450°C phlogopite

LSFM (1.4) 06/11/97 11:20:24 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. 731 observations. 58 variables.

Esd of an observation of unit weight = 3.616

Unweighted R factor = 0.119 Weighted R factor = 0.129

ä ³Fo³ = 1.30295E+04

ä ³³Fo³-³Fc³³ = 1.55308E+03

ä W*DELý = 8.79818E+03

ä W*Foý = 5.24817E+05

Scale factor:	New	Old	Shift	Error	SHFT/ERR
	0.99723	0.99717	0.00006	0.00503	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)	0.08659	0.08661	-0.00001	0.00519	0.00
6	U(2,2)	0.09226	0.09224	0.00002	0.00595	0.00
7	U(3,3)	0.06892	0.06893	-0.00001	0.00437	0.00
	U(1,2)	0.00000				
9	U(1,3)	0.01328	0.01327	0.00001	0.00402	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	0.07676	0.07680	-0.00004 (0.0002)	0.00045 (0.0024)	-0.08
12	y	0.16678	0.16676	0.00002 (0.0002)	0.00031 (0.0028)	0.07
13	z	0.22956	0.22961	-0.00005 (0.0005)	0.00024 (0.0025)	-0.20
14	U(1,1)	0.02060	0.02061	-0.00001	0.00091	-0.01
15	U(2,2)	0.03080	0.03079	0.00001	0.00118	0.01
16	U(3,3)	0.02321	0.02322	-0.00001	0.00096	-0.01
17	U(1,2)	0.00028	0.00028	0.00000	0.00105	0.00
18	U(1,3)	0.00278	0.00279	-0.00001	0.00080	-0.01
19	U(2,3)	-0.00014	-0.00014	0.00000	0.00100	0.00

Total shift = 0.0005

Atom no. 3 MG 1 (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)	0.01590	0.01590	0.00000	0.00223	0.00
24	U(2,2)	0.03002	0.03002	0.00000	0.00299	0.00
25	U(3,3)	0.02580	0.02580	0.00000	0.00257	0.00
	U(1,2)	0.00000				
27	U(1,3)	0.00432	0.00434	-0.00002	0.00202	-0.01
	U(2,3)	0.00000				

Total shift = 0.0000

Atom no. 4 MG 2 (electron count = 12.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	0.50000				
	x	0.00000				
30	y	0.33172	0.33172	0.00000 (0.0000)	0.00053 (0.0049)	0.01
	z	0.50000				
32	U(1,1)	0.01572	0.01572	0.00000	0.00150	0.00
33	U(2,2)	0.03018	0.03019	-0.00001	0.00207	0.00
34	U(3,3)	0.02388	0.02389	0.00000	0.00171	0.00
	U(1,2)	0.00000				
36	U(1,3)	0.00181	0.00182	-0.00001	0.00137	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	0.13201	0.13200	0.00001 (0.0001)	0.00178 (0.0095)	0.01
	y	0.50000				
40	z	0.39784	0.39770	0.00014 (0.0014)	0.00098 (0.0100)	0.14
41	U(1,1)	0.03584	0.03585	-0.00001	0.00426	0.00
42	U(2,2)	0.04728	0.04727	0.00001	0.00518	0.00
43	U(3,3)	0.04613	0.04612	0.00000	0.00481	0.00
	U(1,2)	0.00000				
45	U(1,3)	0.00457	0.00458	-0.00001	0.00387	0.00
	U(2,3)	0.00000				

Total shift = 0.0014

Atom no. 6 O 1 (electron count = 8.0)

Parameter		New	Old	Shift	Error	SHFT/ERR
	Mult.	0.50000				
47	x	0.01792	0.01858	-0.00066 (0.0035)	0.00223 (0.0118)	-0.30
	y	0.00000				
49	z	0.17265	0.17253	0.00012 (0.0012)	0.00110 (0.0113)	0.11
50	U(1,1)	0.04560	0.04559	0.00001	0.00562	0.00
51	U(2,2)	0.02915	0.02921	-0.00006	0.00485	-0.01
52	U(3,3)	0.03819	0.03818	0.00001	0.00515	0.00
	U(1,2)	0.00000				

54	U(1,3)	0.00126	0.00125	0.00000		0.00463		0.00
	U(2,3)	0.00000						
	Total shift =	0.0035						

Atom no. 7 O 2 (electron count = 8.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	1.00000						
56	x	0.32733	0.32694	0.00039	(0.0020)	0.00134	(0.0071)	0.29
57	y	0.22886	0.22861	0.00025	(0.0023)	0.00091	(0.0084)	0.28
58	z	0.17333	0.17321	0.00012	(0.0012)	0.00073	(0.0075)	0.16
59	U(1,1)	0.03199	0.03204	-0.00005		0.00309		-0.01
60	U(2,2)	0.04278	0.04274	0.00003		0.00402		0.01
61	U(3,3)	0.03986	0.03983	0.00003		0.00340		0.01
62	U(1,2)	-0.00905	-0.00902	-0.00002		0.00323		-0.01
63	U(1,3)	0.00891	0.00892	-0.00001		0.00271		0.00
64	U(2,3)	-0.00785	-0.00784	-0.00001		0.00333		0.00
	Total shift =	0.0032						

Atom no. 8 O 3 (electron count = 8.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	1.00000						
65	x	0.13153	0.13172	-0.00019	(0.0010)	0.00116	(0.0061)	-0.16
66	y	0.16726	0.16735	-0.00009	(0.0008)	0.00080	(0.0073)	-0.11
67	z	0.39326	0.39336	-0.00010	(0.0010)	0.00061	(0.0063)	-0.16
68	U(1,1)	0.02271	0.02273	-0.00002		0.00251		-0.01
69	U(2,2)	0.03496	0.03497	-0.00002		0.00329		0.00
70	U(3,3)	0.02550	0.02549	0.00001		0.00267		0.01
71	U(1,2)	0.00183	0.00186	-0.00002		0.00276		-0.01
72	U(1,3)	0.00220	0.00220	0.00000		0.00223		0.00
73	U(2,3)	-0.00113	-0.00110	-0.00003		0.00276		-0.01
	Total shift =	0.0015						

Largest parameter shift/error = 0.30
Average parameter shift/error = 0.04

LSFM (1.4) 06/11/97 11:20:28 Elapsed time = 0.1 min

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

The space group is number 12 -- C12/m1

Refinement cycle no. 2. 731 observations. 58 variables.

Esd of an observation of unit weight = 3.615

Unweighted R factor = 0.119 Weighted R factor = 0.129

ä ³Fo³ = 1.30303E+04

ä ³³Fo³-³Fc³³ = 1.54934E+03

ä W*DELý = 8.79274E+03

```
ä W*Foý =       5.24817E+05

Scale factor:      New       Old          Shift          Error       SHFT/ERR
                 0.99722   0.99723       -0.00001       0.00503       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)   0.08659    0.08659    0.00000              0.00519               0.00
  6  U(2,2)   0.09226    0.09226    0.00000              0.00595               0.00
  7  U(3,3)   0.06892    0.06892    0.00000              0.00437               0.00
     U(1,2)   0.00000
  9  U(1,3)   0.01328    0.01328    0.00000              0.00402               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        0.07676    0.07676    0.00000 (0.0000 )    0.00045 (0.0024 )     0.00
 12  y        0.16678    0.16678    0.00000 (0.0000 )    0.00031 (0.0028 )     0.00
 13  z        0.22956    0.22956    0.00000 (0.0000 )    0.00024 (0.0025 )     0.00
 14  U(1,1)   0.02060    0.02060    0.00000              0.00091               0.00
 15  U(2,2)   0.03080    0.03080    0.00000              0.00118               0.00
 16  U(3,3)   0.02321    0.02321    0.00000              0.00096               0.00
 17  U(1,2)   0.00028    0.00028    0.00000              0.00105               0.00
 18  U(1,3)   0.00278    0.00278    0.00000              0.00080               0.00
 19  U(2,3)  -0.00014   -0.00014    0.00000              0.00100               0.00
     Total shift =  0.0000

Atom no.  3   MG 1     (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)   0.01590    0.01590    0.00000              0.00223               0.00
 24  U(2,2)   0.03002    0.03002    0.00000              0.00299               0.00
 25  U(3,3)   0.02580    0.02580    0.00000              0.00257               0.00
     U(1,2)   0.00000
 27  U(1,3)   0.00432    0.00432    0.00000              0.00202               0.00
     U(2,3)   0.00000
     Total shift =  0.0000

Atom no.  4   MG 2     (electron count = 12.0)
Parameter       New         Old          Shift                Error          SHFT/ERR
     Mult.    0.50000
     x        0.00000
```

