300°C phlogopite

LSFM (1.4) 06/11/97 10:54:15 Elapsed time = 0.1 min

PHLOG21 ..... Demonstration Copy - Not for Resale .....

The space group is number 12 -- C12/m1

Russell & Guggenheim

Refinement cycle no. 1. 732 observations. 58 variables.

Esd of an observation of unit weight = 3.991

Unweighted R factor = 0.133 Weighted R factor = 0.139

ä ³Fo³ = 1.33976E+04

ä ³³Fo³-³Fc³³ = 1.78385E+03

ä W*DELý = 1.07334E+04

ä W*Foý = 5.52633E+05

Scale factor:	New	Old	Shift	Error	SHFT/ERR
	0.97430	0.97380	0.00051	0.00542	0.09

Atom no. 1 K (electron count = 19.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	0.25000				
	x	0.00000				
	y	0.50000				
	z	0.00000				
5	U(1,1)	0.07033	0.07048	-0.00015	0.00446	-0.03
6	U(2,2)	0.07941	0.07917	0.00024	0.00523	0.05
7	U(3,3)	0.05336	0.05345	-0.00009	0.00368	-0.03
	U(1,2)	0.00000				
9	U(1,3)	0.00870	0.00873	-0.00003	0.00347	-0.01
	U(2,3)	0.00000				
	Total shift =	0.0000				

Atom no. 2 SI (electron count = 14.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	1.00000				
11	x	0.07688	0.07685	0.00003 (0.0002)	0.00049 (0.0026)	0.07
12	y	0.16683	0.16687	-0.00004 (0.0004)	0.00034 (0.0031)	-0.12
13	z	0.22900	0.22898	0.00002 (0.0002)	0.00026 (0.0026)	0.06
14	U(1,1)	0.02004	0.02002	0.00002	0.00099	0.02
15	U(2,2)	0.03153	0.03164	-0.00011	0.00130	-0.09
16	U(3,3)	0.01960	0.01961	-0.00001	0.00101	-0.01
17	U(1,2)	0.00029	0.00030	-0.00001	0.00113	-0.01
18	U(1,3)	0.00137	0.00140	-0.00003	0.00088	-0.03
19	U(2,3)	-0.00036	-0.00035	-0.00001	0.00108	-0.01
	Total shift =	0.0004				

Atom no. 3 MG1 (electron count = 12.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	0.25000				
	x	0.00000				
	y	0.00000				
	z	0.50000				
23	U(1,1)	0.01557	0.01540	0.00017	0.00243	0.07
24	U(2,2)	0.02937	0.02959	-0.00022	0.00321	-0.07
25	U(3,3)	0.02067	0.02079	-0.00013	0.00264	-0.05
	U(1,2)	0.00000				
27	U(1,3)	0.00209	0.00214	-0.00005	0.00218	-0.02
	U(2,3)	0.00000				

Total shift = 0.0000

Atom no. 4 MG2 (electron count = 12.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	0.50000				
	x	0.00000				
30	y	0.33191	0.33190	0.00001 (0.0001)	0.00058 (0.0053)	0.02
	z	0.50000				
32	U(1,1)	0.01503	0.01514	-0.00011	0.00162	-0.07
33	U(2,2)	0.03065	0.03062	0.00003	0.00226	0.01
34	U(3,3)	0.01960	0.01955	0.00005	0.00176	0.03
	U(1,2)	0.00000				
36	U(1,3)	0.00085	0.00081	0.00003	0.00147	0.02
	U(2,3)	0.00000				

Total shift = 0.0001

Atom no. 5 F (electron count = 9.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	0.50000				
38	x	0.13098	0.13106	-0.00008 (0.0004)	0.00187 (0.0099)	-0.04
	y	0.50000				
40	z	0.39774	0.39771	0.00003 (0.0003)	0.00100 (0.0102)	0.03
41	U(1,1)	0.03224	0.03310	-0.00086	0.00442	-0.20
42	U(2,2)	0.04510	0.04505	0.00005	0.00538	0.01
43	U(3,3)	0.03722	0.03746	-0.00024	0.00467	-0.05
	U(1,2)	0.00000				
45	U(1,3)	0.00086	0.00162	-0.00075	0.00395	-0.19
	U(2,3)	0.00000				

Total shift = 0.0004

Atom no. 6 O1 (electron count = 8.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	0.50000				
47	x	0.01010	0.01960	-0.00950 (0.0504)	0.00228 (0.0121)	-4.16
	y	0.00000				
49	z	0.17187	0.17164	0.00023 (0.0023)	0.00113 (0.0115)	0.20
50	U(1,1)	0.04008	0.03908	0.00100	0.00547	0.18
51	U(2,2)	0.03091	0.03045	0.00046	0.00521	0.09
52	U(3,3)	0.03308	0.03235	0.00073	0.00508	0.14
	U(1,2)	0.00000				

54	U(1,3)	0.00577	0.00414	0.00163	0.00455	0.36
	U(2,3)	0.00000				
	Total shift =	0.0500				

Atom no. 7 O2 (electron count = 8.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	1.00000				
56	x	0.33190	0.33179	0.00011 (0.0006)	0.00144 (0.0076)	0.08
57	y	0.22518	0.22509	0.00010 (0.0009)	0.00096 (0.0089)	0.10
58	z	0.17311	0.17302	0.00009 (0.0010)	0.00075 (0.0077)	0.13
59	U(1,1)	0.03086	0.03109	-0.00024	0.00329	-0.07
60	U(2,2)	0.04165	0.04126	0.00040	0.00418	0.10
61	U(3,3)	0.03300	0.03317	-0.00017	0.00338	-0.05
62	U(1,2)	-0.00910	-0.00902	-0.00008	0.00342	-0.02
63	U(1,3)	0.00699	0.00709	-0.00010	0.00283	-0.04
64	U(2,3)	-0.00988	-0.00995	0.00007	0.00341	0.02
	Total shift =	0.0014				

Atom no. 8 O3 (electron count = 8.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	1.00000				
65	x	0.13139	0.13136	0.00003 (0.0001)	0.00124 (0.0066)	0.02
66	y	0.16750	0.16746	0.00004 (0.0004)	0.00085 (0.0078)	0.05
67	z	0.39341	0.39342	-0.00002 (0.0002)	0.00064 (0.0066)	-0.03
68	U(1,1)	0.02229	0.02200	0.00029	0.00270	0.11
69	U(2,2)	0.03316	0.03321	-0.00006	0.00347	-0.02
70	U(3,3)	0.02138	0.02133	0.00004	0.00273	0.02
71	U(1,2)	0.00273	0.00324	-0.00051	0.00294	-0.17
72	U(1,3)	0.00166	0.00138	0.00028	0.00239	0.12
73	U(2,3)	-0.00075	-0.00033	-0.00041	0.00287	-0.14
	Total shift =	0.0004				

Largest parameter shift/error = 4.16
Average parameter shift/error = 0.14

LSFM (1.4) 06/11/97 10:54:18 Elapsed time = 0.1 min

PHLOG21 ..... Demonstration Copy - Not for Resale .....

The space group is number 12 -- C12/m1

Refinement cycle no. 2. 732 observations. 58 variables.

Esd of an observation of unit weight = 3.939

Unweighted R factor = 0.129 Weighted R factor = 0.137

ä ³Fo³ = 1.34046E+04

ä ³³Fo³-³Fc³³ = 1.72273E+03

ä W*DELý = 1.04556E+04

ä W*Foý = 5.53207E+05

Scale factor:	New	Old	Shift	Error	SHFT/ERR
	0.97368	0.97430	-0.00062	0.00535	-0.12

Atom no. 1 K (electron count = 19.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	0.25000				
	x	0.00000				
	y	0.50000				
	z	0.00000				
5	U(1,1)	0.07085	0.07033	0.00051	0.00439	0.12
6	U(2,2)	0.07948	0.07941	0.00006	0.00518	0.01
7	U(3,3)	0.05351	0.05336	0.00015	0.00363	0.04
	U(1,2)	0.00000				
9	U(1,3)	0.00906	0.00870	0.00036	0.00342	0.11
	U(2,3)	0.00000				
	Total shift =	0.0000				

Atom no. 2 SI (electron count = 14.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	1.00000				
11	x	0.07686	0.07688	-0.00002 (0.0001)	0.00049 (0.0026)	-0.04
12	y	0.16683	0.16683	0.00000 (0.0000)	0.00033 (0.0031)	0.00
13	z	0.22899	0.22900	-0.00001 (0.0001)	0.00025 (0.0026)	-0.04
14	U(1,1)	0.02000	0.02004	-0.00004	0.00098	-0.04
15	U(2,2)	0.03158	0.03153	0.00005	0.00128	0.04
16	U(3,3)	0.01961	0.01960	0.00002	0.00099	0.02
17	U(1,2)	0.00030	0.00029	0.00001	0.00112	0.01
18	U(1,3)	0.00136	0.00137	-0.00001	0.00086	-0.02
19	U(2,3)	-0.00037	-0.00036	-0.00001	0.00106	-0.01
	Total shift =	0.0001				

Atom no. 3 MG1 (electron count = 12.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	0.25000				
	x	0.00000				
	y	0.00000				
	z	0.50000				
23	U(1,1)	0.01561	0.01557	0.00003	0.00240	0.01
24	U(2,2)	0.02937	0.02937	0.00000	0.00315	0.00
25	U(3,3)	0.02085	0.02067	0.00019	0.00260	0.07
	U(1,2)	0.00000				
27	U(1,3)	0.00224	0.00209	0.00015	0.00215	0.07
	U(2,3)	0.00000				
	Total shift =	0.0000				

Atom no. 4 MG2 (electron count = 12.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	0.50000				
	x	0.00000				

30	y	0.33187	0.33191	-0.00004	(0.0004)	0.00057	(0.0052)	-0.07
	z	0.50000						
32	U(1,1)	0.01505	0.01503	0.00002		0.00160		0.01
33	U(2,2)	0.03073	0.03065	0.00008		0.00223		0.04
34	U(3,3)	0.01956	0.01960	-0.00005		0.00174		-0.03
	U(1,2)	0.00000						
36	U(1,3)	0.00077	0.00085	-0.00008		0.00145		-0.05
	U(2,3)	0.00000						
	Total shift = 0.0004							

Atom no. 5 F (electron count = 9.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	0.50000						
38	x	0.13090	0.13098	-0.00008	(0.0004)	0.00184	(0.0097)	-0.05
	y	0.50000						
40	z	0.39763	0.39774	-0.00010	(0.0011)	0.00098	(0.0101)	-0.11
41	U(1,1)	0.03263	0.03224	0.00039		0.00431		0.09
42	U(2,2)	0.04515	0.04510	0.00005		0.00529		0.01
43	U(3,3)	0.03736	0.03722	0.00014		0.00459		0.03
	U(1,2)	0.00000						
45	U(1,3)	0.00117	0.00086	0.00031		0.00388		0.08
	U(2,3)	0.00000						
	Total shift = 0.0011							

