
4	6	1	27.474	27.319	-27.449	-0.125	0.130	-0.947	0.999
4	7	1	29.026	29.466	29.509	0.275	0.309	1.915	0.999
4	8	1	23.413	23.447	23.509	0.054	0.030	0.816	0.999
4	9	1	18.452	18.299	-18.274	-0.481	-0.034	-0.710	0.999
4	10	1	5.122	5.123	-5.040	-0.927	-0.015	-0.324	0.999
4	11	1	1.707	1.384	-1.274	-0.481	-0.015	-0.324	0.999
4	12	1	5.572	5.123	-5.040	-0.927	-0.015	-0.324	0.999
4	13	1	36.662	37.788	-38.255	-0.188	0.177	-0.997	0.999
4	14	1	63.166	63.404	-65.564	-0.405	-0.123	-1.238	0.999
4	15	2	15.938	16.051	-16.083	-0.405	-0.113	-1.113	0.999
4	16	2	6.746	6.572	-6.551	-0.331	-0.117	-0.461	0.999
4	17	2	6.331	6.063	-5.853	-0.270	-0.067	-0.673	0.999
4	18	2	5.921	5.871	-5.728	-0.158	-0.049	-0.473	0.999
4	19	2	27.391	28.127	28.214	0.100	0.194	0.673	0.999
4	20	2	13.202	13.008	13.009	0.235	0.194	0.673	0.999
4	21	2	1.447	1.579	-1.409	-0.135	-0.267	-0.991	0.999
4	22	2	7.059	6.834	-6.830	-0.232	-0.381	-1.244	0.999
4	23	3	12.193	12.500	-12.515	-0.013	0.307	0.307	0.999
4	24	3	20.078	20.692	-20.739	-0.921	-0.622	-2.800	0.999
4	25	3	10.818	11.220	-11.212	-0.277	-0.393	-1.492	0.999
4	26	3	26.252	26.646	-26.742	-0.598	-0.393	-1.492	0.999
4	27	3	9.903	9.608	-9.695	-0.844	-0.705	-3.804	0.991
4	28	3	23.903	24.608	-24.695	-0.792	-0.705	-3.804	0.991

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STRUCTURE FACTORS

H	K	L	FIBS)	FICALC)	AICALC)	BICALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
4	6	3	30.396	31.325	-31.459	-1.986	-0.929	-8.9921	0.9875
4	7	3	6.913	7.267	-7.248	-0.559	-0.354	-2.2530	0.9994
4	8	3	20.017	20.496	20.423	-0.248	-0.477	-4.2350	0.9994
4	9	3	21.629	21.780	-21.683	0.582	-0.152	-0.2671	0.9952
4	10	3	22.418	22.235	-21.803	-0.865	-0.817	-6.8031	0.9952
4	11	3	19.404	19.672	-19.651	-0.750	-0.351	-2.8810	0.9947
4	12	3	19.666	19.165	-17.603	0.388	-0.606	-4.7048	0.9961
4	13	3	73.290	75.735	-78.532	0.445	-0.131	-0.2210	1.0000
4	14	4	17.313	17.552	-17.568	0.839	-0.444	-2.2144	0.9972
4	15	4	12.517	12.448	-12.448	0.380	-0.237	-2.3594	0.9959
4	16	4	12.517	15.331	-12.338	-0.078	0.277	1.4291	0.9998
4	17	4	17.303	18.441	-18.125	3.644	0.186	-6.3481	0.9980
4	18	4	16.795	16.071	-16.100	0.488	-0.644	-7.0070	0.9685
4	19	4	14.537	14.735	-14.949	1.044	-0.768	-3.4044	0.9968
4	20	4	14.436	14.935	-14.745	-0.360	-0.058	-3.4061	0.9976
4	21	4	20.187	20.779	-20.740	-0.889	-0.342	-3.0061	0.9955
4	22	4	22.502	22.242	-22.245	-0.222	-0.055	-0.3999	0.9989
4	23	4	5.447	5.270	-5.271	0.370	-0.322	-2.1301	0.9949
4	24	4	5.396	5.079	-5.284	0.265	-0.109	-0.4902	0.9997
4	25	4	3.488	3.158	-3.809	0.083	0.016	0.0139	1.0000
4	26	5	8.929	8.275	-8.269	0.861	0.330	1.4389	0.9999
4	27	5	3.022	3.158	-3.157	0.395	0.246	1.0222	0.9996
4	28	5	10.476	10.337	-10.327	0.709	-0.102	-0.7937	0.9982
4	29	5	24.487	24.445	-24.445	0.360	-0.442	-0.3449	0.9998
4	30	5	28.324	28.865	-28.923	1.057	-0.541	-0.3495	0.9937
4	31	5	24.166	24.659	-24.171	0.957	-0.010	-0.3445	0.9915
4	32	5	10.657	10.653	-10.653	0.709	0.038	0.0440	0.9915
4	33	5	26.027	27.741	-26.741	0.957	-0.086	-0.0145	0.9942
4	34	5	16.662	17.364	-17.364	0.416	-0.486	-4.3457	0.9936
4	35	5	12.831	12.712	-12.712	0.918	-0.528	-0.6389	0.9973
4	36	6	17.943	17.104	-17.104	0.773	-0.053	-1.1105	0.9985
4	37	6	45.592	44.826	-44.826	0.772	0.273	-1.4811	0.9997
4	38	6	10.227	9.828	-9.828	0.772	0.164	-1.5083	0.9967
4	39	6	4.833	4.579	-4.579	0.306	0.060	1.0278	0.9990
4	40	6	9.721	9.566	-9.566	0.419	0.254	1.4235	0.9998
4	41	6	33.857	33.396	-33.476	0.328	-0.058	-0.5218	0.9991
4	42	6	38.858	38.276	-38.276	0.541	0.058	1.2356	0.9996
4	43	6	21.011	21.276	-21.264	1.541	-0.161	-0.4401	0.9959
4	44	6	19.332	18.902	-18.902	0.982	0.033	-0.4384	0.9999
4	45	6	12.518	12.841	-12.813	0.022	-0.387	-1.8771	0.9996
4	46	7	18.518	18.119	-18.119	0.742	0.000	-2.3704	0.9994
4	47	7	14.429	14.992	-14.992	0.176	0.435	3.5578	0.9982
4	48	7	9.448	9.201	-9.201	0.349	0.000	0.5304	0.9970
4	49	7	14.915	14.717	-14.717	0.733	0.000	0.6029	0.9981
4	50	7	19.536	19.125	-19.091	0.569	0.491	1.6029	0.9968
4	51	7	16.222	16.016	-16.002	0.422	0.206	1.1489	0.9997
4	52	7	13.169	13.076	-12.946	1.905	0.093	0.7042	0.9985

