

LSFM (1.4) 06/10/97 10:17:15 Elapsed time = 0.1 min

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

600°C  
Phlogopite

The space group is number 12 -- C12/m1

Refinement cycle no. 1. 852 observations. 58 variables.

Russell &  
Guggenheim

Esd of an observation of unit weight = 3.371

Unweighted R factor = 0.069 Weighted R factor = 0.096

$\ddot{a}^3 Fo^3 = 2.20419E+04$

$\ddot{a}^3 Fo^3 - Fo^3 = 1.52900E+03$

$\ddot{a} W \cdot DEL \dot{y} = 9.02408E+03$

$\ddot{a} W \cdot Fo \dot{y} = 9.71687E+05$

Scale factor:	New	Old	Shift	Error	SHFT/ERR
	1.23808	1.23809	-0.00001	0.00344	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)	0.09184	0.09181	0.00002	0.00426	0.00	
6	U(2,2)	0.10544	0.10560	-0.00016	0.00529	-0.03	
7	U(3,3)	0.08637	0.08637	0.00001	0.00418	0.00	
	U(1,2)	0.00000					
9	U(1,3)	0.01539	0.01542	-0.00002	0.00355	-0.01	
	U(2,3)	0.00000					
Total shift = 0.0000							

Atom no.	2	SI	(electron count = 14.0)			Error	SHFT/ERR
Parameter		New	Old	Shift	Error	SHFT/ERR	
Mult.		1.00000					
11	x	0.07708	0.07708	0.00000 (0.0000 )	0.00034 (0.0018 )	0.00	
12	y	0.16668	0.16671	-0.00003 (0.0002 )	0.00023 (0.0021 )	-0.11	
13	z	0.23018	0.23025	-0.00007 (0.0007 )	0.00020 (0.0021 )	-0.33	
14	U(1,1)	0.01620	0.01626	-0.00006	0.00069	-0.08	
15	U(2,2)	0.02302	0.02297	0.00005	0.00088	0.05	
16	U(3,3)	0.03162	0.03163	0.00000	0.00087	0.00	
17	U(1,2)	-0.00045	-0.00041	-0.00004	0.00096	-0.04	
18	U(1,3)	0.00541	0.00547	-0.00006	0.00065	-0.10	
19	U(2,3)	0.00033	0.00038	-0.00004	0.00110	-0.04	
Total shift = 0.0007							

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)	0.01509	0.01504	0.00005	0.00187	0.03	
24	U(2,2)	0.02120	0.02122	-0.00002	0.00234	-0.01	
25	U(3,3)	0.03331	0.03328	0.00003	0.00248	0.01	
		U(1,2)	0.00000				
27	U(1,3)	0.00673	0.00659	0.00014	0.00179	0.08	
		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	0.33173	0.33165	0.00008 (0.0007 )	0.00040 (0.0037 )	0.20	
		z	0.50000				
32	U(1,1)	0.01311	0.01317	-0.00006	0.00117	-0.05	
33	U(2,2)	0.02073	0.02075	-0.00002	0.00155	-0.01	
34	U(3,3)	0.03124	0.03116	0.00008	0.00154	0.05	
		U(1,2)	0.00000				
36	U(1,3)	0.00445	0.00443	0.00002	0.00114	0.01	
		U(2,3)	0.00000				
		Total shift =	0.0007				

Atom no.	5	F	(electron count = 9.0)				
Parameter		New	Old	Shift	Error	SHFT/ERR	
		Mult.	0.50000				
38	x	0.13117	0.13181	-0.00064 (0.0034 )	0.00137 (0.0073 )	-0.46	
		y	0.50000				
40	z	0.39759	0.39767	-0.00008 (0.0008 )	0.00080 (0.0082 )	-0.10	
41	U(1,1)	0.03666	0.03657	0.00009	0.00349	0.03	
42	U(2,2)	0.05021	0.05018	0.00003	0.00457	0.01	
43	U(3,3)	0.05986	0.05990	-0.00004	0.00449	-0.01	
		U(1,2)	0.00000				
45	U(1,3)	0.00764	0.00765	-0.00001	0.00335	0.00	
		U(2,3)	0.00000				
		Total shift =	0.0033				

Atom no.	6	O 1	(electron count = 8.0)				
Parameter		New	Old	Shift	Error	SHFT/ERR	
		Mult.	0.50000				
47	x	0.02379	0.02484	-0.00105 (0.0056 )	0.00164 (0.0087 )	-0.64	
		y	0.00000				
49	z	0.17314	0.17309	0.00005 (0.0006 )	0.00085 (0.0087 )	0.06	
50	U(1,1)	0.04494	0.04498	-0.00004	0.00444	-0.01	
51	U(2,2)	0.02222	0.02233	-0.00012	0.00382	-0.03	
52	U(3,3)	0.04520	0.04504	0.00016	0.00468	0.03	
		U(1,2)	0.00000				

54 U(1,3) 0.00043 0.00033 0.00010 0.00391 0.03  
 U(2,3) 0.00000  
 Total shift = 0.0055

Atom no. 7 O 2 (electron count = 8.0)  
 Parameter New Old Shift Error SHFT/ERR  
 Mult. 1.00000  
 56 x 0.32535 0.32518 0.00017 (0.0009 ) 0.00095 (0.0050 ) 0.18  
 57 y 0.23340 0.23305 0.00035 (0.0032 ) 0.00069 (0.0064 ) 0.51  
 58 z 0.17316 0.17299 0.00017 (0.0018 ) 0.00057 (0.0058 ) 0.30  
 59 U(1,1) 0.02631 0.02625 0.00006 0.00232 0.03  
 60 U(2,2) 0.04173 0.04176 -0.00004 0.00330 -0.01  
 61 U(3,3) 0.05008 0.05010 -0.00001 0.00307 0.00  
 62 U(1,2) -0.01823 -0.01816 -0.00008 0.00243 -0.03  
 63 U(1,3) 0.01098 0.01092 0.00006 0.00215 0.03  
 64 U(2,3) -0.00266 -0.00261 -0.00005 0.00290 -0.02  
 Total shift = 0.0037

Atom no. 8 O 3 (electron count = 8.0)  
 Parameter New Old Shift Error SHFT/ERR  
 Mult. 1.00000  
 65 x 0.13115 0.13107 0.00008 (0.0004 ) 0.00086 (0.0046 ) 0.09  
 66 y 0.16727 0.16740 -0.00013 (0.0012 ) 0.00063 (0.0058 ) -0.20  
 67 z 0.39279 0.39251 0.00028 (0.0029 ) 0.00048 (0.0049 ) 0.59  
 68 U(1,1) 0.02117 0.02115 0.00001 0.00199 0.01  
 69 U(2,2) 0.03226 0.03228 -0.00002 0.00273 -0.01  
 70 U(3,3) 0.03147 0.03137 0.00010 0.00236 0.04  
 71 U(1,2) -0.00097 -0.00101 0.00004 0.00240 0.02  
 72 U(1,3) 0.00459 0.00453 0.00007 0.00187 0.04  
 73 U(2,3) -0.00125 -0.00127 0.00001 0.00251 0.01  
 Total shift = 0.0031

Largest parameter shift/error = 0.64  
 Average parameter shift/error = 0.08

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The space group is number 12 -- C12/m1

Refinement cycle no. 2. 852 observations. 58 variables.

Esd of an observation of unit weight = 3.368

Unweighted R factor = 0.069 Weighted R factor = 0.096

$\ddot{a}^3 \text{Fo}^3 = 2.20417\text{E}+04$

$\ddot{a}^3 \text{Fo}^3 - \text{Fc}^3 = 1.52288\text{E}+03$

$\ddot{a} \text{W*DEL} \acute{y} = 9.00762\text{E}+03$



W\*Fo $\bar{y}$  = 9.71676E+05

Scale factor:	New	Old	Shift	Error	SHFT/ERR
	1.23812	1.23808	0.00004	0.00343	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)	0.09183	0.09184	0.00000	0.00426	0.00	
6	U(2,2)	0.10544	0.10544	0.00000	0.00528	0.00	
7	U(3,3)	0.08638	0.08637	0.00000	0.00417	0.00	
		U(1,2)	0.00000				
9	U(1,3)	0.01540	0.01539	0.00000	0.00354	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	0.07708	0.07708	0.00000 (0.0000 )	0.00034 (0.0018 )	0.00	
12	y	0.16668	0.16668	0.00000 (0.0000 )	0.00023 (0.0021 )	0.00	
13	z	0.23018	0.23018	0.00000 (0.0000 )	0.00020 (0.0021 )	0.00	
14	U(1,1)	0.01620	0.01620	0.00000	0.00069	0.00	
15	U(2,2)	0.02302	0.02302	-0.00001	0.00088	-0.01	
16	U(3,3)	0.03162	0.03162	-0.00001	0.00087	-0.01	
17	U(1,2)	-0.00045	-0.00045	0.00000	0.00096	0.00	
18	U(1,3)	0.00541	0.00541	0.00000	0.00065	0.00	
19	U(2,3)	0.00033	0.00033	0.00000	0.00110	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)	0.01509	0.01509	0.00000	0.00187	0.00	
24	U(2,2)	0.02120	0.02120	0.00000	0.00234	0.00	
25	U(3,3)	0.03331	0.03331	0.00000	0.00248	0.00	
		U(1,2)	0.00000				
27	U(1,3)	0.00673	0.00673	0.00000	0.00179	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	0.33173	0.33173	0.00000	(0.0000 )	0.00040	(0.0037 )	0.00
	z	0.50000						
32	U(1,1)	0.01311	0.01311	0.00000		0.00117		0.00
33	U(2,2)	0.02074	0.02073	0.00000		0.00155		0.00
34	U(3,3)	0.03124	0.03124	0.00000		0.00154		0.00
	U(1,2)	0.00000						
36	U(1,3)	0.00445	0.00445	0.00000		0.00113		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	0.13118	0.13117	0.00000	(0.0000 )	0.00137	(0.0073 )	0.00	
	y	0.50000							
40	z	0.39759	0.39759	0.00000	(0.0000 )	0.00080	(0.0082 )	0.00	
41	U(1,1)	0.03665	0.03666	-0.00001		0.00349		0.00	
42	U(2,2)	0.05021	0.05021	0.00000		0.00457		0.00	
43	U(3,3)	0.05996	0.05986	0.00010		0.00448		0.02	
	U(1,2)	0.00000							
45	U(1,3)	0.00776	0.00764	0.00012		0.00334		0.03	
	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	0.02379	0.02379	0.00000	(0.0000 )	0.00164	(0.0087 )	0.00	
	y	0.00000							
49	z	0.17314	0.17314	0.00000	(0.0000 )	0.00085	(0.0087 )	0.00	
50	U(1,1)	0.04488	0.04494	-0.00006		0.00444		-0.01	
51	U(2,2)	0.02227	0.02222	0.00005		0.00381		0.01	
52	U(3,3)	0.04517	0.04520	-0.00003		0.00468		-0.01	
	U(1,2)	0.00000							
54	U(1,3)	0.00040	0.00043	-0.00004		0.00391		-0.01	
	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	0.32535	0.32535	0.00000	(0.0000 )	0.00095	(0.0050 )	0.00	
57	y	0.23340	0.23340	0.00000	(0.0000 )	0.00069	(0.0064 )	0.00	
58	z	0.17316	0.17316	0.00000	(0.0000 )	0.00057	(0.0058 )	0.00	
59	U(1,1)	0.02627	0.02631	-0.00004		0.00232		-0.02	
60	U(2,2)	0.04180	0.04173	0.00008		0.00330		0.02	
61	U(3,3)	0.05007	0.05008	-0.00002		0.00306		-0.01	
62	U(1,2)	-0.01833	-0.01823	-0.00010		0.00243		-0.04	
63	U(1,3)	0.01095	0.01098	-0.00004		0.00215		-0.02	
64	U(2,3)	-0.00271	-0.00266	-0.00006		0.00290		-0.02	
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	0.13115	0.13115	0.00000	(0.0000 )	0.00086	(0.0046 )	0.00	
66	y	0.16727	0.16727	0.00000	(0.0000 )	0.00063	(0.0058 )	0.00	
67	z	0.39279	0.39279	0.00000	(0.0000 )	0.00048	(0.0049 )	0.00	
68	U(1,1)	0.02116	0.02117	-0.00001		0.00199		0.00	
69	U(2,2)	0.03227	0.03226	0.00001		0.00272		0.00	
70	U(3,3)	0.03137	0.03147	-0.00010		0.00236		-0.04	
71	U(1,2)	-0.00096	-0.00097	0.00000		0.00240		0.00	
72	U(1,3)	0.00456	0.00459	-0.00004		0.00187		-0.02	
73	U(2,3)	-0.00125	-0.00125	0.00001		0.00251		0.00	
Total shift =		0.0000							

Largest parameter shift/error = 0.04

Average parameter shift/error = 0.01

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

No.	h	k	l	Fo	Fc	sin $\theta$ /l	Fo-Fc	w(Fo-Fc)	Flag
---	-	-	-	-----	-----	-----	-----	-----	----
1	-2	0	9	12.443	12.445	0.45355	-0.002	-0.002	
2	-2	0	10	36.500	35.955	0.49904	0.545	0.545	
3	-2	2	9	22.992	23.283	0.46645	-0.292	-0.292	
4	-1	3	9	44.077	44.764	0.46883	-0.687	-0.687	
5	0	4	9	19.055	18.920	0.49628	0.135	0.135	
6	0	4	8	16.071	16.895	0.45228	-0.824	-0.824	
7	1	3	8	12.344	12.751	0.45411	-0.407	-0.407	
8	1	3	9	35.992	35.511	0.49960	0.482	0.482	
9	0	2	9	3.430	4.393	0.45902	-0.963	0.000	omit
10	-1	1	9	6.401	7.156	0.44280	-0.755	-0.755	
11	0	2	10	7.354	5.802	0.50729	1.553	1.553	
12	-1	1	10	4.371	3.053	0.49098	1.318	0.000	omit
13	-3	1	10	6.228	6.269	0.53036	-0.042	0.000	omit
14	-2	2	11	11.304	9.880	0.55600	1.424	1.424	
15	-2	2	10	11.428	11.440	0.51079	-0.012	-0.012	
16	-1	3	10	1.783	5.199	0.51457	-3.416	0.000	omit
17	-1	5	10	4.494	3.754	0.55878	0.741	0.000	omit
18	-1	1	11	10.499	10.043	0.53940	0.457	0.457	
19	-2	0	11	15.328	17.027	0.54523	-1.699	-1.699	
20	0	2	11	10.598	10.861	0.55578	-0.263	-0.263	
21	0	4	10	5.708	3.547	0.54123	2.161	0.000	omit
22	1	3	10	15.501	16.947	0.54580	-1.446	-1.446	
23	1	5	9	3.442	3.606	0.54503	-0.164	0.000	omit
24	1	5	8	5.794	6.013	0.50365	-0.218	0.000	omit
25	1	7	7	4.779	2.395	0.53514	2.384	0.000	omit
26	2	6	7	3.281	2.511	0.53564	0.770	0.000	omit
27	2	8	3	5.918	5.567	0.50845	0.351	0.000	omit
28	2	8	4	13.211	13.763	0.52822	-0.552	-0.552	
29	2	8	5	5.980	5.077	0.55174	0.903	0.000	omit
30	2	4	8	7.453	8.040	0.51742	-0.586	-0.586	
31	2	4	9	1.065	1.085	0.55925	-0.020	0.000	omit