Atom no. 6 O1 (electron count = 8.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	0.50000						
47	x	0.00975	0.01010	-0.00035	(0.0019)	0.00227	(0.0120)	-0.16
	y	0.00000						
49	z	0.17170	0.17187	-0.00017	(0.0017)	0.00112	(0.0115)	-0.15
50	U(1,1)	0.03953	0.04008	-0.00056		0.00548		-0.10
51	U(2,2)	0.03038	0.03091	-0.00053		0.00520		-0.10
52	U(3,3)	0.03257	0.03308	-0.00051		0.00505		-0.10
	U(1,2)	0.00000						
54	U(1,3)	0.00474	0.00577	-0.00103		0.00452		-0.23
	U(2,3)	0.00000						
	Total shift = 0.0023							

Atom no. 7 O2 (electron count = 8.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	1.00000						
56	x	0.33180	0.33190	-0.00010	(0.0005)	0.00142	(0.0075)	-0.07
57	y	0.22517	0.22518	-0.00001	(0.0001)	0.00095	(0.0088)	-0.02
58	z	0.17303	0.17311	-0.00009	(0.0009)	0.00074	(0.0076)	-0.12
59	U(1,1)	0.03109	0.03086	0.00024		0.00323		0.07
60	U(2,2)	0.04176	0.04165	0.00010		0.00414		0.02
61	U(3,3)	0.03320	0.03300	0.00020		0.00333		0.06
62	U(1,2)	-0.00908	-0.00910	0.00002		0.00338		0.01
63	U(1,3)	0.00722	0.00699	0.00024		0.00279		0.08
64	U(2,3)	-0.01004	-0.00988	-0.00016		0.00337		-0.05
	Total shift = 0.0010							

Atom no. 8 O3 (electron count = 8.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	1.00000						
65	x	0.13143	0.13139	0.00005	(0.0002)	0.00123	(0.0065)	0.04
66	y	0.16750	0.16750	0.00000	(0.0000)	0.00084	(0.0077)	0.01
67	z	0.39346	0.39341	0.00005	(0.0005)	0.00064	(0.0065)	0.08
68	U(1,1)	0.02218	0.02229	-0.00011		0.00267		-0.04
69	U(2,2)	0.03322	0.03316	0.00006		0.00343		0.02
70	U(3,3)	0.02139	0.02138	0.00002		0.00270		0.01
71	U(1,2)	0.00306	0.00273	0.00034		0.00291		0.12
72	U(1,3)	0.00155	0.00166	-0.00011		0.00237		-0.05
73	U(2,3)	-0.00059	-0.00075	0.00016		0.00284		0.06

Total shift = 0.0005

Largest parameter shift/error = 0.23
Average parameter shift/error = 0.05

LSFM (1.4) 06/11/97 10:54:22 Elapsed time = 0.1 min

PHLOG21 ..... Demonstration Copy - Not for Resale .....

The space group is number 12 -- C12/m1

Refinement cycle no. 3. 732 observations. 58 variables.

Esd of an observation of unit weight = 3.935

Unweighted R factor = 0.128 Weighted R factor = 0.137

ä ³Fo³ = 1.33960E+04

ä ³³Fo³-³Fc³³ = 1.72093E+03

ä W*DELý = 1.04385E+04

ä W*Foý = 5.52499E+05

Scale factor:	New	Old	Shift	Error	SHFT/ERR
	0.97372	0.97368	0.00004	0.00535	0.01

Atom no. 1 K (electron count = 19.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	0.25000				
	x	0.00000				
	y	0.50000				
	z	0.00000				
5	U(1,1)	0.07094	0.07085	0.00010	0.00442	0.02
6	U(2,2)	0.07908	0.07948	-0.00040	0.00518	-0.08
7	U(3,3)	0.05352	0.05351	0.00001	0.00363	0.00
	U(1,2)	0.00000				
9	U(1,3)	0.00903	0.00906	-0.00003	0.00343	-0.01
	U(2,3)	0.00000				

Total shift = 0.0000

Atom no. 2 SI (electron count = 14.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	1.00000						
11	x	0.07686	0.07686	0.00000	(0.0000)	0.00049	(0.0026)	0.00
12	y	0.16686	0.16683	0.00003	(0.0003)	0.00033	(0.0031)	0.09
13	z	0.22898	0.22899	0.00000	(0.0000)	0.00025	(0.0026)	0.00
14	U(1,1)	0.01998	0.02000	-0.00002		0.00098		-0.02
15	U(2,2)	0.03166	0.03158	0.00008		0.00128		0.06
16	U(3,3)	0.01961	0.01961	0.00000		0.00099		0.00
17	U(1,2)	0.00030	0.00030	0.00000		0.00112		0.00
18	U(1,3)	0.00137	0.00136	0.00001		0.00086		0.02
19	U(2,3)	-0.00037	-0.00037	0.00001		0.00106		0.01

Total shift = 0.0003

Atom no. 3 MG1 (electron count = 12.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	0.25000				
	x	0.00000				
	y	0.00000				
	z	0.50000				
23	U(1,1)	0.01556	0.01561	-0.00004	0.00240	-0.02
24	U(2,2)	0.02957	0.02937	0.00020	0.00315	0.06
25	U(3,3)	0.02084	0.02085	-0.00001	0.00260	0.00
	U(1,2)	0.00000				
27	U(1,3)	0.00227	0.00224	0.00002	0.00215	0.01
	U(2,3)	0.00000				

Total shift = 0.0000

Atom no. 4 MG2 (electron count = 12.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	0.50000						
	x	0.00000						
30	y	0.33191	0.33187	0.00004	(0.0004)	0.00057	(0.0052)	0.07
	z	0.50000						
32	U(1,1)	0.01507	0.01505	0.00002		0.00160		0.01
33	U(2,2)	0.03062	0.03073	-0.00011		0.00223		-0.05
34	U(3,3)	0.01956	0.01956	0.00000		0.00174		0.00
	U(1,2)	0.00000						
36	U(1,3)	0.00076	0.00077	-0.00001		0.00145		-0.01
	U(2,3)	0.00000						

Total shift = 0.0004

Atom no. 5 F (electron count = 9.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	0.50000						
38	x	0.13094	0.13090	0.00004	(0.0002)	0.00184	(0.0098)	0.02
	y	0.50000						
40	z	0.39767	0.39763	0.00004	(0.0004)	0.00098	(0.0101)	0.04
41	U(1,1)	0.03261	0.03263	-0.00002		0.00433		0.00
42	U(2,2)	0.04525	0.04515	0.00010		0.00530		0.02

43	U(3,3)	0.03740	0.03736	0.00004		0.00460			0.01
	U(1,2)	0.00000							
45	U(1,3)	0.00119	0.00117	0.00002		0.00389			0.01
	U(2,3)	0.00000							
	Total shift = 0.0004								

Atom no. 6 O1 (electron count = 8.0)

Parameter		New	Old	Shift		Error			SHFT/ERR
	Mult.	0.50000							
47	x	0.00968	0.00975	-0.00007	(0.0004)	0.00226	(0.0120)		-0.03
	y	0.00000							
49	z	0.17166	0.17170	-0.00004	(0.0004)	0.00111	(0.0114)		-0.03
50	U(1,1)	0.03962	0.03953	0.00009		0.00544			0.02
51	U(2,2)	0.03031	0.03038	-0.00007		0.00514			-0.01
52	U(3,3)	0.03249	0.03257	-0.00008		0.00501			-0.02
	U(1,2)	0.00000							
54	U(1,3)	0.00463	0.00474	-0.00012		0.00450			-0.03
	U(2,3)	0.00000							
	Total shift = 0.0005								

Atom no. 7 O2 (electron count = 8.0)

Parameter		New	Old	Shift		Error			SHFT/ERR
	Mult.	1.00000							
56	x	0.33180	0.33180	-0.00001	(0.0000)	0.00142	(0.0075)		-0.01
57	y	0.22512	0.22517	-0.00005	(0.0004)	0.00095	(0.0088)		-0.05
58	z	0.17302	0.17303	-0.00001	(0.0001)	0.00074	(0.0076)		-0.01
59	U(1,1)	0.03115	0.03109	0.00006		0.00324			0.02
60	U(2,2)	0.04126	0.04176	-0.00050		0.00415			-0.12
61	U(3,3)	0.03320	0.03320	0.00000		0.00334			0.00
62	U(1,2)	-0.00903	-0.00908	0.00005		0.00339			0.02
63	U(1,3)	0.00717	0.00722	-0.00006		0.00279			-0.02
64	U(2,3)	-0.00996	-0.01004	0.00007		0.00337			0.02
	Total shift = 0.0004								

Atom no. 8 O3 (electron count = 8.0)

Parameter		New	Old	Shift		Error			SHFT/ERR
	Mult.	1.00000							
65	x	0.13141	0.13143	-0.00002	(0.0001)	0.00123	(0.0065)		-0.02
66	y	0.16748	0.16750	-0.00002	(0.0002)	0.00084	(0.0077)		-0.03
67	z	0.39344	0.39346	-0.00002	(0.0002)	0.00063	(0.0065)		-0.03
68	U(1,1)	0.02220	0.02218	0.00002		0.00267			0.01
69	U(2,2)	0.03315	0.03322	-0.00007		0.00343			-0.02
70	U(3,3)	0.02138	0.02139	-0.00002		0.00270			-0.01
71	U(1,2)	0.00321	0.00306	0.00015		0.00290			0.05
72	U(1,3)	0.00155	0.00155	0.00000		0.00236			0.00
73	U(2,3)	-0.00035	-0.00059	0.00024		0.00284			0.09
	Total shift = 0.0003								

Largest parameter shift/error = 0.12
Average parameter shift/error = 0.02

LSFM (1.4) 06/11/97 10:54:25 Elapsed time = 0.1 min

PHLOG21 ..... Demonstration Copy - Not for Resale .....

The space group is number 12 -- C12/m1

Refinement cycle no. 4. 732 observations. 58 variables.