30	y	0.33172	0.33172	0.00000	(0.0000)	0.00053	(0.0049)	0.00
	z	0.50000						
32	U(1,1)	0.01572	0.01572	0.00000		0.00150		0.00
33	U(2,2)	0.03019	0.03018	0.00000		0.00207		0.00
34	U(3,3)	0.02388	0.02388	0.00000		0.00171		0.00
	U(1,2)	0.00000						
36	U(1,3)	0.00181	0.00181	0.00000		0.00137		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	0.13202	0.13201	0.00000	(0.0000)	0.00178	(0.0095)	0.00
	y	0.50000						
40	z	0.39784	0.39784	0.00000	(0.0000)	0.00098	(0.0100)	0.00
41	U(1,1)	0.03585	0.03584	0.00001		0.00426		0.00
42	U(2,2)	0.04729	0.04728	0.00001		0.00517		0.00
43	U(3,3)	0.04607	0.04613	-0.00006		0.00481		-0.01
	U(1,2)	0.00000						
45	U(1,3)	0.00457	0.00457	0.00000		0.00387		0.00
	U(2,3)	0.00000						
	Total shift = 0.0000							

Atom no. 6 O 1 (electron count = 8.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	0.50000						
47	x	0.01792	0.01792	0.00000	(0.0000)	0.00223	(0.0118)	0.00
	y	0.00000						
49	z	0.17265	0.17265	0.00000	(0.0000)	0.00110	(0.0113)	0.00
50	U(1,1)	0.04569	0.04560	0.00010		0.00562		0.02
51	U(2,2)	0.02911	0.02915	-0.00004		0.00484		-0.01
52	U(3,3)	0.03816	0.03819	-0.00002		0.00515		0.00
	U(1,2)	0.00000						
54	U(1,3)	0.00118	0.00126	-0.00008		0.00463		-0.02
	U(2,3)	0.00000						
	Total shift = 0.0000							

Atom no. 7 O 2 (electron count = 8.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	1.00000						
56	x	0.32733	0.32733	0.00000	(0.0000)	0.00134	(0.0071)	0.00
57	y	0.22886	0.22886	0.00000	(0.0000)	0.00091	(0.0084)	0.00
58	z	0.17333	0.17333	0.00000	(0.0000)	0.00073	(0.0075)	0.00
59	U(1,1)	0.03192	0.03199	-0.00007		0.00309		-0.02
60	U(2,2)	0.04291	0.04278	0.00014		0.00402		0.03
61	U(3,3)	0.03984	0.03986	-0.00001		0.00340		0.00
62	U(1,2)	-0.00908	-0.00905	-0.00003		0.00322		-0.01
63	U(1,3)	0.00885	0.00891	-0.00006		0.00271		-0.02
64	U(2,3)	-0.00798	-0.00785	-0.00013		0.00333		-0.04
	Total shift = 0.0000							

Atom no. 8 O 3 (electron count = 8.0)

Parameter		New	Old	Shift		Error		SHFT/ERR
	Mult.	1.00000						
65	x	0.13153	0.13153	0.00000	(0.0000)	0.00116	(0.0061)	0.00
66	y	0.16726	0.16726	0.00000	(0.0000)	0.00080	(0.0073)	0.00
67	z	0.39326	0.39326	0.00000	(0.0000)	0.00061	(0.0063)	0.00
68	U(1,1)	0.02270	0.02271	-0.00001		0.00251		0.00
69	U(2,2)	0.03496	0.03496	0.00000		0.00329		0.00
70	U(3,3)	0.02552	0.02550	0.00002		0.00267		0.01
71	U(1,2)	0.00184	0.00183	0.00000		0.00276		0.00
72	U(1,3)	0.00220	0.00220	0.00000		0.00223		0.00
73	U(2,3)	-0.00112	-0.00113	0.00001		0.00276		0.00

Total shift = 0.0000

Largest parameter shift/error = 0.04
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	23.913	24.823	0.09909	-0.910	-0.912	
2	0	2	0	38.443	38.368	0.10892	0.075	0.075	
3	1	1	0	32.408	31.899	0.11015	0.509	0.511	
4	1	1	-1	17.670	15.951	0.11372	1.719	1.723	
5	0	2	1	8.597	9.761	0.11966	-1.164	-1.168	
6	1	1	1	35.048	37.922	0.12745	-2.875	-2.883	*
7	1	1	-2	57.529	63.274	0.13653	-5.744	-5.760	**
8	0	2	2	69.811	81.120	0.14725	-11.309	-11.340	***
9	0	0	3	86.349	100.128	0.14864	-13.779	-13.818	***
10	1	1	2	75.343	86.023	0.15895	-10.680	-10.710	***
11	1	1	-3	65.932	76.690	0.17106	-10.758	-10.788	***
12	0	2	3	52.186	55.905	0.18427	-3.720	-3.730	*
13	2	0	-1	51.681	54.364	0.18925	-2.682	-2.690	*
14	1	3	0	51.812	52.824	0.18937	-1.012	-1.015	
15	2	0	0	100.174	105.086	0.19150	-4.912	-4.926	**
16	1	3	-1	101.170	103.764	0.19147	-2.594	-2.601	*
17	1	1	3	31.245	31.587	0.19797	-0.342	-0.343	
18	0	0	4	46.126	55.615	0.19818	-9.489	-9.515	***
19	2	0	-2	45.529	40.045	0.19967	5.484	5.499	**
20	1	3	1	48.445	41.652	0.19993	6.793	6.812	**
21	1	3	-2	93.784	88.656	0.20584	5.128	5.143	**
22	2	0	1	94.981	93.424	0.20600	1.558	1.562	
23	1	1	-4	11.501	10.615	0.21163	0.886	0.888	
24	0	4	0	38.433	39.976	0.21784	-1.543	-1.548	
25	2	2	-1	37.787	37.569	0.21835	0.219	0.219	
26	2	2	0	36.918	36.400	0.22031	0.518	0.520	
27	2	0	-3	36.843	34.599	0.22098	2.243	2.250	*
28	1	3	2	37.217	33.914	0.22134	3.303	3.313	*
29	0	4	1	34.644	33.132	0.22340	1.511	1.515	
30	0	2	4	4.209	5.580	0.22614	-1.371	-1.375	
31	2	2	-2	33.549	33.027	0.22745	0.522	0.523	

32	1	3	-3	88.152	87.867	0.23019	0.286	0.287	
33	2	0	2	92.117	91.084	0.23046	1.034	1.036	
34	2	2	1	30.288	30.949	0.23302	-0.661	-0.663	
35	0	4	2	21.003	24.359	0.23932	-3.356	-3.366	*
36	1	1	4	12.546	12.893	0.24090	-0.347	-0.348	
37	2	2	-3	9.017	13.908	0.24636	-4.891	-4.904	**
38	0	0	5	85.905	96.668	0.24773	-10.762	-10.792	***
39	2	0	-4	70.546	68.124	0.25040	2.421	2.428	*
40	1	3	3	70.062	68.076	0.25084	1.986	1.991	
41	2	2	2	7.245	1.125	0.25490	6.121	6.138	**
42	1	1	-5	15.099	12.679	0.25539	2.420	2.427	*
43	1	3	-4	41.474	40.251	0.26175	1.223	1.227	
44	2	0	3	43.251	42.251	0.26210	1.000	1.003	
45	0	4	3	19.133	15.536	0.26372	3.597	3.607	*
46	0	2	5	11.842	9.046	0.27062	2.796	2.804	*
47	2	2	-4	27.309	25.821	0.27307	1.487	1.492	
48	2	2	3	28.199	28.844	0.28383	-0.645	-0.646	
49	2	0	-5	33.448	33.756	0.28545	-0.308	-0.308	
50	1	3	4	33.357	34.605	0.28594	-1.248	-1.252	
51	1	1	5	4.947	1.347	0.28597	3.601	3.611	*
52	3	1	-1	28.665	25.037	0.28803	3.629	3.639	*
53	2	4	-1	31.351	25.743	0.28856	5.608	5.623	**
54	1	5	0	19.428	15.738	0.28864	3.690	3.700	*
55	2	4	0	5.321	3.760	0.29004	1.562	1.566	
56	1	5	-1	22.828	21.737	0.29003	1.091	1.094	
57	3	1	-2	12.388	11.754	0.29217	0.634	0.636	
58	3	1	0	7.360	8.354	0.29236	-0.994	-0.997	
59	0	4	4	23.919	24.196	0.29450	-0.277	-0.277	
60	2	4	-2	10.055	8.462	0.29550	1.592	1.597	
61	1	5	1	31.577	29.454	0.29568	2.123	2.128	*
62	0	0	6	19.949	18.897	0.29728	1.053	1.056	
63	1	3	-5	99.862	106.133	0.29825	-6.271	-6.289	**
64	2	0	4	104.584	110.561	0.29865	-5.976	-5.993	**
65	1	5	-2	27.590	23.779	0.29971	3.811	3.822	*

