

phlogo

208 Lota

LSFM (1.4) 03/03/98 09:16:46 Elapsed time = 0.1 min

PHLOG21 Demonstration Copy - Not for Resale Russell q.

The space group is number 12 -- C12/m1

Guggenheim

Refinement cycle no. 1. 754 observations. 54 variables.

Esd of an observation of unit weight = 3.546

Unweighted R factor = 0.097 Weighted R factor = 0.102

 $\ddot{a}^3 \text{Fo}^3 = 1.78685\text{E}+04$ $\ddot{a}^3 \text{Fo}^3 - {}^3\text{Fc}^3 = 1.73304\text{E}+03$ $\ddot{a} \text{W*DEL} \dot{y} = 8.80403\text{E}+03$ $\ddot{a} \text{W*Fo} \dot{y} = 8.38793\text{E}+05$

Scale factor:	New	Old	Shift	Error	SHFT/ERR
	1.85632	1.85628	0.00004	0.00389	0.01

Atom no.	1	MG1	(electron count = 12.0)				
Parameter		New	Old	Shift	Error	SHFT/ERR	
Mult.		0.25000					
x		0.00000					
y		0.00000					
z		0.50000					
5 B(iso)		0.57322	0.57396	-0.00074	0.05977	-0.01	
Total shift = 0.0000							

Atom no.	2	MG2	(electron count = 12.0)				
Parameter		New	Old	Shift	Error	SHFT/ERR	
Mult.		0.50000					
x		0.00000					
7 y		0.33176	0.33176	0.00000 (0.0000)	0.00034 (0.0031)	0.00	
z		0.50000					
9 U(1,1)		0.00079	0.00079	-0.00001	0.00096	-0.01	
10 U(2,2)		0.00299	0.00299	0.00000	0.00117	0.00	
11 U(3,3)		0.01529	0.01531	-0.00003	0.00119	-0.02	
U(1,2)		0.00000					
13 U(1,3)		0.00073	0.00075	-0.00002	0.00091	-0.02	
U(2,3)		0.00000					
Total shift = 0.0000							

Atom no.	3	K	(electron count = 17.6)				
Parameter		New	Old	Shift	Error	SHFT/ERR	
Mult.		0.25000					
x		0.00000					
v		0.50000					

	z	0.00000					
18	U(1,1)	0.03192	0.03191	0.00001		0.00188	0.00
19	U(2,2)	0.03334	0.03334	0.00000		0.00215	0.00
20	U(3,3)	0.03746	0.03742	0.00003		0.00201	0.02
	U(1,2)	0.00000					
22	U(1,3)	0.00570	0.00568	0.00002		0.00164	0.01
	U(2,3)	0.00000					
Total shift =		0.0000					

Atom no.	4	SI	(electron count = 11.8)				
Parameter		New	Old	Shift		Error	SHFT/ERR
	Mult.	1.00000					
24	x	0.07597	0.07597	0.00000 (0.0000)		0.00031 (0.0017)	-0.01
25	y	0.16678	0.16678	0.00000 (0.0000)		0.00020 (0.0019)	0.00
26	z	0.22811	0.22812	0.00000 (0.0000)		0.00018 (0.0018)	0.00
27	U(1,1)	0.00428	0.00428	0.00000		0.00059	0.01
28	U(2,2)	0.00518	0.00518	0.00000		0.00071	0.00
29	U(3,3)	0.01548	0.01546	0.00002		0.00069	0.03
30	U(1,2)	-0.00013	-0.00013	0.00000		0.00059	0.00
31	U(1,3)	0.00201	0.00199	0.00001		0.00055	0.02
32	U(2,3)	0.00003	0.00003	0.00000		0.00064	0.00
Total shift =		0.0000					

Atom no.	5	O1	(electron count = 8.0)				
Parameter		New	Old	Shift		Error	SHFT/ERR
	Mult.	0.50000					
33	x	0.00005	0.00004	0.00001 (0.0000)		0.00144 (0.0077)	0.01
	y	0.00000					
35	z	0.17133	0.17133	0.00000 (0.0000)		0.00076 (0.0078)	0.00
36	U(1,1)	0.01719	0.01717	0.00002		0.00304	0.01
37	U(2,2)	0.01622	0.01623	-0.00001		0.00334	0.00
38	U(3,3)	0.01998	0.01998	-0.00001		0.00315	0.00
	U(1,2)	0.00000					
40	U(1,3)	0.00224	0.00222	0.00002		0.00263	0.01
	U(2,3)	0.00000					
Total shift =		0.0000					

Atom no.	6	O2	(electron count = 8.0)				
Parameter		New	Old	Shift		Error	SHFT/ERR
	Mult.	1.00000					
42	x	0.33641	0.33641	0.00000 (0.0000)		0.00092 (0.0049)	0.00
43	y	0.22147	0.22147	0.00000 (0.0000)		0.00062 (0.0057)	0.00
44	z	0.17170	0.17170	0.00000 (0.0000)		0.00052 (0.0054)	0.00
45	U(1,1)	0.01151	0.01153	-0.00002		0.00187	-0.01
46	U(2,2)	0.01815	0.01813	0.00001		0.00238	0.01
47	U(3,3)	0.02509	0.02511	-0.00002		0.00222	-0.01
48	U(1,2)	-0.00620	-0.00620	0.00000		0.00186	0.00
49	U(1,3)	0.00578	0.00581	-0.00003		0.00168	-0.02
50	U(2,3)	-0.00420	-0.00421	0.00001		0.00210	0.01
Total shift =		0.0000					

Atom no.	7	O3	(electron count = 8.0)				
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Parameter	New	Old	Shift	Error	SHFT/ERR
Mult.	1.00000				
51 x	0.13172	0.13172	0.00001 (0.0000)	0.00084 (0.0045)	0.01
52 y	0.16763	0.16763	0.00000 (0.0000)	0.00053 (0.0048)	0.00
53 z	0.39253	0.39252	0.00000 (0.0000)	0.00047 (0.0048)	0.01
54 U(1,1)	0.00859	0.00859	0.00000	0.00166	0.00
55 U(2,2)	0.00656	0.00656	-0.00001	0.00190	0.00
56 U(3,3)	0.01811	0.01815	-0.00005	0.00193	-0.02
57 U(1,2)	-0.00030	-0.00030	0.00000	0.00161	0.00
58 U(1,3)	0.00072	0.00074	-0.00002	0.00155	-0.01
59 U(2,3)	0.00031	0.00031	0.00000	0.00178	0.00
Total shift = 0.0001					

Atom no.	8	F	(electron count = 9.0)			Error	SHFT/ERR
Parameter	New	Old	Shift				
Mult.	0.50000						
60 x	0.13069	0.13068	0.00000 (0.0000)	0.00125 (0.0066)	0.00		
y	0.50000						
62 z	0.39836	0.39835	0.00000 (0.0000)	0.00072 (0.0073)	0.00		
63 U(1,1)	0.01695	0.01696	-0.00001	0.00265	0.00		
64 U(2,2)	0.01802	0.01802	0.00000	0.00299	0.00		
65 U(3,3)	0.03110	0.03115	-0.00005	0.00318	-0.02		
U(1,2)	0.00000						
67 U(1,3)	0.00190	0.00193	-0.00003	0.00248	-0.01		
U(2,3)	0.00000						
Total shift = 0.0000							

Largest parameter shift/error = 0.03

Average parameter shift/error = 0.01

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
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1	0	0	2	21.580	14.361	0.09909	7.219	7.219	**
2	0	2	0	38.816	33.916	0.10892	4.900	4.900	**
3	1	1	0	31.663	26.863	0.11015	4.800	4.800	**
4	1	1	-1	16.845	13.426	0.11372	3.419	3.419	*
5	0	2	1	9.783	10.518	0.11966	-0.735	-0.735	
6	1	1	1	35.967	36.317	0.12745	-0.350	-0.350	
7	1	1	-2	58.264	62.698	0.13654	-4.434	-4.434	**
8	0	2	2	70.896	80.604	0.14725	-9.708	-9.708	***
9	0	0	3	86.737	102.695	0.14864	-15.958	-15.958	***
10	1	1	2	76.613	86.072	0.15895	-9.459	-9.459	***
11	1	1	-3	67.186	78.181	0.17106	-10.995	-10.995	***
12	0	2	3	53.762	58.042	0.18427	-4.280	-4.280	**
13	2	0	-1	53.277	52.307	0.18925	0.971	0.971	
14	1	3	0	55.002	52.977	0.18937	2.025	2.025	*
15	2	0	0	112.637	116.624	0.19150	-3.987	-3.987	*
16	1	3	-1	112.529	115.390	0.19147	-2.862	-2.862	*
17	1	1	3	33.442	34.930	0.19797	-1.489	-1.489	
18	0	0	4	43.967	52.153	0.19818	-8.186	-8.186	***

