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Perskovite-type MgSi O₃: Single-crystal X-ray diffraction study

Horiuchi, et al.

To be deposited: Structure tables

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For

MgSiO₃ (perovskite-type): Single Crystal X-ray Diffraction Study

Hiroyuki HORIUCHI

Mineralogical Institute, Faculty of Science, University of Tokyo,
Hongo, Bunkyo-ku, Tokyo 113, Japan,

Eiji ITO

Institute for Study of the Earth's Interior, Okayama University
Misasa, Tottori-ken 682-02, Japan

and

Donald J. WEIDNER

Department of Earth and Space Science, State University of New York
at Stony Brook, Stony Brook, New York, 11794, U. S. A.

REFINEMENT OF THE STRUCTURE OF Hg-SI-O(3) PEROVSKITE HgK-alpha.

REAL CELL 4.77560 4.92920 6.89680 90.00000 90.00000 90.00000
 RECIPROCAL CELL 0.20941 0.20287 0.14499 0.0 0.0 0.0
 SYMMETRY CARDS

SCATTERING CURVES
 LABEL A(1) B(1) A(2) B(2) A(3) B(3) A(4) B(4) C
 1/2 X X 1/2 -Z 0
 1/2 -X 1/2 -Y 1/2 Z 0
 1/2 -X 1/2 Y 1/2 Z 0
 1/2 -X 1/2 Y 1/2 Z 0

FOR TH CYCLE ATOM Hg 5.420400 2.827500 2.173500 79.261093 1.226900 0.390800 2.307300 7.193700 0.658600
 SI 6.291500 2.438600 3.035300 32.333694 1.989100 0.678500 1.541000 81.693695 1.140700
 OX 3.048500 13.277100 2.286800 5.701100 1.546300 0.323900 0.867000 32.908905 0.250800

EXTINCTION CORRECTION ISOTROPIC

R-STAR

0.0

0.0

ATOM 1 Hg SCALE FACTOR 1 EQUIPOINT FRACTION 1 OCCUPANCY SPECIES 1

3.8287 0.0000 3.8287 0.00453 0.00

ATOM 2 SI EQUIPOINT FRACTION = 0.500 OCCUPANCY SPECIES 2

1.00000 0.5000000 0.5000000 0.0001076 0.00

ATOM 3 OX1 EQUIPOINT FRACTION = 0.500 OCCUPANCY SPECIES 3

1.00000 0.1027651 0.4659905 0.0002115 0.00

BETA11 0.0029624 0.0029815 0.0010007 0.0000573 0.00
 BETA22 0.0010007 0.0000359 0.0000220 0.0000860 0.00
 BETA12 0.0000000 0.0000000 0.0000000 0.0000000 0.00
 BETA13 0.0000000 0.0000000 0.0000000 0.0000000 0.00
 BETA23 0.0000000 0.0000000 0.0000000 0.0000000 0.00
 X 0.5000000 0.0000000 0.0000000 0.0000000 0.00
 Y 0.0000000 0.0000000 0.0000000 0.0000000 0.00
 Z 0.0029624 0.0029815 0.0010007 0.0000573 0.00
 BETA11 0.0037628 0.0047175 0.0008952 0.0001102 0.00
 BETA22 0.0000000 0.0000000 0.0000000 0.0000000 0.00
 BETA12 0.0000000 0.0000000 0.0000000 0.0000000 0.00
 BETA13 0.0000000 0.0000000 0.0000000 0.0000000 0.00
 BETA23 0.0000000 0.0000000 0.0000000 0.0000000 0.00
 X 0.1027651 0.4659905 0.0002115 0.0001453 0.00
 Y 0.2500000 0.0037628 0.0003031 0.0003236 0.00
 Z 0.0047175 0.0008952 0.0001476 0.0002420 0.00