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
66	2	4	1	46.576	43.133	0.29982	3.442	3.452	*
67	1	1	-6	5.998	7.975	0.30095	-1.977	-1.982	
68	3	1	-3	54.031	54.585	0.30441	-0.554	-0.556	
69	3	1	1	36.842	36.881	0.30479	-0.039	-0.039	
70	2	2	-5	12.690	13.222	0.30553	-0.532	-0.533	
71	2	4	-3	40.695	39.878	0.31030	0.817	0.819	
72	1	5	2	54.750	52.438	0.31056	2.312	2.319	*
73	0	2	6	16.764	18.550	0.31660	-1.786	-1.791	
74	1	5	-3	37.175	36.939	0.31693	0.235	0.236	
75	2	4	2	44.197	43.607	0.31712	0.589	0.591	
76	2	2	4	2.027	1.191	0.31789	0.837	0.839	
77	3	1	-4	26.715	26.979	0.32386	-0.264	-0.265	
78	3	1	2	31.244	30.654	0.32439	0.590	0.591	
79	2	0	-6	73.558	77.433	0.32431	-3.875	-3.885	*
80	1	3	5	73.287	76.445	0.32482	-3.157	-3.166	*

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
81	3	3	-1	133.823	132.181	0.32664	1.642	1.647	
82	0	6	0	131.952	123.506	0.32676	8.445	8.469	***
83	0	4	5	14.899	14.886	0.32989	0.013	0.013	
84	3	3	-2	54.170	50.230	0.33029	3.940	3.951	*
85	3	3	0	54.832	50.109	0.33046	4.723	4.736	**
86	0	6	1	53.247	45.625	0.33050	7.622	7.644	**
87	2	4	-4	19.438	19.061	0.33190	0.377	0.378	
88	1	5	3	9.204	7.407	0.33223	1.797	1.802	
89	1	1	6	26.458	27.322	0.33233	-0.864	-0.867	
90	1	3	-6	48.262	46.795	0.33808	1.467	1.471	
91	2	0	5	49.401	49.777	0.33852	-0.375	-0.376	
92	1	5	-4	9.285	9.442	0.34054	-0.157	-0.158	
93	2	4	3	7.223	7.554	0.34081	-0.331	-0.332	
94	3	3	-3	4.742	4.757	0.34117	-0.014	-0.014	
95	0	6	2	4.463	3.859	0.34146	0.605	0.606	
96	3	3	1	4.730	5.506	0.34150	-0.776	-0.778	
97	2	2	-6	26.870	28.848	0.34211	-1.978	-1.984	
98	0	0	7	46.754	51.250	0.34682	-4.496	-4.508	**
99	1	1	-7	29.631	30.204	0.34761	-0.573	-0.574	
100	3	1	-5	17.038	16.929	0.34930	0.109	0.109	
101	3	1	3	2.360	2.162	0.34996	0.198	0.199	
102	2	2	5	41.171	41.506	0.35561	-0.334	-0.335	
103	3	3	-4	30.856	26.167	0.35863	4.688	4.701	**
104	0	6	3	30.955	24.448	0.35898	6.508	6.526	**
105	2	4	-5	7.229	6.653	0.35908	0.577	0.578	
106	3	3	2	31.251	27.259	0.35910	3.992	4.003	**
107	1	5	4	22.176	20.961	0.35946	1.215	1.218	
108	0	2	7	27.409	28.674	0.36352	-1.266	-1.269	
109	2	0	-7	103.312	110.017	0.36576	-6.704	-6.723	**
110	1	3	6	104.259	111.313	0.36629	-7.053	-7.073	**
111	0	4	6	47.602	47.061	0.36855	0.541	0.542	
112	1	5	-5	9.963	6.732	0.36933	3.231	3.240	*
113	2	4	4	21.364	19.825	0.36966	1.539	1.543	
114	4	0	-1	57.567	54.670	0.37751	2.897	2.905	*
115	2	6	-1	57.671	52.083	0.37761	5.588	5.603	**
116	4	0	-2	83.587	80.209	0.37849	3.377	3.387	*
117	2	6	0	85.152	73.425	0.37874	11.727	11.760	***
118	1	1	7	19.127	19.378	0.37948	-0.251	-0.252	
119	3	1	-6	16.115	15.257	0.37954	0.858	0.860	
120	1	3	-7	22.577	23.199	0.38021	-0.622	-0.624	
121	3	1	4	6.354	4.755	0.38029	1.599	1.603	
122	2	0	6	23.114	24.762	0.38067	-1.648	-1.652	
123	2	2	-7	47.740	48.397	0.38163	-0.658	-0.659	
124	3	3	-5	57.167	53.357	0.38176	3.810	3.821	*
125	0	6	4	58.792	49.514	0.38216	9.278	9.304	***
126	3	3	3	59.633	52.806	0.38236	6.827	6.846	**
127	2	6	-2	6.878	5.818	0.38294	1.060	1.063	
128	4	0	0	5.374	6.548	0.38299	-1.173	-1.176	
129	4	0	-3	80.033	75.926	0.38589	4.107	4.119	**
130	2	6	1	84.889	69.306	0.38628	15.583	15.627	***

131	2	4	-6	1.255	1.467	0.39068	-0.212	-0.212	
132	1	5	5	7.997	6.325	0.39111	1.672	1.677	
133	3	5	-1	29.934	25.895	0.39261	4.038	4.050	**
134	4	2	-1	18.883	17.595	0.39291	1.288	1.291	
135	1	7	0	29.364	26.637	0.39306	2.727	2.734	*
136	4	2	-2	24.967	24.067	0.39385	0.900	0.903	
137	1	7	-1	5.036	2.673	0.39408	2.363	2.370	*
138	2	6	-3	65.522	53.711	0.39447	11.811	11.844	***
139	4	0	1	65.109	59.367	0.39467	5.742	5.758	**
140	1	1	-8	8.876	8.765	0.39496	0.112	0.112	
141	3	5	-2	12.224	10.677	0.39566	1.547	1.551	
142	3	5	0	11.768	12.539	0.39580	-0.771	-0.773	
143	2	2	6	41.382	41.602	0.39595	-0.220	-0.220	
144	0	0	8	48.545	55.308	0.39637	-6.763	-6.782	**
145	4	2	0	26.157	24.794	0.39818	1.363	1.367	
146	1	7	1	2.598	1.654	0.39826	0.944	0.946	
147	4	0	-4	10.810	10.805	0.39934	0.005	0.005	
148	2	6	2	11.517	9.275	0.39986	2.242	2.248	*
149	4	2	-3	15.083	13.014	0.40096	2.069	2.075	*
150	1	7	-2	37.384	33.712	0.40126	3.672	3.683	*
151	1	5	-6	6.816	5.730	0.40219	1.086	1.089	
152	2	4	5	5.555	5.165	0.40256	0.390	0.391	
153	3	5	-3	45.249	41.925	0.40478	3.324	3.333	*
154	3	5	1	24.069	20.176	0.40507	3.893	3.904	*
155	2	0	-8	29.171	30.248	0.40901	-1.077	-1.080	
156	1	7	2	29.090	24.782	0.40942	4.308	4.320	**
157	4	2	1	43.686	42.102	0.40942	1.584	1.589	
158	1	3	7	30.341	29.828	0.40955	0.513	0.515	
159	0	4	7	28.916	28.511	0.40956	0.405	0.406	
160	3	3	-6	27.682	26.973	0.40960	0.710	0.712	
161	0	6	5	28.715	26.539	0.41005	2.176	2.182	*
162	3	3	4	28.423	27.561	0.41030	0.862	0.865	
163	0	2	8	2.145	1.479	0.41106	0.666	0.668	
164	2	6	-4	17.079	11.828	0.41167	5.251	5.266	**
165	4	0	2	17.338	14.619	0.41200	2.719	2.726	*
166	3	1	-7	16.544	16.846	0.41351	-0.303	-0.303	
167	4	2	-4	28.666	27.855	0.41393	0.811	0.814	
168	1	7	-3	35.835	32.095	0.41428	3.740	3.751	*
169	3	1	5	12.924	12.555	0.41434	0.369	0.370	
170	4	0	-5	35.636	34.867	0.41826	0.769	0.771	
171	2	6	3	37.127	32.566	0.41889	4.561	4.573	**
172	3	5	-4	21.712	19.033	0.41960	2.679	2.686	*
173	3	5	2	26.545	24.001	0.42001	2.544	2.552	*
174	2	2	-8	12.441	12.961	0.42326	-0.520	-0.522	
175	1	3	-8	14.570	14.618	0.42394	-0.048	-0.048	
176	2	0	7	14.261	15.179	0.42442	-0.918	-0.921	
177	2	4	-7	16.445	15.884	0.42571	0.561	0.563	
178	1	7	3	18.122	16.739	0.42610	1.382	1.386	
179	1	5	6	26.564	24.962	0.42617	1.602	1.607	
180	4	2	2	5.317	4.278	0.42616	1.039	1.042	
181	1	1	8	5.879	6.876	0.42718	-0.998	-1.000	