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STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
4	0	8	42.197	39.869	40.006	3.399	2.328	21.0858	0.9841
4	1	8	16.181	15.174	15.175	0.0383	1.006	8.24337	0.9480
4	2	8	44.635	44.498	44.498	-0.137	0.0367	0.6197	0.9198
4	3	8	7.185	6.789	6.789	0.391	0.0391	2.3152	0.9196
4	4	8	35.259	35.254	35.254	-0.004	0.0004	17.3095	0.9900
4	5	8	5.344	27.456	15.571	1.0786	0.0786	0.4636	0.9998
4	6	8	16.320	21.811	15.839	0.494	0.0306	5.0910	0.9876
4	7	8	15.156	54.228	12.325	0.0533	0.0938	0.0108	0.9959
4	8	8	14.156	14.228	14.309	0.0407	0.0432	0.2590	0.9527
4	9	8	2.889	2.836	2.836	0.047	0.199	0.0877	0.9971
4	0	8	41.363	41.830	42.128	0.702	0.463	0.3964	0.9999
4	1	8	18.603	18.633	18.671	0.069	0.0326	0.1340	0.9778
4	2	8	19.943	15.633	18.671	0.110	0.0388	0.1620	0.9976
4	3	8	3.010	49.214	2.283	0.4495	0.204	0.0670	0.9960
4	4	8	9.040	2.472	4.744	0.445	0.369	0.1650	0.9997
4	5	8	3.511	3.152	3.172	0.348	0.231	0.0670	0.9999
4	6	8	4.883	4.042	4.042	0.846	0.318	0.0670	0.9999
4	7	8	17.041	16.990	17.006	0.001	0.028	1.0670	0.9999
4	8	8	16.836	15.064	15.058	0.793	0.501	0.8617	0.9954
4	9	8	28.430	28.044	28.044	0.386	0.051	0.2522	0.9991
4	0	8	15.534	15.044	15.044	0.491	0.055	3.8168	0.9964
4	1	8	2.334	2.334	2.334	0.000	0.000	0.8146	0.9889
4	2	8	11.811	11.906	11.906	0.095	0.095	0.8810	0.9971
4	3	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	4	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	5	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	6	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	7	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	8	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	9	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	0	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	1	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	2	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	3	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	4	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	5	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	6	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	7	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	8	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	9	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	0	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	1	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	2	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	3	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	4	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	5	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	6	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	7	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	8	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	9	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	0	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	1	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	2	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	3	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	4	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	5	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	6	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	7	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	8	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	9	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	0	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	1	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	2	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	3	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	4	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	5	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	6	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	7	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	8	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	9	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	0	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	1	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	2	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	3	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	4	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	5	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	6	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	7	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	8	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	9	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	0	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	1	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	2	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	3	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	4	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	5	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	6	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	7	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	8	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	9	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	0	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	1	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	2	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	3	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	4	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	5	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	6	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	7	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	8	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	9	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	0	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	1	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	2	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	3	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	4	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	5	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	6	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	7	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	8	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	9	8	11.527	10.922	10.922	0.605	0.267	0.7700	0.9971
4	0</								

