

TITLE RANCOURT BIOTITE HEAT TREATED (RANO) IN C2/M  
 CELL 0.71073 5.3099 9.185 10.093 90.00 100.069 90.00  
 ZERR 1.00 0.0005 0.001 0.002 0.00 0.01 0.00  
 LATT 7  
 SYMM -X, Y, -Z  
 SFAC A1 7.061625 0.797640 7.172649 11.666479 0.556002 200.176666 =  
 1.668019 27.350302 1.416414 0.167 0.232 978.7 2.27  
 SFAC M1 8.283765 4.405341 2.261523 13.374294 3.813178 0.537183 =  
 1.132520 80.185349 1.721814 0.159 0.392 1627.6 1.60  
 SFAC M2 8.283765 4.405341 2.261523 13.374294 3.813178 0.537183 =  
 1.132520 80.185349 1.721814 0.159 0.392 1627.6 1.60  
 SFAC T1 5.040259 3.147538 0.858992 80.787247 3.329262 1.128188 =  
 1.344917 31.146509 1.297733 0.068 0.066 284.6 1.17  
 SFAC O-1 4.191600 12.857300 1.639690 4.172360 1.526730 47.017900 =  
 -20.307000 -0.014040 21.941200 0.008 0.006 30.48 0.66  
 SFAC OH,F 4.321104 11.077127 1.914772 3.651860 1.403507 39.875435 =  
 -20.567442 -0.012152 22.198444 0.011 0.008 41.2 0.66  
 UNIT 2.0 2.0 4.0 8.0 22.0 4.0  
 L.S. 4  
 LIST 7,1  
 FVAR 1.41725  
 A 1 10.00000 10.50000 10.00000 10.25000 0.03008 0.02822 =  
 0.03776 10.00000 0.00638 10.00000  
 M1 2 10.00000 10.00000 10.50000 10.25000 0.01377 0.01307 =  
 0.02727 10.00000 0.00566 10.00000  
 M2 3 10.00000 0.34201 10.50000 10.50000 0.00806 0.01301 =  
 0.02127 10.00000 0.00212 10.00000  
 T 4 0.07339 0.16734 0.22325 11.00000 0.00765 0.00727 =  
 0.01736 0.00002 0.00249 -0.00005  
 O1 5 0.03124 10.00000 0.16625 10.50000 0.02636 0.00993 =  
 0.02226 10.00000 0.00332 10.00000  
 O2 5 0.31560 0.23796 0.16434 11.00000 0.01638 0.02438 =  
 0.02471 -0.00156 0.00493 -0.00491  
 O3 5 0.12920 0.16943 0.38929 11.00000 0.00914 0.01146 =  
 0.01649 0.00079 0.00224 0.00076  
 OH 6 0.13545 10.50000 0.40021 10.50000 0.01299 0.01256 =  
 0.02189 10.00000 0.00396 10.00000

END *h k l F<sub>0</sub> σ(F<sub>0</sub>) F<sub>c</sub> 8(πsinθ/λ)<sup>2</sup>*  
 DATA GENERATED BY LIST 7 INSTRUCTION

2	0	0	143.77	0.28	136.00	2.89	x
4	0	0	23.14	0.12	22.97	11.55	
6	0	0	20.35	0.21	20.42	26.00	
1	1	0	29.97	0.46	30.27	0.96	
5	1	0	25.19	0.16	25.17	18.29	
7	1	0	19.47	0.68	20.84	35.62	
0	2	0	41.56	0.05	35.05	0.94	—
2	2	0	49.52	1.18	49.38	3.82	
4	2	0	29.52	0.70	29.36	12.49	
6	2	0	18.34	0.45	18.35	26.93	
1	3	0	40.40	0.75	32.44	2.83	—
3	3	0	73.33	2.00	71.20	8.61	
5	3	0	76.19	1.27	76.34	20.16	
7	3	0	33.32	0.54	34.60	37.49	
0	4	0	45.81	0.07	42.96	3.74	
2	4	0	17.74	0.33	15.70	6.63	
4	4	0	13.00	0.27	13.39	15.30	
6	4	0	23.97	0.68	25.02	29.74	
1	5	0	33.91	0.09	33.64	6.57	
3	5	0	15.09	0.54	15.96	12.35	
5	5	0	16.61	1.08	17.41	23.90	

After Anisot.

Heat-treated Fe-rich  
 phlogopite data

standard  
 deviations  
 at end.