19	2	0	-2	55.988	48.868	0.19967	7.120	7.120	**
20	1	3	1	58.428	48.999	0.19993	9.429	9.429	***
21	1	3	-2	88.075	84.817	0.20584	3.257	3.257	*
22	2	0	1	91.027	85.085	0.20600	5.942	5.942	**
23	1	1	-4	13.701	12.213	0.21163	1.489	1.489	
24	0	4	0	41.934	41.750	0.21784	0.184	0.184	
25	2	2	-1	39.824	40.098	0.21835	-0.274	-0.274	
26	2	2	0	40.829	38.346	0.22031	2.483	2.483	*
27	2	0	-3	42.603	38.898	0.22098	3.706	3.706	*
28	1	3	2	43.133	37.600	0.22134	5.533	5.533	**
29	0	4	1	38.955	36.119	0.22340	2.836	2.836	*
30	0	2	4	2.798	2.260	0.22614	0.539	0.539	
31	2	2	-2	38.985	37.551	0.22745	1.434	1.434	
32	1	3	-3	96.042	101.341	0.23019	-5.299	-5.299	**
33	2	0	2	102.175	102.691	0.23046	-0.516	-0.516	
34	2	2	1	36.755	36.354	0.23302	0.401	0.401	
35	0	4	2	27.818	32.385	0.23932	-4.567	-4.567	**
36	1	1	4	10.362	10.280	0.24090	0.081	0.081	
37	2	2	-3	15.699	21.373	0.24636	-5.674	-5.674	**
38	0	0	5	88.639	103.002	0.24773	-14.363	-14.363	***
39	2	0	-4	78.257	77.276	0.25041	0.980	0.980	
40	1	3	3	77.532	77.415	0.25084	0.118	0.118	
41	2	2	2	2.283	5.545	0.25490	-3.262	-3.262	*
42	1	1	-5	13.175	9.754	0.25539	3.421	3.421	*
43	1	3	-4	47.452	47.012	0.26175	0.440	0.440	
44	2	0	3	50.140	48.755	0.26210	1.384	1.384	
45	0	4	3	14.609	10.708	0.26372	3.901	3.901	*
46	0	2	5	10.489	7.613	0.27062	2.876	2.876	*
47	2	2	-4	24.166	24.092	0.27307	0.074	0.074	
48	2	2	3	26.769	27.076	0.28383	-0.307	-0.307	
49	2	0	-5	45.110	46.282	0.28546	-1.172	-1.172	
50	1	3	4	44.786	45.207	0.28594	-0.421	-0.421	
51	1	1	5	4.279	1.021	0.28597	3.258	3.258	*
52	3	1	-1	27.073	22.728	0.28803	4.345	4.345	**
53	2	4	-1	31.783	26.067	0.28856	5.717	5.717	**
54	1	5	0	16.557	11.041	0.28864	5.516	5.516	**
55	2	4	0	3.444	3.326	0.29004	0.118	0.118	
56	1	5	-1	25.915	22.543	0.29003	3.372	3.372	*
57	3	1	-2	22.464	20.980	0.29217	1.484	1.484	
58	3	1	0	9.648	8.902	0.29236	0.746	0.746	
59	0	4	4	23.873	24.067	0.29450	-0.195	-0.195	
60	2	4	-2	7.907	7.339	0.29550	0.567	0.567	
61	1	5	1	45.799	40.732	0.29568	5.067	5.067	**
62	0	0	6	27.130	28.545	0.29727	-1.415	-1.415	
63	1	3	-5	104.375	116.579	0.29825	-12.204	-12.204	***
64	2	0	4	110.261	118.019	0.29865	-7.758	-7.758	**
65	1	5	-2	28.936	27.475	0.29971	1.461	1.461	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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66	2	4	1	60.432	56.682	0.29982	3.749	3.749	*
67	1	1	-6	6.874	7.646	0.30095	-0.772	-0.772	

68	3	1	-3	67.397	68.763	0.30442	-1.366	-1.366	
69	3	1	1	38.549	39.168	0.30479	-0.620	-0.620	
70	2	2	-5	12.363	12.965	0.30553	-0.602	-0.602	
71	2	4	-3	44.461	47.083	0.31030	-2.622	-2.622	*
72	1	5	2	67.864	66.128	0.31056	1.736	1.736	
73	0	2	6	18.268	21.604	0.31660	-3.336	-3.336	*
74	1	5	-3	42.782	43.107	0.31693	-0.325	-0.325	
75	2	4	2	54.354	55.354	0.31712	-1.000	-1.000	
76	2	2	4	2.200	0.587	0.31789	1.613	1.613	
77	3	1	-4	32.173	33.409	0.32386	-1.236	-1.236	
78	3	1	2	38.740	38.766	0.32439	-0.026	-0.026	
79	2	0	-6	87.690	94.964	0.32431	-7.274	-7.274	**
80	1	3	5	88.264	95.949	0.32482	-7.686	-7.686	**
81	3	3	-1	168.017	164.311	0.32664	3.706	3.706	*
82	0	6	0	166.196	162.775	0.32676	3.421	3.421	*
83	0	4	5	16.364	17.114	0.32989	-0.750	-0.750	
84	3	3	-2	58.517	50.970	0.33029	7.547	7.547	**
85	3	3	0	59.645	51.317	0.33046	8.329	8.329	***
86	0	6	1	58.725	51.790	0.33050	6.935	6.935	**
87	2	4	-4	25.903	25.029	0.33190	0.874	0.874	
88	1	5	3	12.090	10.322	0.33223	1.768	1.768	
89	1	1	6	29.053	29.216	0.33232	-0.163	-0.163	
90	1	3	-6	50.316	51.260	0.33808	-0.944	-0.944	
91	2	0	5	51.629	51.428	0.33852	0.200	0.200	
92	1	5	-4	16.612	15.121	0.34054	1.491	1.491	
93	2	4	3	7.834	8.108	0.34081	-0.274	-0.274	
94	3	3	-3	7.241	6.682	0.34117	0.559	0.559	
95	0	6	2	6.952	6.925	0.34146	0.027	0.027	
96	3	3	1	7.305	6.487	0.34150	0.817	0.817	
97	2	2	-6	28.275	33.147	0.34211	-4.872	-4.872	**
98	0	0	7	48.849	53.820	0.34682	-4.971	-4.971	**
99	1	1	-7	33.959	36.544	0.34761	-2.585	-2.585	*
100	3	1	-5	19.734	19.764	0.34930	-0.029	-0.029	
101	3	1	3	5.563	4.227	0.34995	1.336	1.336	
102	2	2	5	45.132	46.553	0.35561	-1.421	-1.421	
103	3	3	-4	38.568	33.546	0.35863	5.021	5.021	**
104	0	6	3	39.438	32.445	0.35898	6.993	6.993	**
105	2	4	-5	1.680	0.575	0.35908	1.105	1.105	
106	3	3	2	39.388	33.972	0.35910	5.416	5.416	**
107	1	5	4	26.557	24.224	0.35946	2.333	2.333	*
108	0	2	7	32.309	34.260	0.36352	-1.951	-1.951	
109	2	0	-7	112.249	123.732	0.36576	-11.483	-11.483	***
110	1	3	6	114.120	126.627	0.36629	-12.507	-12.507	***
111	0	4	6	53.001	55.046	0.36855	-2.045	-2.045	*
112	1	5	-5	3.871	1.248	0.36933	2.623	2.623	*
113	2	4	4	24.753	22.742	0.36966	2.011	2.011	*
114	4	0	-1	69.384	65.779	0.37751	3.605	3.605	*
115	2	6	-1	74.880	65.390	0.37761	9.490	9.490	***
116	4	0	-2	103.008	96.643	0.37849	6.365	6.365	**
117	2	6	0	113.462	95.622	0.37874	17.840	17.840	****
118	1	1	7	24.596	27.344	0.37948	-2.748	-2.748	*
119	3	1	-6	18.248	17.262	0.37954	0.987	0.987	

120	1	3	-7	20.385	22.274	0.38021	-1.889	-1.889	
121	3	1	4	2.009	2.210	0.38028	-0.201	-0.201	
122	2	0	6	21.186	22.283	0.38067	-1.098	-1.098	
123	2	2	-7	54.271	57.128	0.38163	-2.857	-2.857	*
124	3	3	-5	67.801	64.051	0.38176	3.750	3.750	*
125	0	6	4	71.278	63.360	0.38216	7.918	7.918	**
126	3	3	3	71.375	63.925	0.38235	7.451	7.451	**
127	2	6	-2	7.055	6.346	0.38294	0.709	0.709	
128	4	0	0	5.838	6.256	0.38299	-0.418	-0.418	
129	4	0	-3	89.849	82.781	0.38589	7.068	7.068	**
130	2	6	1	100.191	83.482	0.38628	16.709	16.709	****