BETA23 EQUPOINT FRACTION = 1.000 0.0
 OCCUPANCY SPECIES 3 0.0
 X 0.1960875 0.0000000 0.0000000 0.0001466 0.00
 Y 0.2013562 0.0000000 0.0000000 0.2013562 0.00
 Z 0.5530811 0.0000000 0.0000000 0.5530811 0.00
 BETA11 0.0037188 0.0000000 0.0000000 0.0037188 0.00
 BETA22 0.0036682 0.0000000 0.0000000 0.0036682 0.00
 BETA33 0.0017949 0.0000000 0.0000000 0.0017949 0.00
 BETA12 0.0006995 0.0000000 0.0006995 0.0006995 0.00
 BETA13 0.0002925 0.0000000 0.0002925 0.0002925 0.00
 BETA23 0.0004794 0.0000000 0.0004795 0.0001308 0.00

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

FORTH CYCLE
 CORRELATION COEFFICIENTS WITH LARGEST MAGNITUDES

PARAMETERS	VALUE	PARAMETERS	VALUE	PARAMETERS	VALUE	PARAMETERS	VALUE			
1	0.2800	1	0.2614	1	10	0.2556	16	17	-0.2407	
23	-0.2334	17	18	-0.2274	1	6	0.2168	16	18	-0.2150
23	-0.2047	1	4	0.2041	24	25	-0.1969	4	5	-0.1969
5	-0.1931	4	6	-0.1800	8	9	-0.1750	1	5	0.1684
9	-0.1652	8	10	-0.1460	1	24	0.1428	1	23	0.1348

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
2	0	0	61.241	43.181	7	3	0	3.134	3.086	2	7	0	7.809	7.770
4	0	0	42.442	42.988	8	3	0	3.761	3.702	3	7	0	7.809	7.770
6	0	0	29.566	30.292	9	3	0	10.029	9.682	4	7	0	12.212	12.212
8	0	0	10.970	10.717	0	4	0	44.976	45.753	5	7	0	4.414	4.307
10	0	0	20.947	21.288	1	4	0	24.708	25.689	6	7	0	22.671	22.417
1	1	0	22.986	22.796	2	4	0	24.969	24.771	7	7	0	1.802	1.802
2	1	0	27.137	25.866	3	4	0	2.089	2.121	0	8	0	6.086	6.237
3	1	0	8.880	8.621	4	4	0	19.667	19.506	1	8	0	3.761	3.518
4	1	0	20.163	20.769	5	4	0	3.030	3.046	2	8	0	8.906	8.812
5	1	0	4.257	4.526	6	4	0	14.339	14.266	3	8	0	9.951	9.913
6	1	0	7.600	7.857	7	4	0	7.653	7.383	4	8	0	1.358	1.358
7	1	0	7.888	8.219	8	4	0	9.167	9.064	5	8	0	3.421	3.472
8	1	0	6.294	6.448	9	5	0	5.015	4.924	6	8	0	0.0	0.0
9	1	0	8.306	8.028	1	5	0	23.297	23.306	7	8	0	2.298	2.298
10	1	0	3.108	2.825	2	5	0	3.630	3.770	8	9	0	14.052	13.675
1	2	0	45.968	47.966	3	5	0	32.099	32.379	9	9	0	1.645	1.348
2	2	0	15.932	14.964	4	5	0	2.194	1.656	0	9	0	17.551	16.998
3	2	0	78.328	79.370	5	5	0	3.265	2.661	1	9	0	8.906	8.923
4	2	0	16.324	16.335	6	5	0	5.877	6.267	2	10	0	10.108	9.854
5	2	0	28.245	28.245	7	5	0	16.898	17.052	3	10	0	8.723	8.911
6	2	0	5.433	5.290	8	5	0	7.183	7.093	4	10	0	1.332	0.875
7	2	0	16.376	16.291	9	5	0	8.332	8.454	5	10	0	3.291	3.106
8	2	0	3.578	3.175	0	6	0	7.235	7.452	6	10	0	3.030	3.030
9	2	0	23.741	23.914	1	6	0	9.324	9.313	7	10	0	3.918	3.918
10	2	0	6.296	6.563	2	6	0	13.477	13.545	8	10	0	12.014	11.667
1	3	0	7.026	6.901	3	6	0	8.462	8.707	9	10	0	7.156	7.245
2	3	0	34.372	34.712	4	6	0	3.918	3.553	0	11	0	13.562	13.562
3	3	0	6.190	6.188	5	6	0	8.227	8.238	1	11	0	3.526	3.533
4	3	0	0.0	0.821	6	6	0	6.675	6.654	2	11	0	11.805	11.664
5	3	0	17.917	18.020	7	6	0	4.344	4.344	3	11	0	26.743	25.656
6	3	0	13.346	13.528	8	7	0	25.961	26.199	4	11	0	15.129	15.129