32	3	7	5	11.230	11.636	0.56040	-0.407	-0.407	
33	3	7	4	7.887	8.739	0.53571	-0.852	-0.852	
34	3	7	3	11.267	12.132	0.51462	-0.865	-0.865	
35	4	6	0	1.610	0.171	0.50344	1.439	0.000	omit
36	4	6	-1	20.466	18.568	0.49929	1.898	1.898	
37	3	7	2	7.664	6.840	0.49759	0.824	0.824	
38	3	5	4	6.253	6.711	0.46454	-0.459	-0.459	
39	2	4	7	5.794	4.907	0.47706	0.887	0.000	omit
40	2	6	6	10.871	10.764	0.50168	0.107	0.107	
41	3	5	5	5.980	4.770	0.49281	1.210	0.000	omit
42	3	7	0	2.117	2.665	0.47733	-0.548	0.000	omit
43	3	7	1	22.435	21.882	0.48504	0.553	0.553	
44	2	8	2	14.313	14.006	0.49288	0.306	0.306	
45	2	6	4	76.491	75.288	0.44268	1.203	1.203	
46	2	6	5	15.712	15.073	0.47050	0.638	0.638	
47	1	5	7	13.681	12.290	0.46389	1.391	1.391	
48	0	0	9	15.303	17.667	0.44591	-2.364	-2.364	*
49	0	0	10	24.317	22.250	0.49546	2.066	2.066	*
50	1	1	9	2.451	0.615	0.47526	1.836	0.000	omit
51	2	2	8	23.958	24.239	0.48180	-0.281	-0.281	
52	3	3	6	40.784	42.863	0.47684	-2.080	-2.080	*
53	3	3	5	15.130	15.478	0.44205	-0.349	-0.349	
54	3	1	7	5.138	6.228	0.49044	-1.090	0.000	omit
55	2	0	8	43.260	44.122	0.46933	-0.862	-0.862	
56	3	1	6	14.758	13.536	0.45127	1.223	1.223	
57	4	0	4	63.466	60.974	0.46092	2.492	2.492	*
58	4	0	5	59.207	58.003	0.49109	1.204	1.204	
59	4	2	5	18.089	19.328	0.50302	-1.239	-1.239	
60	3	5	6	9.014	7.769	0.52424	1.245	1.245	
61	3	5	7	5.336	6.605	0.55831	-1.269	0.000	omit
62	3	3	8	3.677	0.656	0.55321	3.021	0.000	omit
63	1	1	10	9.732	8.970	0.52361	0.762	0.762	
64	0	0	11	30.842	31.179	0.54500	-0.338	-0.338	
65	2	2	9	2.278	3.250	0.52647	-0.971	0.000	omit

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
---	-	-	-	-----	-----	-----	-----	-----	----
66	2	0	9	2.204	6.010	0.51508	-3.806	0.000	omit
67	3	1	8	3.962	3.482	0.53134	0.480	0.000	omit
68	4	0	7	2.266	1.209	0.55975	1.057	0.000	omit
69	4	0	6	19.253	18.728	0.52420	0.525	0.525	
70	4	2	6	12.889	12.233	0.53540	0.656	0.656	
71	3	3	7	42.690	44.246	0.51406	-1.555	-1.555	
72	4	4	4	8.147	8.788	0.50981	-0.641	-0.641	
73	5	1	4	6.265	6.085	0.55186	0.180	0.000	omit
74	5	1	3	9.571	10.046	0.52829	-0.475	-0.475	
75	5	3	3	55.505	54.985	0.55028	0.520	0.520	
76	5	3	2	8.221	7.413	0.53128	0.808	0.808	
77	5	3	1	16.999	17.588	0.51635	-0.589	-0.589	
78	5	5	0	12.790	12.838	0.55076	-0.049	-0.049	
79	5	5	-1	5.596	5.859	0.54545	-0.262	0.000	omit
80	4	6	1	30.953	29.928	0.51238	1.025	1.025	



81	4	6	2	20.726	21.124	0.52585	-0.398	-0.398	
82	4	6	3	6.946	4.946	0.54352	2.000	2.000	*
83	4	4	5	22.819	24.227	0.53723	-1.408	-1.408	
84	5	1	2	4.891	3.869	0.50846	1.022	0.000	omit
85	4	2	4	9.534	10.241	0.47362	-0.708	-0.708	
86	4	2	3	21.803	23.465	0.44778	-1.662	-1.662	
87	5	1	1	16.294	15.495	0.49284	0.798	0.798	
88	5	1	0	15.452	14.745	0.48183	0.707	0.707	
89	5	1	-1	9.620	10.112	0.47575	-0.491	-0.491	
90	5	3	0	58.996	59.329	0.50585	-0.333	-0.333	
91	5	3	-1	38.840	36.537	0.50006	2.303	2.303	*
92	4	4	0	13.582	14.057	0.44061	-0.475	-0.475	
93	4	4	1	11.997	10.305	0.45079	1.693	1.693	
94	4	4	3	14.127	14.891	0.48590	-0.764	-0.764	
95	4	4	2	9.595	11.313	0.46605	-1.717	-1.717	
96	3	5	0	9.818	12.241	0.39580	-2.423	-2.423	*
97	3	5	1	22.980	23.467	0.40507	-0.488	-0.488	
98	3	5	2	22.781	24.367	0.42001	-1.586	-1.586	
99	3	5	3	2.798	1.551	0.44006	1.247	0.000	omit
100	2	4	6	24.193	24.432	0.43860	-0.239	-0.239	
101	2	4	5	4.841	5.143	0.40256	-0.302	0.000	omit
102	1	5	5	7.317	7.376	0.39111	-0.058	-0.058	
103	1	5	6	23.140	22.805	0.42617	0.335	0.335	
104	2	6	3	32.327	33.956	0.41889	-1.629	-1.629	
105	2	6	0	77.246	79.658	0.37874	-2.411	-2.411	*
106	2	6	1	74.708	76.013	0.38628	-1.305	-1.305	
107	2	6	2	8.048	6.057	0.39986	1.991	1.991	
108	1	3	4	28.663	29.780	0.28594	-1.118	-1.118	
109	2	4	4	19.154	20.589	0.36966	-1.436	-1.436	
110	2	4	3	6.054	7.349	0.34081	-1.295	-1.295	
111	2	4	2	40.425	43.247	0.31712	-2.822	-2.822	*
112	2	4	1	41.291	42.393	0.29982	-1.102	-1.102	
113	2	4	0	7.218	6.405	0.29004	0.814	0.814	
114	1	3	0	49.475	53.157	0.18937	-3.682	-3.682	*
115	1	3	1	39.905	38.510	0.19993	1.394	1.394	
116	1	3	2	32.885	34.228	0.22134	-1.344	-1.344	
117	1	3	3	65.150	67.232	0.25084	-2.082	-2.082	*
118	1	5	3	8.382	7.507	0.33223	0.875	0.875	
119	1	5	4	19.624	20.018	0.35946	-0.393	-0.393	
120	1	3	6	97.836	105.476	0.36629	-7.640	-7.640	**
121	1	3	7	28.502	28.952	0.40955	-0.450	-0.450	
122	0	2	7	24.453	25.264	0.36352	-0.811	-0.811	
123	0	2	8	3.417	3.449	0.41106	-0.032	0.000	omit
124	-2	0	8	28.204	28.858	0.40901	-0.654	-0.654	
125	-1	1	8	7.243	6.208	0.39496	1.035	1.035	
126	-1	1	7	27.189	28.545	0.34761	-1.356	-1.356	
127	-2	2	8	10.239	10.024	0.42326	0.216	0.216	
128	-1	3	8	12.827	12.421	0.42394	0.406	0.406	
129	-1	3	7	22.373	24.456	0.38021	-2.083	-2.083	*
130	0	4	7	25.022	25.479	0.40956	-0.456	-0.456	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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131	0	4	6	43.817	45.543	0.36855	-1.726	-1.726	
132	-1	1	6	5.212	7.401	0.30095	-2.189	-2.189	*
133	-1	1	5	14.944	13.756	0.25539	1.188	1.188	
134	-1	1	4	10.735	8.936	0.21163	1.799	1.799	
135	0	2	3	50.255	54.117	0.18427	-3.861	-3.861	*
136	0	2	4	4.544	5.897	0.22614	-1.353	-1.353	
137	0	2	5	11.614	9.508	0.27062	2.106	2.106	*
138	0	0	2	24.255	25.473	0.09909	-1.218	-1.218	
139	1	3	5	67.354	71.334	0.32482	-3.980	-3.980	*
140	0	2	6	15.477	17.757	0.31660	-2.281	-2.281	*
141	0	0	7	43.260	48.350	0.34682	-5.090	-5.090	**
142	0	0	5	83.016	90.680	0.24773	-7.664	-7.664	**
143	0	0	4	45.513	54.128	0.19818	-8.615	-8.615	***
144	0	0	3	87.127	97.678	0.14864	-10.552	-10.552	***
145	0	0	6	17.346	16.786	0.29728	0.560	0.560	
146	1	1	6	24.441	25.252	0.33233	-0.811	-0.811	
147	1	1	5	4.742	2.405	0.28597	2.337	0.000	omit
148	1	1	4	12.765	13.002	0.24090	-0.237	-0.237	
149	1	1	3	29.826	30.869	0.19797	-1.043	-1.043	
150	1	1	2	74.139	84.895	0.15895	-10.756	-10.756	***
151	2	2	3	27.140	29.763	0.28383	-2.623	-2.623	*
152	2	0	2	94.927	89.425	0.23046	5.502	5.502	**
153	2	0	3	41.688	39.381	0.26210	2.307	2.307	*
154	2	0	4	105.637	106.867	0.29865	-1.231	-1.231	
155	2	2	4	2.130	1.324	0.31789	0.805	0.000	omit
156	1	1	7	16.876	15.975	0.37948	0.901	0.901	
157	0	0	8	43.594	51.022	0.39637	-7.428	-7.428	**
158	1	1	8	5.386	6.419	0.42718	-1.034	0.000	omit
159	2	2	7	4.482	5.021	0.43818	-0.539	0.000	omit
160	2	2	6	37.825	38.920	0.39595	-1.095	-1.095	
161	2	2	5	38.889	40.290	0.35561	-1.400	-1.400	
162	2	0	7	12.864	13.252	0.42442	-0.388	-0.388	
163	2	0	6	23.017	24.287	0.38067	-1.270	-1.270	
164	2	0	5	48.497	47.829	0.33852	0.668	0.668	
165	3	3	4	24.738	25.132	0.41030	-0.395	-0.395	
166	3	1	5	12.233	11.847	0.41434	0.386	0.386	
167	3	1	4	7.577	6.612	0.38029	0.965	0.965	
168	3	1	3	4.284	4.019	0.34996	0.265	0.000	omit
169	4	0	3	15.650	14.032	0.43433	1.618	1.618	
170	4	0	2	16.417	14.113	0.41200	2.305	2.305	*
171	4	0	0	7.057	7.779	0.38299	-0.722	-0.722	
172	4	0	1	68.208	64.130	0.39467	4.078	4.078	**
173	4	2	0	23.462	24.023	0.39818	-0.561	-0.561	
174	4	2	-1	20.726	20.578	0.39291	0.148	0.148	
175	4	2	1	41.279	42.662	0.40942	-1.383	-1.383	
176	4	2	2	5.151	3.985	0.42616	1.166	0.000	omit
177	3	3	3	55.022	54.267	0.38236	0.755	0.755	
178	3	3	2	28.675	27.425	0.35910	1.250	1.250	
179	3	1	1	38.827	38.638	0.30479	0.190	0.190	
180	3	1	0	6.624	7.111	0.29236	-0.487	-0.487	
181	2	0	0	106.379	104.210	0.19150	2.170	2.170	*