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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131	2	4	-6	5.228	7.221	0.39068	-1.993	-1.993	
132	1	5	5	9.275	5.993	0.39110	3.282	3.282	*
133	3	5	-1	37.217	30.687	0.39261	6.530	6.530	**
134	4	2	-1	18.352	14.544	0.39291	3.808	3.808	*
135	1	7	0	38.294	31.517	0.39306	6.778	6.778	**
136	4	2	-2	33.440	31.716	0.39385	1.724	1.724	
137	1	7	-1	3.128	1.215	0.39408	1.913	1.913	
138	2	6	-3	75.571	61.942	0.39447	13.629	13.629	***
139	4	0	1	72.898	63.678	0.39466	9.220	9.220	***
140	1	1	-8	13.524	13.700	0.39496	-0.176	-0.176	
141	3	5	-2	25.685	21.801	0.39566	3.884	3.884	*
142	3	5	0	19.223	16.277	0.39580	2.946	2.946	*
143	2	2	6	50.106	52.460	0.39594	-2.353	-2.353	*
144	0	0	8	54.270	62.419	0.39637	-8.149	-8.149	***
145	4	2	0	43.553	39.025	0.39818	4.528	4.528	**
146	1	7	1	4.449	3.293	0.39826	1.156	1.156	
147	4	0	-4	22.898	20.810	0.39934	2.088	2.088	*
148	2	6	2	25.119	22.834	0.39986	2.285	2.285	*
149	4	2	-3	15.642	14.507	0.40097	1.135	1.135	
150	1	7	-2	60.078	53.343	0.40126	6.735	6.735	**
151	1	5	-6	11.746	11.593	0.40219	0.153	0.153	
152	2	4	5	8.080	7.693	0.40255	0.387	0.387	
153	3	5	-3	68.097	61.932	0.40479	6.165	6.165	**
154	3	5	1	28.760	25.900	0.40507	2.860	2.860	*
155	2	0	-8	28.479	30.534	0.40901	-2.055	-2.055	*
156	1	7	2	39.016	35.578	0.40942	3.438	3.438	*
157	4	2	1	64.950	62.689	0.40942	2.261	2.261	*
158	0	4	7	38.352	38.940	0.40956	-0.589	-0.589	
159	1	3	7	29.944	32.406	0.40955	-2.462	-2.462	*
160	3	3	-6	39.676	39.823	0.40961	-0.146	-0.146	
161	0	6	5	42.263	41.340	0.41005	0.923	0.923	
162	3	3	4	41.604	42.396	0.41030	-0.792	-0.792	
163	0	2	8	2.460	3.263	0.41106	-0.802	-0.802	
164	2	6	-4	28.759	23.195	0.41168	5.564	5.564	**
165	4	0	2	28.058	24.266	0.41200	3.793	3.793	*
166	3	1	-7	21.246	21.490	0.41352	-0.244	-0.244	
167	4	2	-4	38.506	37.013	0.41393	1.493	1.493	
168	1	7	-3	55.167	49.423	0.41428	5.745	5.745	**

169	3	1	5	17.665	17.692	0.41434	-0.026	-0.026	
170	4	0	-5	40.061	37.835	0.41826	2.225	2.225	*
171	2	6	3	43.731	39.612	0.41889	4.119	4.119	**
172	3	5	-4	32.703	31.215	0.41960	1.488	1.488	
173	3	5	2	38.521	37.018	0.42001	1.503	1.503	
174	2	2	-8	19.817	22.153	0.42326	-2.336	-2.336	*
175	1	3	-8	18.898	19.825	0.42394	-0.927	-0.927	
176	2	0	7	18.430	20.667	0.42442	-2.237	-2.237	*
177	2	4	-7	20.584	20.399	0.42572	0.185	0.185	
178	1	7	3	31.483	27.077	0.42610	4.406	4.406	**
179	1	5	6	35.620	34.010	0.42617	1.610	1.610	
180	4	2	2	10.643	8.935	0.42616	1.709	1.709	
181	1	1	8	4.219	5.609	0.42718	-1.391	-1.391	
182	4	2	-5	20.143	19.386	0.43221	0.757	0.757	
183	1	7	-4	11.989	11.092	0.43261	0.898	0.898	
184	2	6	-5	24.208	22.066	0.43389	2.143	2.143	*
185	4	0	3	23.408	22.258	0.43433	1.150	1.150	
186	0	8	0	9.059	6.869	0.43568	2.190	2.190	*
187	4	4	-1	1.838	0.486	0.43586	1.352	1.352	
188	4	4	-2	3.193	3.507	0.43671	-0.314	-0.314	
189	1	5	-7	23.829	23.039	0.43819	0.790	0.790	
190	2	2	7	2.612	2.234	0.43817	0.378	0.378	
191	0	8	1	16.540	14.085	0.43849	2.455	2.455	*
192	2	4	6	38.141	38.263	0.43859	-0.123	-0.123	
193	3	5	-5	24.674	23.709	0.43954	0.965	0.965	
194	3	5	3	10.269	8.941	0.44006	1.328	1.328	
195	4	4	0	18.786	18.662	0.44061	0.124	0.124	

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196	3	3	-7	8.173	8.436	0.44127	-0.263	-0.263	
197	0	6	6	9.236	9.034	0.44175	0.202	0.202	
198	4	0	-6	102.965	99.777	0.44195	3.187	3.187	*
199	3	3	5	9.356	8.488	0.44204	0.868	0.868	
200	2	6	4	107.561	101.031	0.44268	6.530	6.530	**
201	1	1	-9	6.427	4.760	0.44280	1.667	1.667	
202	4	4	-3	27.039	26.367	0.44313	0.672	0.672	
203	0	0	9	20.039	23.199	0.44591	-3.160	-3.160	*
204	0	8	2	31.956	26.685	0.44681	5.271	5.271	**
205	1	7	4	5.195	3.971	0.44766	1.224	1.224	
206	4	2	3	32.961	30.411	0.44778	2.550	2.550	*
207	3	1	-8	36.189	36.157	0.45039	0.032	0.032	
208	4	4	1	23.872	25.931	0.45079	-2.059	-2.059	*
209	3	1	6	19.613	19.208	0.45127	0.405	0.405	
210	0	4	8	14.953	13.509	0.45228	1.444	1.444	
211	2	0	-9	12.487	13.165	0.45355	-0.678	-0.678	
212	1	3	8	13.354	13.874	0.45410	-0.519	-0.519	
213	4	4	-4	18.867	17.976	0.45489	0.890	0.890	
214	4	2	-6	2.042	2.868	0.45518	-0.826	-0.826	
215	1	7	-5	32.312	27.991	0.45562	4.321	4.321	**
216	0	2	9	2.809	5.268	0.45902	-2.459	-2.459	*
217	0	8	3	10.451	9.612	0.46034	0.839	0.839	