10.395	10.162	5.589	5.028	5.570	25.570	25.922
1.802	1.466	2.759	1.992	1.992	13.608	13.693
3.213	2.829	4.376	4.620	20.607	20.553	20.553
4.727	4.820	3.526	3.524	2.351	2.674	2.674
0.0	0.057	1.858	1.858	19.510	19.793	19.793
1.959	1.858	3.526	3.443	1.802	1.579	1.579
4.205	3.778	3.918	3.992	15.906	15.333	15.333
4.432	4.043	1.045	0.993	3.343	3.430	3.430
19.432	18.432	5.433	4.979	7.548	7.548	7.548
20.921	21.008	2.899	3.000	9.037	8.995	8.995
2.403	2.016	2.429	2.221	2.221	2.221	2.221
12.261	14.282	0.183	0.875	0.875	0.961	0.961
5.145	5.858	20.921	20.662	0.914	1.018	1.018
7.496	7.330	25.570	23.841	4.675	5.005	5.005
6.843	6.636	17.473	18.093	11.988	11.784	11.784
4.074	4.188	16.037	16.238	7.104	7.236	7.236
6.843	6.857	3.082	3.066	1.907	1.103	1.103
1.228	0.930	6.377	6.377	13.869	13.085	13.085
7.548	7.378	49.099	49.099	22.644	22.644	22.644
31.499	28.008	15.201	14.821	2.194	2.194	2.194
12.119	11.946	61.456	62.026	7.261	6.851	6.851
10.349	10.253	12.563	12.810	13.764	13.579	13.579
9.037	9.303	38.159	38.364	0.470	0.516	0.516
2.899	3.226	11.440	11.417	9.429	8.831	8.831
3.630	3.764	24.055	23.772	4.101	4.101	4.101
0.0	0.224	0.0	0.381	7.888	7.407	7.407
5.406	5.496	9.429	9.055	4.989	4.694	4.694
20.581	20.704	1.226	0.230	3.787	3.514	3.514
1.698	1.541	32.700	30.422	0.966	0.183	0.183
42.798	42.797	22.018	21.106	20.477	20.477	20.477
5.850	5.451	21.809	21.431	19.931	19.931	19.931
18.230	18.592	3.239	3.105	8.175	8.175	8.175
1.280	0.925	14.783	14.899	2.168	1.742	1.742
12.145	12.378	3.056	2.948	42.076	42.076	42.076
4.153	4.276	5.198	4.769	51.778	51.778	51.778
1.802	0.748	9.716	9.673	8.175	8.562	8.562
0.0	0.690	10.447	10.226	12.641	12.708	12.708
21.730	22.024	2.429	1.843	24.029	23.267	23.267
5.824	5.824	2.429	2.117	13.921	13.842	13.842
11.179	11.158	39.047	39.371	8.671	8.865	8.865
3.317	3.365	9.611	9.725	14.940	15.178	15.178
3.944	3.777	27.450	26.991	14.391	14.578	14.578
1.384	0.404	9.742	9.740	1.306	1.306	1.306
5.198	4.746	37.506	37.685	3.343	3.690	3.690
3.787	3.587	2.533	1.909	1.045	1.048	1.048
5.720	5.637	8.018	7.939	2.742	2.771	2.771
0.810	0.763	7.105	7.594	4.623	4.325	4.325
1.149	1.149	21.156	21.510	28.051	27.287	27.287
11.518	11.834	7.313	7.625	13.608	13.199	13.199
3.552	3.535	15.718	15.718	5.041	4.892	4.892
11.231	11.156	15.566	15.888	12.093	12.217	12.217
2.664	2.025	21.913	21.815	14.783	15.024	15.024
7.653	7.005	5.824	5.647	4.336	3.954	3.954
0.340	0.166	16.010	15.890	10.447	10.359	10.359
3.709	3.840	4.231	4.340	13.085	13.085	13.085
9.794	9.814	5.459	5.328	2.011	1.565	1.565
3.186	2.849	8.018	7.687	1.854	1.854	1.854
4.989	5.038	11.779	11.618	22.409	22.201	22.201
1.489	0.600	3.395	3.337	18.048	18.515	18.515
2.272	1.900	26.353	26.400	21.130	21.349	21.349
3.015	4.730	0.784	0.793	3.996	4.078	4.078
3.186	2.740	7.156	6.778	0.731	0.618	0.618
1.593	0.122	7.183	7.000	5.824	5.901	5.901
2.769	2.550	14.705	14.343	8.802	8.600	8.600
1.358	0.468	6.190	5.976	3.578	3.550	3.550
0.0	0.057	5.976	5.976	4.727	4.482	4.482