182	2	0	1	104.906	97.159	0.20600	7.747	7.747	**
183	2	2	1	28.390	30.380	0.23302	-1.990	-1.990	
184	3	1	2	30.458	30.776	0.32439	-0.318	-0.318	
185	3	3	1	3.727	2.811	0.34150	0.916	0.000	omit
186	2	2	2	8.333	3.863	0.25490	4.469	4.469	**
187	1	1	1	34.432	37.497	0.12745	-3.065	-3.065	*
188	1	1	0	34.246	32.489	0.11015	1.758	1.758	
189	2	2	0	36.760	36.651	0.22031	0.109	0.109	
190	3	3	0	54.131	52.781	0.33046	1.350	1.350	
191	3	3	-1	134.188	136.050	0.32664	-1.862	-1.862	
192	3	3	-2	54.081	51.315	0.33029	2.766	2.766	*
193	2	2	-1	37.849	38.628	0.21835	-0.779	-0.779	
194	1	1	-1	18.485	16.119	0.11372	2.366	2.366	*
195	2	2	-2	32.823	33.577	0.22745	-0.755	-0.755	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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196	2	2	-3	7.478	12.184	0.24636	-4.705	-4.705	**
197	3	1	-2	10.301	9.066	0.29217	1.235	1.235	
198	3	1	-1	30.804	28.213	0.28803	2.591	2.591	*
199	2	0	-1	55.183	55.018	0.18925	0.165	0.165	
200	2	0	-2	44.820	38.995	0.19967	5.825	5.825	**
201	3	1	-4	27.065	27.200	0.32386	-0.135	-0.135	
202	3	1	-3	53.809	54.166	0.30441	-0.357	-0.357	
203	4	0	-1	60.148	58.364	0.37751	1.784	1.784	
204	4	0	-2	86.582	84.322	0.37849	2.260	2.260	*
205	4	2	-2	24.119	25.514	0.39385	-1.396	-1.396	
206	4	0	-3	83.994	79.895	0.38589	4.099	4.099	**
207	4	0	-4	9.236	8.124	0.39934	1.112	1.112	
208	4	0	-5	36.574	35.969	0.41826	0.605	0.605	
209	4	2	-4	28.316	28.532	0.41393	-0.217	-0.217	
210	4	2	-3	16.715	15.194	0.40096	1.521	1.521	
211	3	3	-3	4.098	3.694	0.34117	0.404	0.000	omit
212	3	3	-4	29.628	29.010	0.35863	0.619	0.619	
213	3	3	-5	55.938	53.807	0.38176	2.132	2.132	*
214	4	2	-5	6.847	7.066	0.43221	-0.219	-0.219	
215	3	3	-6	25.629	24.954	0.40960	0.675	0.675	
216	3	1	-6	15.959	15.730	0.37954	0.229	0.229	
217	3	1	-5	16.554	16.242	0.34930	0.311	0.311	
218	3	1	-7	15.860	15.498	0.41351	0.362	0.362	
219	2	0	-8	29.257	28.858	0.40901	0.399	0.399	
220	2	0	-7	102.925	106.073	0.36576	-3.148	-3.148	*
221	2	2	-8	10.747	10.024	0.42326	0.723	0.723	
222	2	2	-7	46.380	46.659	0.38163	-0.278	-0.278	
223	1	1	-7	28.526	28.545	0.34761	-0.019	-0.019	
224	1	1	-8	7.961	6.208	0.39496	1.753	1.753	
225	0	0	-8	46.033	51.022	0.39637	-4.989	-4.989	**
226	0	0	-7	45.402	48.350	0.34682	-2.948	-2.948	*
227	1	1	-6	6.005	7.401	0.30095	-1.396	-1.396	
228	1	1	-5	15.501	13.756	0.25539	1.745	1.745	
229	1	1	-4	11.056	8.936	0.21163	2.121	2.121	*
230	1	1	-3	68.146	74.794	0.17106	-6.648	-6.648	**



231	2	2	-5	12.616	14.127	0.30553	-1.511	-1.511	
232	2	2	-6	26.880	27.456	0.34211	-0.577	-0.577	
233	2	0	-6	71.811	73.235	0.32431	-1.424	-1.424	
234	2	0	-5	31.126	31.058	0.28545	0.069	0.069	
235	2	0	-4	71.031	67.464	0.25040	3.567	3.567	*
236	2	2	-4	27.932	27.852	0.27307	0.080	0.080	
237	2	0	-3	36.884	34.943	0.22098	1.940	1.940	
238	1	1	-2	58.897	64.011	0.13653	-5.113	-5.113	**
239	1	3	-3	86.569	87.274	0.23019	-0.705	-0.705	
240	1	3	-4	39.125	37.084	0.26175	2.041	2.041	*
241	1	3	-5	100.944	104.874	0.29825	-3.929	-3.929	*
242	1	3	-1	94.753	101.378	0.19147	-6.625	-6.625	**
243	1	3	-2	93.627	94.969	0.20584	-1.342	-1.342	
244	2	6	-1	53.091	55.024	0.37761	-1.933	-1.933	
245	2	4	-1	28.861	29.427	0.28856	-0.566	-0.566	
246	2	4	-2	10.772	9.614	0.29550	1.158	1.158	
247	2	4	-3	39.694	42.017	0.31030	-2.323	-2.323	*
248	2	4	-4	17.866	18.125	0.33190	-0.259	-0.259	
249	2	4	-5	8.840	9.123	0.35908	-0.283	-0.283	
250	1	3	-6	47.259	48.072	0.33808	-0.813	-0.813	
251	2	4	-6	2.612	1.556	0.39068	1.056	0.000	omit
252	2	4	-7	15.860	15.810	0.42571	0.050	0.050	
253	3	5	-4	19.699	20.509	0.41960	-0.810	-0.810	
254	3	5	-3	39.459	41.422	0.40478	-1.963	-1.963	
255	3	5	-2	8.766	8.217	0.39566	0.549	0.549	
256	3	5	-1	28.786	30.759	0.39261	-1.972	-1.972	
257	2	6	-2	6.153	5.819	0.38294	0.334	0.000	omit
258	2	6	-3	60.717	62.508	0.39447	-1.791	-1.791	
259	2	6	-4	14.152	12.007	0.41167	2.145	2.145	*
260	2	6	-5	14.176	14.107	0.43389	0.069	0.069	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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261	1	5	-6	5.671	6.171	0.40219	-0.500	0.000	omit
262	1	3	-7	22.682	24.456	0.38021	-1.773	-1.773	
263	0	2	-5	11.948	9.508	0.27062	2.440	2.440	*
264	0	0	-6	18.225	16.786	0.29728	1.439	1.439	
265	0	0	-5	85.752	90.680	0.24773	-4.928	-4.928	**
266	0	0	-2	24.453	25.473	0.09909	-1.020	-1.020	
267	0	0	-3	88.687	97.678	0.14864	-8.992	-8.992	***
268	0	0	-4	46.640	54.128	0.19818	-7.488	-7.488	**
269	0	2	-4	4.606	5.897	0.22614	-1.291	-1.291	
270	-1	1	-5	5.089	2.405	0.28597	2.683	2.683	*
271	-2	0	-4	104.349	106.867	0.29865	-2.518	-2.518	*
272	-2	0	4	70.164	67.464	0.25040	2.701	2.701	*
273	-2	0	5	30.594	31.058	0.28545	-0.464	-0.464	
274	-2	0	6	70.474	73.235	0.32431	-2.761	-2.761	*
275	-2	0	-5	47.903	47.829	0.33852	0.074	0.074	
276	-2	0	-6	22.868	24.287	0.38067	-1.419	-1.419	
277	-2	0	-7	12.963	13.252	0.42442	-0.289	-0.289	
278	-1	1	-6	25.121	25.252	0.33233	-0.130	-0.130	
279	0	2	-6	15.997	17.757	0.31660	-1.761	-1.761	

280	0	2	-7	25.654	25.264	0.36352	0.390	0.390	
281	1	3	-8	13.099	12.421	0.42394	0.678	0.678	
282	0	2	-8	1.585	3.449	0.41106	-1.864	0.000	omit
283	-1	1	-8	5.720	6.419	0.42718	-0.699	0.000	omit
284	-1	1	-7	17.495	15.975	0.37948	1.520	1.520	
285	-2	0	7	99.520	106.073	0.36576	-6.552	-6.552	**
286	-3	1	8	22.200	21.584	0.45039	0.615	0.615	
287	-3	1	9	1.993	2.387	0.48950	-0.394	0.000	omit
288	-4	0	8	11.638	11.829	0.50081	-0.191	-0.191	
289	-1	3	-9	38.704	35.511	0.49960	3.193	3.193	*
290	0	4	-9	19.921	18.920	0.49628	1.002	1.002	
291	0	4	-8	16.777	16.895	0.45228	-0.119	-0.119	
292	1	5	-8	1.449	0.482	0.47663	0.967	0.000	omit
293	2	4	-9	8.394	8.308	0.50315	0.086	0.086	
294	1	3	-9	44.040	44.764	0.46883	-0.724	-0.724	
295	0	2	-9	3.417	4.393	0.45902	-0.976	0.000	omit
296	-1	1	-9	2.291	0.615	0.47526	1.675	0.000	omit
297	-2	0	-8	43.384	44.122	0.46933	-0.738	-0.738	
298	-4	0	9	2.278	2.596	0.53471	-0.318	0.000	omit
299	-1	3	-10	16.603	16.947	0.54580	-0.344	-0.344	
300	-2	2	-9	2.229	3.250	0.52647	-1.021	0.000	omit
301	1	5	-9	8.097	7.656	0.51697	0.442	0.442	
302	1	5	-10	5.089	3.754	0.55878	1.335	0.000	omit
303	0	4	-10	6.290	3.547	0.54123	2.743	0.000	omit
304	-2	0	-9	1.919	6.010	0.51508	-4.091	0.000	omit
305	-1	1	-10	10.276	8.970	0.52361	1.306	1.306	
306	0	2	-11	11.539	10.861	0.55578	0.678	0.678	
307	0	2	-10	7.924	5.802	0.50729	2.122	2.122	*
308	1	3	-10	2.513	5.199	0.51457	-2.686	0.000	omit
309	2	4	-10	2.130	0.285	0.54451	1.844	0.000	omit
310	1	5	-7	17.074	16.592	0.43819	0.481	0.481	
311	2	6	-7	54.935	52.988	0.49046	1.948	1.948	
312	2	6	-6	56.755	56.981	0.46038	-0.226	-0.226	
313	3	7	-4	7.862	7.253	0.49724	0.609	0.609	
314	3	7	-3	19.055	18.066	0.48480	0.988	0.988	
315	3	7	-2	3.269	3.236	0.47721	0.033	0.000	omit
316	3	7	-1	14.226	14.511	0.47469	-0.285	-0.285	
317	4	6	-2	37.602	34.749	0.50003	2.853	2.853	*
318	3	5	-5	17.618	17.924	0.43954	-0.306	-0.306	
319	2	4	-8	8.642	7.411	0.46340	1.231	1.231	
320	3	5	-7	9.546	9.533	0.49211	0.013	0.013	
321	3	5	-6	16.541	17.854	0.46393	-1.313	-1.313	
322	4	6	-3	56.545	55.664	0.50565	0.881	0.881	
323	4	6	-4	16.058	15.561	0.51599	0.498	0.498	
324	4	6	-5	8.234	6.557	0.53077	1.676	1.676	
325	4	6	-6	53.920	51.987	0.54963	1.933	1.933	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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326	3	5	-9	1.151	1.325	0.55749	-0.173	0.000	omit
327	3	5	-8	19.599	18.082	0.52348	1.517	1.517	
328	3	7	-5	7.751	7.389	0.51417	0.361	0.361	



329	3	7	-6	5.881	6.620	0.53517	-0.739	0.000	omit
330	2	8	-6	1.647	2.463	0.54313	-0.817	0.000	omit
331	3	7	-7	10.722	10.841	0.55978	-0.118	-0.118	
332	2	6	-9	2.451	1.376	0.55900	1.076	0.000	omit
333	2	6	-8	17.420	15.752	0.52351	1.668	1.668	
334	3	3	-7	15.229	14.126	0.44127	1.103	1.103	
335	3	1	-8	22.583	21.584	0.45039	0.999	0.999	
336	4	0	-7	17.136	16.449	0.46969	0.687	0.687	
337	3	1	-9	1.201	2.387	0.48950	-1.186	0.000	omit
338	2	0	-10	38.766	35.955	0.49904	2.811	2.811	*
339	2	0	-9	12.914	12.445	0.45355	0.469	0.469	
340	3	3	-8	41.663	42.141	0.47600	-0.478	-0.478	
341	2	2	-9	23.970	23.283	0.46645	0.687	0.687	
342	1	1	-9	6.983	7.156	0.44280	-0.173	-0.173	
343	0	0	-9	16.343	17.667	0.44591	-1.324	-1.324	
344	1	1	-10	4.866	3.053	0.49098	1.813	0.000	omit
345	0	0	-10	25.790	22.250	0.49546	3.540	3.540	*
346	1	1	-11	11.056	10.043	0.53940	1.014	1.014	
347	0	0	-11	32.773	31.179	0.54500	1.594	1.594	
348	2	2	-11	11.713	9.880	0.55600	1.833	1.833	
349	2	2	-10	11.923	11.440	0.51079	0.484	0.484	
350	3	3	-10	1.028	0.372	0.55228	0.656	0.000	omit
351	3	3	-9	43.359	43.338	0.51317	0.021	0.021	
352	3	1	-10	6.822	6.269	0.53036	0.553	0.553	
353	2	0	-11	16.318	17.027	0.54523	-0.708	-0.708	
354	4	0	-9	2.526	2.596	0.53471	-0.070	0.000	omit
355	4	0	-8	11.923	11.829	0.50081	0.094	0.094	
356	4	2	-9	1.288	2.779	0.54570	-1.492	0.000	omit
357	4	2	-8	10.821	10.507	0.51252	0.314	0.314	
358	4	4	-7	15.056	15.351	0.51775	-0.295	-0.295	
359	4	4	-8	21.865	21.947	0.54614	-0.081	-0.081	
360	5	3	-6	6.810	6.100	0.54276	0.710	0.000	omit
361	5	5	-4	14.189	12.991	0.55633	1.198	1.198	
362	5	5	-3	7.008	8.097	0.54827	-1.090	-1.090	
363	5	5	-2	9.026	8.896	0.54461	0.130	0.130	
364	5	3	-3	2.476	0.326	0.50314	2.150	0.000	omit
365	5	3	-4	32.092	31.512	0.51191	0.580	0.580	
366	5	3	-5	21.320	21.621	0.52523	-0.301	-0.301	
367	5	1	-7	2.328	2.779	0.54268	-0.451	0.000	omit
368	5	1	-6	14.486	15.086	0.52044	-0.600	-0.600	
369	5	1	-5	1.288	0.143	0.50213	1.145	0.000	omit
370	4	0	-6	83.586	80.347	0.44195	3.239	3.239	*
371	4	2	-6	8.481	8.252	0.45518	0.229	0.229	
372	5	1	-4	22.819	22.460	0.48818	0.359	0.359	
373	5	1	-2	13.793	14.267	0.47479	-0.474	-0.474	
374	5	3	-2	21.221	20.000	0.49915	1.221	1.221	
375	5	1	-3	12.616	12.958	0.47898	-0.341	-0.341	
376	4	2	-7	1.597	1.458	0.48216	0.139	0.000	omit
377	4	4	-6	7.862	8.092	0.49272	-0.230	-0.230	
378	4	4	-5	15.514	16.044	0.47159	-0.530	-0.530	
379	4	4	-4	6.636	4.522	0.45489	2.115	2.115	*
380	4	4	-3	15.959	15.448	0.44313	0.511	0.511	