218	2	6	-6	85.061	79.488	0.46038	5.572	5.572	**
219	4	0	4	85.922	82.810	0.46092	3.112	3.112	*
220	2	4	-8	12.509	13.116	0.46341	-0.607	-0.607	
221	1	5	7	28.049	27.559	0.46388	0.490	0.490	
222	3	5	-6	25.235	23.912	0.46393	1.323	1.323	
223	3	5	4	2.108	1.730	0.46454	0.378	0.378	
224	4	4	2	2.299	2.805	0.46605	-0.505	-0.505	
225	2	2	-9	25.246	27.337	0.46645	-2.091	-2.091	*
226	1	3	-9	61.958	64.073	0.46883	-2.115	-2.115	*
227	2	0	8	59.107	63.886	0.46932	-4.779	-4.779	**
228	4	0	-7	20.030	17.398	0.46970	2.633	2.633	*
229	2	6	5	19.808	17.934	0.47050	1.874	1.874	
230	4	4	-5	11.200	11.660	0.47159	-0.461	-0.461	
231	1	7	5	4.945	4.243	0.47344	0.702	0.702	
232	4	2	4	15.214	13.877	0.47361	1.336	1.336	
233	3	7	-1	8.502	8.757	0.47469	-0.255	-0.255	
234	5	1	-2	7.737	5.632	0.47479	2.105	2.105	*
235	2	8	-1	9.894	9.143	0.47501	0.751	0.751	
236	1	1	9	4.026	2.980	0.47526	1.046	1.046	
237	5	1	-1	5.662	5.707	0.47575	-0.045	-0.045	
238	2	8	0	1.485	1.547	0.47591	-0.062	-0.062	
239	3	3	-8	51.107	51.581	0.47600	-0.474	-0.474	
240	0	6	7	54.608	52.385	0.47651	2.224	2.224	*
241	1	5	-8	2.983	2.251	0.47663	0.732	0.732	
242	3	3	6	53.961	53.529	0.47684	0.432	0.432	
243	2	4	7	18.237	16.399	0.47706	1.838	1.838	
244	3	7	-2	2.525	1.023	0.47721	1.501	1.501	
245	3	7	0	9.913	11.602	0.47733	-1.689	-1.689	
246	0	8	4	17.951	15.557	0.47864	2.394	2.394	*
247	5	1	-3	24.219	21.482	0.47898	2.737	2.737	*
248	2	8	-2	11.416	10.896	0.47926	0.521	0.521	
249	2	2	8	29.466	28.465	0.48180	1.001	1.001	
250	5	1	0	22.020	19.847	0.48183	2.172	2.172	*
251	2	8	1	31.743	31.500	0.48193	0.243	0.243	
252	4	2	-7	5.672	5.656	0.48216	0.016	0.016	
253	1	7	-6	1.993	0.420	0.48264	1.573	1.573	
254	3	7	-3	23.798	25.111	0.48480	-1.313	-1.313	
255	3	7	1	31.650	32.894	0.48504	-1.244	-1.244	
256	4	4	3	12.561	13.996	0.48590	-1.434	-1.434	
257	5	1	-4	33.876	32.159	0.48819	1.717	1.717	
258	2	8	-3	25.599	26.703	0.48852	-1.105	-1.105	
259	3	1	-9	4.808	6.332	0.48950	-1.523	-1.523	
260	2	6	-7	77.426	71.500	0.49046	5.925	5.925	**

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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261	3	1	7	5.560	4.542	0.49043	1.017	1.017	
262	1	1	-10	7.899	6.287	0.49098	1.612	1.612	
263	4	0	5	77.142	75.330	0.49108	1.812	1.812	
264	3	5	-7	15.396	14.686	0.49211	0.710	0.710	
265	4	4	-6	7.612	7.026	0.49273	0.587	0.587	
266	5	1	1	23.150	20.356	0.49284	2.794	2.794	*

267	2	8	2	20.884	21.058	0.49288	-0.174	-0.174	
268	3	5	5	8.571	8.710	0.49281	-0.139	-0.139	
269	0	0	10	39.271	38.877	0.49546	0.394	0.394	
270	0	4	9	24.458	26.092	0.49628	-1.635	-1.635	
271	3	7	-4	11.101	11.772	0.49724	-0.671	-0.671	
272	3	7	2	11.491	11.872	0.49759	-0.381	-0.381	
273	2	0	-10	58.633	59.344	0.49904	-0.711	-0.711	
274	5	3	-2	29.689	34.541	0.49915	-4.853	-4.853	**
275	4	6	-1	31.279	34.919	0.49929	-3.640	-3.640	*
276	1	9	0	39.001	36.178	0.49941	2.823	2.823	*
277	1	3	9	61.377	60.507	0.49960	0.871	0.871	
278	4	6	-2	47.150	49.511	0.50003	-2.360	-2.360	*
279	5	3	-1	44.604	50.363	0.50006	-5.759	-5.759	**
280	1	9	-1	58.864	49.380	0.50021	9.483	9.483	***
281	4	0	-8	11.593	11.417	0.50081	0.176	0.176	
282	0	8	5	1.956	0.429	0.50119	1.527	1.527	
283	2	6	6	11.793	12.351	0.50168	-0.559	-0.559	
284	5	1	-5	1.700	0.964	0.50214	0.736	0.736	
285	2	8	-4	3.713	2.988	0.50252	0.725	0.725	
286	1	7	6	12.575	10.658	0.50279	1.917	1.917	
287	4	2	5	30.482	28.617	0.50302	1.865	1.865	
288	2	4	-9	10.041	11.328	0.50315	-1.286	-1.286	
289	5	3	-3	8.198	7.934	0.50314	0.264	0.264	
290	4	6	0	8.223	6.829	0.50344	1.394	1.394	
291	1	9	1	10.581	6.671	0.50351	3.910	3.910	*
292	1	5	8	3.198	3.854	0.50365	-0.656	-0.656	
293	4	6	-3	67.607	73.363	0.50565	-5.756	-5.756	**
294	5	3	0	63.187	74.621	0.50585	-11.434	-11.434	***
295	1	9	-2	83.423	73.671	0.50588	9.751	9.751	***
296	0	2	10	12.336	12.655	0.50729	-0.319	-0.319	
297	2	8	3	6.943	5.467	0.50844	1.475	1.475	
298	5	1	2	2.881	1.676	0.50846	1.205	1.205	
299	4	4	4	8.401	10.405	0.50980	-2.004	-2.004	*
300	2	2	-10	14.461	14.149	0.51079	0.313	0.313	
301	5	3	-4	30.248	32.504	0.51191	-2.256	-2.256	*
302	4	6	1	31.669	32.168	0.51238	-0.499	-0.499	
303	1	9	2	38.834	31.695	0.51238	7.139	7.139	**
304	4	2	-8	13.153	12.343	0.51252	0.810	0.810	
305	1	7	-7	37.890	34.874	0.51302	3.016	3.016	*
306	3	3	-9	56.996	58.609	0.51317	-1.612	-1.612	
307	0	6	8	60.204	58.956	0.51369	1.248	1.248	
308	3	3	7	60.425	60.333	0.51405	0.092	0.092	
309	3	7	-5	6.014	5.823	0.51418	0.192	0.192	
310	1	3	-10	2.294	2.339	0.51457	-0.044	-0.044	
311	3	7	3	13.681	15.511	0.51462	-1.830	-1.830	
312	2	0	9	1.552	2.892	0.51508	-1.340	-1.340	
313	4	6	-4	21.960	23.790	0.51599	-1.830	-1.830	
314	1	9	-3	20.826	23.650	0.51627	-2.824	-2.824	*
315	5	3	1	20.251	25.336	0.51635	-5.085	-5.085	**
316	1	5	-9	9.913	7.417	0.51697	2.496	2.496	*
317	2	4	8	8.068	6.970	0.51742	1.098	1.098	
318	4	4	-7	17.737	18.268	0.51775	-0.531	-0.531	

319	5	1	-6	17.036	15.877	0.52045	1.158	1.158
320	2	8	-5	4.990	5.935	0.52087	-0.945	-0.945
321	3	5	-8	37.124	35.063	0.52348	2.061	2.061
322	2	6	-8	27.847	26.147	0.52351	1.700	1.700
323	1	1	10	15.658	14.425	0.52361	1.233	1.233
324	4	0	6	28.663	28.123	0.52420	0.541	0.541
325	3	5	6	9.605	10.782	0.52424	-1.178	-1.178