0	4	2.298	2.568	3	2	4	8.322	8.196	5	0	5	4.293	4.292
1	4	8.358	8.518	3	4	26.562	26.510	26.510	0	5	5	16.454	16.567
2	4	25.648	25.763	3	5	3.761	3.761	3.691	9	0	5	2.063	2.203
3	4	1.487	1.541	3	6	16.830	16.840	16.840	1	1	5	2.658	2.661
4	4	14.052	13.989	3	7	0.996	0.990	0.990	1	1	5	17.081	17.409
5	4	0.705	0.707	3	8	17.290	17.028	17.028	1	1	5	19.589	19.597
6	4	6.477	6.543	3	9	2.925	2.925	2.925	3	1	5	5.145	4.671
7	4	1.802	1.781	3	10	23.532	23.532	23.532	4	1	5	9.535	9.553
8	4	9.141	8.878	3	11	1.097	1.097	0.760	6	6	5	4.074	3.860
9	4	3.343	3.631	3	12	9.611	9.611	9.340	7	7	5	8.462	8.400
1	4	19.798	20.235	3	13	1.175	1.175	0.283	8	8	5	1.306	1.113
2	4	4.675	4.771	3	14	9.194	9.194	9.035	9	9	5	1.280	1.228
3	4	9.768	9.687	3	15	7.444	7.444	7.516	10	10	5	1.280	2.642
4	4	10.186	10.166	3	16	6.530	6.530	6.597	11	11	5	2.533	2.642
5	4	3.892	4.025	3	17	5.198	5.198	5.271	12	12	5	20.581	20.442
6	4	9.664	9.670	3	18	8.515	8.515	8.688	13	13	5	19.719	19.770
7	4	4.022	3.777	3	19	8.022	8.022	8.053	14	14	5	3.395	3.316
8	4	0.0	0.370	3	20	6.608	6.608	6.687	15	15	5	9.638	9.519
9	4	14.443	14.817	3	21	25.031	25.031	24.887	16	16	5	5.067	5.300
0	4	4.101	4.042	3	22	6.608	6.608	7.025	17	17	5	3.787	3.953
1	4	0.727	0.245	3	23	16.115	16.115	16.033	18	18	5	2.089	2.011
2	4	2.168	1.873	3	24	3.839	3.839	3.934	19	19	5	6.582	6.487
3	4	13.268	13.150	3	25	11.753	11.753	11.677	20	20	5	10.343	10.282
4	4	1.123	1.111	3	26	2.597	2.597	2.063	21	21	5	25.846	23.916
5	4	11.100	10.922	3	27	10.186	10.186	10.175	22	22	5	0.235	0.392
6	4	2.873	2.136	3	28	0.360	0.360	0.319	23	23	5	3.552	3.475
7	4	3.474	3.723	3	29	23.454	23.454	23.713	24	24	5	14.785	14.892
8	4	11.596	11.592	3	30	3.259	3.259	3.144	25	25	5	11.805	11.503
9	4	3.761	3.689	3	31	20.529	20.529	20.476	26	26	5	7.574	7.956
0	4	0.0	0.0	3	32	9.599	9.599	9.719	27	27	5	0.0	0.252
1	4	8.567	8.403	3	33	1.364	1.364	0.719	28	28	5	5.302	5.334
2	4	3.463	3.344	3	34	6.138	6.138	6.246	29	29	5	24.107	24.411
3	4	3.056	2.791	3	35	11.231	11.231	11.145	30	30	5	2.196	2.000