381	4	4	-2	3.702	4.071	0.43671	-0.369	0.000	omit
382	0	4	-5	14.139	13.798	0.32989	0.341	0.341	
383	0	4	-4	22.843	24.916	0.29450	-2.072	-2.072	*
384	0	2	-2	70.387	80.510	0.14725	-10.123	-10.123	***
385	0	4	-3	19.736	18.173	0.26372	1.563	1.563	
386	0	6	-3	28.130	26.440	0.35898	1.690	1.690	
387	1	5	-1	20.986	21.345	0.29003	-0.359	-0.359	
388	1	5	-3	34.234	35.642	0.31693	-1.408	-1.408	
389	1	5	-4	6.760	5.917	0.34054	0.844	0.844	
390	1	5	-2	26.929	26.610	0.29971	0.319	0.319	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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391	1	5	0	20.280	19.360	0.28864	0.921	0.921	
392	1	5	1	26.595	26.887	0.29568	-0.293	-0.293	
393	1	5	2	48.460	51.195	0.31056	-2.735	-2.735	*
394	1	7	0	27.387	29.829	0.39306	-2.442	-2.442	*
395	1	7	-1	6.810	7.257	0.39408	-0.448	-0.448	
396	1	7	-2	31.708	33.123	0.40126	-1.414	-1.414	
397	0	6	-4	53.982	52.065	0.38216	1.917	1.917	
398	0	6	-5	24.713	22.585	0.41005	2.128	2.128	*
399	0	6	-6	15.018	14.302	0.44175	0.716	0.716	
400	0	4	-6	44.894	45.543	0.36855	-0.648	-0.648	
401	1	5	-5	11.341	10.148	0.36933	1.194	1.194	
402	1	7	-4	8.741	8.968	0.43261	-0.227	-0.227	
403	1	7	-3	31.411	32.784	0.41428	-1.373	-1.373	
404	1	7	2	27.090	26.700	0.40942	0.390	0.390	
405	1	7	1	4.197	0.758	0.39826	3.440	0.000	omit
406	1	7	3	14.424	15.502	0.42610	-1.078	-1.078	
407	0	6	6	15.031	14.302	0.44175	0.729	0.729	
408	0	6	5	24.899	22.585	0.41005	2.313	2.313	*
409	-1	5	7	16.888	16.592	0.43819	0.296	0.296	
410	-2	4	7	15.613	15.810	0.42571	-0.198	-0.198	
411	-2	2	7	44.597	46.659	0.38163	-2.061	-2.061	*
412	-3	3	7	15.588	14.126	0.44127	1.462	1.462	
413	-1	5	6	5.745	6.171	0.40219	-0.426	0.000	omit
414	-2	4	6	2.092	1.556	0.39068	0.536	0.000	omit
415	0	6	3	28.019	26.440	0.35898	1.579	1.579	
416	0	6	4	54.651	52.065	0.38216	2.586	2.586	*
417	-1	5	5	11.787	10.148	0.36933	1.639	1.639	
418	-1	3	6	45.711	48.072	0.33808	-2.361	-2.361	*
419	-2	2	6	26.805	27.456	0.34211	-0.651	-0.651	
420	-1	1	3	69.038	74.794	0.17106	-5.757	-5.757	**
421	0	4	5	13.855	13.798	0.32989	0.056	0.056	
422	0	4	4	23.413	24.916	0.29450	-1.503	-1.503	
423	0	2	2	70.412	80.510	0.14725	-10.098	-10.098	***
424	0	2	1	8.419	9.343	0.11966	-0.924	-0.924	
425	0	4	2	19.079	22.663	0.23932	-3.584	-3.584	*
426	0	4	3	19.897	18.173	0.26372	1.724	1.724	
427	-1	3	4	39.174	37.084	0.26175	2.091	2.091	*
428	-1	3	5	98.654	104.874	0.29825	-6.220	-6.220	**
429	-2	2	5	13.124	14.127	0.30553	-1.003	-1.003	

430	-2	4	4	19.699	18.125	0.33190	1.573	1.573	
431	-1	5	4	7.553	5.917	0.34054	1.636	1.636	
432	-1	3	3	91.732	87.274	0.23019	4.458	4.458	**
433	-1	5	3	38.481	35.642	0.31693	2.839	2.839	*
434	0	6	2	3.739	3.291	0.34146	0.449	0.000	omit
435	0	4	1	33.986	33.407	0.22340	0.579	0.579	
436	-1	5	1	23.153	21.345	0.29003	1.808	1.808	
437	-1	5	2	30.544	26.610	0.29971	3.935	3.935	*
438	-1	3	1	114.167	101.378	0.19147	12.789	12.789	***
439	-1	3	2	107.556	94.969	0.20584	12.587	12.587	***
440	-2	4	2	14.053	9.614	0.29550	4.439	4.439	**
441	-2	4	3	46.974	42.017	0.31030	4.957	4.957	**
442	-3	5	4	22.955	20.509	0.41960	2.446	2.446	*
443	-2	6	4	16.343	12.007	0.41167	4.336	4.336	**
444	-2	6	3	73.705	62.508	0.39447	11.197	11.197	***
445	-2	6	1	62.005	55.024	0.37761	6.982	6.982	**
446	-1	7	2	34.073	33.123	0.40126	0.950	0.950	
447	-2	6	2	7.775	5.819	0.38294	1.956	1.956	
448	-2	4	5	9.818	9.123	0.35908	0.695	0.695	
449	-3	5	5	19.550	17.924	0.43954	1.626	1.626	
450	-2	6	5	15.712	14.107	0.43389	1.605	1.605	
451	-1	7	4	9.534	8.968	0.43261	0.566	0.566	
452	0	8	2	14.857	12.261	0.44681	2.596	2.596	*
453	-1	7	3	34.110	32.784	0.41428	1.326	1.326	
454	-1	5	0	21.630	19.360	0.28864	2.270	2.270	*
455	0	4	0	38.283	40.051	0.21784	-1.769	-1.769	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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456	0	2	0	40.053	39.762	0.10892	0.291	0.291	
457	-1	3	0	53.734	53.157	0.18937	0.577	0.577	
458	-1	5	-1	28.786	26.887	0.29568	1.899	1.899	
459	-1	5	-2	53.066	51.195	0.31056	1.870	1.870	
460	0	4	-2	19.104	22.663	0.23932	-3.559	-3.559	*
461	0	4	-1	33.887	33.407	0.22340	0.480	0.480	
462	0	2	-1	8.469	9.343	0.11966	-0.875	-0.875	
463	0	6	0	127.985	126.916	0.32676	1.068	1.068	
464	0	6	-1	51.642	49.737	0.33050	1.905	1.905	
465	0	6	1	52.001	49.737	0.33050	2.264	2.264	*
466	-1	7	1	7.379	7.257	0.39408	0.122	0.122	
467	-1	7	0	29.096	29.829	0.39306	-0.733	-0.733	
468	-2	6	0	84.328	79.658	0.37874	4.671	4.671	**
469	-1	7	-1	3.702	0.758	0.39826	2.944	0.000	omit
470	-1	7	-2	28.712	26.700	0.40942	2.012	2.012	*
471	-2	6	-1	87.993	76.013	0.38628	11.980	11.980	***
472	-1	5	-3	8.902	7.507	0.33223	1.395	1.395	
473	-1	7	-3	15.501	15.502	0.42610	0.000	0.000	
474	0	6	-2	3.640	3.291	0.34146	0.350	0.000	omit
475	0	8	0	4.532	2.132	0.43568	2.399	0.000	omit
476	0	8	1	9.893	9.928	0.43849	-0.036	-0.036	
477	0	8	-1	9.657	9.928	0.43849	-0.271	-0.271	
478	1	9	3	20.194	18.842	0.52580	1.352	1.352	



479	1	9	-5	51.469	48.436	0.55000	3.032	3.032	*
480	2	8	-5	8.494	9.059	0.52087	-0.566	-0.566	
481	1	7	-7	20.107	19.490	0.51302	0.617	0.617	
482	1	7	-8	5.893	5.123	0.54622	0.771	0.000	omit
483	0	6	-8	42.319	41.629	0.51369	0.690	0.690	
484	0	8	-6	19.971	20.038	0.52744	-0.068	-0.068	
485	0	8	-7	15.563	14.024	0.55687	1.539	1.539	
486	1	9	-4	7.912	5.656	0.53109	2.255	2.255	*
487	1	9	-2	53.524	52.289	0.50588	1.235	1.235	
488	1	9	-3	15.080	12.887	0.51627	2.194	2.194	*
489	1	9	2	29.715	28.654	0.51238	1.061	1.061	
490	1	9	1	1.981	1.447	0.50351	0.534	0.000	omit
491	1	9	-1	35.435	32.161	0.50021	3.275	3.275	*
492	1	9	0	19.476	17.685	0.49941	1.791	1.791	
493	1	7	-5	19.748	21.673	0.45562	-1.925	-1.925	
494	0	6	-7	40.709	40.518	0.47651	0.191	0.191	
495	1	7	-6	1.052	0.789	0.48264	0.264	0.000	omit
496	2	8	-3	18.918	18.676	0.48852	0.243	0.243	
497	2	8	-2	6.513	6.087	0.47926	0.425	0.425	
498	2	8	-1	13.124	14.611	0.47501	-1.487	-1.487	
499	2	8	0	6.785	8.113	0.47591	-1.328	-1.328	
500	2	8	1	19.414	19.456	0.48193	-0.042	-0.042	
501	1	7	4	6.958	6.613	0.44766	0.345	0.345	
502	1	7	5	2.773	2.914	0.47344	-0.141	0.000	omit
503	1	7	6	8.704	7.967	0.50280	0.737	0.737	
504	0	6	7	40.474	40.518	0.47651	-0.044	-0.044	
505	-2	4	9	8.221	8.308	0.50315	-0.087	-0.087	
506	-2	4	8	10.276	7.411	0.46340	2.865	2.865	*
507	-3	3	8	41.328	42.141	0.47600	-0.813	-0.813	
508	-3	3	9	42.022	43.338	0.51317	-1.316	-1.316	
509	-1	7	7	20.862	19.490	0.51302	1.373	1.373	
510	0	8	5	1.634	0.250	0.50119	1.384	0.000	omit
511	0	8	4	16.777	16.346	0.47864	0.431	0.431	
512	1	9	4	6.624	4.622	0.54342	2.002	0.000	omit
513	0	8	7	16.009	14.024	0.55687	1.985	1.985	
514	0	6	8	41.997	41.629	0.51369	0.368	0.368	
515	-1	5	9	8.196	7.656	0.51697	0.541	0.541	
516	-3	5	8	19.500	18.082	0.52348	1.418	1.418	
517	-3	5	9	1.610	1.325	0.55749	0.285	0.000	omit
518	-2	6	9	1.696	1.376	0.55900	0.320	0.000	omit
519	-2	6	8	18.126	15.752	0.52351	2.374	2.374	*
520	-1	7	8	5.955	5.123	0.54622	0.833	0.000	omit

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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521	0	8	6	20.367	20.039	0.52744	0.329	0.329	
522	0	8	3	1.176	3.987	0.46034	-2.811	0.000	omit
523	-1	7	6	1.251	0.789	0.48264	0.462	0.000	omit
524	-1	7	5	21.073	21.673	0.45562	-0.600	-0.600	
525	-2	6	6	60.284	56.981	0.46038	3.303	3.303	*
526	-2	6	7	56.409	52.988	0.49046	3.421	3.421	*
527	-3	5	7	10.252	9.533	0.49211	0.719	0.719	



528	-3	5	6	17.396	17.854	0.46393	-0.458	-0.458	
529	-3	7	3	20.206	18.066	0.48480	2.140	2.140	*
530	-3	7	2	3.541	3.236	0.47721	0.305	0.000	omit
531	-3	7	1	14.585	14.511	0.47469	0.075	0.075	
532	-2	8	3	22.261	18.676	0.48852	3.586	3.586	*
533	-2	8	2	7.132	6.087	0.47926	1.044	1.044	
534	-1	9	2	56.929	52.289	0.50588	4.640	4.640	**
535	-2	8	4	2.229	1.244	0.50252	0.984	0.000	omit
536	-3	7	4	8.456	7.253	0.49724	1.204	1.204	
537	-4	6	6	48.856	51.987	0.54963	-3.131	-3.131	*
538	-3	7	6	6.092	6.620	0.53517	-0.529	0.000	omit
539	-3	7	5	8.345	7.389	0.51417	0.956	0.956	
540	-3	7	7	11.329	10.841	0.55978	0.488	0.488	
541	-2	8	6	2.031	2.463	0.54313	-0.433	0.000	omit
542	-2	8	5	9.657	9.059	0.52087	0.598	0.598	
543	-1	9	5	54.824	48.436	0.55000	6.388	6.388	**
544	-1	9	4	8.159	5.656	0.53109	2.503	2.503	*
545	-1	9	3	16.083	12.887	0.51627	3.197	3.197	*
546	0	10	2	14.833	13.561	0.55354	1.271	1.271	
547	0	10	1	1.610	0.188	0.54685	1.421	0.000	omit
548	0	10	0	8.890	10.040	0.54460	-1.150	-1.150	
549	0	10	-1	1.424	0.188	0.54685	1.236	0.000	omit
550	0	10	-2	14.709	13.561	0.55354	1.148	1.148	
551	-1	7	-6	9.001	7.967	0.50280	1.034	1.034	
552	-2	8	-4	12.852	13.763	0.52822	-0.911	-0.911	
553	-1	9	-4	6.834	4.622	0.54342	2.213	2.213	*
554	-2	8	-3	5.819	5.567	0.50845	0.252	0.000	omit
555	-1	9	-3	20.813	18.842	0.52580	1.971	1.971	
556	-1	9	-2	31.263	28.654	0.51238	2.609	2.609	*
557	-1	9	-1	2.650	1.447	0.50351	1.202	0.000	omit
558	-2	8	1	14.053	14.611	0.47501	-0.558	-0.558	
559	-1	9	1	37.602	32.161	0.50021	5.441	5.441	**
560	-1	9	0	20.578	17.685	0.49941	2.893	2.893	*
561	-2	8	0	7.255	8.113	0.47591	-0.858	-0.858	
562	-2	8	-1	20.268	19.456	0.48193	0.812	0.812	
563	-2	8	-2	14.981	14.006	0.49288	0.975	0.975	
564	0	8	-2	14.659	12.261	0.44681	2.398	2.398	*
565	0	8	-3	1.028	3.987	0.46034	-2.959	0.000	omit
566	0	8	-4	16.578	16.346	0.47864	0.233	0.233	
567	-1	7	-5	2.092	2.914	0.47344	-0.822	0.000	omit
568	-1	7	-4	7.119	6.613	0.44766	0.506	0.506	
569	0	4	-7	26.013	25.479	0.40956	0.534	0.534	
570	-1	3	-7	30.198	28.952	0.40955	1.246	1.246	
571	-1	3	-6	101.786	105.476	0.36629	-3.690	-3.690	*
572	-2	2	-6	38.766	38.920	0.39595	-0.154	-0.154	
573	-3	1	-5	12.517	11.847	0.41434	0.671	0.671	
574	-4	0	-3	15.229	14.032	0.43433	1.197	1.197	
575	-4	0	-2	15.922	14.113	0.41200	1.809	1.809	
576	-3	1	-4	8.221	6.612	0.38029	1.609	1.609	
577	-2	2	-5	40.833	40.290	0.35561	0.544	0.544	
578	-1	5	-5	7.676	7.376	0.39111	0.301	0.301	
579	-1	5	-6	24.094	22.805	0.42617	1.288	1.288	