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
6	1	1	11.5339	11.5000	11.5100	-0.0744	0.0400	0.2681	0.9982
6	2	1	29.7771	29.2633	29.4220	0.0970	0.5077	4.1110	0.9883
6	3	1	5.0695	6.1331	6.1099	-0.0532	-0.4436	-1.4840	0.9995
6	4	1	3.0774	4.2341	4.0688	-1.2014	0.0467	-2.4130	0.9997
6	5	1	15.3225	14.8946	14.9442	-0.8522	0.0379	0.2298	0.9973
6	6	1	11.9326	11.6493	11.7833	0.0887	0.0446	0.0298	0.9983
6	7	1	6.6663	6.4493	6.4333	-0.0449	0.1170	0.8311	0.9995
6	8	1	37.9883	37.8344	38.0788	-0.0449	0.1490	0.1582	0.9984
6	9	1	12.4400	12.4447	12.4288	-0.0447	0.0443	-0.3099	0.9983
6	10	1	12.2500	12.3937	12.2296	-0.1661	0.1473	-0.9049	0.9984
6	11	1	21.2283	22.1622	22.2229	-0.9345	0.0477	-0.1784	0.9939
6	12	1	6.9556	6.7223	6.8338	-0.0861	-0.0477	0.2632	0.9994
6	13	2	7.2287	8.0773	8.0440	-0.8170	-0.5976	-13.6566	0.9994
6	14	2	6.2280	5.2734	5.2200	-0.9599	-0.7871	-4.1988	0.9992
6	15	2	10.7010	10.7384	10.7224	-0.0394	-0.0333	-5.2643	0.9997
6	16	2	12.2655	12.6041	12.3865	-0.3380	-0.0336	-2.2127	0.9983
6	17	2	18.0180	18.6511	18.3715	-0.6396	-0.3227	-2.2730	0.9983
6	18	2	9.4115	9.1332	9.6134	0.1992	0.1833	-1.0912	0.9964
6	19	2	25.0116	24.7810	24.8258	-0.1177	0.2336	1.7874	0.9992
6	20	2	25.9416	24.5600	24.5528	-0.1555	0.3380	1.7167	0.9939
6	21	3	23.9468	24.3995	24.4462	-0.4976	0.6227	1.7196	0.9998
6	22	3	23.7688	24.3974	23.9882	-0.4086	0.3365	-1.1796	0.9998
6	23	3	13.6117	13.9744	13.9152	-0.1896	0.0220	-0.5187	0.9999
6	24	3	17.8961	17.9150	17.9232	-0.1896	0.0220	-0.9699	0.9999
6	25	3	10.6111	10.7770	10.6655	-0.1544	0.0153	-0.1518	0.9966
6	26	3	11.4452	11.7908	11.0207	-0.7772	0.0560	-0.9001	0.9988
6	27	3	36.4977	37.4408	37.6607	-0.9448	0.6511	-0.9901	0.9900
6	28	4	4.7777	5.2220	5.1550	-0.4476	0.9444	-0.3922	0.9865
6	29	4	22.8922	23.7699	23.3485	-0.8822	0.8770	-0.7622	0.9940
6	30	4	16.6572	16.3488	15.1622	-1.2866	0.6990	-0.4052	0.9997
6	31	4	5.5911	6.2222	6.1113	-0.6310	0.5223	-0.4513	0.9997
6	32	4	5.5955	6.1113	6.6669	-0.5716	0.5223	-0.4513	0.9997
6	33	4	48.3355	48.8774	49.1447	-0.8173	0.3144	-0.7019	0.9937
6	34	4	25.0069	25.5800	25.7336	-0.5231	0.1844	-0.9917	0.9963
6	35	4	18.9122	19.5982	19.9499	-1.0370	0.5870	-0.7019	0.9995
6	36	4	12.4483	12.5597	12.6007	-0.1524	0.0710	-0.1114	0.9963
6	37	5	23.9986	23.6334	23.6883	-0.3653	0.0710	-0.8419	0.9944
6	38	5	1.4426	0.6687	0.4229	-0.8152	0.3653	-0.9769	0.9944
6	39	5	4.8443	4.5077	4.3888	-0.3366	0.0338	-0.0625	0.9900
6	40	5	8.3881	8.6666	8.6442	-0.2888	0.3366	-0.5250	0.9900
6	41	5	10.0886	10.2732	10.6442	-0.5556	0.1334	-0.6659	0.9993
6	42	5	19.1888	19.4332	19.3997	-0.2444	0.0244	-0.5250	0.9992
6	43	5	10.0888	10.5499	10.5699	-0.4811	0.0878	-0.1772	0.9974
6	44	5	16.7000	16.3115	16.2883	-0.3885	0.0151	-0.1772	0.9990
6	45	5	10.5583	11.0315	10.9992	-0.4774	0.0268	-0.1155	0.9990
6	46	6	42.3346	41.7774	41.9992	-0.5556	0.0577	-0.7586	0.9997
6	47	6	6.4300	5.9320	5.8885	-0.4978	0.0366	-0.2157	0.9997
6	48	6	4.3300	3.9373	3.9228	-0.4072	0.0366	-0.4157	0.9999
6	49	6	39.1114	37.3433	37.6445	-1.7681	0.7714	-0.2157	0.9821
6	50	6	8.1180	8.4494	8.4490	-0.3389	0.3114	-0.7099	0.9991