4	4	0.0	0.180	3	36	6.660	6.660	6.179	31	31	5	2.325	2.228
5	4	7.345	7.213	3	37	13.536	13.536	13.376	32	32	5	6.216	6.097
6	4	5.433	5.322	3	38	1.802	1.802	1.676	33	33	5	16.219	16.249
7	4	5.250	5.013	3	39	9.977	9.977	9.920	34	34	5	0.992	0.627
8	4	4.283	3.952	3	40	7.966	7.966	7.875	35	35	5	13.111	13.368
9	4	4.127	3.861	3	41	2.877	2.877	2.847	36	36	5	5.537	5.176
0	4	3.448	3.028	3	42	6.817	6.817	6.612	37	37	5	3.892	4.103
1	4	2.664	2.288	3	43	1.985	1.985	2.406	38	38	5	16.742	16.696
2	4	2.142	0.608	3	44	5.772	5.772	5.329	39	39	5	9.925	9.925
3	4	3.813	3.801	3	45	21.130	21.130	21.016	40	40	5	8.515	8.466
4	4	4.127	0.034	3	46	4.649	4.649	4.786	41	41	5	9.847	9.838
5	4	1.515	0.034	3	47	15.697	15.697	15.667	42	42	5	2.821	2.257
6	4	8.436	8.431	3	48	1.201	1.201	0.607	43	43	5	4.850	5.798
7	4	4.675	3.977	3	49	15.305	15.305	14.986	44	44	5	4.362	4.282
8	4	4.754	3.084	3	50	3.004	3.004	3.106	45	45	5	5.563	5.509
9	4	3.259	3.030	3	1	9.316	9.316	9.181	46	46	5	6.843	7.407
0	4	86.158	86.320	3	2	9.316	9.316	9.181	47	47	5	2.063	1.287
1	4	53.673	53.509	3	3	4.074	4.074	3.835	48	48	5	15.175	14.906
2	4	33.170	33.016	3	4	5.170	5.170	5.282	49	49	5	3.964	3.861
3	4	23.227	22.342	3	5	3.996	3.996	3.557	50	50	5	8.306	8.115
4	4	15.514	15.617	3	6	4.518	4.518	4.115	1	6	5	2.377	2.144
5	4	17.107	16.534	3	7	0.856	0.856	0.110	2	7	5	4.257	3.816
6	4	4.727	4.598	3	8	4.518	4.518	4.115	3	8	5	0.496	0.160
7	4	4.858	4.834	3	9	3.317	3.317	3.130	4	9	5	6.765	6.962
8	4	5.041	4.746	3	10	13.660	13.660	13.162	5	10	5	5.380	5.781
9	4	0.836	0.063	3	11	2.742	2.742	2.281	6	11	5	7.391	7.038
0	4	1.201	0.479	3	12	14.156	14.156	13.702	7	12	5	3.589	5.512
1	4	6.112	5.982	3	13	3.735	3.735	3.503	8	13	5	5.250	5.118
2	4	3.552	3.082	3	14	3.259	3.259	2.955	9	14	5	8.384	8.107
3	4	8.332	8.440	3	15	1.280	1.280	1.275	10	15	5	3.918	3.633
4	4	57.251	56.409	3	16	1.384	1.384	1.192	11	16	5	6.530	6.594
5	4	1.541	1.278	3	17	17.839	17.839	17.567	12	17	5	3.421	3.467
6	4	49.912	50.024	3	18	12.798	12.798	13.185	13	18	5	2.847	2.247