580	-2	4	-5	5.497	5.143	0.40256	0.354	0.000	omit
581	-3	1	-2	31.547	30.776	0.32439	0.771	0.771	
582	-3	1	-3	4.692	4.019	0.34996	0.674	0.000	omit
583	-2	2	-3	30.062	29.763	0.28383	0.299	0.299	
584	-2	2	-4	1.944	1.324	0.31789	0.620	0.000	omit
585	-1	3	-4	29.789	29.780	0.28594	0.009	0.009	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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586	-1	1	-2	79.834	84.895	0.15895	-5.061	-5.061	**
587	0	2	-3	51.097	54.117	0.18427	-3.019	-3.019	*
588	-1	3	-5	69.223	71.334	0.32482	-2.111	-2.111	*
589	-1	1	-4	12.926	13.002	0.24090	-0.076	-0.076	
590	-1	1	-3	31.052	30.870	0.19797	0.183	0.183	
591	-2	0	-3	41.304	39.381	0.26210	1.923	1.923	
592	-2	0	-2	93.627	89.425	0.23046	4.202	4.202	**
593	-2	0	-1	103.581	97.159	0.20600	6.422	6.422	**
594	-2	0	0	103.866	104.210	0.19150	-0.344	-0.344	
595	-2	0	1	54.750	55.018	0.18925	-0.268	-0.268	
596	-2	0	2	43.619	38.995	0.19967	4.624	4.624	**
597	-2	0	3	36.426	34.943	0.22098	1.482	1.482	
598	-3	1	4	27.189	27.200	0.32386	-0.011	-0.011	
599	-3	1	3	54.366	54.166	0.30441	0.200	0.200	
600	-2	2	4	30.421	27.852	0.27307	2.568	2.568	*
601	-1	1	2	63.924	64.011	0.13653	-0.087	-0.087	
602	-3	1	2	10.375	9.066	0.29217	1.310	1.310	
603	-3	1	0	6.760	7.111	0.29236	-0.351	-0.351	
604	-3	1	-1	39.558	38.638	0.30479	0.920	0.920	
605	-3	1	5	16.640	16.242	0.34930	0.398	0.398	
606	-3	1	6	15.947	15.730	0.37954	0.217	0.217	
607	-3	1	7	15.786	15.498	0.41351	0.288	0.288	
608	-4	0	5	35.608	35.969	0.41826	-0.361	-0.361	
609	-4	0	4	9.063	8.124	0.39934	0.939	0.939	
610	-4	0	3	82.471	79.895	0.38589	2.576	2.576	*
611	-4	2	5	6.773	7.066	0.43221	-0.294	-0.294	
612	-3	3	6	26.459	24.954	0.40960	1.505	1.505	
613	-4	0	2	85.183	84.322	0.37849	0.861	0.861	
614	-4	0	1	58.204	58.364	0.37751	-0.160	-0.160	
615	-4	0	0	7.144	7.779	0.38299	-0.635	-0.635	
616	-4	0	-1	67.341	64.130	0.39467	3.211	3.211	*
617	-4	2	0	24.416	24.023	0.39818	0.392	0.392	
618	-4	2	2	25.072	25.514	0.39385	-0.442	-0.442	
619	-4	2	1	21.234	20.578	0.39291	0.655	0.655	
620	-4	2	3	17.445	15.194	0.40096	2.251	2.251	*
621	-4	2	4	29.603	28.532	0.41393	1.071	1.071	
622	-3	3	5	60.742	53.807	0.38176	6.935	6.935	**
623	-3	5	1	31.659	30.759	0.39261	0.900	0.900	
624	-4	4	1	1.746	0.856	0.43586	0.890	0.000	omit
625	-4	4	2	4.185	4.071	0.43671	0.113	0.000	omit
626	-3	3	4	32.823	29.010	0.35863	3.813	3.813	*
627	-3	5	3	47.891	41.422	0.40478	6.469	6.469	**
628	-3	5	2	10.153	8.217	0.39566	1.935	1.935	



629	-3	3	3	4.581	3.694	0.34117	0.887	0.000	omit
630	-3	3	2	59.083	51.315	0.33029	7.768	7.768	**
631	-3	1	1	31.114	28.213	0.28803	2.901	2.901	*
632	-1	1	1	20.379	16.119	0.11372	4.261	4.261	**
633	-2	2	3	8.320	12.184	0.24636	-3.863	-3.863	*
634	-2	2	2	37.292	33.577	0.22745	3.715	3.715	*
635	-2	4	1	37.490	29.427	0.28856	8.064	8.064	***
636	-2	2	1	40.648	38.628	0.21835	2.019	2.019	*
637	-3	3	1	139.809	136.050	0.32664	3.759	3.759	*
638	-3	3	0	58.514	52.781	0.33046	5.733	5.733	**
639	-1	1	0	36.005	32.489	0.11015	3.516	3.516	*
640	-2	2	-1	31.906	30.380	0.23302	1.527	1.527	
641	-2	2	-2	9.583	3.863	0.25490	5.720	5.720	**
642	-1	1	-1	39.063	37.497	0.12745	1.565	1.565	
643	-2	4	-3	7.243	7.349	0.34081	-0.106	-0.106	
644	-1	3	-3	68.741	67.232	0.25084	1.508	1.508	
645	-1	3	-2	36.921	34.228	0.22134	2.692	2.692	*
646	-1	3	-1	47.185	38.510	0.19993	8.674	8.674	***
647	-2	4	-2	48.014	43.247	0.31712	4.768	4.768	**
648	-2	4	-1	51.407	42.393	0.29982	9.013	9.013	***
649	-2	4	0	9.014	6.405	0.29004	2.609	2.609	*
650	-3	3	-1	4.123	2.811	0.34150	1.312	0.000	omit

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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651	-2	2	0	39.409	36.651	0.22031	2.758	2.758	*
652	-3	3	-2	32.773	27.425	0.35910	5.348	5.348	**
653	-3	5	0	10.450	12.241	0.39580	-1.791	-1.791	
654	-3	5	-1	27.783	23.467	0.40507	4.316	4.316	**
655	-3	5	-2	27.189	24.367	0.42001	2.822	2.822	*
656	-2	6	-3	36.846	33.956	0.41889	2.891	2.891	*
657	-2	6	-2	9.298	6.057	0.39986	3.241	3.241	*
658	-1	5	-4	20.639	20.018	0.35946	0.622	0.622	
659	-2	4	-4	21.320	20.589	0.36966	0.731	0.731	
660	-3	3	-4	26.917	25.132	0.41030	1.784	1.784	
661	-3	3	-3	61.782	54.267	0.38236	7.515	7.515	**
662	-4	2	-1	43.124	42.662	0.40942	0.462	0.462	
663	-4	2	-2	5.052	3.985	0.42616	1.067	0.000	omit
664	-4	2	-5	19.129	19.328	0.50302	-0.199	-0.199	
665	-3	3	-6	42.307	42.863	0.47684	-0.557	-0.557	
666	-3	3	-5	16.306	15.478	0.44205	0.828	0.828	
667	-2	4	-6	25.901	24.432	0.43860	1.469	1.469	
668	-2	4	-7	8.283	4.907	0.47706	3.376	3.376	*
669	-1	5	-7	14.597	12.290	0.46389	2.307	2.307	*
670	-1	5	-8	6.042	6.013	0.50365	0.029	0.000	omit
671	-2	2	-8	25.208	24.239	0.48180	0.970	0.970	
672	-1	3	-8	13.161	12.751	0.45411	0.410	0.410	
673	-2	2	-7	5.200	5.021	0.43818	0.179	0.000	omit
674	-3	1	-6	14.907	13.536	0.45127	1.371	1.371	
675	-3	1	-7	5.175	6.228	0.49044	-1.053	0.000	omit
676	-3	3	-7	44.263	44.246	0.51406	0.017	0.017	
677	-4	2	-6	13.496	12.233	0.53540	1.263	1.263	

678	-3	5	-7	5.955	6.605	0.55831	-0.650	0.000	omit
679	-2	4	-8	8.333	8.040	0.51742	0.293	0.293	
680	-2	6	-7	1.944	2.511	0.53564	-0.567	0.000	omit
681	-1	7	-7	4.915	2.395	0.53514	2.520	0.000	omit
682	-1	5	-9	4.234	3.606	0.54503	0.628	0.000	omit
683	-3	1	-8	4.234	3.482	0.53134	0.753	0.000	omit
684	-4	0	-7	2.278	1.209	0.55975	1.069	0.000	omit
685	-5	1	-4	6.327	6.085	0.55186	0.242	0.000	omit
686	-5	1	-3	9.657	10.046	0.52829	-0.389	-0.389	
687	-5	1	-2	4.519	3.869	0.50846	0.650	0.000	omit
688	-5	1	-1	16.368	15.495	0.49284	0.873	0.873	
689	-5	1	5	1.449	0.143	0.50213	1.306	0.000	omit
690	-4	4	8	22.249	21.947	0.54614	0.302	0.302	
691	-4	2	8	11.131	10.507	0.51252	0.623	0.623	
692	-4	2	9	1.251	2.779	0.54570	-1.529	0.000	omit
693	-5	1	7	1.052	2.779	0.54268	-1.727	0.000	omit
694	-5	1	6	14.474	15.086	0.52044	-0.612	-0.612	
695	-4	0	-6	19.067	18.728	0.52420	0.340	0.340	
696	-4	0	-5	58.229	58.003	0.49109	0.226	0.226	
697	-4	2	-3	23.685	23.465	0.44778	0.220	0.220	
698	-4	2	-4	9.992	10.241	0.47362	-0.250	-0.250	
699	-5	1	0	15.229	14.745	0.48183	0.484	0.484	
700	-5	1	2	13.694	14.267	0.47479	-0.573	-0.573	
701	-5	1	3	12.654	12.958	0.47898	-0.304	-0.304	
702	-5	1	1	9.434	10.112	0.47575	-0.677	-0.677	
703	-4	0	-4	62.228	60.974	0.46092	1.254	1.254	
704	-5	1	4	22.720	22.460	0.48818	0.260	0.260	
705	-4	0	6	82.137	80.347	0.44195	1.790	1.790	
706	-4	2	6	8.729	8.252	0.45518	0.477	0.477	
707	-4	0	7	16.801	16.449	0.46969	0.352	0.352	
708	-4	2	7	1.548	1.458	0.48216	0.089	0.000	omit
709	-4	4	7	15.959	15.351	0.51775	0.609	0.609	
710	-5	3	6	7.453	6.100	0.54276	1.354	1.354	
711	-5	5	4	7.726	12.991	0.55633	-5.265	-5.265	**
712	-5	3	4	33.974	31.512	0.51191	2.462	2.462	*
713	-5	3	5	22.534	21.621	0.52523	0.912	0.912	
714	-5	3	-1	17.978	17.588	0.51635	0.389	0.389	
715	-5	5	0	5.336	12.838	0.55076	-7.502	0.000	omit

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716	-5	5	1	2.105	5.859	0.54545	-3.754	0.000	omit
717	-5	5	2	4.160	8.896	0.54461	-4.736	0.000	omit
718	-5	5	3	3.652	8.097	0.54827	-4.445	0.000	omit
719	-4	6	5	7.293	6.557	0.53077	0.735	0.735	
720	-4	6	4	13.582	15.561	0.51599	-1.978	-1.978	
721	-4	4	5	17.198	16.044	0.47159	1.154	1.154	
722	-4	4	6	8.320	8.092	0.49272	0.228	0.228	
723	-5	3	3	2.464	0.326	0.50314	2.138	0.000	omit
724	-5	3	2	22.026	20.000	0.49915	2.026	2.026	*
725	-5	3	1	40.028	36.537	0.50006	3.492	3.492	*
726	-5	3	0	62.067	59.329	0.50585	2.738	2.738	*



727	-4	4	3	17.408	15.448	0.44313	1.960	1.960	
728	-4	4	4	7.144	4.522	0.45489	2.622	2.622	*
729	-4	6	3	44.647	55.664	0.50565	-11.017	-11.017	***
730	-4	6	2	26.087	34.749	0.50003	-8.662	-8.662	***
731	-4	6	1	12.356	18.568	0.49929	-6.212	-6.212	**
732	-4	4	0	14.697	14.057	0.44061	0.640	0.640	
733	-4	6	0	1.213	0.171	0.50344	1.042	0.000	omit
734	-4	6	-1	17.854	29.928	0.51238	-12.074	-12.074	***
735	-4	6	-2	11.737	21.124	0.52585	-9.387	-9.387	***
736	-4	6	-3	3.628	4.946	0.54352	-1.318	0.000	omit
737	-3	7	-4	6.005	8.739	0.53571	-2.734	0.000	omit
738	-3	7	-3	9.001	12.132	0.51462	-3.131	-3.131	*
739	-2	8	-5	5.782	5.077	0.55174	0.705	0.000	omit
740	-4	4	-5	24.713	24.227	0.53723	0.486	0.486	
741	-3	5	-6	9.719	7.769	0.52424	1.951	1.951	
742	-4	4	-4	9.100	8.788	0.50981	0.313	0.313	
743	-5	3	-3	59.244	54.985	0.55028	4.260	4.260	**
744	-5	3	-2	8.964	7.413	0.53128	1.551	1.551	
745	-4	4	-1	13.496	10.305	0.45079	3.191	3.191	*
746	-4	4	-2	10.697	11.313	0.46605	-0.616	-0.616	
747	-3	5	-3	2.959	1.551	0.44006	1.408	0.000	omit
748	-3	7	-2	6.624	6.840	0.49759	-0.216	-0.216	
749	-3	7	-1	19.909	21.882	0.48504	-1.973	-1.973	
750	-3	7	0	2.130	2.665	0.47733	-0.535	0.000	omit
751	-2	6	-4	82.781	75.288	0.44268	7.493	7.493	**
752	-2	6	-5	16.876	15.073	0.47050	1.802	1.802	
753	-2	6	-6	11.775	10.764	0.50168	1.011	1.011	
754	-3	5	-4	7.082	6.711	0.46454	0.371	0.371	
755	-3	5	-5	6.451	4.770	0.49281	1.680	1.680	
756	-4	4	-3	15.873	14.891	0.48590	0.981	0.981	
757	-4	2	-7	4.432	4.334	0.57025	0.099	0.000	omit
758	-5	1	-5	13.000	12.271	0.57872	0.729	0.729	
759	-3	3	-9	17.965	15.695	0.59392	2.270	2.270	*
760	-2	4	-10	8.035	7.005	0.60226	1.031	1.031	
761	0	6	-10	17.061	14.123	0.59351	2.938	2.938	*
762	-1	5	-10	6.451	5.218	0.58767	1.233	0.000	omit
763	-1	7	-8	6.711	6.128	0.56996	0.582	0.000	omit
764	-2	6	-8	22.026	20.773	0.57187	1.253	1.253	
765	-4	4	-6	6.797	5.048	0.56767	1.749	0.000	omit
766	-5	3	-5	20.256	19.538	0.59887	0.718	0.718	
767	-4	4	-7	15.105	13.954	0.60065	1.152	1.152	
768	-1	7	-9	1.498	1.210	0.60683	0.288	0.000	omit
769	-1	5	-11	7.045	5.900	0.63131	1.145	0.000	omit
770	-3	3	-10	32.402	28.865	0.63589	3.537	3.537	*
771	-4	2	-8	4.296	4.876	0.60715	-0.580	0.000	omit
772	-6	0	-3	5.002	3.329	0.61801	1.673	0.000	omit
773	-2	6	-9	6.166	7.751	0.60999	-1.585	0.000	omit
774	-3	5	-9	7.033	5.224	0.63261	1.808	0.000	omit
775	-4	4	-8	7.837	7.875	0.63579	-0.037	-0.037	
776	-5	3	-6	1.634	1.236	0.62764	0.399	0.000	omit
777	-6	2	-3	1.659	1.826	0.62753	-0.167	0.000	omit
778	-6	2	-2	10.264	10.021	0.60958	0.243	0.243	