**

H	K	L	FIBBS)	FICALC)	AICALC)	BICALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
7	3	0	23.911	23.770	23.706	2.688	0.141	0.6879	0.9926
7	4	0	6.023	4.595	4.539	0.717	1.429	4.3412	0.9997
7	5	0	2.135	1.814	-1.808	0.147	0.339	0.4251	1.0000
7	6	0	9.233	9.373	-9.332	-0.922	-0.133	0.5251	0.9990
7	7	0	33.886	34.220	34.275	1.889	0.133	-0.5251	0.9873
7	0	1	8.373	8.555	8.500	1.092	-0.193	-0.9669	0.9991
7	1	1	27.262	26.555	-26.609	-1.059	0.215	0.9669	0.9991
7	2	1	12.151	12.366	-12.340	0.972	-0.107	-1.0924	0.9911
7	3	1	9.205	9.587	9.505	1.460	0.381	0.2682	0.9988
7	4	1	11.555	11.479	11.460	0.788	-0.078	-1.9973	0.9988
7	5	1	6.009	5.570	-5.483	0.295	0.438	0.4687	0.9985
7	6	1	2.141	1.888	-1.890	0.428	0.043	1.8449	0.9996
7	7	1	14.876	14.572	14.442	0.588	0.221	1.6208	0.9996
7	0	2	15.340	15.578	15.470	0.585	-0.231	-0.5730	1.0000
7	1	2	7.672	8.278	8.273	0.385	0.606	0.0364	0.9972
7	2	2	4.093	4.418	4.268	0.840	1.674	5.4827	0.9999
7	3	2	5.804	6.321	6.265	0.696	1.006	4.2079	0.9998
7	4	2	8.545	8.937	8.790	1.293	0.573	4.2303	0.9998
7	5	2	12.131	12.331	12.340	0.153	0.392	2.2353	0.9992
7	6	2	17.848	17.874	17.879	0.976	0.290	1.2555	0.9985
7	7	2	11.891	12.374	12.818	1.007	0.520	1.4579	0.9994
7	0	3	9.671	9.366	-9.294	-1.007	-0.483	-3.0456	0.9965
7	1	3	12.427	12.511	-12.479	0.685	0.697	0.5412	0.9980
7	2	3	9.400	9.913	-9.894	1.217	-0.513	-3.0431	0.9990
7	3	3	13.739	14.886	14.824	1.480	0.084	0.5412	0.9990
7	4	3	29.864	30.728	30.727	0.575	-0.386	-2.9610	1.0000
7	5	4	6.861	7.286	7.279	1.358	0.422	3.9610	0.9906
7	6	4	23.862	24.365	24.310	0.303	-0.504	-3.7634	0.9939
7	7	4	4.966	5.025	3.970	0.663	0.938	3.8639	0.9998

* **

REFINE 108206 CYCLE 4

ALL REFLECTIONS

RESULTS OF STRUCTURE FACTOR CALCULATION

WEIGHTED R	UNWEIGHTED R	NUMERATOR	DENOMINATOR	NUMBER	R
156674.38	587.42	65553232.00	15283.48	773	0.049
				773	0.038

RANGES OF F(OBS)