4	6	347	6	235	3	7	6	567	8	416	6	115	8	854
5	1	175	5	052	5	7	6	653	0	595	1	115	9	246
1	2	5380	5	009	5	7	6	2925	2	193	2	108	3	108
2	9	1724	5	406	5	6	6	2951	3	503	3	287	0	287
3	2	7026	5	723	5	6	6	18570	4	615	4	164	6	107
4	9	4989	5	4708	5	6	6	5067	5	006	5	742	2	286
0	0	5015	5	833	5	6	6	13294	6	939	6	089	5	089
0	0	12772	6	672	6	6	6	31160	7	570	7	642	7	642
0	0	9324	6	397	6	6	6	12772	8	549	8	022	8	022
4	4	11257	6	1260	6	6	6	0	129	1	8	422	9	422
6	6	8149	6	407	6	6	6	4597	2	487	2	630	0	630
8	0	6582	6	167	6	6	6	2325	3	570	3	013	7	013
1	1	37662	6	035	6	6	6	1724	4	1570	4	369	8	369
2	1	5067	6	93	6	6	6	1124	5	1355	5	519	9	519
3	1	37662	6	035	6	6	6	15227	6	14828	6	2925	0	878
1	1	5067	6	93	6	6	6	2168	7	2045	7	2925	1	892
2	1	37558	6	316	6	6	6	6086	8	5835	8	29775	2	929
4	4	5406	6	048	6	6	6	3039	9	3627	9	29775	3	240
5	4	32857	6	904	6	6	6	6086	0	627	0	964	4	666
4	4	1776	6	517	6	6	6	10108	1	0067	1	7630	5	666
6	6	17134	6	810	6	6	6	10787	2	10829	2	10761	6	308
7	1	3604	6	810	6	6	6	7783	3	7721	3	19693	7	803
8	1	8201	6	578	6	6	6	4283	4	4046	4	14025	8	025
9	0	8384	6	024	6	6	6	9664	5	684	5	6086	9	086
0	1	1097	6	508	6	6	6	9272	6	9266	6	2063	0	888
1	2	3630	6	520	6	6	6	1750	7	1596	7	804	1	888
2	2	7078	6	247	6	6	6	2847	8	2554	8	376	2	888
3	2	15488	6	444	6	6	6	0026	9	0189	9	106	3	888
4	2	3239	6	988	6	6	6	2351	0	2049	0	481	4	888
5	2	12328	6	881	6	6	6	13190	1	3323	1	541	5	888
6	2	1254	6	775	6	6	6	4910	2	5044	2	802	6	888
7	2	1933	6	448	6	6	6	3683	3	563	3	802	7	888
8	2	2925	6	126	6	6	6	7313	4	7231	4	182	8	888
9	1	30506	6	601	6	6	6	9794	5	589	5	182	9	888
1	2	1619	6	693	6	6	6	2116	6	7879	6	182	0	888
2	3	15802	6	802	6	6	6	10552	7	8079	7	182	1	888
3	3	4388	6	104	6	6	6	2194	8	1338	8	182	2	888
4	3	10604	6	592	6	6	6	11126	9	1086	9	182	3	888
5	4	9194	6	295	6	6	6	12484	0	678	0	182	4	888
6	4	16611	6	814	6	6	6	2272	1	902	1	164	5	888
7	4	4727	6	766	6	6	6	3709	2	3795	2	164	6	888
8	4	15723	6	723	6	6	6	6216	3	6170	3	164	7	888
9	4	3395	6	395	6	6	6	3421	4	2967	4	164	8	888
0	4	12145	6	145	6	6	6	1802	5	1732	5	164	9	888
1	4	3050	6	030	6	6	6	4884	6	5069	6	164	0	888
2	4	7522	6	522	6	6	6	15436	7	1754	7	164	1	888
3	4	13712	6	712	6	6	6	2011	8	1754	8	164	2	888
4	5	3213	6	213	6	6	6	9291	9	1032	9	164	3	888
5	5	10317	6	033	6	6	6	1384	0	885	0	164	4	888
6	5	0836	6	833	6	6	6	5172	1	5013	1	164	5	888
7	5	16193	6	193	6	6	6	1933	2	1956	2	164	6	888
8	5	5328	6	1402	6	6	6	6334	3	6760	3	164	7	888
9	5	6138	6	154	6	6	6	13503	4	3555	4	164	8	888
0	6	6107	6	685	6	6	6	3108	5	2790	5	164	9	888
1	6	6007	6	608	6	6	6	6556	6	4499	6	164	0	888
2	6	16167	6	662	6	6	6	7757	7	7457	7	164	1	888
3	6	0104	6	422	6	6	6	2560	8	2027	8	164	2	888
4	6	17551	6	7952	6	6	6	7391	9	3076	9	164	3	888
5	6	81567	6	8364	6	6	6	3650	0	3076	0	164	4	888
6	6	15802	6	677	6	6	6	9194	1	3285	1	164	5	888
7	6	2153	6	677	6	6	6	3213	2	1108	2	164	6	888
8	6	12060	6	677	6	6	6	0	108	3	164	7	888	
9	6	2925	6	677	6	6	6	1663	4	1386	4	164	8	888
0	6	4153	6	677	6	6	6	10526	5	10026	5	164	9	888
1	6	4649	6	677	6	6	6	1123	6	0748	6	164	0	888
2	6	4649	6	677	6	6	6	1123	7	0748	7	164	1	888