779	-6	0	0	2.934	3.464	0.57449	-0.529	0.000	omit
780	-6	0	1	20.949	20.289	0.56794	0.660	0.660	

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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781	-6	0	2	57.139	57.668	0.56568	-0.529	-0.529	
782	-6	2	3	4.816	6.221	0.57809	-1.405	0.000	omit
783	-6	2	4	13.285	12.717	0.58433	0.568	0.568	
784	-5	3	7	28.700	26.950	0.56411	1.750	1.750	
785	-6	0	3	31.523	33.220	0.56774	-1.698	-1.698	
786	-6	0	-1	16.207	16.006	0.58517	0.201	0.201	
787	-6	0	4	6.797	8.288	0.57409	-1.490	0.000	omit
788	-6	0	5	14.350	14.691	0.58458	-0.341	-0.341	
789	-4	2	10	5.299	5.119	0.58121	0.180	0.000	omit
790	-5	1	8	15.093	15.981	0.56837	-0.889	-0.889	
791	-4	2	11	4.705	3.978	0.61865	0.726	0.000	omit
792	-5	1	10	8.172	7.748	0.62838	0.423	0.423	
793	-5	1	9	7.094	6.392	0.59707	0.702	0.000	omit
794	-6	0	6	35.571	37.409	0.59901	-1.838	-1.838	
795	-6	0	7	11.614	11.528	0.61708	0.086	0.086	
796	-6	0	-2	26.186	25.158	0.59977	1.028	1.028	
797	-6	2	6	13.161	13.290	0.60883	-0.129	-0.129	
798	-6	2	7	4.036	4.937	0.62662	-0.901	0.000	omit
799	-5	3	9	16.096	14.767	0.61662	1.328	1.328	
800	-5	3	8	50.119	48.317	0.58887	1.802	1.802	
801	-5	5	6	6.104	10.378	0.58485	-4.274	0.000	omit
802	-6	4	2	4.618	18.154	0.60617	-13.536	0.000	omit
803	-6	2	2	6.785	7.270	0.57607	-0.485	0.000	omit
804	-6	2	1	1.090	2.056	0.57829	-0.967	0.000	omit
805	-6	2	0	9.509	8.354	0.58472	1.155	1.155	
806	-5	7	1	1.275	12.632	0.60721	-11.357	0.000	omit
807	-5	7	2	1.350	15.142	0.60645	-13.792	0.000	omit
808	-5	5	5	1.820	3.414	0.56861	-1.594	0.000	omit
809	-5	7	4	1.746	18.047	0.61700	-16.302	0.000	omit
810	-6	4	1	0.854	2.752	0.60829	-1.898	0.000	omit
811	-6	4	0	4.779	19.974	0.61440	-15.195	0.000	omit
812	-5	5	8	9.583	14.274	0.62787	-4.691	-4.691	**
813	-6	4	5	3.430	9.933	0.62385	-6.504	0.000	omit
814	-6	4	3	2.340	8.057	0.60810	-5.717	0.000	omit
815	-6	4	4	4.296	12.036	0.61403	-7.740	0.000	omit
816	-6	4	-1	2.105	8.434	0.62440	-6.330	0.000	omit
817	-5	5	-1	3.207	7.516	0.56042	-4.309	0.000	omit
818	-5	5	-2	1.857	5.717	0.57421	-3.860	0.000	omit
819	-4	8	-1	1.127	8.660	0.58786	-7.533	0.000	omit
820	-4	6	-4	13.496	25.361	0.56500	-11.866	-11.866	***
821	-5	3	-4	26.830	25.972	0.57295	0.858	0.858	
822	-5	5	-3	3.157	9.569	0.59183	-6.411	0.000	omit
823	-4	6	-5	22.682	46.313	0.58986	-23.631	-23.631	****
824	-3	7	-5	7.949	11.636	0.56040	-3.688	-3.688	*
825	-3	7	-6	7.590	10.296	0.58823	-2.706	-2.706	*
826	-2	8	-6	12.542	13.558	0.57856	-1.016	-1.016	
827	-3	9	-3	3.764	33.697	0.59979	-29.933	0.000	omit



828	-3	9	-4	0.854	9.007	0.61798	-8.153	0.000	omit
829	-5	7	-2	1.015	1.554	0.63317	-0.539	0.000	omit
830	-5	7	-1	1.102	12.885	0.62069	-11.783	0.000	omit
831	-6	4	-2	2.328	11.166	0.63811	-8.839	0.000	omit
832	-5	5	-5	3.454	11.377	0.63726	-7.922	0.000	omit
833	-5	5	-4	1.771	6.766	0.61297	-4.995	0.000	omit
834	-4	6	-6	7.218	15.236	0.61771	-8.018	-8.018	***
835	-3	7	-7	2.959	4.502	0.61878	-1.542	0.000	omit
836	-2	8	-7	1.251	0.206	0.60824	1.045	0.000	omit
837	-2	8	-9	1.449	0.444	0.67463	1.005	0.000	omit
838	-1	7	-11	4.940	4.788	0.68538	0.152	0.000	omit
839	-2	6	-11	13.793	12.358	0.69058	1.434	1.434	
840	-3	7	-9	2.179	1.451	0.68657	0.728	0.000	omit
841	-6	2	-6	7.751	8.390	0.69991	-0.639	0.000	omit
842	-3	3	-11	8.815	7.356	0.67887	1.460	1.460	
843	0	8	-11	10.413	9.434	0.69775	0.978	0.978	
844	-2	4	-12	5.089	5.280	0.69091	-0.191	0.000	omit
845	-4	2	-10	4.259	4.653	0.68575	-0.394	0.000	omit

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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846	-6	0	-6	27.251	27.955	0.69138	-0.704	-0.704	
847	-5	1	-8	1.560	1.092	0.67490	0.468	0.000	omit
848	-6	2	-4	11.737	12.383	0.64878	-0.645	-0.645	
849	-6	2	-5	8.630	8.479	0.67301	0.151	0.151	
850	-5	3	-7	24.057	24.214	0.65888	-0.157	-0.157	
851	-4	4	-9	6.513	5.375	0.67274	1.137	0.000	omit
852	-3	5	-10	7.590	7.184	0.67216	0.406	0.000	omit
853	-2	6	-10	1.424	1.297	0.64964	0.127	0.000	omit
854	-1	7	-10	8.035	6.560	0.64539	1.475	1.475	
855	-2	4	-11	4.705	4.321	0.64620	0.384	0.000	omit
856	-4	2	-9	3.355	2.500	0.64575	0.855	0.000	omit
857	-5	1	-7	8.617	7.715	0.64062	0.902	0.902	
858	-6	0	-5	21.197	21.172	0.66414	0.025	0.025	
859	-6	0	-4	11.812	10.636	0.63957	1.176	1.176	
860	-7	1	0	10.462	9.870	0.67245	0.592	0.592	
861	-7	1	1	3.851	3.884	0.66562	-0.033	0.000	omit
862	-7	1	2	9.794	11.034	0.66244	-1.240	-1.240	
863	-7	1	3	5.448	5.981	0.66295	-0.533	0.000	omit
864	-7	1	4	9.781	10.810	0.66716	-1.029	-1.029	
865	-5	5	9	2.674	2.606	0.65397	0.069	0.000	omit
866	-6	0	8	13.892	13.200	0.63849	0.692	0.692	
867	-6	0	9	27.895	29.818	0.66293	-1.924	-1.924	
868	-6	2	8	12.765	13.838	0.64772	-1.073	-1.073	
869	-6	2	9	11.106	10.827	0.67182	0.279	0.279	
870	-5	1	11	3.640	3.744	0.66191	-0.104	0.000	omit
871	-5	3	10	7.008	7.099	0.64698	-0.091	0.000	omit
872	-5	3	11	16.269	16.344	0.67960	-0.075	-0.075	
873	-6	2	10	6.513	6.794	0.69860	-0.282	0.000	omit
874	-6	0	10	22.831	22.726	0.69006	0.105	0.105	
875	-7	1	7	8.073	9.209	0.70096	-1.136	-1.136	
876	-7	1	6	4.866	4.051	0.68631	0.814	0.000	omit

877	-7	1	5	8.593	8.365	0.67499	0.228	0.228	
878	-7	3	6	2.588	9.383	0.70338	-6.795	0.000	omit
879	-7	1	-2	7.132	6.874	0.69655	0.258	0.000	omit
880	-6	4	8	2.043	3.247	0.67463	-1.204	0.000	omit
881	-6	4	9	2.588	3.283	0.69780	-0.695	0.000	omit
882	-5	5	10	6.525	7.937	0.68267	-1.412	0.000	omit
883	-6	4	7	3.219	6.831	0.65440	-3.612	0.000	omit
884	-5	7	6	1.783	13.308	0.64283	-11.525	0.000	omit
885	-6	6	4	1.486	7.914	0.66057	-6.428	0.000	omit
886	-6	6	5	1.498	20.668	0.66971	-19.170	0.000	omit
887	-7	3	2	2.749	13.453	0.68011	-10.705	0.000	omit
888	-6	6	-1	1.473	20.054	0.67022	-18.581	0.000	omit
889	-6	6	2	3.454	49.233	0.65327	-45.778	0.000	omit
890	-6	6	3	1.337	13.486	0.65506	-12.149	0.000	omit
891	-5	9	3	0.768	2.157	0.68315	-1.389	0.000	omit
892	-5	9	1	1.411	23.335	0.68089	-21.924	0.000	omit
893	-6	6	-2	1.449	19.255	0.68301	-17.806	0.000	omit
894	-6	6	6	1.535	19.309	0.68234	-17.773	0.000	omit
895	-7	3	4	6.859	30.285	0.68471	-23.425	-23.425	****
896	-7	3	3	5.089	26.516	0.68061	-21.427	0.000	omit
897	-7	3	1	1.473	3.824	0.68321	-2.351	0.000	omit
898	-7	3	0	4.470	25.805	0.68986	-21.336	0.000	omit
899	-7	3	-1	1.325	9.812	0.69997	-8.487	0.000	omit
900	-5	9	0	0.768	27.335	0.68515	-26.568	0.000	omit
901	-3	9	-7	2.377	20.244	0.69123	-17.867	0.000	omit
902	-4	8	-6	1.312	3.342	0.68162	-2.029	0.000	omit
903	-4	6	-8	6.587	14.875	0.68084	-8.288	0.000	omit
904	-5	7	-5	0.904	4.423	0.69086	-3.520	0.000	omit
905	-5	5	-7	2.105	8.031	0.69395	-5.926	0.000	omit
906	-6	4	-5	1.300	9.234	0.69895	-7.933	0.000	omit
907	-6	4	-3	1.969	11.709	0.65528	-9.740	0.000	omit
908	-2	8	-8	7.243	7.626	0.64038	-0.383	-0.383	
909	-3	7	-8	4.259	5.835	0.65168	-1.576	0.000	omit
910	-4	6	-7	2.848	6.695	0.64815	-3.847	0.000	omit

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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911	-4	8	-5	0.817	16.294	0.65649	-15.477	0.000	omit
912	-3	9	-5	1.139	12.453	0.63949	-11.314	0.000	omit
913	-3	9	-6	2.699	26.398	0.66402	-23.699	0.000	omit
914	-2	12	-3	0.879	6.103	0.70412	-5.224	0.000	omit
915	-1	11	-6	1.325	4.925	0.68290	-3.600	0.000	omit
916	-2	12	-2	1.189	1.847	0.69297	-0.659	0.000	omit
917	0	12	-4	5.027	16.547	0.68291	-11.520	0.000	omit
918	0	12	-3	5.138	17.068	0.67021	-11.930	0.000	omit
919	-2	12	0	1.709	19.997	0.68100	-18.289	0.000	omit
920	-2	12	-1	1.424	24.244	0.68522	-22.821	0.000	omit
921	-3	11	-1	1.176	9.351	0.66993	-8.175	0.000	omit
922	-3	11	-2	0.916	3.629	0.67907	-2.713	0.000	omit
923	-3	11	-3	1.090	7.196	0.69165	-6.107	0.000	omit
924	-2	10	-6	2.031	13.317	0.66446	-11.286	0.000	omit
925	-2	10	-5	1.449	7.646	0.64124	-6.197	0.000	omit