Russell & Guggenheim

0	6	0	179.85	0.09	168.35	8.42
2	6	0	118.42	2.37	117.08	11.31
4	6	0	15.56	0.24	16.37	19.98
1	7	0	11.75	0.52	12.46	12.19
3	7	0	11.43	0.46	11.88	17.96
5	7	0	16.60	0.68	17.48	29.52
0	8	0	17.23	0.24	18.15	14.97
2	8	0	5.32	0.88	5.29	17.86
4	8	0	23.83	0.82	24.57	26.53
1	9	0	23.90	0.15	24.02	19.67
3	9	0	40.02	1.05	40.39	25.45
5	9	0	39.81	1.27	41.69	37.01
0	10	0	17.39	0.26	16.17	23.40
1	11	0	28.30	0.26	29.66	29.03
3	11	0	6.16	0.92	5.22	34.81
0	12	0	81.14	0.15	79.39	33.69
2	12	0	38.64	0.21	40.95	36.58
-6	0	1	31.52	0.20	31.92	25.40
-4	0	1	62.49	0.46	58.46	11.22
-2	0	1	39.44	0.13	30.91	2.82
2	0	1	135.06	0.09	128.11	3.35
4	0	1	85.98	0.64	82.80	12.29
6	0	1	27.77	0.44	28.32	27.00
-5	1	1	13.28	0.39	13.26	17.82
-3	1	1	31.22	0.28	27.76	6.53
-1	1	1	23.13	0.21	19.96	1.02
1	1	1	30.13	0.33	31.75	1.29
3	1	1	46.63	0.48	45.62	7.33
5	1	1	26.01	0.50	26.01	19.15
-6	2	1	6.86	0.42	7.10	26.34
-4	2	1	21.73	0.38	22.17	12.16
-2	2	1	45.24	0.85	41.94	3.76
0	2	1	3.50	0.44	1.53	1.14
2	2	1	38.10	0.89	35.95	4.29
4	2	1	51.44	0.69	50.97	13.22
-5	3	1	63.74	1.25	63.71	19.70
-3	3	1	174.55	5.15	170.55	8.41
-1	3	1	138.88	1.23	134.82	2.89
1	3	1	9.63	0.12	2.98	3.16
3	3	1	32.37	0.94	32.72	9.20
5	3	1	34.51	0.78	34.96	21.02
7	3	1	19.39	0.49	20.25	38.62
-6	4	1	8.53	0.49	8.62	29.14
-4	4	1	16.65	0.24	16.95	14.97
-2	4	1	14.89	0.13	13.86	6.57
0	4	1	46.78	0.05	50.75	3.94
2	4	1	58.28	1.10	55.74	7.10
4	4	1	27.48	0.80	27.09	16.03
6	4	1	22.28	0.47	22.61	30.74
-3	5	1	18.33	0.16	18.15	12.15
-1	5	1	8.53	0.24	6.83	6.64
1	5	1	45.42	0.35	44.21	6.90
3	5	1	42.07	1.13	42.82	12.95
5	5	1	26.25	0.70	27.45	24.77
-6	6	1	20.91	1.04	21.51	33.82
-4	6	1	21.70	0.79	22.19	19.65
-2	6	1	63.46	0.82	60.60	11.25
0	6	1	59.02	0.55	68.46	8.62
2	6	1	98.07	1.80	95.46	11.78
4	6	1	40.97	1.29	41.36	20.71

6	6	1	34.42	1.02	35.75	35.42
-5	7	1	18.58	0.27	20.05	29.05
-3	7	1	21.59	0.42	21.96	17.77
-1	7	1	14.51	0.33	14.32	12.25
1	7	1	5.88	0.63	5.56	12.52
3	7	1	26.41	0.53	27.36	18.56
5	7	1	14.24	0.24	15.02	30.38
-4	8	1	8.11	0.54	7.94	26.20
-2	8	1	27.59	0.13	27.36	17.80
0	8	1	5.34	0.43	5.68	15.17
2	8	1	19.48	0.17	19.76	18.33
4	8	1	8.24	0.37	8.86	27.26
-5	9	1	40.89	1.36	42.47	36.54
-3	9	1	82.46	1.17	84.62	25.25
-1	9	1	57.91	0.54	57.80	19.74
1	9	1	13.58	0.39	13.21	20.01
5	9	1	15.03	1.08	16.51	37.87
-2	10	1	11.27	0.44	12.35	26.22
0	10	1	8.44	0.80	10.25	23.60
2	10	1	23.89	0.21	24.63	26.75
4	10	1	27.60	0.94	29.02	35.68
-1	11	1	6.40	0.67	5.33	29.10
1	11	1	17.25	0.20	15.58	29.37
3	11	1	30.82	0.21	31.69	35.41
-2	12	1	18.08	0.24	19.62	36.52
0	12	1	15.54	0.23	17.38	33.89
2	12	1	38.34	0.55	39.56	37.05
-6	0	2	88.00	0.53	89.13	25.20
-4	0	2	121.82	0.83	118.35	11.29
-2	0	2	10.08	0.10	3.48	3.16
0	0	2	12.09	0.45	22.04	0.80
2	0	2	123.69	0.36	119.58	4.22
4	0	2	22.85	0.19	22.80	13.42
6	0	2	43.22	0.12	43.06	28.39
-7	1	2	8.33	0.74	9.40	34.56
-5	1	2	9.11	0.28	9.20	17.76
-3	1	2	16.18	0.26	14.54	6.74
-1	1	2	67.50	0.30	65.40	1.49
1	1	2	93.11	0.94	91.53	2.02
3	1	2	44.05	0.51	42.45	8.33
5	1	2	6.65	0.70	6.41	20.42
-4	2	2	16.15	0.34	15.66	12.23
-2	2	2	46.76	0.81	47.42	4.09
0	2	2	76.81	0.67	86.87	1.74
4	2	2	17.72	0.31	18.28	14.35
6	2	2	10.15	0.28	10.23	29.33
-7	3	2	14.16	0.27	14.45	36.43
-5	3	2	20.48	0.23	19.84	19.63
-3	3	2	74.48	1.77	72.96	8.61
-1	3	2	130.03	0.64	126.23	3.36
1	3	2	59.03	0.87	59.72	3.89
3	3	2	46.22	1.26	45.45	10.20
5	3	2	23.99	0.47	24.46	22.29
-6	4	2	18.67	0.33	20.38	28.95
-4	4	2	7.17	0.34	7.44	15.04
-2	4	2	4.44	0.61	5.24	6.90
0	4	2	18.69	0.21	22.26	4.54
2	4	2	48.22	1.15	48.06	7.96
4	4	2	16.52	0.77	16.73	17.16
6	4	2	10.38	0.56	12.05	32.14