Esd of an observation of unit weight = 3.935

Unweighted R factor = 0.128 Weighted R factor = 0.137

ä ³Fo³ = 1.33966E+04

ä ³³Fo³-³Fc³³ = 1.72108E+03

ä W*DELý = 1.04385E+04

ä W*Foý = 5.52550E+05

Scale factor:	New	Old	Shift	Error	SHFT/ERR
	0.97372	0.97372	-0.00001	0.00534	0.00

Atom no. 1 K (electron count = 19.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	0.25000				
	x	0.00000				
	y	0.50000				
	z	0.00000				
5	U(1,1)	0.07095	0.07094	0.00001	0.00442	0.00
6	U(2,2)	0.07907	0.07908	0.00000	0.00516	0.00
7	U(3,3)	0.05351	0.05352	-0.00001	0.00363	0.00
	U(1,2)	0.00000				
9	U(1,3)	0.00903	0.00903	0.00000	0.00343	0.00
	U(2,3)	0.00000				

Total shift = 0.0000

Atom no. 2 SI (electron count = 14.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	1.00000				
11	x	0.07686	0.07686	0.00000 (0.0000)	0.00049 (0.0026)	0.00
12	y	0.16686	0.16686	0.00000 (0.0000)	0.00033 (0.0031)	0.00
13	z	0.22898	0.22898	0.00000 (0.0000)	0.00025 (0.0026)	0.00
14	U(1,1)	0.01998	0.01998	0.00000	0.00098	0.00
15	U(2,2)	0.03166	0.03166	0.00000	0.00128	0.00
16	U(3,3)	0.01961	0.01961	0.00000	0.00099	0.00
17	U(1,2)	0.00029	0.00030	0.00000	0.00112	0.00
18	U(1,3)	0.00137	0.00137	0.00000	0.00086	0.00
19	U(2,3)	-0.00037	-0.00037	0.00000	0.00106	0.00

Total shift = 0.0000

Atom no. 3 MG1 (electron count = 12.0)

Parameter	New	Old	Shift	Error	SHFT/ERR

	Mult.	0.25000						
	x	0.00000						
	y	0.00000						
	z	0.50000						
23	U(1,1)	0.01556	0.01556	0.00000		0.00240		0.00
24	U(2,2)	0.02955	0.02957	-0.00001		0.00316		0.00
25	U(3,3)	0.02085	0.02084	0.00001		0.00260		0.00
	U(1,2)	0.00000						
27	U(1,3)	0.00227	0.00227	0.00000		0.00215		0.00
	U(2,3)	0.00000						
	Total shift =	0.0000						

Atom no. 4 MG2 (electron count = 12.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	0.50000						
	x	0.00000						
30	y	0.33191	0.33191	0.00000	(0.0000)	0.00057	(0.0052)	0.00
	z	0.50000						
32	U(1,1)	0.01507	0.01507	0.00000		0.00160		0.00
33	U(2,2)	0.03063	0.03062	0.00001		0.00222		0.01
34	U(3,3)	0.01955	0.01956	0.00000		0.00174		0.00
	U(1,2)	0.00000						
36	U(1,3)	0.00076	0.00076	0.00000		0.00145		0.00
	U(2,3)	0.00000						
	Total shift =	0.0000						

Atom no. 5 F (electron count = 9.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	0.50000						
38	x	0.13094	0.13094	0.00000	(0.0000)	0.00184	(0.0098)	0.00
	y	0.50000						
40	z	0.39767	0.39767	0.00000	(0.0000)	0.00098	(0.0101)	0.00
41	U(1,1)	0.03262	0.03261	0.00000		0.00433		0.00
42	U(2,2)	0.04524	0.04525	0.00000		0.00531		0.00
43	U(3,3)	0.03740	0.03740	0.00000		0.00460		0.00
	U(1,2)	0.00000						
45	U(1,3)	0.00120	0.00119	0.00000		0.00389		0.00
	U(2,3)	0.00000						
	Total shift =	0.0000						

Atom no. 6 O1 (electron count = 8.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	0.50000						
47	x	0.00967	0.00968	-0.00001	(0.0000)	0.00226	(0.0120)	0.00
	y	0.00000						
49	z	0.17166	0.17166	0.00000	(0.0000)	0.00111	(0.0114)	0.00
50	U(1,1)	0.03961	0.03962	0.00000		0.00544		0.00
51	U(2,2)	0.03032	0.03031	0.00002		0.00513		0.00
52	U(3,3)	0.03249	0.03249	0.00000		0.00501		0.00
	U(1,2)	0.00000						
54	U(1,3)	0.00461	0.00463	-0.00002		0.00450		0.00
	U(2,3)	0.00000						

Total shift = 0.0000

Atom no. 7 O2 (electron count = 8.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	1.00000						
56	x	0.33179	0.33180	0.00000	(0.0000)	0.00142	(0.0075)	0.00
57	y	0.22511	0.22512	-0.00001	(0.0001)	0.00095	(0.0087)	-0.01
58	z	0.17302	0.17302	0.00000	(0.0000)	0.00074	(0.0076)	0.00
59	U(1,1)	0.03117	0.03115	0.00002		0.00324		0.01
60	U(2,2)	0.04126	0.04126	0.00000		0.00412		0.00
61	U(3,3)	0.03320	0.03320	0.00000		0.00334		0.00
62	U(1,2)	-0.00904	-0.00903	-0.00001		0.00337		0.00
63	U(1,3)	0.00716	0.00717	0.00000		0.00279		0.00
64	U(2,3)	-0.00997	-0.00996	-0.00001		0.00336		0.00

Total shift = 0.0001

Atom no. 8 O3 (electron count = 8.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	1.00000						
65	x	0.13141	0.13141	0.00000	(0.0000)	0.00123	(0.0065)	0.00
66	y	0.16748	0.16748	0.00000	(0.0000)	0.00084	(0.0077)	0.00
67	z	0.39344	0.39344	0.00000	(0.0000)	0.00063	(0.0065)	0.00
68	U(1,1)	0.02220	0.02220	0.00000		0.00267		0.00
69	U(2,2)	0.03315	0.03315	0.00000		0.00342		0.00
70	U(3,3)	0.02138	0.02138	0.00000		0.00269		0.00
71	U(1,2)	0.00321	0.00321	0.00000		0.00290		0.00
72	U(1,3)	0.00155	0.00155	0.00000		0.00236		0.00
73	U(2,3)	-0.00034	-0.00035	0.00000		0.00283		0.00

Total shift = 0.0000

Largest parameter shift/error = 0.01
Average parameter shift/error = 0.00

The calculations have converged with a shift/error less than 0.100

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
1	0	0	2	23.160	23.907	0.09909	-0.747	-0.747	
2	0	2	0	37.546	37.432	0.10892	0.115	0.115	
3	1	1	0	31.118	30.621	0.11015	0.497	0.497	
4	1	1	-1	17.159	15.432	0.11372	1.727	1.727	
5	0	2	1	8.979	10.331	0.11966	-1.352	-1.352	
6	1	1	1	34.798	37.948	0.12745	-3.150	-3.150	*
7	1	1	-2	57.289	63.465	0.13653	-6.175	-6.175	**
8	0	2	2	69.553	81.584	0.14725	-12.031	-12.031	***
9	0	0	3	87.167	101.507	0.14864	-14.339	-14.339	***
10	1	1	2	75.242	86.481	0.15895	-11.239	-11.239	***
11	1	1	-3	66.356	77.888	0.17106	-11.532	-11.532	***
12	0	2	3	52.719	57.257	0.18427	-4.537	-4.537	**
13	2	0	-1	50.386	53.772	0.18925	-3.386	-3.386	*
14	1	3	0	50.635	52.114	0.18937	-1.479	-1.479	
15	2	0	0	102.195	109.202	0.19150	-7.007	-7.007	**

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
16	1	3	-1	103.446	106.445	0.19147	-2.999	-2.999	*
17	1	1	3	32.226	32.648	0.19797	-0.421	-0.421	
18	0	0	4	45.765	55.397	0.19818	-9.632	-9.632	***
19	2	0	-2	49.107	42.830	0.19967	6.278	6.278	**
20	1	3	1	51.970	44.609	0.19993	7.362	7.362	**
21	1	3	-2	89.179	84.043	0.20584	5.136	5.136	**
22	2	0	1	90.343	89.141	0.20600	1.201	1.201	
23	1	1	-4	12.316	12.207	0.21163	0.109	0.109	
24	0	4	0	38.199	39.519	0.21784	-1.320	-1.320	
25	2	2	-1	37.027	36.850	0.21835	0.177	0.177	
26	2	2	0	37.185	36.760	0.22031	0.426	0.426	
27	2	0	-3	38.721	35.936	0.22098	2.785	2.785	*
28	1	3	2	39.076	34.401	0.22134	4.675	4.675	**
29	0	4	1	34.738	33.403	0.22340	1.334	1.334	
30	0	2	4	3.197	4.754	0.22614	-1.557	-1.557	
31	2	2	-2	34.607	34.017	0.22745	0.591	0.591	
32	1	3	-3	90.168	90.575	0.23019	-0.407	-0.407	
33	2	0	2	93.889	94.673	0.23046	-0.784	-0.784	
34	2	2	1	31.762	32.119	0.23302	-0.357	-0.357	
35	0	4	2	22.880	26.499	0.23932	-3.619	-3.619	*
36	1	1	4	11.805	11.849	0.24090	-0.044	-0.044	
37	2	2	-3	11.285	16.204	0.24636	-4.920	-4.920	**
38	0	0	5	87.776	100.557	0.24773	-12.781	-12.781	***
39	2	0	-4	73.094	69.452	0.25040	3.642	3.642	*
40	1	3	3	72.268	70.918	0.25084	1.350	1.350	
41	2	2	2	5.054	2.388	0.25490	2.666	2.666	*
42	1	1	-5	14.303	11.630	0.25539	2.673	2.673	*
43	1	3	-4	43.977	42.448	0.26175	1.530	1.530	
44	2	0	3	45.780	44.259	0.26210	1.521	1.521	
45	0	4	3	16.953	13.054	0.26372	3.899	3.899	*
46	0	2	5	11.325	8.423	0.27062	2.902	2.902	*
47	2	2	-4	25.861	24.134	0.27307	1.728	1.728	
48	2	2	3	27.113	27.372	0.28383	-0.259	-0.259	
49	2	0	-5	38.405	38.295	0.28545	0.109	0.109	
50	1	3	4	37.758	38.718	0.28594	-0.960	-0.960	
51	1	1	5	4.622	0.828	0.28597	3.795	3.795	*
52	3	1	-1	26.855	23.130	0.28803	3.726	3.726	*
53	2	4	-1	30.566	23.977	0.28856	6.589	6.589	**
54	1	5	0	17.399	13.164	0.28864	4.236	4.236	**
55	2	4	0	2.512	0.608	0.29004	1.904	1.904	
56	1	5	-1	23.071	21.194	0.29003	1.876	1.876	
57	3	1	-2	15.765	14.728	0.29217	1.037	1.037	
58	3	1	0	8.204	8.620	0.29236	-0.416	-0.416	
59	0	4	4	23.647	23.787	0.29450	-0.140	-0.140	
60	2	4	-2	8.203	7.088	0.29550	1.115	1.115	
61	1	5	1	35.638	32.441	0.29568	3.197	3.197	*
62	0	0	6	23.019	22.046	0.29728	0.973	0.973	
63	1	3	-5	100.721	107.384	0.29825	-6.662	-6.662	**
64	2	0	4	105.219	112.076	0.29865	-6.856	-6.856	**
65	1	5	-2	26.670	22.809	0.29971	3.861	3.861	*