926	-1	11	-4	0.904	3.136	0.64338	-2.232	0.000	omit
927	0	12	-2	2.130	6.948	0.66099	-4.819	0.000	omit
928	0	12	-1	5.014	10.892	0.65540	-5.877	0.000	omit
929	0	12	0	16.343	39.871	0.65352	-23.527	-23.527	****
930	0	12	1	5.794	10.892	0.65540	-5.097	0.000	omit
931	0	12	2	2.625	6.948	0.66099	-4.323	0.000	omit
932	-3	11	3	1.090	6.751	0.66976	-5.662	0.000	omit
933	-1	11	5	3.999	13.236	0.64895	-9.237	0.000	omit
934	0	12	3	8.134	17.068	0.67021	-8.933	-8.933	***
935	-2	10	7	2.179	11.520	0.65603	-9.341	0.000	omit
936	-3	9	8	3.479	18.659	0.66342	-15.180	0.000	omit
937	-4	8	8	1.238	11.039	0.66380	-9.801	0.000	omit
938	-2	12	3	1.151	20.543	0.68987	-19.392	0.000	omit
939	-3	9	9	4.333	23.755	0.69057	-19.421	0.000	omit
940	-4	6	10	22.039	23.564	0.65781	-1.526	-1.526	
941	-2	8	10	2.612	2.261	0.66246	0.351	0.000	omit
942	-3	7	10	6.624	5.715	0.65088	0.909	0.000	omit
943	-1	9	9	23.017	21.611	0.65829	1.406	1.406	
944	0	10	8	5.584	4.622	0.67357	0.962	0.000	omit
945	0	10	7	7.775	6.764	0.64566	1.011	1.011	
946	1	11	5	4.185	4.052	0.66158	0.133	0.000	omit
947	0	8	10	1.808	0.827	0.65977	0.980	0.000	omit
948	1	9	8	6.785	6.414	0.64789	0.371	0.000	omit
949	-1	7	11	4.643	3.950	0.65827	0.693	0.000	omit
950	-3	5	12	5.138	5.066	0.67123	0.073	0.000	omit
951	-4	4	11	1.919	3.421	0.64678	-1.502	0.000	omit
952	-4	4	12	8.890	8.385	0.68422	0.505	0.505	
953	-1	7	12	2.848	2.359	0.69866	0.489	0.000	omit
954	-2	6	12	6.673	4.228	0.67617	2.445	0.000	omit
955	1	11	6	6.178	4.925	0.68290	1.254	0.000	omit
956	0	10	9	7.057	5.539	0.70387	1.519	0.000	omit
957	-3	7	11	4.804	2.636	0.68574	2.168	0.000	omit
958	-4	6	11	3.219	1.152	0.69111	2.067	0.000	omit
959	-2	8	11	6.376	4.707	0.69792	1.670	0.000	omit
960	-1	11	7	3.504	8.695	0.69046	-5.191	0.000	omit
961	0	12	5	4.915	7.235	0.69890	-2.320	0.000	omit
962	0	12	4	8.952	16.547	0.68291	-7.595	-7.595	**
963	2	12	3	7.713	6.103	0.70412	1.611	0.000	omit
964	2	12	2	2.575	1.847	0.69297	0.728	0.000	omit
965	2	12	1	27.561	24.244	0.68522	3.316	3.316	*
966	2	10	-8	3.516	1.840	0.68109	1.677	0.000	omit
967	2	12	-4	7.701	7.679	0.69985	0.022	0.000	omit
968	1	11	-7	9.150	8.695	0.69046	0.455	0.455	
969	0	10	-9	6.760	5.539	0.70387	1.221	0.000	omit
970	0	12	-5	2.563	7.235	0.69890	-4.672	0.000	omit
971	2	12	-3	21.989	20.543	0.68987	1.446	1.446	
972	2	12	-2	3.974	1.511	0.68335	2.463	0.000	omit
973	2	12	0	22.905	19.997	0.68100	2.908	2.908	*
974	1	11	4	4.631	3.136	0.64338	1.495	0.000	omit
975	2	12	-1	12.926	10.044	0.68037	2.882	2.882	*

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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976	3	11	-3	8.407	6.751	0.66976	1.655	1.655		
977	2	10	-7	11.094	11.520	0.65603	-0.426	-0.426		
978	1	9	-9	22.509	21.611	0.65829	0.898	0.898		
979	0	8	-10	1.832	0.827	0.65977	1.005	0.000	omit	
980	-1	9	-8	6.847	6.414	0.64789	0.433	0.000	omit	
981	-1	9	-9	15.477	14.152	0.68055	1.325	1.325		
982	0	10	-8	5.287	4.622	0.67357	0.665	0.000	omit	
983	0	10	-7	7.577	6.764	0.64566	0.813	0.813		
984	1	11	-5	13.136	13.236	0.64895	-0.100	-0.100		
985	-1	9	-6	45.910	42.142	0.58967	3.768	3.768	*	
986	-1	9	-7	15.117	13.417	0.61748	1.700	1.700		
987	0	10	-5	4.643	5.865	0.59830	-1.222	0.000	omit	
988	-1	11	-2	2.390	11.596	0.61739	-9.207	0.000	omit	
989	-1	11	2	3.826	15.985	0.61201	-12.159	0.000	omit	
990	-1	11	0	2.872	15.032	0.60667	-12.160	0.000	omit	
991	-1	11	1	1.870	6.374	0.60733	-4.504	0.000	omit	
992	-2	10	-3	0.953	11.155	0.60439	-10.201	0.000	omit	
993	-2	10	-4	1.189	8.088	0.62112	-6.900	0.000	omit	
994	-3	9	-2	1.077	11.564	0.58524	-10.487	0.000	omit	
995	-3	9	0	3.083	29.526	0.56811	-26.444	0.000	omit	
996	-3	9	1	5.522	47.925	0.56590	-42.403	-42.403	!#\$?	
997	0	10	-3	3.033	2.788	0.56452	0.245	0.000	omit	
998	-1	9	-5	26.001	22.983	0.56485	3.018	3.018	*	
999	0	10	-4	8.444	8.024	0.57954	0.420	0.420		
1000	-2	10	-1	0.805	10.298	0.58226	-9.493	0.000	omit	
1001	0	10	3	3.170	2.788	0.56452	0.382	0.000	omit	
1002	-1	11	3	3.628	11.338	0.62062	-7.710	0.000	omit	
1003	-1	11	4	1.114	3.836	0.63301	-2.722	0.000	omit	
1004	-2	10	5	1.931	8.060	0.61488	-6.129	0.000	omit	
1005	-3	9	7	1.585	9.364	0.63896	-7.779	0.000	omit	
1006	-4	6	9	1.832	1.933	0.62665	-0.101	0.000	omit	
1007	-4	8	7	0.879	9.107	0.64065	-8.228	0.000	omit	
1008	-4	8	6	1.498	6.016	0.62060	-4.518	0.000	omit	
1009	-4	8	5	1.052	6.823	0.60395	-5.770	0.000	omit	
1010	-3	9	5	3.368	22.642	0.59940	-19.274	0.000	omit	
1011	-3	9	6	0.854	1.689	0.61751	-0.835	0.000	omit	
1012	-2	10	4	1.052	3.673	0.59941	-2.621	0.000	omit	
1013	-2	10	3	1.337	4.393	0.58773	-3.056	0.000	omit	
1014	-3	9	2	2.204	16.605	0.56801	-14.401	0.000	omit	
1015	-3	9	4	1.857	13.928	0.58494	-12.071	0.000	omit	
1016	-4	8	3	1.090	8.220	0.58200	-7.130	0.000	omit	
1017	-4	6	7	22.175	24.528	0.57218	-2.353	-2.353	*	
1018	-4	6	8	17.185	18.234	0.59798	-1.049	-1.049		
1019	-3	7	8	8.840	8.216	0.58755	0.625	0.625		
1020	-2	8	7	14.672	13.165	0.56886	1.507	1.507		
1021	-1	9	6	25.121	22.268	0.57258	2.854	2.854	*	
1022	-2	8	8	3.355	2.249	0.59758	1.107	0.000	omit	
1023	-4	4	9	3.566	4.077	0.57739	-0.511	0.000	omit	
1024	-4	4	10	14.115	13.595	0.61106	0.519	0.519		
1025	-3	5	10	5.175	4.249	0.59369	0.927	0.000	omit	
1026	-1	9	7	18.857	16.825	0.59842	2.031	2.031	*	



1027	0	10	5	5.076	5.865	0.59830	-0.788	0.000	omit
1028	0	10	4	8.654	8.024	0.57954	0.631	0.631	
1029	1	9	5	26.236	22.983	0.56485	3.253	3.253	*
1030	1	9	6	46.454	42.142	0.58967	4.312	4.312	**
1031	0	8	8	11.143	11.464	0.58900	-0.320	-0.320	
1032	-1	7	9	5.411	4.776	0.58175	0.635	0.000	omit
1033	-2	6	10	18.064	16.589	0.59650	1.475	1.475	
1034	-3	3	11	16.529	14.870	0.59296	1.658	1.658	
1035	-2	8	9	8.184	6.874	0.62891	1.310	1.310	
1036	-3	7	9	5.844	5.669	0.61804	0.175	0.000	omit
1037	0	10	6	11.019	9.753	0.62046	1.266	1.266	
1038	1	11	3	4.073	4.592	0.62857	-0.519	0.000	omit
1039	-1	9	8	1.362	2.341	0.62711	-0.979	0.000	omit
1040	-1	7	10	1.894	2.567	0.61921	-0.673	0.000	omit

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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1041	-2	6	11	12.815	12.728	0.63565	0.087	0.087	
1042	0	8	9	11.217	9.866	0.62342	1.351	1.351	
1043	1	9	7	15.043	13.417	0.61748	1.626	1.626	
1044	2	10	5	7.466	7.646	0.64124	-0.180	0.000	omit
1045	2	10	4	7.354	8.088	0.62112	-0.734	-0.734	
1046	2	10	3	10.995	11.155	0.60439	-0.160	-0.160	
1047	2	10	2	6.092	3.664	0.59136	2.427	0.000	omit
1048	2	10	1	10.611	10.298	0.58226	0.313	0.313	
1049	2	10	-4	3.306	3.673	0.59941	-0.368	0.000	omit
1050	1	7	-9	5.633	4.776	0.58175	0.858	0.000	omit
1051	2	10	-1	6.290	5.746	0.57655	0.544	0.000	omit
1052	2	10	-2	5.658	4.911	0.58005	0.747	0.000	omit
1053	2	10	-3	6.822	4.393	0.58773	2.429	0.000	omit
1054	1	9	-6	23.376	22.268	0.57258	1.108	1.108	
1055	1	9	-7	18.126	16.825	0.59842	1.301	1.301	
1056	0	8	-8	10.883	11.464	0.58900	-0.580	-0.580	
1057	0	8	-9	10.970	9.866	0.62342	1.103	1.103	
1058	1	9	-8	1.176	2.341	0.62711	-1.165	0.000	omit
1059	2	10	-6	3.813	3.666	0.63385	0.147	0.000	omit
1060	2	10	-5	8.692	8.060	0.61488	0.632	0.632	
1061	1	11	-4	3.714	3.836	0.63301	-0.122	0.000	omit
1062	1	11	2	13.780	11.596	0.61739	2.184	2.184	*
1063	1	11	-2	15.613	15.985	0.61201	-0.372	-0.372	
1064	0	10	-6	10.462	9.753	0.62046	0.709	0.709	
1065	1	11	-3	12.654	11.338	0.62062	1.316	1.316	
1066	1	11	0	14.226	15.032	0.60667	-0.806	-0.806	
1067	1	11	-1	7.713	6.374	0.60733	1.340	1.340	
1068	3	11	2	4.309	3.629	0.67907	0.680	0.000	omit
1069	4	10	2	1.548	0.671	0.68289	0.876	0.000	omit
1070	4	10	3	8.890	8.589	0.69659	0.301	0.301	
1071	3	11	3	7.862	7.196	0.69165	0.666	0.000	omit
1072	3	9	7	22.323	20.244	0.69123	2.079	2.079	*
1073	2	10	7	1.362	1.972	0.69045	-0.610	0.000	omit
1074	4	8	6	4.532	3.342	0.68162	1.190	0.000	omit
1075	3	7	9	2.699	1.451	0.68657	1.248	0.000	omit

1076	5	9	2	8.605	7.847	0.70414	0.758	0.758	
1077	5	9	1	3.504	1.847	0.69294	1.657	0.000	omit
1078	5	9	0	28.873	27.335	0.68515	1.538	1.538	
1079	5	9	-1	23.871	23.335	0.68089	0.536	0.536	
1080	4	10	-1	8.778	9.700	0.66265	-0.922	-0.922	
1081	4	10	0	5.683	5.946	0.66579	-0.263	0.000	omit
1082	4	10	1	10.128	9.272	0.67257	0.856	0.856	
1083	3	7	8	6.574	5.835	0.65168	0.739	0.000	omit
1084	3	9	6	26.496	26.398	0.66402	0.098	0.098	
1085	4	8	5	15.452	16.294	0.65649	-0.842	-0.842	
1086	3	11	-1	10.623	10.783	0.66248	-0.160	-0.160	
1087	3	11	0	1.275	1.997	0.66437	-0.721	0.000	omit
1088	3	11	1	10.153	9.351	0.66993	0.802	0.802	
1089	2	10	6	14.152	13.317	0.66446	0.835	0.835	
1090	2	8	8	8.890	7.626	0.64038	1.264	1.264	
1091	1	9	9	16.343	14.152	0.68055	2.191	2.191	*
1092	1	7	11	4.668	4.788	0.68538	-0.121	0.000	omit
1093	0	8	11	10.512	9.434	0.69775	1.077	1.077	
1094	-1	5	13	7.763	7.475	0.69040	0.288	0.000	omit
1095	-4	2	13	1.622	2.232	0.69808	-0.610	0.000	omit
1096	-3	1	14	5.361	5.686	0.70504	-0.325	0.000	omit
1097	-2	0	14	18.708	17.340	0.68662	1.368	1.368	
1098	-2	2	14	7.788	6.417	0.69521	1.371	0.000	omit
1099	-1	1	14	2.130	1.429	0.68563	0.701	0.000	omit
1100	0	4	13	7.057	6.634	0.67994	0.423	0.000	omit
1101	2	6	11	12.963	12.358	0.69058	0.605	0.605	
1102	1	7	10	7.392	6.560	0.64539	0.831	0.000	omit
1103	0	6	12	8.518	7.329	0.67843	1.189	1.189	
1104	-1	5	12	4.457	3.788	0.64571	0.670	0.000	omit
1105	-2	4	13	4.705	4.903	0.67523	-0.199	0.000	omit