6344.80	38585664.00	455	0.017
14001.61	15688674.00	185	0.030
17716.83	65298880.00	77	0.052
45511.65	2883324.00	34	0.126
8211.89	1102447.00	13	0.086
17267.14	339214.38	4	0.226
36589.86	339214.38	4	0.328
11050.32	84803.63	1	0.361

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

95609.88	3816164.00	45	0.158
31336.91	5512238.00	65	0.075
8449.83	7038701.00	83	0.035
5527.70	8310758.00	98	0.026
3398.41	8734776.00	103	0.020
3364.59	10261240.00	1121	0.018
3172.73	10346043.00	1122	0.018
5833.98	11533297.00	136	0.022

UNREJECTED REFLECTIONS

WEIGHTED R	UNWEIGHTED R				
156592.19	551.21	65553184.00	15211.66	723	0.049
				723	0.036

RANGES OF F(OBS)

6261.72	36720656.00	405	0.013
14001.61	16773635.00	185	0.029
17716.83	6981459.00	77	0.050
45511.65	3082722.00	34	0.122
8211.89	1178687.00	13	0.083
17267.14	362673.19	4	0.218
36589.86	362673.19	4	0.318
11050.32	90668.25	1	0.349

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

95595.63	3717400.00	41	0.160
31336.42	5802771.00	64	0.073
8431.53	6981459.00	77	0.035
5522.16	8522820.00	94	0.020
3385.17	8794824.00	97	0.020
3354.00	9973512.00	110	0.018
3168.22	10426854.00	115	0.017
5817.84	11333537.00	125	0.023