182	4	2	-5	8.766	8.136	0.43221	0.630	0.632	
183	1	7	-4	10.091	9.888	0.43261	0.202	0.203	
184	2	6	-5	16.215	13.819	0.43389	2.396	2.402	*
185	4	0	3	16.021	13.917	0.43433	2.104	2.110	*
186	0	8	0	5.126	1.582	0.43568	3.544	3.554	*
187	4	4	-1	1.495	0.426	0.43586	1.069	1.072	
188	4	4	-2	3.504	4.424	0.43671	-0.920	-0.922	
189	1	5	-7	18.419	15.915	0.43819	2.503	2.510	*
190	2	2	7	4.059	3.222	0.43818	0.837	0.839	
191	0	8	1	10.571	8.976	0.43849	1.595	1.599	
192	2	4	6	28.083	26.516	0.43860	1.567	1.572	
193	3	5	-5	19.344	18.531	0.43954	0.813	0.816	
194	3	5	3	1.407	0.709	0.44006	0.698	0.700	
195	4	4	0	14.740	13.132	0.44061	1.608	1.612	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
196	3	3	-7	14.071	14.087	0.44127	-0.015	-0.015	
197	0	6	6	14.790	13.626	0.44175	1.164	1.167	
198	4	0	-6	83.548	79.436	0.44195	4.112	4.124	**
199	3	3	5	14.934	14.554	0.44205	0.380	0.381	
200	2	6	4	84.751	73.795	0.44268	10.956	10.986	***
201	1	1	-9	6.982	7.399	0.44280	-0.418	-0.419	
202	4	4	-3	17.589	14.668	0.44313	2.921	2.929	*
203	0	0	9	17.427	18.441	0.44591	-1.014	-1.017	
204	0	8	2	17.177	13.420	0.44681	3.757	3.767	*
205	1	7	4	4.900	2.705	0.44766	2.195	2.201	*
206	4	2	3	24.630	23.859	0.44778	0.771	0.773	
207	3	1	-8	24.902	24.084	0.45039	0.818	0.820	
208	4	4	1	14.527	12.113	0.45079	2.414	2.421	*
209	3	1	6	15.255	14.854	0.45127	0.401	0.402	
210	0	4	8	17.232	16.176	0.45228	1.056	1.059	
211	2	0	-9	13.041	13.576	0.45355	-0.535	-0.537	
212	1	3	8	13.524	13.708	0.45411	-0.184	-0.185	
213	4	4	-4	8.468	6.769	0.45489	1.699	1.704	
214	4	2	-6	6.258	5.462	0.45518	0.796	0.798	
215	1	7	-5	23.041	20.873	0.45562	2.168	2.174	*
216	0	2	9	3.557	5.019	0.45902	-1.462	-1.467	
217	2	6	-6	61.814	55.673	0.46038	6.142	6.159	**
218	4	0	4	65.283	62.712	0.46092	2.572	2.579	*
219	2	4	-8	9.922	8.030	0.46340	1.892	1.897	
220	1	5	7	17.240	15.763	0.46389	1.477	1.481	
221	3	5	-6	17.914	17.469	0.46393	0.444	0.446	
222	3	5	4	5.086	4.070	0.46454	1.016	1.018	
223	4	4	2	8.758	8.659	0.46605	0.099	0.099	
224	2	2	-9	24.659	24.413	0.46645	0.246	0.247	
225	1	3	-9	48.945	48.544	0.46883	0.401	0.402	
226	2	0	8	47.240	50.369	0.46933	-3.129	-3.138	*
227	4	0	-7	17.332	15.337	0.46969	1.995	2.000	*
228	2	6	5	17.497	14.301	0.47050	3.196	3.205	*
229	4	4	-5	15.135	13.922	0.47159	1.212	1.216	
230	1	7	5	1.656	1.079	0.47344	0.577	0.579	

231	4	2	4	10.572	10.048	0.47362	0.524	0.525	
232	3	7	-1	9.776	11.669	0.47469	-1.893	-1.899	
233	5	1	-2	12.002	11.898	0.47479	0.104	0.104	
234	2	8	-1	10.227	11.211	0.47501	-0.984	-0.987	
235	1	1	9	2.416	1.151	0.47526	1.265	1.269	
236	5	1	-1	8.607	8.626	0.47575	-0.019	-0.019	
237	2	8	0	4.602	4.206	0.47591	0.396	0.397	
238	3	3	-8	43.564	42.965	0.47600	0.600	0.601	
239	0	6	7	45.114	40.325	0.47651	4.788	4.802	**
240	1	5	-8	1.846	0.757	0.47663	1.088	1.091	
241	3	3	6	44.421	44.103	0.47684	0.318	0.319	
242	2	4	7	9.557	7.394	0.47706	2.163	2.169	*
243	3	7	-2	2.059	3.072	0.47721	-1.013	-1.016	
244	3	7	0	2.382	2.969	0.47733	-0.587	-0.588	
245	0	8	4	17.228	14.499	0.47864	2.729	2.736	*
246	5	1	-3	13.618	12.633	0.47898	0.986	0.988	
247	2	8	-2	5.263	4.793	0.47926	0.471	0.472	
248	5	1	0	14.913	13.489	0.48183	1.424	1.428	
249	2	2	8	26.755	26.622	0.48180	0.133	0.133	
250	2	8	1	16.535	17.989	0.48193	-1.455	-1.459	
251	4	2	-7	2.248	1.620	0.48216	0.628	0.630	
252	1	7	-6	1.306	0.528	0.48264	0.779	0.781	
253	3	7	-3	14.234	15.892	0.48480	-1.658	-1.663	
254	3	7	1	17.371	21.837	0.48504	-4.466	-4.479	**
255	4	4	3	14.751	13.526	0.48590	1.225	1.228	
256	5	1	-4	23.046	20.862	0.48818	2.183	2.189	*
257	2	8	-3	15.960	16.141	0.48852	-0.181	-0.182	
258	3	1	-9	1.371	0.503	0.48950	0.868	0.871	
259	2	6	-7	59.539	51.488	0.49046	8.052	8.074	***
260	3	1	7	5.609	6.327	0.49044	-0.717	-0.719	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
261	1	1	-10	5.346	4.294	0.49098	1.052	1.055	
262	4	0	5	61.649	61.034	0.49109	0.615	0.617	
263	3	5	-7	10.684	10.468	0.49211	0.216	0.217	
264	4	4	-6	7.844	7.077	0.49272	0.768	0.770	
265	2	8	2	11.408	13.051	0.49288	-1.642	-1.647	
266	3	5	5	6.454	5.270	0.49281	1.184	1.187	
267	5	1	1	16.335	15.057	0.49284	1.278	1.281	
268	0	0	10	29.308	27.715	0.49546	1.593	1.598	
269	0	4	9	21.411	21.028	0.49628	0.382	0.383	
270	3	7	-4	6.284	8.094	0.49724	-1.810	-1.815	
271	3	7	2	5.965	6.722	0.49759	-0.757	-0.759	
272	2	0	-10	42.869	42.403	0.49904	0.466	0.467	
273	5	3	-2	22.293	20.165	0.49915	2.128	2.134	*
274	4	6	-1	15.477	19.221	0.49929	-3.744	-3.755	*
275	1	9	0	18.673	18.101	0.49941	0.573	0.574	
276	1	3	9	44.365	42.894	0.49960	1.472	1.476	
277	4	6	-2	27.140	31.651	0.50003	-4.511	-4.523	**
278	5	3	-1	38.718	33.829	0.50006	4.889	4.903	**
279	1	9	-1	32.604	26.760	0.50021	5.844	5.860	**