| --- | - | - | - | ----- | ----- | ------ | ----- | -------- | ---- |
66	2	4	1	50.213	45.925	0.29982	4.288	4.288	**
67	1	1	-6	6.367	8.510	0.30095	-2.142	-2.142	*
68	3	1	-3	57.405	57.521	0.30441	-0.116	-0.116	
69	3	1	1	35.424	36.383	0.30479	-0.959	-0.959	
70	2	2	-5	12.420	12.557	0.30553	-0.138	-0.138	
71	2	4	-3	40.688	39.085	0.31030	1.603	1.603	
72	1	5	2	57.288	53.535	0.31056	3.753	3.753	*
73	0	2	6	17.415	19.759	0.31660	-2.343	-2.343	*
74	1	5	-3	37.520	37.536	0.31693	-0.017	-0.017	
75	2	4	2	46.707	45.600	0.31712	1.107	1.107	
76	2	2	4	2.221	0.685	0.31789	1.536	1.536	
77	3	1	-4	27.707	28.581	0.32386	-0.874	-0.874	
78	3	1	2	33.079	32.373	0.32439	0.706	0.706	
79	2	0	-6	79.143	82.979	0.32431	-3.836	-3.836	*
80	1	3	5	78.657	81.930	0.32482	-3.273	-3.273	*
81	3	3	-1	136.922	135.983	0.32664	0.939	0.939	
82	0	6	0	134.986	126.761	0.32676	8.225	8.225	***
83	0	4	5	15.424	15.504	0.32989	-0.080	-0.080	
84	3	3	-2	52.801	47.798	0.33029	5.003	5.003	**
85	3	3	0	53.481	48.537	0.33046	4.944	4.944	**
86	0	6	1	51.861	44.016	0.33050	7.845	7.845	**
87	2	4	-4	21.291	20.378	0.33190	0.913	0.913	
88	1	5	3	9.707	8.004	0.33223	1.703	1.703	
89	1	1	6	27.567	28.863	0.33233	-1.296	-1.296	
90	1	3	-6	48.940	46.604	0.33808	2.335	2.335	*
91	2	0	5	49.993	50.290	0.33852	-0.297	-0.297	
92	1	5	-4	11.839	11.889	0.34054	-0.050	-0.050	
93	2	4	3	7.525	7.742	0.34081	-0.217	-0.217	
94	3	3	-3	5.490	6.144	0.34117	-0.654	-0.654	
95	0	6	2	4.879	4.412	0.34146	0.467	0.467	
96	3	3	1	5.169	5.165	0.34150	0.003	0.003	
97	2	2	-6	27.108	29.700	0.34211	-2.592	-2.592	*
98	0	0	7	48.126	51.753	0.34682	-3.627	-3.627	*
99	1	1	-7	31.477	31.542	0.34761	-0.065	-0.065	
100	3	1	-5	17.975	17.381	0.34930	0.594	0.594	
101	3	1	3	1.927	0.181	0.34996	1.746	1.746	
102	2	2	5	42.348	42.970	0.35561	-0.621	-0.621	
103	3	3	-4	32.303	27.289	0.35863	5.014	5.014	**
104	0	6	3	32.329	25.220	0.35898	7.109	7.109	**
105	2	4	-5	4.092	3.441	0.35908	0.651	0.651	
106	3	3	2	32.484	28.245	0.35910	4.240	4.240	**
107	1	5	4	23.478	21.738	0.35946	1.740	1.740	
108	0	2	7	29.446	31.152	0.36352	-1.706	-1.706	
109	2	0	-7	107.018	112.718	0.36576	-5.699	-5.699	**
110	1	3	6	107.416	115.481	0.36629	-8.066	-8.066	***
111	0	4	6	48.832	48.530	0.36855	0.302	0.302	
112	1	5	-5	7.445	4.176	0.36933	3.269	3.269	*
113	2	4	4	22.316	19.699	0.36966	2.616	2.616	*
114	4	0	-1	57.949	54.293	0.37751	3.656	3.656	*
115	2	6	-1	57.771	51.149	0.37761	6.621	6.621	**
116	4	0	-2	85.064	80.355	0.37849	4.709	4.709	**

117	2	6	0	86.823	73.544	0.37874	13.279	13.279	***
118	1	1	7	21.310	22.185	0.37948	-0.875	-0.875	
119	3	1	-6	16.841	15.756	0.37954	1.085	1.085	
120	1	3	-7	21.368	21.896	0.38021	-0.527	-0.527	
121	3	1	4	3.813	1.751	0.38029	2.062	2.062	*
122	2	0	6	22.016	23.885	0.38067	-1.870	-1.870	
123	2	2	-7	50.118	50.798	0.38163	-0.680	-0.680	
124	3	3	-5	58.787	53.494	0.38176	5.294	5.294	**
125	0	6	4	60.863	49.900	0.38216	10.963	10.963	***
126	3	3	3	61.323	53.940	0.38236	7.383	7.383	**
127	2	6	-2	6.506	5.518	0.38294	0.989	0.989	
128	4	0	0	5.922	6.573	0.38299	-0.651	-0.651	
129	4	0	-3	79.317	73.342	0.38589	5.975	5.975	**
130	2	6	1	84.236	67.248	0.38628	16.988	16.988	****

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
131	2	4	-6	2.056	4.031	0.39068	-1.975	-1.975	
132	1	5	5	8.514	4.858	0.39111	3.656	3.656	*
133	3	5	-1	29.768	25.238	0.39261	4.530	4.530	**
134	4	2	-1	17.284	14.995	0.39291	2.289	2.289	*
135	1	7	0	29.546	26.079	0.39306	3.467	3.467	*
136	4	2	-2	26.907	25.153	0.39385	1.753	1.753	
137	1	7	-1	2.866	0.549	0.39408	2.317	2.317	*
138	2	6	-3	64.847	50.777	0.39447	14.069	14.069	***
139	4	0	1	64.237	57.183	0.39467	7.054	7.054	**
140	1	1	-8	10.748	11.230	0.39496	-0.482	-0.482	
141	3	5	-2	15.823	12.788	0.39566	3.034	3.034	*
142	3	5	0	13.228	13.260	0.39580	-0.031	-0.031	
143	2	2	6	44.454	44.106	0.39595	0.348	0.348	
144	0	0	8	51.422	58.413	0.39637	-6.991	-6.991	**
145	4	2	0	30.318	28.398	0.39818	1.921	1.921	
146	1	7	1	2.692	2.882	0.39826	-0.190	-0.190	
147	4	0	-4	14.251	13.520	0.39934	0.731	0.731	
148	2	6	2	14.942	13.129	0.39986	1.813	1.813	
149	4	2	-3	13.950	11.550	0.40096	2.400	2.400	*
150	1	7	-2	41.734	36.209	0.40126	5.525	5.525	**
151	1	5	-6	8.379	6.701	0.40219	1.678	1.678	
152	2	4	5	6.295	5.826	0.40256	0.468	0.468	
153	3	5	-3	50.069	45.442	0.40478	4.627	4.627	**
154	3	5	1	23.321	19.935	0.40507	3.386	3.386	*
155	2	0	-8	28.723	30.313	0.40901	-1.590	-1.590	
156	1	7	2	29.672	25.016	0.40942	4.656	4.656	**
157	4	2	1	47.800	45.449	0.40942	2.350	2.350	*
158	0	4	7	32.082	31.717	0.40956	0.365	0.365	
159	1	3	7	29.933	30.506	0.40955	-0.572	-0.572	
160	3	3	-6	31.057	29.898	0.40960	1.159	1.159	
161	0	6	5	32.235	30.069	0.41005	2.166	2.166	*
162	3	3	4	32.054	31.853	0.41030	0.202	0.202	
163	0	2	8	2.042	0.932	0.41106	1.110	1.110	
164	2	6	-4	19.700	13.418	0.41167	6.281	6.281	**
165	4	0	2	19.932	18.126	0.41200	1.806	1.806	

166	3	1	-7	17.888	17.641	0.41351	0.246	0.246	
167	4	2	-4	30.126	28.260	0.41393	1.866	1.866	
168	1	7	-3	39.245	34.072	0.41428	5.173	5.173	**
169	3	1	5	14.134	14.278	0.41434	-0.145	-0.145	
170	4	0	-5	36.004	34.518	0.41826	1.486	1.486	
171	2	6	3	37.699	32.494	0.41889	5.205	5.205	**
172	3	5	-4	23.632	20.849	0.41960	2.782	2.782	*
173	3	5	2	29.013	26.401	0.42001	2.612	2.612	*
174	2	2	-8	15.158	15.698	0.42326	-0.540	-0.540	
175	1	3	-8	16.252	16.832	0.42394	-0.581	-0.581	
176	2	0	7	15.925	18.380	0.42442	-2.455	-2.455	*
177	2	4	-7	17.186	16.808	0.42571	0.379	0.379	
178	1	7	3	21.198	18.743	0.42610	2.456	2.456	*
179	4	2	2	6.355	5.381	0.42616	0.974	0.974	
180	1	5	6	29.420	27.367	0.42617	2.052	2.052	*
181	1	1	8	5.285	6.354	0.42718	-1.070	-1.070	
182	4	2	-5	12.423	11.383	0.43221	1.040	1.040	
183	1	7	-4	10.527	9.610	0.43261	0.917	0.917	
184	2	6	-5	17.848	14.718	0.43389	3.130	3.130	*
185	4	0	3	17.420	15.758	0.43433	1.662	1.662	
186	0	8	0	6.183	2.432	0.43568	3.751	3.751	*
187	4	4	-1	1.217	0.643	0.43586	0.574	0.574	
188	4	4	-2	3.162	3.852	0.43671	-0.690	-0.690	
189	1	5	-7	19.825	16.470	0.43819	3.355	3.355	*
190	2	2	7	2.197	0.652	0.43818	1.546	1.546	
191	0	8	1	11.300	8.944	0.43849	2.356	2.356	*
192	2	4	6	30.876	28.901	0.43860	1.975	1.975	
193	3	5	-5	20.577	18.630	0.43954	1.947	1.947	
194	3	5	3	3.777	3.208	0.44006	0.569	0.569	
195	4	4	0	14.997	13.910	0.44061	1.088	1.088	

No.	h	k	l	Fo	Fc	sinθ/λ	Fo-Fc	w(Fo-Fc)	Flag
196	3	3	-7	11.745	12.124	0.44127	-0.380	-0.380	
197	0	6	6	12.498	11.609	0.44175	0.890	0.890	
198	4	0	-6	87.120	81.481	0.44195	5.639	5.639	**
199	3	3	5	12.853	11.903	0.44205	0.951	0.951	
200	2	6	4	87.926	75.285	0.44268	12.641	12.641	***
201	1	1	-9	7.024	6.429	0.44280	0.596	0.596	
202	4	4	-3	19.457	15.752	0.44313	3.705	3.705	*
203	0	0	9	18.666	19.677	0.44591	-1.011	-1.011	
204	0	8	2	19.655	15.695	0.44681	3.960	3.960	*
205	1	7	4	1.686	0.289	0.44766	1.397	1.397	
206	4	2	3	26.558	25.583	0.44778	0.974	0.974	
207	3	1	-8	28.971	27.400	0.45039	1.571	1.571	
208	4	4	1	16.388	15.262	0.45079	1.125	1.125	
209	3	1	6	16.171	16.212	0.45127	-0.041	-0.041	
210	0	4	8	16.324	14.588	0.45228	1.737	1.737	
211	2	0	-9	12.812	13.159	0.45355	-0.347	-0.347	
212	1	3	8	13.378	14.183	0.45411	-0.805	-0.805	
213	4	4	-4	11.082	9.374	0.45489	1.708	1.708	
214	4	2	-6	3.317	2.144	0.45518	1.173	1.173	