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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326	5	3	-5	24.907	27.663	0.52523	-2.756	-2.756	*
327	1	9	3	24.011	25.941	0.52580	-1.930	-1.930	
328	4	6	2	27.121	27.913	0.52585	-0.792	-0.792	
329	2	2	9	3.435	4.963	0.52647	-1.527	-1.527	
330	0	8	6	31.163	26.456	0.52744	4.707	4.707	**
331	5	1	3	6.752	6.209	0.52828	0.543	0.543	
332	2	8	4	15.110	15.206	0.52821	-0.095	-0.095	
333	3	1	-10	7.101	8.079	0.53037	-0.979	-0.979	
334	4	6	-5	6.683	6.987	0.53077	-0.304	-0.304	
335	1	9	-4	6.777	8.290	0.53110	-1.513	-1.513	
336	5	3	2	6.273	8.669	0.53128	-2.396	-2.396	*
337	3	1	8	3.415	4.262	0.53133	-0.847	-0.847	
338	4	0	-9	2.265	0.814	0.53472	1.452	1.452	
339	1	7	7	6.149	5.641	0.53514	0.509	0.509	
340	3	7	-6	1.448	0.480	0.53518	0.967	0.967	
341	4	2	6	30.183	29.005	0.53540	1.178	1.178	
342	2	6	7	3.965	1.326	0.53563	2.638	2.638	*
343	3	7	4	6.386	6.440	0.53571	-0.054	-0.054	
344	4	4	5	25.655	31.830	0.53723	-6.175	-6.175	**
345	1	1	-11	16.308	17.741	0.53940	-1.433	-1.433	
346	0	4	10	8.371	7.995	0.54123	0.376	0.376	
347	5	1	-7	3.176	1.773	0.54268	1.402	1.402	
348	5	3	-6	7.998	7.783	0.54276	0.214	0.214	
349	2	8	-6	4.585	4.315	0.54314	0.270	0.270	
350	1	9	4	10.470	7.318	0.54342	3.151	3.151	*
351	4	6	3	8.743	7.819	0.54352	0.924	0.924	
352	2	4	-10	4.939	4.483	0.54451	0.456	0.456	
353	5	5	-2	2.469	1.232	0.54461	1.237	1.237	
354	1	5	9	4.802	4.214	0.54502	0.589	0.589	
355	0	0	11	43.521	43.258	0.54500	0.263	0.263	
356	2	0	-11	12.559	14.766	0.54523	-2.207	-2.207	*
357	5	5	-1	2.450	0.539	0.54545	1.912	1.912	
358	4	2	-9	2.487	3.394	0.54570	-0.907	-0.907	
359	1	3	10	13.381	14.778	0.54580	-1.397	-1.397	
360	4	4	-8	30.235	31.790	0.54614	-1.556	-1.556	
361	1	7	-8	21.463	18.176	0.54622	3.286	3.286	*
362	5	5	-3	13.217	13.980	0.54827	-0.763	-0.763	
363	4	6	-6	75.218	82.686	0.54963	-7.468	-7.468	**
364	1	9	-5	94.134	82.987	0.55000	11.147	11.147	***
365	5	3	3	82.717	85.510	0.55028	-2.793	-2.793	*
366	5	5	0	18.563	21.038	0.55076	-2.475	-2.475	*
367	2	8	5	14.052	13.360	0.55174	0.692	0.692	

368	5	1	4	16.482	15.461	0.55185	1.022	1.022	
369	3	3	-10	1.387	1.107	0.55228	0.280	0.280	
370	0	6	9	2.855	0.596	0.55282	2.259	2.259	*
371	3	3	8	6.902	1.314	0.55321	5.588	5.588	**
372	0	2	11	17.719	16.391	0.55578	1.327	1.327	
373	2	2	-11	16.006	14.800	0.55601	1.206	1.206	
374	5	5	-4	17.524	19.722	0.55633	-2.198	-2.198	*
375	0	8	7	30.314	26.252	0.55687	4.062	4.062	**
376	3	5	-9	8.787	9.014	0.55749	-0.227	-0.227	
377	3	5	7	6.318	6.862	0.55831	-0.544	-0.544	
378	1	5	-10	10.939	9.236	0.55878	1.703	1.703	
379	2	6	-9	2.766	0.441	0.55900	2.325	2.325	*
380	2	4	9	1.634	1.286	0.55925	0.348	0.348	
381	4	0	7	1.195	0.424	0.55975	0.771	0.771	
382	3	7	-7	19.157	20.031	0.55978	-0.873	-0.873	
383	3	7	5	20.141	22.198	0.56039	-2.057	-2.057	*
384	5	5	1	10.748	10.381	0.56042	0.367	0.367	
385	1	3	-11	9.449	6.674	0.56096	2.775	2.775	*
386	2	0	10	8.661	6.160	0.56148	2.501	2.501	*
387	5	3	-7	39.015	42.422	0.56412	-3.407	-3.407	*
388	0	10	3	2.228	4.596	0.56452	-2.368	-2.368	*
389	1	9	5	48.487	44.876	0.56485	3.611	3.611	*
390	4	6	4	40.635	45.525	0.56499	-4.890	-4.890	**

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391	6	0	-2	97.919	81.222	0.56568	16.697	16.697	****
392	3	9	-1	77.371	80.563	0.56590	-3.192	-3.192	*
393	4	4	6	12.103	15.319	0.56766	-3.216	-3.216	*
394	6	0	-3	53.391	45.585	0.56774	7.805	7.805	**
395	6	0	-1	23.224	18.395	0.56794	4.829	4.829	**
396	3	9	-2	17.765	19.306	0.56801	-1.541	-1.541	
397	3	9	0	42.844	44.341	0.56811	-1.498	-1.498	
398	5	1	-8	29.010	27.283	0.56837	1.727	1.727	
399	5	5	-5	3.954	5.360	0.56861	-1.406	-1.406	
400	2	8	-7	25.023	25.088	0.56886	-0.065	-0.065	
401	1	7	8	8.664	8.628	0.56995	0.036	0.036	
402	4	2	7	2.960	1.746	0.57025	1.214	1.214	
403	4	0	-10	36.722	36.771	0.57091	-0.049	-0.049	
404	2	6	8	33.397	36.497	0.57187	-3.100	-3.100	*
405	2	2	10	22.997	23.375	0.57195	-0.377	-0.377	
406	1	1	11	14.748	16.085	0.57216	-1.337	-1.337	
407	4	6	-7	24.411	25.926	0.57218	-1.515	-1.515	
408	1	9	-6	23.164	25.463	0.57258	-2.299	-2.299	*
409	3	1	-11	4.799	4.673	0.57260	0.125	0.125	
410	5	3	4	20.735	27.368	0.57295	-6.633	-6.633	**
411	3	1	9	15.454	15.676	0.57359	-0.222	-0.222	
412	6	0	-4	10.871	10.852	0.57409	0.019	0.019	
413	5	5	2	7.240	6.979	0.57421	0.261	0.261	
414	6	0	0	16.912	14.869	0.57449	2.042	2.042	*
415	3	9	-3	13.161	13.282	0.57441	-0.121	-0.121	
416	2	8	1	9.876	9.169	0.57460	0.706	0.706	

417	6	2	-2	8.637	12.657	0.57607	-4.020	-4.020	**
418	4	8	-1	5.086	4.938	0.57648	0.148	0.148	
419	2	10	-1	11.398	11.226	0.57655	0.172	0.172	
420	4	8	-2	7.407	8.798	0.57713	-1.391	-1.391	
421	2	10	0	3.137	0.966	0.57729	2.171	2.171	*
422	4	4	-9	3.708	1.761	0.57739	1.947	1.947	
423	6	2	-3	8.095	11.172	0.57810	-3.077	-3.077	*
424	6	2	-1	0.965	1.700	0.57829	-0.735	-0.735	
425	2	8	6	27.566	26.732	0.57856	0.834	0.834	
426	5	1	5	24.759	22.289	0.57872	2.470	2.470	*
427	0	10	4	5.559	10.457	0.57954	-4.898	-4.898	**
428	2	10	-2	8.595	8.070	0.58005	0.525	0.525	
429	4	8	0	16.595	16.859	0.58009	-0.263	-0.263	
430	4	2	-10	5.306	4.599	0.58121	0.706	0.706	
431	1	7	-9	3.784	2.660	0.58175	1.124	1.124	
432	4	8	-3	14.275	17.348	0.58200	-3.073	-3.073	*
433	2	10	1	24.243	23.459	0.58226	0.784	0.784	
434	6	2	-4	22.483	26.857	0.58433	-4.375	-4.375	**
435	6	0	-5	19.037	15.062	0.58459	3.976	3.976	*
436	6	2	0	13.917	16.365	0.58472	-2.447	-2.447	*
437	5	5	-6	8.855	9.821	0.58485	-0.966	-0.966	
438	3	9	-4	17.227	17.075	0.58494	0.152	0.152	
439	6	0	1	21.255	18.363	0.58517	2.892	2.892	*
440	3	9	2	15.203	14.906	0.58524	0.298	0.298	
441	0	4	11	27.021	24.811	0.58693	2.210	2.210	*
442	2	4	-11	18.753	16.431	0.58714	2.322	2.322	*
443	3	7	-8	16.670	16.818	0.58755	-0.149	-0.149	
444	1	5	10	9.061	7.555	0.58766	1.506	1.506	
445	2	10	-3	18.897	18.641	0.58773	0.256	0.256	
446	4	8	1	23.241	25.904	0.58786	-2.663	-2.663	*
447	1	1	-12	11.379	8.517	0.58801	2.863	2.863	*
448	3	7	6	22.294	23.458	0.58823	-1.163	-1.163	
449	5	3	-8	54.943	61.904	0.58887	-6.961	-6.961	**
450	0	8	8	10.177	8.211	0.58900	1.966	1.966	
451	1	9	6	71.023	63.645	0.58967	7.378	7.378	**
452	4	6	5	58.845	66.166	0.58986	-7.321	-7.321	**
453	4	8	-4	13.050	12.738	0.59101	0.312	0.312	
454	2	10	2	21.032	18.929	0.59136	2.103	2.103	*
455	5	5	3	7.685	9.403	0.59183	-1.718	-1.718	