280	4	0	-8	11.408	11.234	0.50081	0.175	0.175	
281	0	8	5	1.912	0.152	0.50119	1.760	1.765	
282	2	6	6	11.838	10.917	0.50168	0.921	0.923	
283	5	1	-5	2.114	0.644	0.50213	1.470	1.474	
284	2	8	-4	1.526	1.512	0.50252	0.013	0.013	
285	1	7	6	9.278	6.622	0.50280	2.656	2.663	*
286	4	2	5	20.516	19.932	0.50302	0.584	0.586	
287	2	4	-9	8.995	8.425	0.50315	0.570	0.571	
288	5	3	-3	2.897	2.280	0.50314	0.617	0.619	
289	4	6	0	2.692	1.030	0.50344	1.662	1.667	
290	1	9	1	2.035	1.600	0.50351	0.434	0.435	
291	1	5	8	5.745	5.957	0.50365	-0.212	-0.212	
292	4	6	-3	41.161	50.962	0.50565	-9.801	-9.828	***
293	1	9	-2	50.308	46.029	0.50588	4.279	4.291	**
294	5	3	0	58.939	56.124	0.50585	2.815	2.823	*
295	0	2	10	9.060	7.392	0.50729	1.667	1.672	
296	5	1	2	3.979	3.658	0.50846	0.321	0.322	
297	2	8	3	4.366	5.420	0.50845	-1.054	-1.057	
298	4	4	4	8.781	7.631	0.50981	1.150	1.153	
299	2	2	-10	12.691	12.925	0.51079	-0.234	-0.235	
300	5	3	-4	31.368	27.220	0.51191	4.148	4.160	**
301	4	6	1	21.768	25.456	0.51238	-3.688	-3.698	*
302	1	9	2	24.535	21.430	0.51238	3.104	3.113	*
303	4	2	-8	10.790	10.329	0.51252	0.461	0.463	
304	1	7	-7	24.013	21.067	0.51302	2.947	2.955	*
305	3	3	-9	45.696	44.851	0.51317	0.845	0.848	
306	0	6	8	47.286	42.415	0.51369	4.871	4.885	**
307	3	3	7	47.419	46.987	0.51406	0.433	0.434	
308	3	7	-5	5.421	4.969	0.51417	0.452	0.453	
309	1	3	-10	2.708	4.298	0.51457	-1.590	-1.594	
310	3	7	3	8.421	11.103	0.51462	-2.682	-2.690	*
311	2	0	9	1.837	4.852	0.51508	-3.016	-3.024	*
312	4	6	-4	11.778	14.378	0.51599	-2.600	-2.607	*
313	1	9	-3	14.906	12.803	0.51627	2.103	2.109	*
314	5	3	1	16.894	17.041	0.51635	-0.147	-0.148	
315	1	5	-9	8.694	7.197	0.51697	1.497	1.501	
316	2	4	8	8.492	8.460	0.51742	0.031	0.032	
317	4	4	-7	15.517	14.630	0.51775	0.887	0.889	
318	5	1	-6	14.440	13.868	0.52044	0.572	0.574	
319	2	8	-5	6.705	6.140	0.52087	0.565	0.567	
320	3	5	-8	22.313	21.196	0.52348	1.118	1.121	
321	2	6	-8	19.510	17.004	0.52351	2.506	2.513	*
322	1	1	10	11.662	11.556	0.52361	0.106	0.106	
323	4	0	6	20.892	20.508	0.52420	0.384	0.385	
324	3	5	6	9.360	7.276	0.52424	2.084	2.090	*
325	5	3	-5	21.562	18.495	0.52523	3.068	3.076	*

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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326	1	9	3	16.725	15.075	0.52580	1.650	1.654	
327	4	6	2	15.496	17.878	0.52585	-2.382	-2.388	*
328	2	2	9	3.047	3.631	0.52647	-0.583	-0.585	

329	0	8	6	22.200	18.627	0.52744	3.573	3.583	*
330	5	1	3	8.825	8.690	0.52829	0.135	0.136	
331	2	8	4	9.968	11.898	0.52822	-1.930	-1.935	
332	3	1	-10	6.897	7.303	0.53036	-0.406	-0.407	
333	4	6	-5	5.566	6.611	0.53077	-1.045	-1.048	
334	1	9	-4	7.093	4.187	0.53109	2.907	2.915	*
335	5	3	2	7.690	8.482	0.53128	-0.791	-0.794	
336	3	1	8	4.132	4.493	0.53134	-0.361	-0.362	
337	4	0	-9	2.283	2.570	0.53471	-0.287	-0.288	
338	1	7	7	4.889	2.293	0.53514	2.596	2.603	*
339	3	7	-6	3.956	4.471	0.53517	-0.515	-0.516	
340	4	2	6	16.128	14.569	0.53540	1.559	1.563	
341	2	6	7	2.967	1.073	0.53564	1.893	1.898	
342	3	7	4	5.649	7.927	0.53571	-2.278	-2.285	*
343	4	4	5	24.468	23.175	0.53723	1.294	1.297	
344	1	1	-11	12.480	12.731	0.53940	-0.251	-0.252	
345	0	4	10	6.624	4.551	0.54123	2.073	2.079	*
346	5	1	-7	1.590	1.624	0.54268	-0.034	-0.034	
347	5	3	-6	6.866	3.712	0.54276	3.154	3.163	*
348	2	8	-6	1.077	0.421	0.54313	0.656	0.657	
349	1	9	4	5.244	3.771	0.54342	1.473	1.477	
350	4	6	3	6.841	4.220	0.54352	2.620	2.628	*
351	2	4	-10	1.979	0.373	0.54451	1.606	1.611	
352	0	10	0	6.342	5.890	0.54460	0.452	0.454	
353	5	5	-2	8.147	8.377	0.54461	-0.230	-0.231	
354	1	5	9	4.369	5.199	0.54503	-0.830	-0.832	
355	0	0	11	36.224	37.499	0.54500	-1.275	-1.279	
356	2	0	-11	16.271	17.942	0.54523	-1.672	-1.677	
357	5	5	-1	3.194	3.506	0.54545	-0.312	-0.313	
358	4	2	-9	1.610	2.154	0.54570	-0.544	-0.545	
359	1	3	10	16.907	17.726	0.54580	-0.819	-0.821	
360	4	4	-8	23.201	21.186	0.54614	2.015	2.021	*
361	1	7	-8	8.557	7.303	0.54622	1.254	1.257	
362	0	10	1	1.261	0.655	0.54685	0.607	0.608	
363	5	5	-3	5.377	6.333	0.54827	-0.956	-0.958	
364	4	6	-6	40.759	49.934	0.54963	-9.175	-9.200	***
365	1	9	-5	52.394	45.362	0.55000	7.032	7.052	**
366	5	3	3	54.775	55.562	0.55028	-0.787	-0.789	
367	5	5	0	9.497	12.079	0.55076	-2.582	-2.589	*
368	2	8	5	5.270	5.812	0.55174	-0.543	-0.544	
369	5	1	4	7.155	6.170	0.55186	0.985	0.988	
370	3	3	-10	1.147	1.161	0.55228	-0.014	-0.014	
371	0	6	9	1.690	0.629	0.55282	1.061	1.064	
372	3	3	8	4.412	0.772	0.55321	3.641	3.651	*
373	0	10	2	12.553	11.141	0.55354	1.412	1.416	
374	0	2	11	12.620	13.175	0.55578	-0.555	-0.556	
375	2	2	-11	12.610	11.870	0.55600	0.739	0.741	
376	5	5	-4	9.883	12.059	0.55633	-2.176	-2.182	*
377	0	8	7	18.453	15.212	0.55687	3.241	3.250	*
378	3	5	-9	1.110	0.612	0.55749	0.498	0.499	
379	3	5	7	6.290	6.556	0.55831	-0.266	-0.267	
380	1	5	-10	6.038	5.462	0.55878	0.576	0.578	

381	2	6	-9	2.183	0.648	0.55900	1.535	1.539	
382	3	7	-7	8.765	9.934	0.55978	-1.169	-1.173	
383	4	0	7	2.059	1.575	0.55975	0.484	0.485	
384	3	7	5	8.937	11.306	0.56040	-2.369	-2.375	*
385	5	5	1	6.235	7.778	0.56042	-1.543	-1.548	
386	1	3	-11	9.254	8.052	0.56096	1.203	1.206	
387	2	0	10	9.115	8.352	0.56148	0.763	0.765	
388	5	3	-7	29.707	26.814	0.56411	2.893	2.901	*
389	0	10	3	2.334	1.914	0.56452	0.420	0.421	
390	1	9	5	22.188	21.966	0.56485	0.222	0.223	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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391	4	6	4	20.457	25.943	0.56500	-5.486	-5.501	**
392	6	0	-2	58.477	53.209	0.56568	5.268	5.283	**
393	3	9	-1	39.824	42.309	0.56590	-2.485	-2.492	*
394	4	4	6	7.629	6.829	0.56767	0.801	0.803	
395	6	0	-3	32.908	31.035	0.56774	1.873	1.878	
396	6	0	-1	19.717	18.838	0.56794	0.879	0.881	
397	3	9	-2	0.937	12.631	0.56801	-11.694	-11.726	***
398	3	9	0	22.968	26.296	0.56811	-3.329	-3.338	*
399	5	1	-8	16.514	15.049	0.56837	1.464	1.469	
400	2	8	-7	8.845	12.408	0.56886	-3.563	-3.573	*
401	1	7	8	7.490	6.065	0.56996	1.425	1.429	
402	4	2	7	3.766	3.779	0.57025	-0.013	-0.013	
403	2	6	8	24.492	21.999	0.57187	2.493	2.500	*
404	2	2	10	17.192	16.654	0.57195	0.538	0.539	
405	4	6	-7	3.590	20.454	0.57218	-16.864	-16.911	****
406	1	1	11	9.922	10.521	0.57217	-0.599	-0.601	
407	1	9	-6	22.745	18.895	0.57258	3.850	3.860	*
408	3	1	-11	3.859	2.744	0.57260	1.115	1.118	
409	5	3	4	22.714	24.284	0.57295	-1.570	-1.574	
410	3	1	9	9.244	7.882	0.57360	1.362	1.366	
411	6	0	-4	7.609	6.286	0.57409	1.322	1.326	
412	5	5	2	4.604	5.585	0.57421	-0.981	-0.984	
413	6	0	0	4.787	5.461	0.57449	-0.675	-0.677	
414	3	9	1	7.868	7.019	0.57460	0.849	0.852	
415	6	2	-2	5.036	6.631	0.57607	-1.595	-1.599	
416	4	8	-1	3.839	2.721	0.57648	1.118	1.121	
417	2	10	-1	7.200	4.757	0.57655	2.443	2.450	*
418	4	8	-2	0.798	3.901	0.57713	-3.103	-3.112	*
419	4	4	-9	2.533	2.811	0.57739	-0.278	-0.279	
420	6	2	-3	4.039	4.561	0.57809	-0.522	-0.523	
421	6	2	-1	1.566	1.497	0.57829	0.069	0.069	
422	2	8	6	11.340	13.501	0.57856	-2.161	-2.167	*
423	5	1	5	13.962	13.078	0.57872	0.884	0.886	
424	0	10	4	6.911	6.372	0.57954	0.539	0.541	
425	4	8	0	6.648	8.234	0.58009	-1.587	-1.591	
426	2	10	-2	6.013	4.540	0.58005	1.473	1.477	
427	4	2	-10	5.395	4.992	0.58121	0.403	0.404	
428	1	7	-9	5.889	5.001	0.58175	0.888	0.891	
429	4	8	-3	0.888	7.795	0.58200	-6.908	-6.927	**