SUM FCAL 15119.30
STANDARD DEV OF UNIT WEIGHT OBS 15.14

R-FINE 108206 CYCLE - 4
 ESTIMATED STD. DEV. FOR OBS. OF UNIT WEIGHT
 EXTINGUISHION CORRECTION ISOTROPIC

PARAMETER OLD
 15.14

CHANGE

NEW

ERROR

SHIFT/ERROR

ATOM 1 M1

EQUIPOINT FRACTION = 0.500
 OCCUPANCY SPECIES 1
 OCCUPANCY SPECIES 2
 TOTAL OCCUPANCY (FIXED) =

R-STAR 0.1738E 00
 SCALE FACTOR 1 9.2610

0.1738E 00
 9.2610

0.00852

0.00

1

ATOM 2 M2

EQUIPOINT FRACTION = 0.500
 OCCUPANCY SPECIES 1
 OCCUPANCY SPECIES 2
 TOTAL OCCUPANCY (FIXED) =

BETA11 0.00577800
 BETA22 0.0021662
 BETA33 0.0047871
 BETA12 -0.0000283
 BETA13 -0.0007489
 BETA23 -0.00006874

-0.00000000
 -0.00000000
 -0.00000000
 -0.00000000
 -0.00000000
 -0.00000000

0.00577799
 0.0021662
 0.0047871
 -0.0000283
 -0.0007489
 -0.00006874

0.00004221
 0.00009715
 0.0002338
 0.0001858
 0.0002667
 0.0001046

-0.00
 -0.00
 -0.00
 -0.00
 -0.00
 -0.00

2
 3
 4
 5
 6
 7

ATOM 3 S1

EQUIPOINT FRACTION = 0.500
 OCCUPANCY SPECIES 1
 OCCUPANCY SPECIES 2
 TOTAL OCCUPANCY (FIXED) =

BETA11 0.00809
 BETA22 0.99191
 BETA33 1.00000
 BETA12 0.9876623
 BETA13 0.2801470
 BETA23 0.2500000

-0.00000001
 -0.00000000
 -0.00000001
 -0.00000000
 -0.00000001
 -0.00000000

0.00809
 0.99191
 1.00000
 0.9876621
 0.2801470
 0.2500000

0.0002444
 0.0000980
 0.0003705
 0.0001707
 0.0001773
 0.0001614

-0.00
 0.00
 -0.00
 -0.00
 -0.00
 -0.00

8
 9
 10
 11
 12
 13

ATOM 4 O1

EQUIPOINT FRACTION = 0.500
 OCCUPANCY SPECIES 1
 OCCUPANCY SPECIES 2
 TOTAL OCCUPANCY (FIXED) =

BETA11 1.00000
 BETA22 0.4265044
 BETA33 0.0951376
 BETA12 0.2500000
 BETA13 0.0054112
 BETA23 0.0014092

-0.00000001
 0.00000000
 0.00000001
 -0.00000000
 0.00000000
 0.00000000

1.00000
 0.4265043
 0.0951376
 0.2500000
 0.0054113
 0.0014092

0.00004186
 0.0001943
 0.0006759
 0.0001388
 0.0003488
 0.0002640

-0.00
 0.00
 0.00
 -0.00
 -0.00
 0.00

14
 15
 16
 17
 18
 19

BETA11 0.0029444
 BETA22 0.0024576
 BETA33 0.0066857
 BETA12 0.0000627
 BETA13 0.0
 BETA23 0.0

-0.00000001
 0.00000000
 -0.00000001
 -0.00000000
 0.00000000
 0.00000000

0.0029442
 0.0024576
 0.0066859
 0.0000627
 0.0
 0.0

0.0017574
 0.0004258
 0.0010018
 0.00007686
 0.0
 0.0

-0.00
 0.00
 0.00
 -0.00
 0.00
 0.00

20
 21
 22
 23
 24
 25

ATOM 5 02

EQUIPOINT FRACTION = 0.500
OCCUPANCY SPECIES

X
Y
Z
BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

1.000000	-0.0000001	1.000000	0.0010731	-0.00	26
0.2161920	0.0000001	0.2161918	0.0004696	-0.00	27
0.4524900	0.0000000	0.4524900	0.0018196	-0.00	28
0.2500000	0.0000001	0.2500000	0.0003807	0.00	29
0.0057160	0.0000000	0.0057159	0.0009196	-0.00	30
0.0014470	0.0000000	0.0014470	0.0007079	0.00	31
0.0056397	0.0000000	0.0056397			
-0.0001527	0.0000000	-0.0001528			
0.0	0.0000000	0.0			
0.0	0.0000000	0.0			

ATOM 6 03

EQUIPOINT FRACTION = 1.000
OCCUPANCY SPECIES

X
Y
Z
BETA11
BETA22
BETA33
BETA12
BETA13
BETA23

1.000000	0.0000000	1.000000	0.0007888	0.00	32
0.2856678	0.0000000	0.2856678	0.003293	-0.00	33
0.1625297	0.0000000	0.1625296	0.0004964	0.00	34
0.0400593	0.0000001	0.0400593	0.003347	0.00	35
0.0075079	0.0000000	0.0075080	0.002759	0.00	36
0.0018599	0.0000000	0.0018600	0.006491	0.00	37
0.0049291	0.0000000	0.0049291	0.005111	0.00	38
0.0001707	0.0000000	0.0001707	0.0007503	0.00	39
0.0000837	0.0000000	0.0000838	0.0003480	0.00	40
0.0003964	0.0000000	0.0003964			

MAXIMUM SHIFT/ERROR = -0.00
AVERAGE SHIFT/ERROR = 0.00

RFINE 108206 CYCLE 4

CORRELATION COEFFICIENTS WITH LARGEST MAGNITUDES

PARAMETERS	VALUE	PARAMETERS	VALUE	PARAMETERS	VALUE	PARAMETERS	VALUE
1	-0.4804	1	-0.4388	1	-0.3722	17	-0.2633
22	-0.2624	29	-0.2553	11	-0.2545	36	-0.2533
23	-0.2504	35	-0.2469	16	-0.2462	22	-0.2456
17	-0.2456	18	-0.2449	28	-0.2385	16	-0.2365
15	-0.2351	10	-0.2330	10	-0.2275	28	-0.2274

REFINE 108206 CYCLE 4
 BOND DISTANCES BETWEEN, 1.50 AND 2.50 ANG.

ATOM 1	X	Y	Z	ATOM 2	X	Y	Z	DISTANCE	NUMBER
M1	0.0	0.0	0.0	M1	0.0	0.0	0.0	2.18299	1
M2	0.98766	0.28015	0.25000	M1	0.42650	0.09514	0.25000	2.18299	2
SI	0.42650	0.09514	0.25000	M1	0.42650	0.09514	0.25000	2.18299	3
O1	0.75735	0.09142	0.25000	M2	0.98766	0.28015	0.25000	2.14389	4
O2	0.21619	0.45249	0.25000	SI	0.42650	0.09514	0.25000	2.14389	5
O3	0.28567	0.16253	0.04006	M2	0.98766	0.28015	0.25000	2.22794	6
				SI	0.42650	0.09514	0.25000	2.22794	7
				M1	0.50000	0.50000	0.0	2.31831	8
				M2	0.50000	0.50000	0.0	2.31831	9
				SI	0.07350	0.59514	0.25000	2.14658	10
				M1	0.0	0.99514	0.25000	2.14658	11
				M2	0.0	0.99514	0.25000	2.14658	12
				SI	0.0	0.28015	0.25000	2.14658	13
				M1	0.0	0.28015	0.25000	2.14658	14
				M2	0.0	0.28015	0.25000	2.14658	15
				SI	0.0	0.28015	0.25000	2.14658	16
				M1	0.0	0.28015	0.25000	2.14658	17
				M2	0.0	0.28015	0.25000	2.14658	18
				SI	0.0	0.28015	0.25000	2.14658	19
				M1	0.0	0.28015	0.25000	2.14658	20
				M2	0.0	0.28015	0.25000	2.14658	21
				SI	0.0	0.28015	0.25000	2.14658	22
				M1	0.0	0.28015	0.25000	2.14658	23
				M2	0.0	0.28015	0.25000	2.14658	24