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456	2	0	-12	20.442	16.213	0.59197	4.229	4.229	**
457	1	3	11	21.197	18.181	0.59254	3.017	3.017	*
458	3	3	-11	33.132	30.597	0.59296	2.535	2.535	*
459	0	6	10	34.899	32.429	0.59351	2.470	2.470	*
460	3	5	-10	4.884	5.023	0.59369	-0.139	-0.139	
461	3	3	9	35.128	34.141	0.59392	0.987	0.987	
462	3	5	8	1.486	1.080	0.59455	0.406	0.406	
463	0	0	12	31.910	30.238	0.59455	1.672	1.672	
464	6	2	-5	7.524	9.466	0.59465	-1.943	-1.943	
465	6	2	1	12.307	12.694	0.59522	-0.386	-0.386	

466	2	6	-10	37.546	33.180	0.59650	4.366	4.366	**
467	5	1	-9	18.145	16.678	0.59708	1.467	1.467	
468	4	0	8	35.649	34.970	0.59730	0.679	0.679	
469	2	8	-8	8.873	7.828	0.59759	1.046	1.046	
470	4	6	-8	23.687	25.641	0.59799	-1.955	-1.955	
471	1	9	-7	28.866	25.909	0.59842	2.957	2.957	*
472	5	3	5	25.914	26.431	0.59887	-0.517	-0.517	
473	6	0	-6	67.091	58.457	0.59901	8.634	8.634	***
474	2	10	-4	5.365	4.274	0.59941	1.091	1.091	
475	3	9	-5	32.021	32.096	0.59941	-0.074	-0.074	
476	4	8	2	1.374	2.416	0.59964	-1.043	-1.043	
477	3	9	3	55.448	55.191	0.59978	0.257	0.257	
478	6	0	2	40.691	33.066	0.59977	7.624	7.624	**
479	4	4	7	10.746	14.291	0.60064	-3.545	-3.545	*
480	1	5	-11	19.034	18.882	0.60178	0.152	0.152	
481	2	2	-12	26.995	28.155	0.60191	-1.160	-1.160	
482	2	4	10	11.823	12.034	0.60226	-0.212	-0.212	
483	2	10	3	10.952	9.496	0.60439	1.457	1.457	
484	0	2	12	5.254	6.183	0.60444	-0.929	-0.929	
485	5	5	-7	6.219	5.846	0.60472	0.373	0.373	
486	6	4	-2	17.060	20.660	0.60617	-3.600	-3.600	*
487	5	7	-2	11.453	14.120	0.60645	-2.666	-2.666	*
488	1	11	0	12.604	18.594	0.60667	-5.989	-5.989	**
489	1	7	9	8.225	7.923	0.60682	0.301	0.301	
490	4	2	8	5.588	5.567	0.60715	0.021	0.021	
491	5	7	-1	13.458	16.779	0.60721	-3.320	-3.320	*
492	1	11	-1	3.100	5.188	0.60733	-2.088	-2.088	*
493	1	3	-12	41.509	41.163	0.60785	0.347	0.347	
494	6	4	-3	9.282	9.837	0.60810	-0.555	-0.555	
495	2	8	7	7.017	5.761	0.60824	1.256	1.256	
496	6	4	-1	8.372	10.465	0.60829	-2.093	-2.093	*
497	2	0	11	41.908	41.951	0.60837	-0.043	-0.043	
498	5	1	6	1.646	0.523	0.60843	1.123	1.123	
499	6	2	-6	11.753	15.080	0.60883	-3.327	-3.327	*
500	4	0	-11	3.677	5.956	0.60899	-2.279	-2.279	*
501	6	2	2	6.516	6.936	0.60958	-0.421	-0.421	
502	5	7	-3	18.062	20.488	0.60974	-2.426	-2.426	*
503	2	6	9	3.632	6.267	0.60998	-2.635	-2.635	*
504	1	11	1	1.077	0.265	0.61004	0.812	0.812	
505	4	4	-10	14.991	15.026	0.61106	-0.035	-0.035	
506	5	7	0	8.168	9.969	0.61198	-1.801	-1.801	
507	1	11	-2	18.767	32.190	0.61201	-13.422	-13.422	***
508	5	5	4	15.760	17.880	0.61296	-2.120	-2.120	*
509	6	4	-4	17.357	17.052	0.61403	0.305	0.305	
510	6	4	0	32.003	33.784	0.61440	-1.781	-1.781	
511	2	10	-5	6.905	7.234	0.61488	-0.329	-0.329	
512	4	8	3	14.089	14.583	0.61519	-0.494	-0.494	
513	3	1	-12	11.880	10.374	0.61593	1.507	1.507	
514	5	3	-9	25.041	27.322	0.61663	-2.281	-2.281	*
515	3	1	10	18.644	17.796	0.61694	0.848	0.848	
516	6	0	-7	31.095	26.181	0.61708	4.914	4.914	**
517	5	7	-4	28.235	33.506	0.61700	-5.272	-5.272	**

518	1	11	2	16.020	21.451	0.61739	-5.431	-5.431	**
519	1	9	7	32.690	28.364	0.61748	4.325	4.325	**
520	3	9	-6	8.019	7.994	0.61751	0.025	0.025	

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521	4	6	6	26.675	29.038	0.61770	-2.363	-2.363	*
522	3	9	4	27.102	27.249	0.61797	-0.146	-0.146	
523	2	2	11	25.496	22.276	0.61805	3.220	3.220	*
524	6	0	3	10.155	7.921	0.61800	2.235	2.235	*
525	3	7	-9	6.182	6.580	0.61804	-0.398	-0.398	
526	4	2	-11	14.253	12.274	0.61866	1.979	1.979	
527	3	7	7	2.135	2.662	0.61878	-0.527	-0.527	
528	1	7	-10	2.966	4.098	0.61921	-1.132	-1.132	
529	0	10	6	15.148	21.794	0.62046	-6.647	-6.647	**
530	4	8	-6	5.179	6.978	0.62060	-1.799	-1.799	
531	5	7	1	20.104	21.823	0.62069	-1.719	-1.719	
532	1	11	-3	13.848	22.293	0.62062	-8.445	-8.445	***
533	1	1	12	0.910	3.995	0.62088	-3.086	-3.086	*
534	2	10	4	12.753	13.224	0.62111	-0.471	-0.471	
535	0	8	9	14.173	12.415	0.62342	1.758	1.758	
536	6	4	-5	16.930	18.278	0.62386	-1.348	-1.348	
537	6	4	1	16.354	18.265	0.62440	-1.911	-1.911	
538	6	2	-7	6.153	7.887	0.62662	-1.734	-1.734	
539	4	6	-9	3.490	5.347	0.62666	-1.857	-1.857	
540	1	9	-8	3.259	4.236	0.62711	-0.977	-0.977	
541	5	3	6	2.725	4.078	0.62763	-1.352	-1.352	
542	5	5	-8	24.578	27.064	0.62788	-2.486	-2.486	*
543	5	7	-5	5.105	4.766	0.62810	0.338	0.338	
544	5	1	-10	10.629	9.841	0.62838	0.788	0.788	
545	1	11	3	8.725	10.679	0.62857	-1.955	-1.955	
546	2	8	-9	8.734	11.606	0.62891	-2.872	-2.872	*
547	2	4	-12	15.487	16.749	0.63078	-1.262	-1.262	
548	1	5	11	12.744	13.451	0.63131	-0.707	-0.707	
549	3	5	-11	1.377	1.026	0.63171	0.351	0.351	
550	3	5	9	13.506	15.655	0.63261	-2.148	-2.148	*
551	1	11	-4	2.228	3.319	0.63301	-1.091	-1.091	
552	5	7	2	6.107	7.887	0.63316	-1.780	-1.780	
553	0	4	12	17.803	17.140	0.63320	0.663	0.663	
554	2	10	-6	6.330	3.952	0.63385	2.378	2.378	*
555	4	8	4	1.485	2.160	0.63424	-0.675	-0.675	
556	3	3	-12	44.870	43.438	0.63490	1.432	1.432	
557	0	6	11	46.921	43.593	0.63545	3.328	3.328	*
558	2	6	-11	15.519	15.789	0.63565	-0.271	-0.271	
559	4	4	8	6.352	8.310	0.63578	-1.958	-1.958	
560	3	3	10	47.670	45.057	0.63588	2.613	2.613	*
561	4	0	9	14.852	16.062	0.63649	-1.210	-1.210	
562	1	1	-13	6.469	6.206	0.63677	0.264	0.264	
563	5	5	5	22.072	23.827	0.63726	-1.755	-1.755	
564	6	4	-6	3.230	3.438	0.63739	-0.208	-0.208	
565	6	4	2	13.700	15.963	0.63810	-2.263	-2.263	*
566	6	0	-8	18.546	15.689	0.63850	2.856	2.856	*