430	2	10	1	8.587	9.264	0.58226	-0.677	-0.679	
431	6	2	-4	11.189	12.318	0.58433	-1.130	-1.133	
432	6	0	-5	14.619	13.058	0.58458	1.561	1.565	
433	6	2	0	8.533	8.542	0.58472	-0.009	-0.009	
434	5	5	-6	1.047	7.834	0.58485	-6.787	-6.806	**
435	3	9	-4	1.296	11.302	0.58494	-10.005	-10.033	***
436	6	0	1	16.131	15.390	0.58517	0.740	0.742	
437	3	9	2	13.931	9.265	0.58524	4.666	4.679	**
438	0	4	11	19.705	18.832	0.58693	0.873	0.875	
439	2	4	-11	11.159	9.987	0.58714	1.171	1.175	
440	3	7	-8	3.401	6.694	0.58755	-3.294	-3.303	*
441	1	5	10	7.117	6.081	0.58767	1.036	1.039	
442	2	10	-3	8.606	5.189	0.58773	3.417	3.427	*
443	4	8	1	8.706	9.028	0.58786	-0.322	-0.323	
444	1	1	-12	6.392	6.093	0.58801	0.299	0.300	
445	3	7	6	9.374	11.739	0.58823	-2.364	-2.371	*
446	5	3	-8	50.489	44.334	0.58887	6.155	6.172	**
447	0	8	8	11.414	9.238	0.58900	2.176	2.182	*
448	1	9	6	37.427	38.173	0.58967	-0.746	-0.748	
449	4	6	5	35.577	44.785	0.58986	-9.208	-9.234	***
450	2	10	2	5.636	4.989	0.59136	0.647	0.649	
451	5	5	3	6.328	9.000	0.59183	-2.672	-2.680	*
452	2	0	-12	17.461	15.721	0.59197	1.740	1.745	
453	1	3	11	18.080	16.588	0.59254	1.491	1.495	
454	3	3	-11	19.884	18.291	0.59296	1.594	1.598	
455	0	6	10	20.664	17.404	0.59351	3.260	3.269	*

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
456	3	5	-10	5.614	5.657	0.59369	-0.043	-0.043	
457	3	3	9	20.785	19.423	0.59392	1.363	1.366	
458	3	5	8	1.356	0.959	0.59456	0.397	0.398	
459	0	0	12	23.734	21.057	0.59455	2.677	2.684	*
460	6	2	-5	1.097	0.276	0.59465	0.821	0.823	
461	6	2	1	1.626	1.037	0.59522	0.589	0.591	
462	2	6	-10	21.620	18.059	0.59650	3.560	3.570	*
463	5	1	-9	8.566	7.222	0.59707	1.344	1.348	
464	4	0	8	21.520	21.281	0.59730	0.239	0.240	
465	2	8	-8	2.134	2.599	0.59758	-0.465	-0.466	
466	4	6	-8	3.022	17.382	0.59798	-14.361	-14.401	***
467	0	10	5	3.201	3.292	0.59830	-0.091	-0.092	
468	1	9	-7	18.521	17.135	0.59842	1.386	1.390	
469	5	3	5	17.392	19.308	0.59887	-1.917	-1.922	
470	6	0	-6	38.183	33.821	0.59901	4.362	4.374	**
471	3	9	-5	1.685	16.847	0.59940	-15.162	-15.204	***
472	2	10	-4	2.114	1.862	0.59941	0.253	0.253	
473	4	8	2	6.302	5.380	0.59964	0.923	0.925	
474	3	9	3	26.401	29.322	0.59979	-2.921	-2.929	*
475	6	0	2	26.017	22.910	0.59977	3.107	3.116	*
476	4	4	7	13.751	13.834	0.60065	-0.083	-0.083	
477	1	5	-11	11.358	10.338	0.60178	1.020	1.023	
478	2	2	-12	19.017	18.184	0.60191	0.833	0.835	

479	2	4	10	8.825	8.167	0.60226	0.658	0.660	
480	2	10	3	8.185	8.770	0.60439	-0.584	-0.586	
481	0	2	12	0.927	0.549	0.60445	0.379	0.380	
482	6	4	-2	1.047	14.102	0.60617	-13.055	-13.092	***
483	5	7	-2	0.578	10.332	0.60645	-9.753	-9.781	***
484	1	11	0	10.135	11.940	0.60667	-1.804	-1.809	
485	1	7	9	3.002	2.531	0.60683	0.471	0.472	
486	4	2	8	4.713	5.692	0.60715	-0.978	-0.981	
487	5	7	-1	8.377	11.097	0.60721	-2.719	-2.727	*
488	1	11	-1	4.740	4.122	0.60733	0.618	0.620	
489	1	3	-12	29.368	28.019	0.60785	1.349	1.352	
490	2	8	7	1.167	0.976	0.60824	0.191	0.192	
491	6	4	-1	1.827	2.422	0.60829	-0.595	-0.597	
492	2	0	11	29.029	30.085	0.60838	-1.056	-1.059	
493	5	1	6	1.156	1.963	0.60844	-0.807	-0.809	
494	6	2	-6	10.481	10.708	0.60883	-0.227	-0.228	
495	6	2	2	7.370	8.512	0.60958	-1.142	-1.145	
496	2	6	9	6.104	6.683	0.60999	-0.579	-0.581	
497	1	11	1	1.655	1.508	0.61005	0.148	0.148	
498	4	4	-10	14.509	12.844	0.61106	1.665	1.670	
499	5	7	0	6.452	4.173	0.61198	2.279	2.286	*
500	1	11	-2	11.772	14.193	0.61201	-2.421	-2.427	*
501	5	5	4	7.968	6.980	0.61297	0.988	0.991	
502	6	4	-4	1.027	9.648	0.61403	-8.621	-8.645	***
503	6	4	0	14.354	18.199	0.61440	-3.845	-3.855	*
504	2	10	-5	8.865	7.047	0.61488	1.819	1.824	
505	4	8	3	8.471	10.084	0.61519	-1.613	-1.617	
506	3	1	-12	8.347	9.011	0.61593	-0.664	-0.666	
507	5	3	-9	17.910	15.927	0.61662	1.983	1.989	
508	5	7	-4	0.947	15.092	0.61700	-14.145	-14.185	***
509	3	1	10	10.790	11.720	0.61695	-0.930	-0.933	
510	6	0	-7	13.662	11.439	0.61708	2.223	2.229	*
511	1	11	2	14.669	9.276	0.61739	5.393	5.408	**
512	1	9	7	13.425	13.956	0.61748	-0.532	-0.533	
513	4	6	6	12.678	15.965	0.61771	-3.287	-3.296	*
514	3	9	4	13.742	11.041	0.61798	2.701	2.708	*
515	3	7	-9	1.376	4.830	0.61804	-3.454	-3.464	*
516	6	0	3	4.977	3.653	0.61801	1.324	1.327	
517	2	2	11	15.926	14.700	0.61805	1.226	1.229	
518	4	2	-11	6.143	4.825	0.61865	1.318	1.322	
519	3	7	7	3.989	3.791	0.61878	0.197	0.198	
520	1	7	-10	2.204	3.340	0.61921	-1.136	-1.140	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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521	0	10	6	9.293	9.397	0.62046	-0.104	-0.105	
522	4	8	-6	0.688	5.341	0.62060	-4.653	-4.666	**
523	1	11	-3	9.041	10.322	0.62062	-1.281	-1.285	
524	5	7	1	9.745	10.708	0.62069	-0.963	-0.965	
525	1	1	12	3.640	4.833	0.62088	-1.193	-1.196	
526	2	10	4	8.676	6.909	0.62112	1.766	1.771	
527	0	8	9	12.397	10.137	0 62342	2.260	2.267	*