215	1	7	-5	24.865	21.418	0.45562	3.447	3.447	*
216	0	2	9	3.238	4.734	0.45902	-1.496	-1.496	
217	0	8	3	3.278	1.514	0.46034	1.764	1.764	
218	2	6	-6	65.911	57.746	0.46038	8.166	8.166	***
219	4	0	4	69.493	65.893	0.46092	3.600	3.600	*
220	2	4	-8	10.383	8.398	0.46340	1.985	1.985	
221	1	5	7	20.513	18.904	0.46389	1.609	1.609	
222	3	5	-6	20.030	18.945	0.46393	1.085	1.085	
223	3	5	4	2.709	2.347	0.46454	0.361	0.361	
224	4	4	2	5.821	6.443	0.46605	-0.622	-0.622	
225	2	2	-9	24.944	24.300	0.46645	0.644	0.644	
226	1	3	-9	53.702	51.963	0.46883	1.739	1.739	
227	2	0	8	51.640	55.394	0.46933	-3.754	-3.754	*
228	4	0	-7	17.834	14.741	0.46969	3.094	3.094	*
229	2	6	5	17.531	14.434	0.47050	3.098	3.098	*
230	4	4	-5	13.140	11.584	0.47159	1.555	1.555	
231	1	7	5	1.408	0.630	0.47344	0.778	0.778	
232	4	2	4	11.649	9.968	0.47362	1.681	1.681	
233	3	7	-1	8.156	9.055	0.47469	-0.899	-0.899	
234	5	1	-2	10.030	9.299	0.47479	0.732	0.732	
235	2	8	-1	8.769	9.600	0.47501	-0.832	-0.832	
236	1	1	9	3.204	0.657	0.47526	2.547	2.547	*
237	5	1	-1	7.265	6.982	0.47575	0.283	0.283	
238	2	8	0	3.143	1.846	0.47591	1.297	1.297	
239	3	3	-8	45.369	43.257	0.47600	2.112	2.112	*
240	0	6	7	47.215	41.187	0.47651	6.028	6.028	**
241	1	5	-8	1.845	1.425	0.47663	0.420	0.420	
242	3	3	6	46.161	45.408	0.47684	0.753	0.753	
243	2	4	7	12.407	10.495	0.47706	1.912	1.912	
244	3	7	-2	2.493	1.629	0.47721	0.864	0.864	
245	3	7	0	3.929	4.417	0.47733	-0.487	-0.487	
246	0	8	4	16.257	13.331	0.47864	2.926	2.926	*
247	5	1	-3	15.711	14.150	0.47898	1.562	1.562	
248	2	8	-2	5.628	5.555	0.47926	0.073	0.073	
249	5	1	0	15.502	13.541	0.48183	1.961	1.961	
250	2	2	8	27.814	27.053	0.48180	0.761	0.761	
251	2	8	1	17.483	18.271	0.48193	-0.788	-0.788	
252	4	2	-7	3.111	2.770	0.48216	0.342	0.342	
253	1	7	-6	1.323	0.473	0.48264	0.850	0.850	
254	3	7	-3	14.658	15.685	0.48480	-1.027	-1.027	
255	3	7	1	18.603	22.124	0.48504	-3.521	-3.521	*
256	4	4	3	12.406	12.879	0.48590	-0.473	-0.473	
257	5	1	-4	24.791	21.829	0.48818	2.962	2.962	*
258	2	8	-3	15.055	15.447	0.48852	-0.392	-0.392	
259	3	1	-9	1.378	2.005	0.48950	-0.627	-0.627	
260	2	6	-7	62.746	52.528	0.49046	10.218	10.218	***

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
261	3	1	7	5.562	5.554	0.49044	0.008	0.008	
262	1	1	-10	6.412	5.686	0.49098	0.726	0.726	
263	4	0	5	64.798	64.528	0.49109	0.269	0.269	

264	3	5	-7	11.787	10.677	0.49211	1.110	1.110	
265	4	4	-6	7.393	6.614	0.49272	0.779	0.779	
266	2	8	2	11.789	13.463	0.49288	-1.674	-1.674	
267	5	1	1	17.006	15.295	0.49284	1.711	1.711	
268	3	5	5	6.468	6.111	0.49281	0.357	0.357	
269	0	0	10	33.252	32.544	0.49546	0.709	0.709	
270	0	4	9	22.479	22.003	0.49628	0.476	0.476	
271	3	7	-4	6.484	8.164	0.49724	-1.680	-1.680	
272	3	7	2	6.452	6.246	0.49759	0.206	0.206	
273	2	0	-10	48.882	47.699	0.49904	1.182	1.182	
274	5	3	-2	21.352	21.709	0.49915	-0.357	-0.357	
275	4	6	-1	17.449	20.919	0.49929	-3.469	-3.469	*
276	1	9	0	18.986	19.410	0.49941	-0.424	-0.424	
277	1	3	9	50.371	48.866	0.49960	1.505	1.505	
278	4	6	-2	28.930	32.194	0.50003	-3.265	-3.265	*
279	5	3	-1	34.473	34.636	0.50006	-0.163	-0.163	
280	1	9	-1	31.002	27.227	0.50021	3.775	3.775	*
281	4	0	-8	11.252	10.638	0.50081	0.614	0.614	
282	0	8	5	1.915	1.110	0.50119	0.805	0.805	
283	2	6	6	11.232	10.450	0.50168	0.782	0.782	
284	5	1	-5	2.055	0.397	0.50213	1.658	1.658	
285	2	8	-4	1.868	1.704	0.50252	0.164	0.164	
286	1	7	6	9.236	6.248	0.50280	2.988	2.988	*
287	4	2	5	22.919	21.394	0.50302	1.524	1.524	
288	2	4	-9	9.411	8.508	0.50315	0.903	0.903	
289	5	3	-3	4.049	4.268	0.50314	-0.219	-0.219	
290	4	6	0	3.029	2.131	0.50344	0.898	0.898	
291	1	9	1	3.286	2.528	0.50351	0.758	0.758	
292	1	5	8	4.879	5.314	0.50365	-0.434	-0.434	
293	4	6	-3	43.780	50.820	0.50565	-7.040	-7.040	**
294	5	3	0	52.018	56.822	0.50585	-4.804	-4.804	**
295	1	9	-2	47.191	45.663	0.50588	1.528	1.528	
296	0	2	10	10.283	8.834	0.50729	1.449	1.449	
297	5	1	2	3.472	3.600	0.50846	-0.128	-0.128	
298	2	8	3	4.473	5.076	0.50845	-0.603	-0.603	
299	4	4	4	7.639	7.876	0.50981	-0.237	-0.237	
300	2	2	-10	13.375	13.809	0.51079	-0.435	-0.435	
301	5	3	-4	27.016	25.462	0.51191	1.554	1.554	
302	4	6	1	21.773	24.138	0.51238	-2.364	-2.364	*
303	1	9	2	22.724	19.967	0.51238	2.757	2.757	*
304	4	2	-8	10.769	9.983	0.51252	0.786	0.786	
305	1	7	-7	27.206	22.848	0.51302	4.358	4.358	**
306	3	3	-9	48.712	46.571	0.51317	2.141	2.141	*
307	0	6	8	50.391	44.176	0.51369	6.215	6.215	**
308	3	3	7	50.583	49.634	0.51406	0.949	0.949	
309	3	7	-5	4.888	4.441	0.51417	0.448	0.448	
310	1	3	-10	2.226	2.913	0.51457	-0.687	-0.687	
311	3	7	3	8.831	11.032	0.51462	-2.201	-2.201	*
312	2	0	9	1.603	3.565	0.51508	-1.962	-1.962	
313	4	6	-4	12.997	14.624	0.51599	-1.626	-1.626	
314	1	9	-3	14.216	13.661	0.51627	0.556	0.556	
315	5	3	1	15.433	18.272	0.51635	-2.839	-2.839	*

316	1	5	-9	9.037	6.456	0.51697	2.582	2.582	*
317	2	4	8	8.379	7.866	0.51742	0.513	0.513	
318	4	4	-7	15.215	14.586	0.51775	0.629	0.629	
319	5	1	-6	14.479	13.633	0.52044	0.847	0.847	
320	2	8	-5	5.564	4.865	0.52087	0.699	0.699	
321	3	5	-8	26.626	24.194	0.52348	2.432	2.432	*
322	2	6	-8	21.275	18.644	0.52351	2.630	2.630	*
323	1	1	10	13.243	13.886	0.52361	-0.644	-0.644	
324	4	0	6	22.752	22.279	0.52420	0.473	0.473	
325	3	5	6	8.359	7.249	0.52424	1.110	1.110	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
326	5	3	-5	19.761	18.097	0.52523	1.664	1.664	
327	1	9	3	16.792	15.032	0.52580	1.760	1.760	
328	4	6	2	16.428	18.688	0.52585	-2.260	-2.260	*
329	2	2	9	3.171	3.582	0.52647	-0.412	-0.412	
330	0	8	6	23.308	18.830	0.52744	4.478	4.478	**
331	5	1	3	7.668	7.084	0.52829	0.584	0.584	
332	2	8	4	10.190	11.104	0.52822	-0.914	-0.914	
333	3	1	-10	7.130	6.862	0.53036	0.268	0.268	
334	4	6	-5	5.262	6.615	0.53077	-1.353	-1.353	
335	1	9	-4	5.946	4.421	0.53109	1.525	1.525	
336	5	3	2	6.172	8.017	0.53128	-1.845	-1.845	
337	3	1	8	3.844	4.934	0.53134	-1.090	-1.090	
338	4	0	-9	1.706	2.177	0.53471	-0.470	-0.470	
339	3	7	-6	3.515	3.021	0.53517	0.494	0.494	
340	1	7	7	4.595	2.383	0.53514	2.211	2.211	*
341	4	2	6	20.006	18.279	0.53540	1.727	1.727	
342	2	6	7	2.842	0.603	0.53564	2.239	2.239	*
343	3	7	4	5.094	6.254	0.53571	-1.160	-1.160	
344	4	4	5	21.689	23.495	0.53723	-1.807	-1.807	
345	1	1	-11	13.788	14.596	0.53940	-0.808	-0.808	
346	0	4	10	7.381	5.201	0.54123	2.179	2.179	*
347	5	1	-7	1.787	1.056	0.54268	0.731	0.731	
348	5	3	-6	6.243	3.492	0.54276	2.751	2.751	*
349	1	9	4	4.998	3.566	0.54342	1.431	1.431	
350	4	6	3	4.923	4.383	0.54352	0.540	0.540	
351	2	4	-10	3.024	1.228	0.54451	1.796	1.796	
352	5	5	-2	4.427	6.249	0.54461	-1.822	-1.822	
353	0	10	0	2.619	3.504	0.54460	-0.884	-0.884	
354	0	0	11	39.445	40.438	0.54500	-0.992	-0.992	
355	1	5	9	4.743	5.900	0.54503	-1.157	-1.157	
356	2	0	-11	15.141	16.152	0.54523	-1.011	-1.011	
357	5	5	-1	1.944	1.381	0.54545	0.563	0.563	
358	4	2	-9	2.053	2.493	0.54570	-0.440	-0.440	
359	1	3	10	15.786	16.249	0.54580	-0.463	-0.463	
360	4	4	-8	24.372	21.665	0.54614	2.707	2.707	*
361	1	7	-8	12.493	9.997	0.54622	2.496	2.496	*
362	0	10	1	1.429	1.782	0.54685	-0.353	-0.353	
363	5	5	-3	6.590	7.586	0.54827	-0.997	-0.997	
364	4	6	-6	45.517	52.775	0.54963	-7.258	-7.258	**