567	3	9	-7	11.379	11.799	0.63896	-0.420	-0.420	
568	2	0	-13	2.769	1.028	0.63913	1.741	1.741	
569	3	9	5	15.686	16.109	0.63949	-0.423	-0.423	
570	6	0	4	14.517	11.721	0.63956	2.795	2.795	*
571	1	3	12	2.935	1.347	0.63970	1.588	1.588	
572	2	8	8	12.419	11.387	0.64038	1.032	1.032	
573	5	1	7	14.137	12.670	0.64061	1.467	1.467	
574	4	8	-7	9.393	10.909	0.64065	-1.516	-1.516	
575	2	10	5	9.337	8.216	0.64124	1.121	1.121	
576	5	7	-6	16.503	18.846	0.64283	-2.344	-2.344	*
577	0	0	13	25.061	20.536	0.64409	4.525	4.525	**
578	0	0	13	24.893	20.536	0.64409	4.357	4.357	**
579	1	7	10	20.126	16.775	0.64539	3.351	3.351	*
580	0	10	7	9.536	17.244	0.64566	-7.708	-7.708	**
581	4	2	9	3.932	1.995	0.64574	1.937	1.937	
582	1	5	-12	11.783	8.645	0.64571	3.138	3.138	*
583	2	4	11	11.022	9.055	0.64620	1.967	1.967	
584	4	4	-11	1.207	2.497	0.64678	-1.289	-1.289	
585	5	3	-10	10.943	12.461	0.64699	-1.517	-1.517	

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586	6	2	-8	13.899	16.640	0.64772	-2.741	-2.741	*
587	1	9	8	13.978	11.232	0.64789	2.746	2.746	*
588	4	6	7	11.825	11.534	0.64815	0.290	0.290	
589	2	2	-13	8.604	5.037	0.64834	3.567	3.567	*
590	2	2	-13	8.539	5.037	0.64834	3.502	3.502	*
591	4	0	-12	1.095	1.485	0.64862	-0.390	-0.390	
592	6	2	4	11.598	14.787	0.64877	-3.189	-3.189	*
593	1	11	-5	10.340	21.640	0.64895	-11.300	-11.300	***
594	5	7	3	1.355	3.679	0.64919	-2.324	-2.324	*
595	2	6	10	1.251	1.485	0.64964	-0.234	-0.234	
596	3	7	-10	9.282	9.457	0.65089	-0.176	-0.176	
597	3	7	8	9.876	11.237	0.65167	-1.361	-1.361	
598	0	2	13	9.681	10.661	0.65324	-0.980	-0.980	
599	6	6	-2	65.305	73.118	0.65327	-7.812	-7.812	**
600	5	5	-9	9.764	9.437	0.65397	0.327	0.327	
601	6	4	-7	2.135	2.020	0.65441	0.115	0.115	
602	6	6	-3	19.269	22.139	0.65506	-2.870	-2.870	*
603	1	3	-13	53.423	48.617	0.65513	4.806	4.806	**
604	6	6	-1	19.677	22.538	0.65523	-2.861	-2.861	*
605	6	4	3	14.145	16.160	0.65527	-2.015	-2.015	*
606	2	0	12	53.014	51.031	0.65566	1.983	1.983	
607	2	10	-7	17.004	16.889	0.65603	0.114	0.114	
608	4	8	5	22.684	25.785	0.65649	-3.101	-3.101	*
609	4	2	-12	18.333	18.980	0.65770	-0.647	-0.647	
610	4	6	-10	34.917	38.079	0.65781	-3.162	-3.162	*
611	1	7	-11	5.449	5.756	0.65827	-0.308	-0.308	
612	1	9	-9	33.542	37.514	0.65829	-3.972	-3.972	*
613	5	3	7	37.553	39.369	0.65887	-1.815	-1.815	
614	0	8	10	5.284	3.145	0.65977	2.139	2.139	*
615	3	1	-13	7.186	6.797	0.66013	0.390	0.390	

616	6	6	-4	3.063	3.963	0.66057	-0.900	-0.900	
617	6	6	0	3.453	3.748	0.66092	-0.296	-0.296	
618	5	7	-7	6.720	9.590	0.66096	-2.870	-2.870	*
619	3	1	11	3.188	3.144	0.66116	0.045	0.045	
620	5	1	-11	5.709	5.845	0.66192	-0.136	-0.136	
621	3	11	-1	12.307	14.047	0.66248	-1.739	-1.739	
622	2	8	-10	3.416	3.324	0.66246	0.092	0.092	
623	7	1	-2	9.486	8.332	0.66244	1.154	1.154	
624	4	10	-1	7.128	8.266	0.66265	-1.138	-1.138	
625	6	0	-9	52.332	47.920	0.66293	4.412	4.412	**
626	7	1	-3	4.195	4.096	0.66296	0.099	0.099	
627	4	10	-2	3.620	5.583	0.66321	-1.963	-1.963	
628	3	9	-8	26.007	27.421	0.66342	-1.414	-1.414	
629	4	8	-8	16.001	17.427	0.66380	-1.426	-1.426	
630	3	9	6	44.440	47.293	0.66402	-2.853	-2.853	*
631	6	0	5	33.618	29.071	0.66413	4.547	4.547	**
632	3	11	-2	3.341	3.488	0.66428	-0.147	-0.147	
633	5	5	6	2.116	0.765	0.66436	1.351	1.351	
634	3	11	0	6.701	8.844	0.66437	-2.143	-2.143	*
635	2	10	6	26.341	24.512	0.66445	1.829	1.829	
636	2	2	12	1.841	1.199	0.66465	0.641	0.641	
637	7	1	-1	9.170	6.559	0.66562	2.611	2.611	*
638	4	10	0	11.249	11.468	0.66579	-0.218	-0.218	
639	7	1	-4	20.995	19.956	0.66716	1.039	1.039	
640	4	10	-3	11.194	13.767	0.66746	-2.573	-2.573	*
641	5	7	4	3.434	3.403	0.66851	0.031	0.031	
642	3	11	-3	16.057	13.466	0.66976	2.591	2.591	*
643	1	1	13	8.288	6.663	0.66971	1.625	1.625	
644	6	6	-5	18.934	21.442	0.66971	-2.508	-2.508	*
645	3	11	1	19.566	18.074	0.66993	1.491	1.491	
646	6	6	1	19.009	22.171	0.67022	-3.162	-3.162	*
647	3	5	-12	7.564	6.026	0.67123	1.537	1.537	
648	6	2	-9	18.768	21.370	0.67182	-2.603	-2.603	*
649	3	5	10	13.825	16.423	0.67216	-2.599	-2.599	*
650	7	1	0	20.587	17.413	0.67244	3.174	3.174	*

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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651	4	10	1	17.208	18.363	0.67257	-1.155	-1.155	
652	4	4	9	8.354	9.730	0.67273	-1.376	-1.376	
653	6	2	5	15.018	14.650	0.67300	0.368	0.368	
654	0	10	8	5.142	7.043	0.67357	-1.901	-1.901	
655	6	4	-8	6.126	6.015	0.67464	0.111	0.111	
656	5	1	8	4.025	2.414	0.67489	1.612	1.612	
657	7	1	-5	17.802	13.167	0.67499	4.635	4.635	**
658	2	4	-13	3.990	5.808	0.67523	-1.818	-1.818	
659	4	10	-4	13.440	13.167	0.67533	0.273	0.273	
660	6	4	4	8.947	9.336	0.67565	-0.389	-0.389	
661	1	5	12	2.309	0.610	0.67577	1.699	1.699	
662	2	6	-12	10.467	6.974	0.67617	3.493	3.493	*
663	4	0	10	9.925	8.360	0.67704	1.565	1.565	
664	3	3	-13	15.939	14.151	0.67786	1.788	1.788	