528	6	4	1	6.339	7.069	0.62440	-0.731	-0.733	
529	6	2	-7	4.049	4.733	0.62662	-0.684	-0.686	
530	1	9	-8	1.915	1.855	0.62711	0.059	0.060	
531	6	2	3	1.047	2.250	0.62753	-1.202	-1.206	
532	5	3	6	1.905	2.162	0.62764	-0.257	-0.258	
533	5	5	-8	1.586	11.964	0.62787	-10.379	-10.408	***
534	5	1	-10	8.436	7.266	0.62838	1.171	1.174	
535	1	11	3	5.146	4.823	0.62857	0.323	0.324	
536	2	8	-9	5.136	7.326	0.62891	-2.190	-2.196	*
537	2	4	-12	8.845	8.707	0.63078	0.138	0.138	
538	1	5	11	8.064	7.834	0.63131	0.230	0.231	
539	3	5	9	8.321	6.789	0.63261	1.532	1.536	
540	1	11	-4	3.899	3.605	0.63301	0.294	0.295	
541	0	4	12	9.733	7.374	0.63320	2.358	2.365	*
542	2	10	-6	2.963	2.955	0.63385	0.008	0.008	
543	4	8	4	1.386	0.561	0.63425	0.825	0.827	
544	3	3	-12	34.035	32.001	0.63489	2.034	2.040	*
545	0	6	11	34.514	30.601	0.63546	3.912	3.923	*
546	2	6	-11	13.782	12.907	0.63565	0.874	0.877	
547	4	4	8	7.460	8.004	0.63579	-0.543	-0.545	
548	3	3	10	35.392	34.295	0.63589	1.097	1.100	
549	4	0	9	13.782	15.080	0.63649	-1.298	-1.302	
550	1	1	-13	7.160	8.559	0.63677	-1.399	-1.402	
551	5	5	5	9.014	11.568	0.63726	-2.554	-2.561	*
552	6	4	2	7.876	9.702	0.63811	-1.827	-1.832	
553	6	0	-8	14.430	11.379	0.63849	3.051	3.059	*
554	3	9	-7	0.788	7.862	0.63896	-7.074	-7.094	**
555	2	0	-13	4.737	2.519	0.63913	2.218	2.224	*
556	3	9	5	10.340	11.588	0.63949	-1.248	-1.251	
557	6	0	4	11.738	9.621	0.63957	2.116	2.122	*
558	1	3	12	4.896	2.278	0.63970	2.618	2.625	*
559	2	8	8	6.822	7.627	0.64038	-0.805	-0.807	
560	5	1	7	9.603	8.642	0.64062	0.962	0.964	
561	4	8	-7	8.067	5.981	0.64065	2.087	2.093	*
562	2	10	5	5.558	5.662	0.64124	-0.104	-0.105	
563	5	7	-6	9.812	12.764	0.64283	-2.952	-2.960	*
564	1	11	4	3.969	1.458	0.64338	2.511	2.518	*
565	0	0	13	17.810	15.541	0.64410	2.269	2.275	*
566	1	7	10	10.104	8.454	0.64539	1.650	1.655	
567	0	10	7	6.904	6.056	0.64566	0.848	0.850	
568	1	5	-12	5.654	4.498	0.64571	1.156	1.159	
569	4	2	9	3.680	2.825	0.64575	0.854	0.857	
570	2	4	11	5.416	5.295	0.64620	0.121	0.122	
571	4	4	-11	2.978	3.386	0.64678	-0.408	-0.409	
572	5	3	-10	7.684	6.368	0.64698	1.315	1.319	
573	6	2	-8	12.420	11.912	0.64772	0.508	0.509	
574	1	9	8	5.857	6.298	0.64789	-0.441	-0.442	
575	4	6	7	5.695	6.321	0.64815	-0.626	-0.628	
576	2	2	-13	2.670	0.728	0.64834	1.942	1.947	
577	4	0	-12	2.264	1.274	0.64862	0.990	0.992	
578	6	2	4	9.251	11.192	0.64878	-1.940	-1.946	
579	1	11	-5	8.901	11.435	0.64895	-2.535	-2.542	*

No.	h	k	l	Fo	Fc	sinθ/λ	Fo-Fc	w(Fo-Fc)	Flag
580	5	7	3	5.215	3.826	0.64919	1.389	1.393	
581	2	6	10	2.436	1.889	0.64964	0.547	0.549	
582	3	7	-10	5.465	4.826	0.65088	0.639	0.641	
583	3	7	8	7.599	6.668	0.65168	0.931	0.933	
584	0	2	13	8.686	8.664	0.65324	0.022	0.022	
585	6	6	-2	35.028	40.833	0.65327	-5.805	-5.821	**
586	0	12	0	4.009	30.950	0.65352	-26.941	-27.016	****
587	5	5	-9	4.228	3.169	0.65397	1.059	1.062	
588	6	4	-7	5.265	4.761	0.65440	0.505	0.506	
589	6	6	-3	10.662	12.827	0.65506	-2.166	-2.172	*
590	1	3	-13	37.416	33.510	0.65513	3.906	3.917	*
591	6	4	3	7.722	10.738	0.65528	-3.016	-3.024	*
592	6	6	-1	10.983	13.406	0.65523	-2.422	-2.429	*
593	0	12	1	1.060	8.896	0.65540	-7.836	-7.858	**
594	2	0	12	37.635	35.864	0.65566	1.771	1.776	
595	2	10	-7	8.819	9.690	0.65603	-0.871	-0.874	
596	4	8	5	11.963	14.326	0.65649	-2.363	-2.369	*
597	4	2	-12	9.299	9.036	0.65770	0.262	0.263	
598	4	6	-10	18.480	21.925	0.65781	-3.445	-3.455	*
599	1	9	-9	24.576	20.375	0.65829	4.200	4.212	**
600	1	7	-11	4.846	4.221	0.65827	0.625	0.627	
601	5	3	7	21.095	24.931	0.65888	-3.836	-3.847	*
602	0	8	10	2.196	0.442	0.65977	1.754	1.759	
603	3	1	-13	2.461	1.378	0.66013	1.083	1.086	
604	6	6	-4	6.362	4.628	0.66057	1.734	1.739	
605	6	6	0	6.641	4.624	0.66092	2.017	2.023	*
606	0	12	2	0.874	4.490	0.66099	-3.617	-3.627	*
607	5	7	-7	5.724	4.833	0.66095	0.891	0.893	
608	1	11	5	3.680	2.614	0.66158	1.066	1.069	
609	5	1	-11	4.131	3.600	0.66191	0.531	0.532	
610	3	11	-1	7.978	8.079	0.66248	-0.101	-0.101	
611	7	1	-2	6.973	9.104	0.66244	-2.131	-2.137	*
612	2	8	-10	2.284	2.158	0.66246	0.126	0.126	
613	4	10	-1	6.232	6.541	0.66265	-0.309	-0.310	
614	6	0	-9	31.368	28.205	0.66293	3.162	3.171	*
615	7	1	-3	3.574	3.702	0.66295	-0.128	-0.128	
616	3	9	-8	1.436	14.955	0.66342	-13.519	-13.557	***
617	3	9	6	21.438	24.757	0.66402	-3.319	-3.328	*
618	6	0	5	22.622	21.113	0.66414	1.509	1.513	
619	3	11	0	2.114	2.289	0.66437	-0.175	-0.175	
620	2	10	6	11.043	12.256	0.66446	-1.213	-1.217	
621	2	2	12	4.268	5.865	0.66465	-1.597	-1.601	
622	7	1	-1	2.843	3.159	0.66562	-0.316	-0.317	
623	4	10	0	6.312	5.261	0.66579	1.051	1.054	
624	7	1	-4	8.131	9.174	0.66716	-1.043	-1.046	
625	5	7	4	1.386	0.300	0.66851	1.086	1.089	
626	1	1	13	6.582	7.018	0.66971	-0.436	-0.437	
627	6	6	-5	13.500	15.503	0.66971	-2.003	-2.009	*
628	3	11	-3	6.580	5.675	0.66976	0.905	0.908	