365	1	9	-5	50.764	47.457	0.55000	3.306	3.306	*
366	5	3	3	51.797	58.809	0.55028	-7.012	-7.012	**
367	5	5	0	10.453	11.808	0.55076	-1.355	-1.355	
368	2	8	5	6.586	6.984	0.55174	-0.398	-0.398	
369	5	1	4	9.650	8.439	0.55186	1.211	1.211	
370	0	6	9	1.826	0.566	0.55282	1.260	1.260	
371	3	3	8	5.798	1.362	0.55321	4.436	4.436	**
372	0	10	2	8.173	10.721	0.55354	-2.548	-2.548	*
373	0	2	11	14.820	14.948	0.55578	-0.128	-0.128	
374	2	2	-11	13.851	13.064	0.55600	0.788	0.788	
375	5	5	-4	10.591	12.115	0.55633	-1.524	-1.524	
376	0	8	7	20.947	16.782	0.55687	4.165	4.165	**
377	3	5	-9	3.453	3.333	0.55749	0.120	0.120	
378	3	5	7	5.985	5.693	0.55831	0.291	0.291	
379	1	5	-10	7.736	6.892	0.55878	0.844	0.844	
380	2	6	-9	1.817	0.483	0.55900	1.334	1.334	
381	2	4	9	1.091	0.277	0.55925	0.814	0.814	
382	3	7	-7	10.071	11.092	0.55978	-1.021	-1.021	
383	4	0	7	1.687	0.530	0.55975	1.157	1.157	
384	3	7	5	10.590	13.088	0.56040	-2.498	-2.498	*
385	5	5	1	9.250	7.409	0.56042	1.841	1.841	
386	1	3	-11	9.348	7.793	0.56096	1.555	1.555	
387	2	0	10	9.192	8.617	0.56148	0.575	0.575	
388	5	3	-7	24.460	28.191	0.56411	-3.731	-3.731	*
389	0	10	3	1.644	1.254	0.56452	0.390	0.390	
390	1	9	5	23.644	23.853	0.56485	-0.210	-0.210	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
391	4	6	4	22.816	27.961	0.56500	-5.145	-5.145	**
392	6	0	-2	63.243	54.624	0.56568	8.619	8.619	***
393	3	9	-1	42.896	42.897	0.56590	-0.001	-0.001	
394	4	4	6	8.222	8.931	0.56767	-0.710	-0.710	
395	6	0	-3	35.959	31.570	0.56774	4.390	4.390	**
396	6	0	-1	18.916	17.369	0.56794	1.547	1.547	
397	3	9	-2	1.052	11.717	0.56801	-10.665	-10.665	***
398	3	9	0	24.935	26.843	0.56811	-1.908	-1.908	
399	5	1	-8	19.309	16.914	0.56837	2.395	2.395	*
400	2	8	-7	6.057	13.748	0.56886	-7.691	-7.691	**
401	1	7	8	7.722	6.068	0.56996	1.654	1.654	
402	4	2	7	2.043	2.148	0.57025	-0.105	-0.105	
403	2	6	8	25.765	24.360	0.57187	1.405	1.405	
404	2	2	10	19.104	19.242	0.57195	-0.138	-0.138	
405	4	6	-7	2.522	18.799	0.57218	-16.277	-16.277	****
406	1	1	11	11.577	12.730	0.57217	-1.153	-1.153	
407	1	9	-6	19.738	17.752	0.57258	1.986	1.986	
408	3	1	-11	3.866	2.576	0.57260	1.290	1.290	
409	5	3	4	19.778	23.818	0.57295	-4.039	-4.039	**
410	3	1	9	11.276	10.307	0.57360	0.968	0.968	
411	6	0	-4	8.238	6.444	0.57409	1.794	1.794	
412	5	5	2	6.631	5.965	0.57421	0.666	0.666	
413	3	9	-3	0.643	6.655	0.57441	-6.012	-6.012	**

414	6	0	0	7.610	7.039	0.57449	0.571	0.571	
415	3	9	1	6.204	6.775	0.57460	-0.571	-0.571	
416	6	2	-2	3.311	7.569	0.57607	-4.258	-4.258	**
417	4	8	-1	4.138	2.900	0.57648	1.238	1.238	
418	2	10	-1	5.607	5.323	0.57655	0.284	0.284	
419	4	8	-2	0.769	5.036	0.57713	-4.266	-4.266	**
420	2	10	0	1.604	0.955	0.57729	0.650	0.650	
421	6	2	-3	2.590	4.447	0.57809	-1.857	-1.857	
422	6	2	-1	1.363	1.227	0.57829	0.136	0.136	
423	2	8	6	13.350	14.659	0.57856	-1.309	-1.309	
424	5	1	5	15.925	14.770	0.57872	1.156	1.156	
425	0	10	4	4.520	5.934	0.57954	-1.414	-1.414	
426	2	10	-2	5.979	4.155	0.58005	1.823	1.823	
427	4	8	0	11.256	9.538	0.58009	1.718	1.718	
428	4	2	-10	5.209	4.748	0.58121	0.462	0.462	
429	1	7	-9	5.222	4.089	0.58175	1.133	1.133	
430	4	8	-3	0.584	7.997	0.58200	-7.413	-7.413	**
431	2	10	1	10.136	10.681	0.58226	-0.545	-0.545	
432	6	2	-4	8.160	14.188	0.58433	-6.029	-6.029	**
433	6	0	-5	14.703	12.990	0.58458	1.713	1.713	
434	6	2	0	8.921	9.808	0.58472	-0.887	-0.887	
435	5	5	-6	1.071	7.437	0.58485	-6.366	-6.366	**
436	3	9	-4	1.071	10.570	0.58494	-9.499	-9.499	***
437	6	0	1	16.320	14.811	0.58517	1.509	1.509	
438	3	9	2	9.968	8.496	0.58524	1.471	1.471	
439	0	4	11	21.811	20.848	0.58693	0.963	0.963	
440	2	4	-11	13.642	12.251	0.58714	1.390	1.390	
441	3	7	-8	2.561	7.613	0.58755	-5.052	-5.052	**
442	1	5	10	7.654	6.857	0.58767	0.797	0.797	
443	2	10	-3	10.760	6.365	0.58773	4.395	4.395	**
444	4	8	1	10.969	10.878	0.58786	0.091	0.091	
445	1	1	-12	8.238	7.411	0.58801	0.827	0.827	
446	3	7	6	11.373	13.614	0.58823	-2.241	-2.241	*
447	5	3	-8	38.364	44.178	0.58887	-5.814	-5.814	**
448	0	8	8	10.556	7.263	0.58900	3.293	3.293	*
449	1	9	6	38.265	38.553	0.58967	-0.288	-0.288	
450	4	6	5	37.527	46.533	0.58986	-9.007	-9.007	***
451	2	10	2	10.740	6.933	0.59136	3.807	3.807	*
452	5	5	3	6.223	7.999	0.59183	-1.777	-1.777	
453	2	0	-12	18.793	16.744	0.59197	2.049	2.049	*
454	1	3	11	19.396	18.146	0.59254	1.250	1.250	
455	3	3	-11	23.622	21.825	0.59296	1.797	1.797	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
456	0	6	10	24.777	21.243	0.59351	3.534	3.534	*
457	3	5	-10	5.355	5.142	0.59369	0.214	0.214	
458	3	3	9	24.987	23.408	0.59392	1.579	1.579	
459	0	0	12	26.845	24.347	0.59455	2.498	2.498	*
460	6	2	-5	1.422	2.071	0.59465	-0.649	-0.649	
461	6	2	1	3.641	3.666	0.59522	-0.025	-0.025	
462	2	6	-10	25.239	20.405	0.59650	4.834	4.834	**

463	5	1	-9	10.896	8.938	0.59707	1.957	1.957	
464	4	0	8	25.414	25.408	0.59730	0.006	0.006	
465	2	8	-8	2.093	3.057	0.59758	-0.963	-0.963	
466	4	6	-8	2.551	17.539	0.59798	-14.988	-14.988	***
467	0	10	5	1.349	1.727	0.59830	-0.378	-0.378	
468	1	9	-7	17.395	17.291	0.59842	0.104	0.104	
469	5	3	5	16.976	19.953	0.59887	-2.978	-2.978	*
470	6	0	-6	43.009	35.505	0.59901	7.504	7.504	**
471	3	9	-5	1.646	16.187	0.59940	-14.541	-14.541	***
472	4	8	2	4.557	3.696	0.59964	0.861	0.861	
473	3	9	3	29.756	30.313	0.59979	-0.557	-0.557	
474	6	0	2	27.128	23.157	0.59977	3.971	3.971	*
475	4	4	7	11.601	13.440	0.60065	-1.839	-1.839	
476	1	5	-11	13.807	12.473	0.60178	1.334	1.334	
477	2	2	-12	21.802	21.117	0.60191	0.685	0.685	
478	2	4	10	9.578	9.128	0.60226	0.450	0.450	
479	2	10	3	7.794	8.135	0.60439	-0.341	-0.341	
480	0	2	12	2.512	1.846	0.60445	0.666	0.666	
481	6	4	-2	1.149	13.411	0.60617	-12.262	-12.262	***
482	5	7	-2	1.091	9.408	0.60645	-8.317	-8.317	***
483	1	11	0	7.063	11.573	0.60667	-4.510	-4.510	**
484	1	7	9	4.493	4.149	0.60683	0.344	0.344	
485	4	2	8	5.336	5.920	0.60715	-0.584	-0.584	
486	5	7	-1	8.804	11.101	0.60721	-2.297	-2.297	*
487	1	11	-1	3.720	3.328	0.60733	0.391	0.391	
488	1	3	-12	33.700	31.579	0.60785	2.122	2.122	*
489	6	4	-3	0.867	6.831	0.60810	-5.965	-5.965	**
490	2	8	7	3.145	1.686	0.60824	1.459	1.459	
491	6	4	-1	4.469	3.616	0.60829	0.853	0.853	
492	2	0	11	33.252	34.754	0.60838	-1.501	-1.501	
493	6	2	-6	6.397	9.776	0.60883	-3.378	-3.378	*
494	6	2	2	6.271	7.542	0.60958	-1.271	-1.271	
495	5	7	-3	0.740	11.300	0.60974	-10.560	-10.560	***
496	2	6	9	5.076	6.161	0.60999	-1.085	-1.085	
497	1	11	1	1.363	1.236	0.61005	0.127	0.127	
498	4	4	-10	13.846	12.287	0.61106	1.559	1.559	
499	5	7	0	6.193	4.367	0.61198	1.826	1.826	
500	1	11	-2	8.653	14.709	0.61201	-6.057	-6.057	**
501	5	5	4	7.395	9.379	0.61297	-1.984	-1.984	
502	6	4	-4	0.954	9.155	0.61403	-8.201	-8.201	***
503	6	4	0	16.606	19.653	0.61440	-3.046	-3.046	*
504	2	10	-5	7.994	6.137	0.61488	1.858	1.858	
505	4	8	3	9.080	10.903	0.61519	-1.824	-1.824	
506	3	1	-12	9.406	9.688	0.61593	-0.282	-0.282	
507	5	3	-9	15.307	17.750	0.61662	-2.444	-2.444	*
508	5	7	-4	0.730	16.148	0.61700	-15.418	-15.418	***
509	3	1	10	13.311	13.989	0.61695	-0.679	-0.679	
510	6	0	-7	17.478	14.032	0.61708	3.447	3.447	*
511	1	11	2	7.738	8.991	0.61739	-1.254	-1.254	
512	1	9	7	15.167	15.643	0.61748	-0.476	-0.476	
513	4	6	6	14.872	17.729	0.61771	-2.857	-2.857	*
514	3	9	4	12.572	12.922	0.61798	-0.350	-0.350	