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100																																																																																																																																																																																																																																																																																																																						
12.824	0.949	18.048	4.518	5.642	8.149	2.351	2.063	6.112	0.862	3.421	3.395	8.462	4.336	8.044	4.179	4.989	0.862	2.272	2.037	0.653	3.448	3.970	6.530	2.716	6.765	3.030	4.153	5.380	11.466	3.500	5.061	5.276	5.276	2.977	2.533	2.533	2.636	6.007	2.194	5.694	3.082	9.376	0.601	7.548	2.873	10.578	2.220	4.623	4.623	1.750	1.881	1.541	0.313	0.401	1.959	5.093	2.690	7.130	1.332	6.164	0.653	2.429	0.0	0.0	1.645	1.071	10.682	12.197	7.653	12.657	18.048	4.518	5.642	8.149	2.351	2.063	6.112	0.862	3.421	3.395	8.462	4.336	8.044	4.179	4.989	0.862	2.272	2.037	0.653	3.448	3.970	6.530	2.716	6.765	3.030	4.153	5.380	11.466	3.500	5.061	5.276	5.276	2.977	2.533	2.533	2.636	6.007	2.194	5.694	3.082	9.376	0.601	7.548	2.873	10.578	2.220	4.623	4.623	1.750	1.881	1.541	0.313	0.401	1.959	5.093	2.690	7.130	1.332	6.164	0.653	2.429	0.0	0.0	1.645	1.071	10.682	12.197	7.653	4.231	20.033	6.503	19.536	8.997	23.141	5.119	10.917	10.065	3.709	1.175	5.720	11.727	2.560	11.231	2.664	11.440	1.776	22.671	4.623	9.350	8.044	13.451	4.336	10.944	12.067	0.0	10.421	1.489	8.593	11.100	3.134	3.096	0.548	16.324	8.906	4.440	12.667	8.880	11.074	2.769	5.250	9.011	2.194	5.694	2.769	10.957	8.716	2.136	5.822	5.822	2.151	2.092	7.122	5.641	3.301	3.233	0.488	0.089	6.332	5.904	0.836	4.571	4.672	2.291	3.023	9.421	9.480	2.262	1.816	5.927	3.988	3.661	4.260	20.188	6.870	19.951	9.009	23.129	5.248	10.874	10.962	3.706	0.492	6.300	12.081	2.290	11.234	2.949	11.143	1.760	23.120	4.761	9.314	8.069	13.514	4.479	11.339	12.012	0.785	10.781	0.957	8.208	10.665	2.963	2.403	0.009	16.570	8.987	4.444	13.092	8.716	10.957	2.136	5.822	5.822	2.151	2.092	7.122	5.641	3.301	3.233	0.488	0.089	6.332	5.904	0.836	4.571	4.672	2.291	3.023	9.421	9.480	2.262	1.816	5.927	3.988	3.661	1.045	1.953	3.657	8.384	0.0	0.619	4.545	4.205	2.899	3.213	0.0	5.694	2.481	5.877	16.977	22.357	9.742	6.059	9.559	3.004	1.672	4.884	1.541	5.302	5.302	24.603	4.942	12.249	2.455	9.794	0.418	8.645	3.815	9.220	3.237	0.287	11.805	2.664	11.880	11.675	4.712	5.798	12.772	3.004	3.787	4.466	4.921	9.220	2.795	5.198	3.735	3.996	3.354	5.354	5.250	3.813	1.280	5.824	5.171	4.962	6.869	7.352	6.482	3.108	4.545	3.813	8.149	4.037	5.102	1.621	3.597	8.402	0.489	8.585	4.500	3.971	3.005	3.692	0.393	5.872	1.947	5.266	17.452	23.020	9.545	6.009	9.789	2.871	1.611	4.817	1.635	5.172	25.077	4.857	12.619	1.189	9.995	0.646	8.806	3.823	9.125	2.987	1.310	11.819	2.257	11.880	6.732	6.009	12.746	2.820	3.789	4.946	6.724	0.941	2.861	5.111	3.911	4.591	5.778	5.866	3.656	0.489	6.027	5.054	4.985	7.352	6.482	2.625	5.102	4.037	4.537	1.009	7.001