REFINE 108206 CYCLE 4
 BOND ANGLES

CENTRAL ATOM X Y Z
 M1 0.0 0.0 0.0

ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
01	01	179.931
01	02	93.739
01	03	86.261
01	03	85.189
01	01	94.811
01	02	86.261
01	03	93.739
01	01	94.811
01	02	85.139
02	02	180.000
02	03	107.675
02	03	72.325
02	03	72.325
03	03	107.675
03	03	179.944

CENTRAL ATOM X Y Z
 M2 0.98766 0.28015 0.25000

ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
01	02	177.926
01	03	80.711
01	03	91.250
01	03	91.250
01	03	80.711
01	03	97.586
02	03	89.867
02	03	89.867
02	03	97.586
02	03	89.867
02	03	97.927
02	03	156.196
03	03	68.740
03	03	114.784
03	03	156.196
03	03	87.927

CENTRAL ATOM X Y Z
 S1 0.42650 0.09514 0.25000

ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
02	03	102.706
02	01	113.331
02	03	102.706
03	01	115.392
03	03	105.775
03	01	115.392

CENTRAL ATOM X Y Z
 O1 0.75735 0.09142 0.25000

ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
M2 8	SI 15	117.933
M2 8	MI 17	96.961
SI 15	MI 18	96.961
SI 17	MI 17	123.541
	MI 18	123.541
	MI 18	91.111

CENTRAL ATOM X Y Z
 02 0.21619 0.45249 0.25000

ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
MI 20	MI 21	93.263
MI 20	SI 22	122.449
MI 21	SI 22	93.257
MI 21	SI 23	122.449
MI 22	SI 23	93.257
	SI 23	123.869

CENTRAL ATOM X Y Z
 03 0.28567 0.16253 0.04006

ATOM 1 NUMBER	ATOM 2 NUMBER	ANGLE
MI 1	SI 15	90.859
MI 1	MI 22	94.966
MI 15	MI 24	114.252
SI 15	MI 22	92.611
SI 15	MI 24	127.071
M2 22	MI 24	127.670

RFINE 108206 CYCLE 4

ELLIPSOIDS OF VIBRATION

ELLIPSOID FOR M1

EQUIVALENT ISOTROPIC B = 0.7551

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.079546	29.96	79.13	62.46
2	0.093520	60.43	117.68	137.33
3	0.116684	94.37	149.90	60.29

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM M1

ATOM	X	Y	Z	RAW	LOWER	AT	NON-CORR	UPPER	DISPLACEMENT ALONG BOND
01	-0.24265	0.09142	0.25000	2.18299	2.18299	2.19220	2.20141	2.20141	0.09348
01	0.24265	-0.09142	-0.25000	2.18299	2.18299	2.19220	2.20141	2.20141	0.09348
02	-0.28381	0.04751	-0.25000	2.14389	2.14392	2.15265	2.16137	2.16137	0.09100
02	0.28381	-0.04751	0.25000	2.14389	2.14392	2.15265	2.16137	2.16137	0.09100
03	0.28567	0.16253	0.04006	2.22794	2.22794	2.23643	2.24491	2.24491	0.09772
03	-0.28567	-0.16253	-0.04006	2.22794	2.22794	2.23643	2.24491	2.24491	0.09772

ELLIPSOID FOR M2

EQUIVALENT ISOTROPIC B = 0.6762

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.087003	56.24	146.24	90.00
2	0.090891	146.23	123.77	90.00
3	0.099298	90.60	90.00	0.0

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM M2

ATOM	X	Y	Z	RAW	LOWER	AT	NON-CORR	UPPER	DISPLACEMENT ALONG BOND
01	0.75735	0.09142	0.25000	2.29221	2.29221	2.30020	2.30818	2.30818	0.09011
02	1.21619	0.45249	0.25000	2.13812	2.13813	2.14660	2.15508	2.15508	0.09022
03	1.28567	0.31831	0.04006	2.14658	2.14663	2.15514	2.16366	2.16366	0.09129
03	0.78567	0.33747	0.04006	2.14658	2.14663	2.15514	2.16366	2.16366	0.09607
03	1.28567	0.16253	0.45994	2.31831	2.31832	2.32620	2.33407	2.33407	0.09607
03	0.78567	0.33747	0.04006	2.14658	2.14663	2.15514	2.16366	2.16366	0.09607
03	1.28567	0.16253	0.45994	2.31831	2.31832	2.32620	2.33407	2.33407	0.09129