515	3	7	-9	1.412	4.600	0.61804	-3.188	-3.188	*
516	6	0	3	5.590	4.146	0.61801	1.443	1.443	
517	2	2	11	18.958	17.111	0.61805	1.847	1.847	
518	4	2	-11	8.608	6.609	0.61865	1.999	1.999	
519	3	7	7	3.213	3.683	0.61878	-0.470	-0.470	
520	1	7	-10	2.795	3.487	0.61921	-0.692	-0.692	

No.	h	k	l	Fo	Fc	sinθ/λ	Fo-Fc	w(Fo-Fc)	Flag
521	0	10	6	7.027	10.638	0.62046	-3.611	-3.611	*
522	4	8	-6	0.691	4.651	0.62060	-3.959	-3.959	*
523	1	11	-3	6.381	11.053	0.62062	-4.672	-4.672	**
524	5	7	1	11.036	11.371	0.62069	-0.335	-0.335	
525	1	1	12	2.619	3.960	0.62088	-1.341	-1.341	
526	2	10	4	6.664	7.260	0.62112	-0.596	-0.596	
527	0	8	9	12.382	10.118	0.62342	2.264	2.264	*
528	6	4	1	7.912	7.920	0.62440	-0.008	-0.008	
529	6	2	-7	2.931	5.240	0.62662	-2.309	-2.309	*
530	1	9	-8	1.943	2.195	0.62711	-0.252	-0.252	
531	6	2	3	1.246	2.072	0.62753	-0.825	-0.825	
532	5	3	6	1.854	2.020	0.62764	-0.165	-0.165	
533	5	5	-8	1.685	13.688	0.62787	-12.004	-12.004	***
534	5	1	-10	8.900	6.699	0.62838	2.200	2.200	*
535	1	11	3	4.781	5.678	0.62857	-0.897	-0.897	
536	2	8	-9	3.379	7.986	0.62891	-4.607	-4.607	**
537	2	4	-12	10.614	10.559	0.63078	0.055	0.055	
538	1	5	11	9.484	9.797	0.63131	-0.314	-0.314	
539	3	5	-11	1.227	1.911	0.63171	-0.684	-0.684	
540	3	5	9	9.019	8.833	0.63261	0.186	0.186	
541	1	11	-4	2.532	3.117	0.63301	-0.586	-0.586	
542	5	7	2	2.736	2.466	0.63317	0.270	0.270	
543	0	4	12	12.425	9.850	0.63320	2.575	2.575	*
544	2	10	-6	3.013	2.642	0.63385	0.371	0.371	
545	3	3	-12	37.303	34.263	0.63489	3.040	3.040	*
546	0	6	11	37.858	32.788	0.63546	5.070	5.070	**
547	2	6	-11	14.236	12.604	0.63565	1.632	1.632	
548	4	4	8	6.855	7.660	0.63579	-0.806	-0.806	
549	3	3	10	38.942	37.188	0.63589	1.755	1.755	
550	4	0	9	14.275	15.130	0.63649	-0.855	-0.855	
551	1	1	-13	7.264	8.491	0.63677	-1.227	-1.227	
552	5	5	5	11.102	13.196	0.63726	-2.094	-2.094	*
553	6	4	2	8.649	10.042	0.63811	-1.392	-1.392	
554	6	0	-8	14.635	10.920	0.63849	3.715	3.715	*
555	3	9	-7	0.906	7.687	0.63896	-6.781	-6.781	**
556	2	0	-13	3.749	2.174	0.63913	1.575	1.575	
557	3	9	5	15.200	11.388	0.63949	3.812	3.812	*
558	6	0	4	11.748	9.480	0.63957	2.268	2.268	*
559	1	3	12	4.226	1.925	0.63970	2.301	2.301	*
560	2	8	8	7.388	7.485	0.64038	-0.096	-0.096	
561	5	1	7	10.521	9.904	0.64062	0.617	0.617	
562	4	8	-7	0.818	5.143	0.64065	-4.325	-4.325	**
563	2	10	5	5.510	4.809	0.64124	0.701	0.701	

564	5	7	-6	10.747	12.850	0.64283	-2.103	-2.103	*
565	1	11	4	2.512	0.802	0.64338	1.710	1.710	
566	0	0	13	20.516	18.346	0.64410	2.170	2.170	*
567	1	7	10	12.743	10.614	0.64539	2.130	2.130	*
568	0	10	7	5.714	6.678	0.64566	-0.964	-0.964	
569	4	2	9	3.365	3.166	0.64575	0.199	0.199	
570	1	5	-12	7.391	5.563	0.64571	1.828	1.828	
571	2	4	11	7.043	6.096	0.64620	0.947	0.947	
572	4	4	-11	2.415	3.006	0.64678	-0.591	-0.591	
573	5	3	-10	7.977	6.769	0.64698	1.208	1.208	
574	6	2	-8	10.938	11.094	0.64772	-0.156	-0.156	
575	1	9	8	6.732	6.485	0.64789	0.247	0.247	
576	4	6	7	9.026	7.266	0.64815	1.760	1.760	
577	2	2	-13	4.654	2.612	0.64834	2.042	2.042	*
578	6	2	4	9.034	10.981	0.64878	-1.947	-1.947	
579	1	11	-5	5.787	11.421	0.64895	-5.634	-5.634	**
580	5	7	3	3.982	2.797	0.64919	1.186	1.186	
581	2	6	10	1.609	1.610	0.64964	-0.001	-0.001	
582	3	7	-10	2.006	4.885	0.65088	-2.879	-2.879	*
583	3	7	8	6.138	7.818	0.65168	-1.680	-1.680	
584	0	2	13	9.143	8.817	0.65324	0.326	0.326	
585	6	6	-2	38.575	40.533	0.65327	-1.957	-1.957	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
586	0	12	0	4.129	30.154	0.65352	-26.025	-26.025	****
587	6	4	-7	3.807	3.440	0.65440	0.367	0.367	
588	6	6	-3	11.743	13.268	0.65506	-1.524	-1.524	
589	1	3	-13	43.223	38.542	0.65513	4.681	4.681	**
590	6	4	3	8.552	10.774	0.65528	-2.221	-2.221	*
591	6	6	-1	12.152	13.723	0.65523	-1.571	-1.571	
592	0	12	1	1.257	9.326	0.65540	-8.069	-8.069	***
593	2	0	12	43.730	42.056	0.65566	1.674	1.674	
594	2	10	-7	9.073	9.195	0.65603	-0.121	-0.121	
595	4	8	5	13.200	14.683	0.65649	-1.482	-1.482	
596	4	2	-12	11.441	11.050	0.65770	0.391	0.391	
597	4	6	-10	3.778	22.191	0.65781	-18.413	-18.413	****
598	1	9	-9	23.473	20.975	0.65829	2.497	2.497	*
599	1	7	-11	4.002	4.011	0.65827	-0.009	-0.009	
600	5	3	7	21.898	27.165	0.65888	-5.267	-5.267	**
601	0	8	10	2.522	0.164	0.65977	2.358	2.358	*
602	3	1	-13	3.924	2.516	0.66013	1.408	1.408	
603	6	6	-4	3.900	3.365	0.66057	0.535	0.535	
604	0	12	2	0.852	3.006	0.66099	-2.154	-2.154	*
605	6	6	0	5.813	3.522	0.66092	2.291	2.291	*
606	5	7	-7	4.522	5.195	0.66095	-0.673	-0.673	
607	1	11	5	2.843	1.769	0.66158	1.074	1.074	
608	5	1	-11	4.284	4.179	0.66191	0.105	0.105	
609	2	8	-10	1.168	2.324	0.66246	-1.155	-1.155	
610	3	11	-1	8.098	7.189	0.66248	0.909	0.909	
611	7	1	-2	6.385	7.988	0.66244	-1.603	-1.603	
612	4	10	-1	7.994	5.762	0.66265	2.232	2.232	*

613	7	1	-3	3.508	3.074	0.66295	0.435	0.435	
614	6	0	-9	35.484	29.764	0.66293	5.720	5.720	**
615	3	9	-8	1.344	14.448	0.66342	-13.104	-13.104	***
616	3	9	6	24.399	26.164	0.66402	-1.765	-1.765	
617	6	0	5	23.579	21.749	0.66414	1.830	1.830	
618	3	11	0	2.970	2.764	0.66437	0.206	0.206	
619	5	5	6	0.955	1.269	0.66437	-0.314	-0.314	
620	2	10	6	17.507	13.052	0.66446	4.456	4.456	**
621	2	2	12	3.515	5.054	0.66465	-1.539	-1.539	
622	7	1	-1	4.148	3.437	0.66562	0.711	0.711	
623	4	10	0	5.271	5.394	0.66579	-0.123	-0.123	
624	7	1	-4	8.742	9.704	0.66716	-0.962	-0.962	
625	5	7	4	1.431	0.106	0.66851	1.325	1.325	
626	1	1	13	7.585	7.634	0.66971	-0.049	-0.049	
627	3	11	-3	10.604	6.045	0.66976	4.558	4.558	**
628	6	6	-5	13.715	14.322	0.66971	-0.607	-0.607	
629	3	11	1	9.158	7.878	0.66993	1.280	1.280	
630	6	6	1	13.550	14.578	0.67022	-1.028	-1.028	
631	0	12	3	1.496	10.241	0.67021	-8.745	-8.745	***
632	3	5	-12	5.969	5.328	0.67123	0.641	0.641	
633	6	2	-9	12.507	11.164	0.67182	1.343	1.343	
634	3	5	10	9.669	10.804	0.67216	-1.135	-1.135	
635	7	1	0	8.423	8.392	0.67245	0.031	0.031	
636	4	10	1	8.867	7.601	0.67257	1.266	1.266	
637	4	4	9	6.375	7.114	0.67274	-0.739	-0.739	
638	6	2	5	7.655	8.359	0.67301	-0.704	-0.704	
639	0	10	8	3.186	4.980	0.67357	-1.794	-1.794	
640	2	8	9	0.691	0.496	0.67463	0.195	0.195	
641	6	4	-8	2.952	3.838	0.67463	-0.886	-0.886	
642	5	1	8	2.395	1.100	0.67490	1.294	1.294	
643	7	1	-5	7.555	7.333	0.67499	0.222	0.222	
644	2	4	-13	4.830	5.345	0.67523	-0.516	-0.516	
645	6	4	4	5.998	5.421	0.67565	0.577	0.577	
646	2	6	-12	8.481	6.261	0.67617	2.220	2.220	*
647	4	0	10	8.364	8.208	0.67704	0.156	0.156	
648	3	3	-13	11.626	8.870	0.67786	2.756	2.756	*
649	0	6	12	11.860	9.114	0.67843	2.746	2.746	*
650	3	3	11	11.817	11.396	0.67887	0.420	0.420	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
651	3	11	2	4.263	3.301	0.67907	0.962	0.962	
652	5	3	-11	20.490	17.611	0.67960	2.880	2.880	*
653	0	4	13	7.916	7.313	0.67994	0.603	0.603	
654	7	3	-2	12.932	12.654	0.68011	0.278	0.278	
655	2	12	-1	10.834	10.611	0.68037	0.224	0.224	
656	1	9	9	15.859	15.001	0.68055	0.858	0.858	
657	7	3	-3	21.243	23.915	0.68061	-2.672	-2.672	*
658	4	6	8	15.589	18.817	0.68084	-3.228	-3.228	*
659	5	9	-1	20.472	19.501	0.68089	0.971	0.971	
660	2	12	0	18.550	16.450	0.68100	2.100	2.100	*
661	2	10	-8	6.018	3.061	0.68109	2.957	2.957	*