629	3	11	1	11.219	7.957	0.66993	3.262	3.271	*
630	6	6	1	19.157	15.903	0.67022	3.253	3.263	*
631	0	12	3	1.790	11.669	0.67021	-9.880	-9.907	***
632	3	5	-12	5.521	5.442	0.67123	0.079	0.079	
633	6	2	-9	12.303	10.213	0.67182	2.090	2.095	*
634	3	5	10	9.069	9.017	0.67216	0.052	0.052	
635	7	1	0	7.693	7.976	0.67245	-0.284	-0.285	
636	4	10	1	10.830	7.433	0.67257	3.397	3.407	*
637	4	4	9	6.570	5.976	0.67274	0.594	0.595	
638	6	2	5	7.145	8.153	0.67301	-1.008	-1.011	
639	0	10	8	4.682	4.603	0.67357	0.079	0.080	
640	2	8	9	1.416	0.477	0.67463	0.939	0.941	
641	6	4	-8	2.560	3.742	0.67463	-1.183	-1.186	
642	5	1	8	1.965	0.907	0.67490	1.058	1.061	
643	7	1	-5	7.185	7.247	0.67499	-0.062	-0.062	
644	2	4	-13	5.235	5.549	0.67523	-0.314	-0.315	
645	6	4	4	5.445	5.238	0.67565	0.207	0.207	
646	1	5	12	1.955	2.274	0.67578	-0.320	-0.320	
647	2	6	-12	7.519	5.615	0.67617	1.904	1.909	
648	4	0	10	7.439	6.938	0.67704	0.502	0.503	
649	3	3	-13	9.773	8.077	0.67786	1.696	1.701	
650	0	6	12	9.942	8.054	0.67843	1.888	1.894	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
651	3	3	11	10.073	9.322	0.67887	0.751	0.753	
652	3	11	2	3.765	3.237	0.67907	0.528	0.530	
653	5	3	-11	18.852	16.182	0.67960	2.670	2.678	*
654	0	4	13	7.818	7.589	0.67994	0.230	0.230	
655	7	3	-2	10.575	11.200	0.68011	-0.626	-0.628	
656	2	12	-1	14.978	9.680	0.68037	5.298	5.313	**
657	1	9	9	13.596	13.750	0.68055	-0.154	-0.155	
658	7	3	-3	18.510	22.429	0.68061	-3.919	-3.930	*
659	5	9	-1	17.762	18.729	0.68089	-0.967	-0.969	
660	4	6	8	13.163	16.342	0.68084	-3.178	-3.187	*
661	2	10	-8	4.946	2.534	0.68109	2.412	2.419	*
662	2	12	0	18.472	15.933	0.68100	2.539	2.546	*
663	4	8	6	5.814	3.875	0.68162	1.938	1.944	
664	5	7	-8	8.536	8.007	0.68221	0.530	0.531	
665	6	6	-6	14.417	16.048	0.68234	-1.631	-1.635	
666	5	5	-10	6.603	7.254	0.68267	-0.652	-0.654	
667	1	11	6	4.735	3.756	0.68290	0.979	0.982	
668	7	1	1	1.476	0.851	0.68281	0.625	0.626	
669	0	12	4	2.045	11.860	0.68291	-9.815	-9.842	***
670	6	6	2	14.492	16.641	0.68301	-2.149	-2.155	*
671	7	3	-1	3.281	2.550	0.68321	0.730	0.733	
672	2	12	-2	3.470	2.600	0.68335	0.870	0.872	
673	4	4	-12	10.122	9.189	0.68422	0.933	0.935	
674	7	3	-4	21.459	26.388	0.68471	-4.929	-4.943	**
675	5	9	0	20.700	21.768	0.68515	-1.069	-1.072	
676	2	12	1	20.904	18.500	0.68522	2.404	2.410	*
677	1	7	11	6.135	5.449	0.68538	0.686	0.688	

678	1	1	-14	2.399	2.288	0.68563	0.112	0.112	
679	3	7	-11	2.224	4.012	0.68574	-1.789	-1.794	
680	4	2	10	4.792	5.445	0.68575	-0.653	-0.655	
681	7	1	-6	3.984	4.087	0.68631	-0.103	-0.103	
682	3	7	9	3.042	1.430	0.68657	1.611	1.616	
683	2	0	-14	22.808	22.286	0.68662	0.522	0.524	
684	1	3	13	23.395	22.406	0.68720	0.988	0.991	
685	4	0	-13	15.736	15.262	0.68953	0.474	0.476	
686	5	9	-4	1.167	17.601	0.68964	-16.434	-16.480	****
687	7	3	0	17.888	21.334	0.68986	-3.446	-3.455	*
688	2	12	-3	17.394	15.280	0.68987	2.114	2.120	*
689	6	0	-10	24.713	21.401	0.69006	3.312	3.321	*
690	1	11	-7	9.065	8.554	0.69046	0.511	0.512	
691	1	5	-13	8.795	8.849	0.69040	-0.053	-0.053	
692	2	6	11	16.082	14.900	0.69058	1.182	1.185	
693	3	9	-9	2.184	22.058	0.69057	-19.874	-19.930	****
694	5	7	5	5.475	4.318	0.69086	1.156	1.160	
695	2	4	12	5.116	5.857	0.69091	-0.740	-0.742	
696	4	6	-11	0.997	0.454	0.69111	0.544	0.545	
697	3	9	7	17.201	18.434	0.69123	-1.233	-1.236	
698	6	0	6	31.069	28.870	0.69138	2.199	2.205	*
699	1	9	-10	1.673	1.159	0.69161	0.514	0.515	
700	3	11	3	8.526	6.125	0.69165	2.401	2.408	*
701	5	3	8	1.795	0.192	0.69226	1.603	1.607	
702	7	3	-5	3.321	3.926	0.69234	-0.605	-0.606	
703	5	9	1	3.520	2.920	0.69294	0.600	0.602	
704	2	12	2	2.178	1.504	0.69297	0.675	0.677	
705	5	5	7	7.031	8.338	0.69395	-1.307	-1.311	
706	2	2	-14	8.851	8.053	0.69521	0.798	0.800	
707	4	10	3	9.493	6.795	0.69659	2.699	2.706	*
708	7	1	2	5.149	5.769	0.69655	-0.620	-0.622	
709	5	1	-12	5.106	3.725	0.69736	1.381	1.385	
710	0	8	11	12.307	9.889	0.69775	2.418	2.425	*
711	6	4	-9	4.109	2.197	0.69780	1.911	1.917	
712	2	8	-11	5.275	5.688	0.69792	-0.413	-0.414	
713	4	2	-13	2.676	2.712	0.69808	-0.035	-0.036	
714	6	6	-7	10.780	7.773	0.69825	3.007	3.015	*
715	1	7	-12	3.061	3.106	0.69866	-0.045	-0.045	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
716	6	2	-10	5.802	5.306	0.69860	0.496	0.497	
717	6	4	5	10.710	9.586	0.69895	1.124	1.127	
718	0	12	5	0.776	6.726	0.69890	-5.950	-5.967	**
719	6	6	3	10.730	8.220	0.69907	2.510	2.517	*
720	2	12	-4	8.566	4.679	0.69985	3.887	3.898	*
721	7	3	1	6.456	8.290	0.69997	-1.834	-1.840	
722	6	2	6	5.777	7.377	0.69991	-1.601	-1.605	
723	7	1	-7	6.568	7.607	0.70096	-1.039	-1.041	
724	4	10	-6	1.227	3.469	0.70137	-2.242	-2.249	*
725	0	2	14	2.074	1.458	0.70214	0.616	0.618	
726	2	0	13	1.167	0.584	0.70326	0.582	0.584	

727	7	3	-6	6.942	8.764	0.70338	-1.823	-1.828	
728	0	10	9	6.149	5.398	0.70387	0.751	0.753	
729	2	12	3	9.334	5.882	0.70412	3.452	3.462	*
730	5	9	2	9.234	7.684	0.70414	1.550	1.554	
731	3	1	-14	6.228	6.156	0.70504	0.072	0.072	

LSFM (1.4) 06/11/97 11:20:29 Elapsed time = 0.0 min

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

The space group is number 12 -- C12/m1

After refinement cycle no. 2. 731 observations. 73 variables.

Esd of an observation of unit weight = 3.656

Unweighted R factor = 0.119 Weighted R factor = 0.129

ä ³Fo³ = 1.30301E+04

ä ³³Fo³-³Fc³³ = 1.54933E+03

ä W*DELý = 8.79270E+03

ä W*Foý = 5.24817E+05

Largest parameter shift/error = 0.04
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	3.616	0.119	0.129	0.30	0.04
2	3.656	0.119	0.129	0.04	0.00
3	0.000	0.000	0.000	0.00	0.00
4	0.000	0.000	0.000	0.00	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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