RESULTS	ALL REFLECTIONS	NUMERATOR	DENOMINATOR	NUMBER	R
0	0	1.280	1.026	671	0.012
2	0	2.951	2.744	159	0.023
1	1	9.429	9.442	41	0.054
2	1	2.298	0.882	14	0.098
3	1	12.641	13.037	6	0.107
0	2	0.0	0.931	2	0.074
1	2	1.280	1.050	0	0.0
2	2	3.004	3.545	0	0.0
1	3	7.261	7.068	2	0.087

WEIGHTED R	UNWEIGHTED R	NUMERATOR	DENOMINATOR	NUMBER	R
9170.50	264.78	15756316.0	7569.22	895	0.024
				895	0.035

RANGES OF F(OBS)

1573.48	11812835.0	671	0.012
1434.72	2799166.00	159	0.023
2130.31	721797.69	41	0.054
2360.36	246467.44	14	0.098
1211.90	105628.87	6	0.107
194.05	35209.64	2	0.074
0.0	0.0	0	0.0
267.01	35209.64	2	0.087

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

6680.28	045031.44	48	0.089
671.37	1337966.00	76	0.022
266.05	1690062.00	96	0.013
201.83	1918924.00	109	0.010
262.45	218297.00	124	0.011
382.34	2288626.00	130	0.013
351.75	2623118.00	149	0.012
355.79	2869585.00	163	0.011

UNREJECTED REFLECTIONS

WEIGHTED R	UNWEIGHTED R	NUMERATOR	DENOMINATOR	NUMBER	R
9170.50	264.78	15756316.0	7569.22	895	0.024
				895	0.035

RANGES OF F(OBS)

1573.48	11812835.0	671	0.012
1434.72	2799166.00	159	0.023
2130.31	721797.69	41	0.054
2360.36	246467.44	14	0.098
1211.90	105628.87	6	0.107
194.05	35209.64	2	0.074
0.0	0.0	0	0.0
267.01	35209.64	2	0.087

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

6680.28	045031.44	48	0.089
671.37	1337966.00	76	0.022
266.05	1690062.00	96	0.013
201.83	1918924.00	109	0.010
262.45	218297.00	124	0.011
382.34	2288626.00	130	0.013
351.75	2623118.00	149	0.012
355.79	2869585.00	163	0.011

SUM FCAL

7494.49