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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1106	-3	3	13	8.494	7.560	0.67786	0.933	0.933	
1107	-4	2	12	7.392	7.609	0.65770	-0.218	0.000	omit
1108	-3	1	13	2.390	0.391	0.66013	1.999	0.000	omit
1109	-1	3	13	31.188	26.571	0.65513	4.618	4.618	**
1110	0	2	13	7.070	7.245	0.65324	-0.175	0.000	omit
1111	1	5	12	1.362	3.067	0.67578	-1.705	0.000	omit
1112	2	6	10	1.746	1.297	0.64964	0.449	0.000	omit
1113	0	0	13	14.758	11.656	0.64410	3.102	3.102	*
1114	1	1	13	5.782	5.246	0.66971	0.536	0.000	omit
1115	2	2	12	4.172	5.248	0.66465	-1.075	0.000	omit
1116	2	4	11	3.987	4.321	0.64620	-0.334	0.000	omit
1117	3	5	10	7.540	7.184	0.67216	0.357	0.000	omit
1118	4	6	7	6.711	6.695	0.64815	0.015	0.000	omit
1119	4	4	9	6.537	5.375	0.67274	1.162	0.000	omit
1120	5	3	7	23.512	24.214	0.65888	-0.702	-0.702	
1121	5	1	7	8.815	7.715	0.64062	1.101	1.101	
1122	4	2	9	3.504	2.500	0.64575	1.004	0.000	omit
1123	2	0	12	31.077	27.707	0.65566	3.370	3.370	*
1124	0	0	14	1.560	0.449	0.69364	1.111	0.000	omit



1125	0	2	14	1.870	1.339	0.70214	0.531	0.000	omit
1126	1	3	13	19.278	17.212	0.68720	2.065	2.065	*
1127	2	4	12	4.482	5.280	0.69091	-0.798	0.000	omit
1128	4	6	8	16.492	14.875	0.68084	1.617	1.617	
1129	3	3	11	8.494	7.356	0.67887	1.138	1.138	
1130	4	2	10	3.801	4.653	0.68575	-0.852	0.000	omit
1131	4	0	10	6.314	4.986	0.67704	1.329	0.000	omit
1132	5	1	8	2.080	1.092	0.67490	0.988	0.000	omit
1133	6	0	6	28.303	27.955	0.69138	0.348	0.348	
1134	5	5	7	9.026	8.031	0.69395	0.995	0.995	
1135	6	4	5	9.212	9.234	0.69895	-0.022	-0.022	
1136	5	7	5	5.312	4.423	0.69086	0.888	0.000	omit
1137	6	6	3	9.806	9.160	0.69907	0.646	0.646	
1138	6	6	2	19.377	19.255	0.68301	0.122	0.122	
1139	6	4	4	4.990	5.683	0.67565	-0.693	0.000	omit
1140	7	3	-1	4.296	3.824	0.68321	0.472	0.000	omit
1141	7	3	0	24.292	25.805	0.68986	-1.513	-1.513	
1142	7	3	1	8.828	9.812	0.69997	-0.984	-0.984	
1143	7	1	1	1.610	0.727	0.68281	0.883	0.000	omit
1144	7	1	2	6.834	6.874	0.69655	-0.039	0.000	omit
1145	6	2	6	7.652	8.390	0.69991	-0.739	0.000	omit
1146	6	2	5	8.333	8.479	0.67301	-0.146	-0.146	
1147	6	0	5	21.494	21.172	0.66414	0.322	0.322	
1148	6	2	4	11.601	12.383	0.64878	-0.782	-0.782	
1149	6	4	3	10.078	11.709	0.65528	-1.630	-1.630	
1150	7	1	0	10.140	9.870	0.67245	0.270	0.270	
1151	7	1	-1	3.652	3.884	0.66562	-0.231	0.000	omit
1152	6	6	-1	15.303	14.084	0.65523	1.219	1.219	
1153	6	6	0	6.834	7.998	0.66092	-1.164	0.000	omit
1154	6	6	1	18.609	20.054	0.67022	-1.445	-1.445	
1155	5	7	3	6.030	6.416	0.64919	-0.386	0.000	omit
1156	2	6	8	20.627	20.773	0.57187	-0.146	-0.146	
1157	3	7	6	11.180	10.296	0.58823	0.884	0.884	
1158	4	6	4	26.880	25.361	0.56500	1.518	1.518	
1159	4	8	1	10.635	8.660	0.58786	1.975	1.975	
1160	4	8	0	8.766	9.216	0.58009	-0.451	-0.451	
1161	4	8	-1	3.256	2.454	0.57648	0.802	0.000	omit
1162	3	9	-1	52.212	47.925	0.56590	4.286	4.286	**
1163	3	9	0	29.207	29.526	0.56811	-0.319	-0.319	
1164	3	9	1	6.574	7.610	0.57460	-1.035	0.000	omit
1165	3	9	2	13.161	11.564	0.58524	1.597	1.597	
1166	2	8	6	14.337	13.558	0.57856	0.780	0.780	
1167	1	7	8	6.624	6.128	0.56996	0.496	0.000	omit
1168	4	8	2	6.946	8.319	0.59964	-1.373	0.000	omit
1169	4	8	3	10.747	11.001	0.61519	-0.254	-0.254	
1170	4	8	4	1.857	1.032	0.63425	0.825	0.000	omit

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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1171	4	6	5	46.950	46.313	0.58986	0.636	0.636	
1172	3	5	8	1.387	0.735	0.59456	0.651	0.000	omit
1173	3	5	9	6.401	5.224	0.63261	1.177	0.000	omit

1174	3	9	3	33.244	33.697	0.59979	-0.454	-0.454	
1175	3	9	4	10.995	9.007	0.61798	1.987	1.987	
1176	3	9	5	13.471	12.453	0.63949	1.018	1.018	
1177	2	8	7	1.164	0.206	0.60824	0.958	0.000	omit
1178	3	7	7	4.073	4.502	0.61878	-0.428	0.000	omit
1179	2	6	9	5.547	7.751	0.60999	-2.204	0.000	omit
1180	1	5	10	6.141	5.218	0.58767	0.923	0.000	omit
1181	2	4	10	7.379	7.005	0.60226	0.374	0.374	
1182	1	3	11	15.712	13.115	0.59254	2.597	2.597	*
1183	0	4	11	16.950	15.924	0.58693	1.026	1.026	
1184	-1	1	12	5.014	4.797	0.58801	0.217	0.000	omit
1185	-2	0	12	15.538	12.775	0.59197	2.763	2.763	*
1186	-3	1	11	3.628	2.280	0.57260	1.348	0.000	omit
1187	-2	2	12	16.108	14.865	0.60191	1.242	1.242	
1188	-2	4	11	9.261	7.656	0.58714	1.605	1.605	
1189	-1	3	11	8.494	6.772	0.56096	1.722	1.722	
1190	-1	5	11	9.174	8.312	0.60178	0.863	0.863	
1191	0	6	10	16.715	14.123	0.59351	2.592	2.592	*
1192	1	7	9	2.315	1.210	0.60683	1.105	0.000	omit
1193	0	6	11	30.284	27.201	0.63546	3.083	3.083	*
1194	-1	3	12	24.738	23.724	0.60785	1.014	1.014	
1195	-2	4	12	6.847	7.290	0.63078	-0.444	0.000	omit
1196	-3	3	12	29.888	28.436	0.63489	1.453	1.453	
1197	-3	1	12	7.577	7.815	0.61593	-0.237	-0.237	
1198	-2	0	13	4.593	2.188	0.63913	2.405	0.000	omit
1199	-1	1	13	6.513	7.480	0.63677	-0.968	0.000	omit
1200	0	2	12	1.325	0.138	0.60445	1.187	0.000	omit
1201	0	4	12	7.491	5.331	0.63320	2.159	0.000	omit
1202	1	3	12	4.606	2.017	0.63970	2.588	0.000	omit
1203	1	5	11	6.178	5.900	0.63131	0.278	0.000	omit
1204	0	0	12	19.822	16.890	0.59455	2.932	2.932	*
1205	1	1	11	8.234	8.040	0.57217	0.194	0.194	
1206	2	2	10	15.155	13.586	0.57195	1.568	1.568	
1207	3	3	9	16.838	15.695	0.59392	1.143	1.143	
1208	4	4	7	14.276	13.954	0.60065	0.322	0.322	
1209	4	4	6	6.401	5.048	0.56767	1.353	0.000	omit
1210	5	3	5	19.092	19.538	0.59887	-0.446	-0.446	
1211	5	1	5	12.765	12.271	0.57872	0.494	0.494	
1212	4	2	7	4.333	4.334	0.57025	0.000	0.000	omit
1213	4	0	8	18.238	17.124	0.59730	1.114	1.114	
1214	3	1	9	7.491	6.131	0.57360	1.360	1.360	
1215	2	0	10	8.258	6.420	0.56148	1.838	1.838	
1216	2	0	11	24.837	23.646	0.60838	1.191	1.191	
1217	1	1	12	2.823	4.796	0.62088	-1.973	0.000	omit
1218	2	2	11	13.186	11.699	0.61805	1.487	1.487	
1219	3	3	10	30.198	28.865	0.63589	1.333	1.333	
1220	4	4	8	7.751	7.875	0.63579	-0.124	-0.124	
1221	4	6	6	15.464	15.236	0.61771	0.228	0.228	
1222	3	1	10	8.853	9.276	0.61695	-0.423	-0.423	
1223	4	0	9	12.852	13.617	0.63649	-0.765	-0.765	
1224	4	2	8	3.925	4.876	0.60715	-0.951	0.000	omit
1225	5	1	6	1.845	2.485	0.60844	-0.640	0.000	omit



1226	6	0	4	12.171	10.636	0.63957	1.535	1.535	
1227	5	3	6	1.647	1.236	0.62764	0.411	0.000	omit
1228	5	7	0	6.797	6.491	0.61198	0.306	0.000	omit
1229	5	7	1	13.161	12.885	0.62069	0.277	0.277	
1230	5	7	2	1.981	1.554	0.63317	0.427	0.000	omit
1231	5	5	4	6.859	6.766	0.61297	0.093	0.000	omit
1232	5	5	5	11.230	11.377	0.63726	-0.147	-0.147	
1233	6	4	2	10.499	11.166	0.63811	-0.667	-0.667	
1234	6	2	3	1.944	1.826	0.62753	0.117	0.000	omit
1235	6	0	3	5.089	3.329	0.61801	1.759	0.000	omit

No.	h	k	l	Fo	Fc	siné/l	Fo-Fc	w(Fo-Fc)	Flag
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1236	6	2	2	10.128	10.021	0.60958	0.107	0.107	
1237	6	4	1	8.333	8.434	0.62440	-0.102	-0.102	
1238	6	4	0	18.696	19.974	0.61440	-1.278	-1.278	
1239	6	4	-1	2.229	2.752	0.60829	-0.523	0.000	omit
1240	6	2	1	1.721	0.387	0.59522	1.334	0.000	omit
1241	5	7	-1	11.242	12.632	0.60721	-1.390	-1.390	
1242	5	5	1	8.914	7.516	0.56042	1.399	1.399	
1243	5	5	2	6.178	5.717	0.57421	0.461	0.000	omit
1244	5	5	3	9.100	9.569	0.59183	-0.468	-0.468	
1245	5	3	4	25.035	25.972	0.57295	-0.937	-0.937	
1246	6	2	0	9.744	8.354	0.58472	1.390	1.390	
1247	6	2	-1	2.352	2.056	0.57829	0.296	0.000	omit
1248	6	0	-1	21.308	20.289	0.56794	1.019	1.019	
1249	6	0	0	3.331	3.464	0.57449	-0.133	0.000	omit
1250	6	0	1	16.331	16.006	0.58517	0.325	0.325	
1251	6	0	2	26.186	25.158	0.59977	1.028	1.028	
1252	6	6	-5	18.931	20.668	0.66971	-1.737	-1.737	
1253	5	7	-7	5.200	6.972	0.66095	-1.772	0.000	omit
1254	5	7	-6	13.025	13.308	0.64283	-0.283	-0.283	
1255	6	6	-2	48.336	49.233	0.65327	-0.896	-0.896	
1256	6	6	-3	14.697	13.486	0.65506	1.211	1.211	
1257	6	6	-4	6.698	7.914	0.66057	-1.215	0.000	omit
1258	6	2	-8	12.530	13.838	0.64772	-1.308	-1.308	
1259	6	4	-8	3.306	3.247	0.67463	0.059	0.000	omit
1260	6	4	-7	5.695	6.831	0.65440	-1.136	0.000	omit
1261	7	1	-4	9.756	10.810	0.66716	-1.054	-1.054	
1262	7	1	-3	5.807	5.981	0.66295	-0.174	0.000	omit
1263	7	1	-2	9.496	11.034	0.66244	-1.537	-1.537	
1264	7	3	-2	14.053	13.453	0.68011	0.599	0.599	
1265	7	3	-3	25.060	26.516	0.68061	-1.456	-1.456	
1266	7	3	-4	29.752	30.285	0.68471	-0.533	-0.533	
1267	7	1	-5	8.518	8.365	0.67499	0.153	0.153	
1268	7	1	-6	4.680	4.051	0.68631	0.629	0.000	omit
1269	7	1	-7	7.850	9.209	0.70096	-1.359	0.000	omit
1270	7	3	-6	8.890	9.383	0.70338	-0.493	-0.493	
1271	7	3	-5	3.194	2.677	0.69234	0.518	0.000	omit
1272	6	6	-6	19.439	19.309	0.68234	0.130	0.130	
1273	5	7	-8	7.491	7.890	0.68221	-0.400	0.000	omit
1274	6	6	-7	10.004	9.388	0.69825	0.616	0.616	

1275	6	4	-9	3.640	3.283	0.69780	0.357	0.000	omit
1276	6	0	-9	28.786	29.818	0.66293	-1.032	-1.032	
1277	6	2	-9	11.193	10.827	0.67182	0.366	0.366	
1278	5	3	-10	7.392	7.099	0.64698	0.292	0.000	omit

LSFM (1.4)      06/10/97      10:17:20      Elapsed time =    0.0 min

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

The space group is number    12    --    C12/m1

After refinement cycle no. 2.    852 observations.    73 variables.

Esd of an observation of unit weight =    3.401

Unweighted R factor =    0.069    Weighted R factor =    0.096

$\bar{a}^3 Fo^3 =$             2.20425E+04

$\bar{a}^3 Fo^3 - \bar{a}^3 Fc^3 =$     1.52314E+03

$\bar{a} W \cdot DEL \bar{y} =$             9.00818E+03

$\bar{a} W \cdot Fo \bar{y} =$             9.71742E+05

Largest parameter shift/error =    0.04

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	3.371	0.069	0.096	0.64	0.08
2	3.401	0.069	0.096	0.04	0.01
3	0.000	0.000	0.000	0.00	0.00
4	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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