665	0	6	12	16.308	14.784	0.67843	1.525	1.525	
666	3	11	-4	9.207	8.818	0.67882	0.389	0.389	
667	3	3	11	16.582	15.107	0.67887	1.476	1.476	
668	3	11	2	9.783	9.359	0.67907	0.423	0.423	
669	5	3	-11	27.808	29.617	0.67961	-1.809	-1.809	
670	0	4	13	7.343	8.856	0.67994	-1.513	-1.513	
671	7	3	-2	30.109	29.231	0.68011	0.878	0.878	
672	5	9	-2	25.116	29.009	0.68022	-3.893	-3.893	*
673	2	12	-1	24.726	28.667	0.68037	-3.941	-3.941	*
674	1	9	9	34.379	29.680	0.68055	4.699	4.699	**
675	7	3	-3	45.294	45.825	0.68062	-0.531	-0.531	
676	4	6	8	29.274	31.223	0.68083	-1.949	-1.949	
677	5	9	-1	38.945	44.922	0.68089	-5.977	-5.977	**
678	2	10	-8	9.894	8.099	0.68109	1.795	1.795	
679	2	12	0	39.781	42.576	0.68100	-2.795	-2.795	*
680	4	8	6	12.864	12.554	0.68162	0.310	0.310	
681	5	7	-8	13.718	16.217	0.68221	-2.499	-2.499	*
682	6	6	-6	30.388	33.623	0.68234	-3.235	-3.235	*
683	5	5	-10	12.289	12.931	0.68268	-0.643	-0.643	
684	1	11	6	10.006	12.323	0.68290	-2.317	-2.317	*
685	4	10	2	2.246	1.898	0.68289	0.348	0.348	
686	7	1	1	3.546	1.808	0.68281	1.737	1.737	
687	6	6	2	30.481	33.712	0.68300	-3.232	-3.232	*
688	5	9	-3	2.320	3.086	0.68315	-0.766	-0.766	
689	7	3	-1	2.970	2.426	0.68321	0.544	0.544	
690	2	12	-2	2.413	3.059	0.68335	-0.646	-0.646	
691	4	4	-12	15.173	15.228	0.68423	-0.055	-0.055	
692	7	3	-4	43.716	44.233	0.68471	-0.516	-0.516	
693	5	9	0	37.850	44.370	0.68515	-6.520	-6.520	**
694	2	12	1	39.465	44.633	0.68522	-5.168	-5.168	**
695	1	7	11	12.638	12.855	0.68537	-0.217	-0.217	
696	1	1	-14	3.350	3.991	0.68563	-0.640	-0.640	
697	1	1	-14	3.100	3.991	0.68563	-0.891	-0.891	
698	4	2	10	7.614	8.338	0.68574	-0.723	-0.723	
699	3	7	-11	8.966	8.544	0.68574	0.422	0.422	
700	7	1	-6	4.599	5.048	0.68631	-0.448	-0.448	
701	3	7	9	4.771	4.104	0.68657	0.667	0.667	
702	4	10	-5	3.360	3.076	0.68668	0.284	0.284	
703	2	0	-14	32.868	32.241	0.68663	0.627	0.627	
704	2	0	-14	33.228	32.241	0.68663	0.987	0.987	
705	1	3	13	34.686	33.403	0.68720	1.284	1.284	
706	4	0	-13	23.891	24.194	0.68953	-0.304	-0.304	
707	5	9	-4	31.149	36.762	0.68964	-5.613	-5.613	**
708	4	8	-9	1.169	0.942	0.68974	0.227	0.227	
709	7	3	0	37.219	38.473	0.68986	-1.253	-1.253	
710	2	12	-3	27.344	34.557	0.68987	-7.214	-7.214	**
711	6	0	-10	38.426	33.473	0.69006	4.952	4.952	**
712	2	10	7	6.757	5.212	0.69045	1.545	1.545	
713	1	5	-13	10.346	9.810	0.69040	0.537	0.537	
714	1	11	-7	8.502	20.352	0.69046	-11.850	-11.850	***
715	3	9	-9	46.334	47.322	0.69057	-0.988	-0.988	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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716	2	6	11	22.469	26.444	0.69057	-3.976	-3.976	*
717	5	7	5	7.945	8.913	0.69085	-0.968	-0.968	
718	2	4	12	2.458	2.418	0.69090	0.039	0.039	
719	4	6	-11	6.646	4.919	0.69112	1.727	1.727	
720	3	9	7	33.154	36.005	0.69123	-2.851	-2.851	*
721	6	0	6	58.438	50.912	0.69138	7.526	7.526	**
722	3	11	-5	6.794	6.484	0.69132	0.310	0.310	
723	3	11	3	10.303	11.698	0.69165	-1.395	-1.395	
724	1	9	-10	6.117	4.836	0.69161	1.280	1.280	
725	5	3	8	5.620	4.812	0.69225	0.808	0.808	
726	7	3	-5	5.476	4.201	0.69234	1.275	1.275	
727	2	12	2	5.513	6.520	0.69297	-1.007	-1.007	
728	5	9	1	5.031	5.858	0.69294	-0.827	-0.827	
729	0	0	14	4.483	6.356	0.69364	-1.873	-1.873	
730	0	0	14	4.548	6.356	0.69364	-1.808	-1.808	
731	5	5	7	14.071	15.278	0.69395	-1.207	-1.207	
732	2	2	-14	10.556	8.607	0.69521	1.949	1.949	
733	7	1	2	8.650	7.051	0.69655	1.599	1.599	
734	4	10	3	10.414	11.182	0.69659	-0.768	-0.768	
735	5	1	-12	8.632	5.923	0.69737	2.709	2.709	*
736	0	8	11	20.717	16.785	0.69774	3.932	3.932	*
737	6	4	-9	6.646	5.871	0.69781	0.775	0.775	
738	2	8	-11	10.226	11.608	0.69792	-1.382	-1.382	
739	4	2	-13	7.518	5.567	0.69808	1.951	1.951	
740	6	6	-7	16.206	16.697	0.69826	-0.492	-0.492	
741	6	2	-10	1.671	2.742	0.69861	-1.072	-1.072	
742	1	7	-12	6.974	5.234	0.69866	1.740	1.740	
743	6	4	5	20.104	21.281	0.69894	-1.177	-1.177	
744	6	6	3	16.354	18.359	0.69907	-2.005	-2.005	*
745	5	9	-5	10.265	11.289	0.69958	-1.024	-1.024	
746	2	12	-4	8.576	11.141	0.69985	-2.565	-2.565	*
747	6	2	6	7.110	7.553	0.69991	-0.443	-0.443	
748	7	3	1	12.642	11.918	0.69997	0.724	0.724	
749	7	1	-7	7.480	11.164	0.70096	-3.684	-3.684	*
750	4	10	-6	3.676	5.901	0.70137	-2.226	-2.226	*
751	0	2	14	2.906	3.617	0.70214	-0.712	-0.712	
752	1	3	-14	4.349	2.984	0.70272	1.364	1.364	
753	2	0	13	3.894	2.150	0.70326	1.743	1.743	
754	7	3	-6	16.224	16.391	0.70339	-0.167	-0.167	

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PHLOG21 Demonstration Copy - Not for Resale

The space group is number 12 -- C12/m1

After refinement cycle no. 1. 754 observations. 68 variables.

Esd of an observation of unit weight = 3.582

Unweighted R factor = 0.097 Weighted R factor = 0.102

$\bar{a}^3 \text{Fo}^3 = 1.78689\text{E}+04$

$\bar{a}^3 \text{Fo}^3 - \text{Fc}^3 = 1.73276\text{E}+03$

$\bar{a} \text{W*DEL} \bar{y} = 8.80433\text{E}+03$

$\bar{a} \text{W*Fo} \bar{y} = 8.38828\text{E}+05$

Largest parameter shift/error = 0.03

Average parameter shift/error = 0.01

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

Cycle	Error	R1	R2	Max.shift	Av.shift
1	3.582	0.097	0.102	0.03	0.01
2	0.000	0.000	0.000	0.00	0.00
3	0.000	0.000	0.000	0.00	0.00

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-1M 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 $1.81 \times 10^{-5} \text{ }^\circ\text{C}^{-1}$, and 1.40 and $1.34 \times 10^{-5} \text{ }^\circ\text{C}^{-1}$ 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 $\alpha_c = 1.81 \times 10^{-5} \text{ }^\circ\text{C}^{-1}$). The OH-rich octahedra ($M1$, $M2$) 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-1M 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 ($M1$, $M2$) 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-1M 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 $1.81 \times 10^{-5} \text{ }^\circ\text{C}^{-1}$, et celle des dimensions a et b , 1.40 and $1.34 \times 10^{-5} \text{ }^\circ\text{C}^{-1}$, 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 $\alpha_c = 1.81 \times 10^{-5} \text{ }^\circ\text{C}^{-1}$). Les octaèdres riches en OH ($M1$, $M2$) 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 aplatissement général avec une augmentation en température. Nous avons aussi affiné la structure à température ambiante d'un échantillon de phlogopite-1M 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 ($M1$, $M2$) et le site inter-feuillet sont aplatis dans les échantillons de ce mica, chauffé ou non, mais l'échantillon chauffé montre un aplatissement 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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