662	4	8	6	5.580	5.407	0.68162	0.173	0.173	
663	5	7	-8	7.168	8.431	0.68221	-1.263	-1.263	
664	6	6	-6	16.300	16.614	0.68234	-0.314	-0.314	
665	5	5	-10	1.315	7.449	0.68267	-6.134	-6.134	**
666	7	1	1	2.123	0.749	0.68281	1.374	1.374	
667	1	11	6	4.565	3.947	0.68290	0.617	0.617	
668	0	12	4	1.796	11.740	0.68291	-9.944	-9.944	***
669	6	6	2	16.426	17.370	0.68301	-0.944	-0.944	
670	7	3	-1	2.767	2.749	0.68321	0.018	0.018	
671	2	12	-2	2.999	2.354	0.68335	0.645	0.645	
672	4	4	-12	10.945	9.874	0.68422	1.070	1.070	
673	7	3	-4	23.614	25.732	0.68471	-2.118	-2.118	*
674	5	9	0	31.841	22.142	0.68515	9.698	9.698	***
675	2	12	1	20.360	18.497	0.68522	1.863	1.863	
676	1	7	11	7.576	6.447	0.68538	1.129	1.129	
677	1	1	-14	3.272	2.450	0.68563	0.822	0.822	
678	4	2	10	5.263	5.964	0.68575	-0.701	-0.701	
679	3	7	-11	1.792	4.594	0.68574	-2.802	-2.802	*
680	7	1	-6	3.650	3.924	0.68631	-0.274	-0.274	
681	3	7	9	3.457	1.954	0.68657	1.502	1.502	
682	2	0	-14	25.988	25.329	0.68662	0.659	0.659	
683	1	3	13	27.137	26.004	0.68720	1.134	1.134	
684	5	9	-4	0.935	17.244	0.68964	-16.309	-16.309	****
685	7	3	0	19.615	22.118	0.68986	-2.503	-2.503	*
686	2	12	-3	15.129	14.978	0.68987	0.151	0.151	
687	6	0	-10	26.378	21.114	0.69006	5.264	5.264	**
688	1	11	-7	4.165	9.178	0.69046	-5.014	-5.014	**
689	1	5	-13	9.688	9.513	0.69040	0.175	0.175	
690	2	10	7	1.772	1.079	0.69045	0.693	0.693	
691	2	6	11	17.232	17.299	0.69058	-0.067	-0.067	
692	3	9	-9	2.386	23.712	0.69057	-21.326	-21.326	****
693	5	7	5	5.774	4.666	0.69086	1.108	1.108	
694	2	4	12	4.283	5.335	0.69091	-1.052	-1.052	
695	4	6	-11	1.178	2.060	0.69111	-0.882	-0.882	
696	3	9	7	18.545	19.276	0.69123	-0.732	-0.732	
697	6	0	6	35.951	32.152	0.69138	3.799	3.799	*
698	3	11	3	8.929	5.888	0.69165	3.041	3.041	*
699	1	9	-10	2.405	2.535	0.69161	-0.130	-0.130	
700	5	3	8	2.681	0.717	0.69226	1.964	1.964	
701	7	3	-5	3.496	3.523	0.69234	-0.028	-0.028	
702	5	9	1	2.528	2.947	0.69294	-0.419	-0.419	
703	2	12	2	2.265	1.752	0.69297	0.513	0.513	
704	0	0	14	1.315	2.836	0.69364	-1.522	-1.522	
705	5	5	7	8.014	9.659	0.69395	-1.645	-1.645	
706	2	2	-14	9.688	8.543	0.69521	1.145	1.145	
707	7	1	2	5.092	5.784	0.69655	-0.693	-0.693	
708	4	10	3	7.060	6.062	0.69659	0.998	0.998	
709	0	8	11	14.027	10.483	0.69775	3.544	3.544	*
710	6	4	-9	3.205	1.957	0.69780	1.247	1.247	
711	2	8	-11	3.807	6.731	0.69792	-2.924	-2.924	*
712	4	2	-13	3.574	3.806	0.69808	-0.233	-0.233	
713	6	6	-7	12.074	8.262	0.69825	3.812	3.812	*

714	6	2	-10	2.892	4.250	0.69860	-1.358	-1.358	
715	1	7	-12	3.778	3.612	0.69866	0.166	0.166	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
716	0	12	5	0.701	6.675	0.69890	-5.974	-5.974	**
717	6	4	5	9.528	10.935	0.69895	-1.407	-1.407	
718	6	6	3	8.639	8.650	0.69907	-0.011	-0.011	
719	5	9	-5	0.691	5.275	0.69958	-4.584	-4.584	**
720	2	12	-4	4.807	3.913	0.69985	0.894	0.894	
721	7	3	1	6.789	8.238	0.69997	-1.449	-1.449	
722	6	2	6	5.394	6.578	0.69991	-1.184	-1.184	
723	7	1	-7	6.149	7.593	0.70096	-1.445	-1.445	
724	4	10	-6	0.974	2.846	0.70137	-1.872	-1.872	
725	0	2	14	2.376	1.876	0.70214	0.500	0.500	
726	1	3	-14	1.373	0.790	0.70272	0.583	0.583	
727	2	0	13	1.383	0.550	0.70326	0.833	0.833	
728	7	3	-6	8.116	9.991	0.70338	-1.875	-1.875	
729	0	10	9	5.136	5.938	0.70387	-0.802	-0.802	
730	5	9	2	11.071	8.476	0.70414	2.595	2.595	*
731	2	12	3	7.388	6.507	0.70412	0.881	0.881	
732	3	1	-14	5.862	5.637	0.70504	0.225	0.225	

LSFM (1.4) 06/11/97 10:54:26 Elapsed time = 0.0 min

PHLOG21 ..... Demonstration Copy - Not for Resale .....

The space group is number 12 -- C12/m1

After refinement cycle no. 4. 732 observations. 73 variables.

Esd of an observation of unit weight = 3.980

Unweighted R factor = 0.128 Weighted R factor = 0.137

ä ³Fo³ = 1.33965E+04

ä ³³Fo³-³Fc³³ = 1.72102E+03

ä W*DELý = 1.04383E+04

ä W*Foý = 5.52542E+05

Largest parameter shift/error = 0.01
Average parameter shift/error = 0.00

The calculations have converged with a shift/error less than 0.100

Cycle Error R1 R2 Max.shift Av.shift

1	3.991	0.133	0.139	4.16	0.14
2	3.939	0.129	0.137	0.23	0.05
3	3.935	0.128	0.137	0.12	0.02
4	3.980	0.128	0.137	0.01	0.00

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CRYSTAL STRUCTURES OF NEAR-END-MEMBER PHLOGOPITE AT HIGH TEMPERATURES AND HEAT-TREATED Fe-RICH PHLOGOPITE: THE INFLUENCE OF THE O,OH,F SITE

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ABSTRACT

The crystal structure of end-member phlogopite-1*M* from White Well, Australia, was determined by refinement using single-crystal X-ray data to 600°C (R = 0.069, wR = 0.096 at 600°C). Cell parameters were refined at 20, 150, and thereafter at 50°C intervals to 600°C. The rate of expansion of the metric unit-cell dimensions is linear. The expansivity of the c dimension is 1.81 $\times 10^{-5}$ °C^{-1}, and 1.40 and 1.34 $\times 10^{-5}$ °C^{-1} for the a and b dimensions, respectively (compared to fluorophlogopite in a previous study: 24° to 600°C, $\alpha_a = 0.86$, $\alpha_b = 0.75$, and $\alpha_c = 1.81 \times 10^{-5}$ °C^{-1}). The OH-rich octahedra (*M*1, *M*2) expand without changing shape significantly at elevated temperatures, in contrast to F-rich octahedra in fluorophlogopite, which become elongate approximately along the c axis. The interlayer site becomes elongate in phlogopite with increasing temperature relative to fluorophlogopite, although the site shows general flattening with increasing temperature. We also refined the room-temperature structure of a sample of Fe-rich phlogopite-1*M* sample from Silver Crater, near Bancroft, Ontario, and the same phlogopite after heat treatment at 904°C for 24 hours (untreated: R = 0.039, wR = 0.043; heat-treated: R = 0.039, wR = 0.047). In contrast to earlier studies, there was no change in Fe site occupancy from the octahedra to the tetrahedra. The octahedra (*M*1, *M*2) and the interlayer site are flattened in both the heated and unheated samples, but the heated sample shows significant flattening in all these sites over the unheated sample.

Keywords: phlogopite, heat-treated phlogopite, crystal structure.

SOMMAIRE

Nous avons déterminé la structure cristalline d'un échantillon de phlogopite-1*M* de White Well, Australie, dont la composition est proche du pôle, par affinement de données prélevées sur cristal unique jusqu'à 600°C (R = 0.069, wR = 0.096 à 600°C). Les paramètres réticulaires ont été affinés à 20, 150, et ensuite à chaque tranche de 50°C jusqu'à 600°C. Le taux d'expansion des paramètres réticulaires est linéaire. L'expansivité de la dimension c est 1.81 $\times 10^{-5}$ °C^{-1}, et celle des dimensions a et b, 1.40 and 1.34 $\times 10^{-5}$ °C^{-1}, respectivement (on peut comparer ces données à celles de la fluorophlogopite, déterminées antérieurement: entre 24° et 600°C, $\alpha_a = 0.86$, $\alpha_b = 0.75$, et $\alpha_c = 1.81 \times 10^{-5}$ °C^{-1}). Les octaèdres riches en OH (*M*1, *M*2) augmentent en volume sans changer de forme aux températures élevées, contrairement aux octaèdres riches en F dans la fluorophlogopite, qui deviennent allongés le long de l'axe c. Le site inter-feuillet devient allongé dans la phlogopite à mesure qu'augmente la température, relativement à la fluorophlogopite, quoique le site montre un applatissement général avec une augmentation en température. Nous avons aussi affiné la structure à température ambiante d'un échantillon de phlogopite-1*M* riche en Fe provenant de Silver Crater, près de Bancroft, en Ontario, et du même mica après chauffage à 904°C pour 24 heures (sans chauffage: R = 0.039, wR = 0.043; après chauffage: R = 0.039, wR = 0.047). Contrairement aux résultats antérieurs, il n'y a pas eu de changement dans l'occupation des sites par le Fe, par exemple un transfert de site octaédrique à site tétraédrique. Les octaèdres (*M*1, *M*2) et le site inter-feuillet sont applatis dans les échantillons de ce mica, chauffé ou non, mais l'échantillon chauffé montre un applatissement nettement accru à tous ces sites par rapport à l'échantillon non chauffé.

(Traduit par la Rédaction)

Mots-clés: phlogopite, phlogopite chauffé, structure cristalline.

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