ELLIPSOID FOR S1

EQUIVALENT ISOTROPIC B = 0.6139

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.080495	8.74	98.74	90.00
2	0.089663	98.43	171.57	90.00
3	0.093840	90.00	90.00	0.00

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM SI

ATOM	X	Y	Z	RAW	LOWER	DISTANCES RIDDING	AT	NON-CORR	UPPER	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C	DISPLACEMENT ALONG BOND
O2	0.28381	-0.04751	0.25000	1.66298	1.66301	1.66374	1.67300	1.65207	1.68299	0.09514	0.25000	0.08901	0.08901
O3	0.28567	0.16253	0.04006	1.64119	1.64132	1.64284	1.65207	1.62695	1.66283	0.09038	0.09038	0.08065	0.08065
O1	0.75735	0.09142	0.25000	1.61333	1.61371	1.61652	1.62695	1.62695	1.64019	0.08065	0.08065	0.09038	0.09038
O3	0.28567	0.16253	0.45994	1.64119	1.64132	1.64284	1.65207	1.62695	1.66283	0.09038	0.09038	0.08065	0.08065

ELLIPSOID FOR O1

EQUIVALENT ISOTROPIC B = 0.8072

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.059516	0.90	90.90	90.00
2	0.114731	90.00	90.00	180.00
3	0.118164	89.10	0.90	90.00

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM O1

ATOM	X	Y	Z	RAW	LOWER	DISTANCES RIDDING	AT	NON-CORR	UPPER	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C	DISPLACEMENT ALONG BOND
M2	0.98766	0.28015	0.25000	2.29221	2.29221	2.29253	2.30020	2.26995	2.30818	0.09142	0.25000	0.10771	0.10771
SI	0.42650	0.09514	0.25000	1.61333	1.61371	1.61652	1.62695	1.62695	1.64019	0.05952	0.05952	0.08661	0.08661
M1	1.00000	0.0	0.0	2.18299	2.18299	2.18306	2.19220	2.19220	2.20141	0.10206	0.10206	0.09104	0.09104

ELLIPSOID FOR O2

EQUIVALENT ISOTROPIC B = 0.6897

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.082290	15.42	74.57	90.00
2	0.091267	74.57	164.57	90.00
3	0.105374	90.00	90.00	0.0

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM O2

ATOM	X	Y	Z	RAW	LOWER	DISTANCES RIDDING	AT	NON-CORR	UPPER	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C	DISPLACEMENT ALONG BOND
M1	0.50000	0.50000	0.0	2.14389	2.14392	2.14465	2.15265	2.14660	2.16137	0.45249	0.25000	0.09521	0.09521
M1	0.50000	0.50000	0.0	2.14389	2.14392	2.14465	2.15265	2.14660	2.16137	0.45249	0.25000	0.09521	0.09521
M2	-0.01234	0.28015	0.25000	2.13813	2.13813	2.13846	2.14660	2.14660	2.15508	0.08661	0.08661	0.09521	0.09521
SI	0.07350	0.59514	0.25000	1.66298	1.66301	1.66374	1.67300	1.67300	1.68299	0.09104	0.09104	0.09104	0.09104

ELLIPSOID FOR 03

EQUIVALENT ISOTROPIC B = 0.7714

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.093077	62.97	125.36	47.38
2	0.095089	28.17	82.22	116.89
3	0.107722	80.30	36.61	55.10

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BOUNDS FROM 03

ATOM	X	Y	Z	RAW	LOWER	DISTANCES RIDING	AT	NON-CORR	UPPER	DISPLACEMENT ALONG BUND
M1	0.0	0.0	0.0	2.22794	2.22794	2.22804	2.23643	2.24491	2.24491	0.10314
SI	0.42650	0.09514	0.25000	1.64119	1.64132	1.64284	1.65207	1.66283	1.66283	0.09357
M2	-0.01234	0.28015	0.25000	2.31832	2.31833	2.31871	2.32622	2.33408	2.33408	0.10052
M2	0.48766	0.21985	-0.25000	2.14658	2.14663	2.14747	2.15214	2.16365	2.16365	0.09496

PARAMETERS WRITTEN OUT TO UNIT 10.

SUMMARY OF ERRORS FOR THIS JOB ERROR NUMBER NUMBER OF ERRORS

209 1