-5	5	2	15.34	0.44	16.67	23.37
-3	5	2	4.23	0.61	4.21	12.35
-1	5	2	27.90	0.22	25.57	7.11
1	5	2	56.99	0.34	53.71	7.64
3	5	2	23.79	0.60	24.30	13.95
-6	6	2	79.19	2.47	83.98	33.63
-4	6	2	59.78	1.80	60.29	19.71
-2	6	2	16.51	0.18	17.14	11.58
0	6	2	26.58	0.09	28.21	9.22
2	6	2	23.90	0.33	23.89	12.64
4	6	2	34.67	0.82	34.93	21.84
6	6	2	29.44	0.81	29.91	36.81
-3	7	2	8.95	0.33	7.63	17.97
-1	7	2	51.69	0.38	50.03	12.72
1	7	2	52.48	0.48	50.92	13.25
3	7	2	29.38	0.78	29.96	19.56
5	7	2	12.08	0.26	12.31	31.65
-4	8	2	11.94	0.28	12.30	26.27
-2	8	2	24.62	0.27	24.63	18.13
0	8	2	35.35	0.16	37.26	15.77
2	8	2	40.18	0.95	40.14	19.19
-5	9	2	15.78	0.38	16.24	36.48
-3	9	2	27.91	0.35	27.60	25.45
-1	9	2	73.69	0.83	71.61	20.21
1	9	2	39.69	0.26	37.86	20.74
3	9	2	23.87	0.55	23.85	27.05
5	9	2	18.70	0.38	18.65	39.13
-4	10	2	11.58	0.30	12.40	34.69
0	10	2	15.52	0.47	17.05	24.20
-3	11	2	8.31	0.43	8.91	34.81
-1	11	2	15.89	0.22	16.59	29.57
1	11	2	11.60	0.43	12.74	30.10
0	12	2	5.09	0.58	3.43	34.49
2	12	2	13.26	0.31	13.13	37.91
-6	0	3	46.21	0.18	47.31	25.41
-4	0	3	104.33	0.55	101.46	11.76
-2	0	3	59.91	0.20	60.53	3.89
0	0	3	118.31	2.74	139.20	1.80x
2	0	3	65.56	0.20	64.47	5.48
6	0	3	8.77	0.34	9.29	30.19
-7	1	3	5.36	0.57	4.57	34.63
-5	1	3	15.44	0.22	15.75	18.09
-3	1	3	59.40	0.48	58.45	7.34
-1	1	3	73.88	0.11	76.99	2.36
1	1	3	34.19	0.30	36.21	3.15
5	1	3	9.40	0.42	9.37	22.08
-6	2	3	9.75	0.33	10.37	26.34
-4	2	3	20.72	0.20	20.32	12.70
-2	2	3	12.84	0.27	13.21	4.83
0	2	3	52.46	0.61	55.38	2.73
2	2	3	35.20	0.61	35.18	6.42
4	2	3	16.28	0.16	16.41	15.88
-7	3	3	43.20	0.51	43.95	36.50
-5	3	3	16.11	0.18	15.75	19.97
-3	3	3	30.79	0.70	31.14	9.21
-1	3	3	120.70	0.47	119.38	4.23
1	3	3	86.47	1.01	87.46	5.03
3	3	3	80.10	1.66	78.16	11.60
5	3	3	90.21	1.49	89.99	23.95
-4	4	3	29.03	0.98	28.58	15.50

-2	4	3	62.64	0.76	61.45	7.63
0	4	3	7.96	0.38	6.18	5.54
2	4	3	12.94	0.17	12.06	9.23
4	4	3	6.46	0.41	6.99	18.69
6	4	3	6.97	0.51	7.07	33.93
-5	5	3	18.55	0.29	19.11	23.71
-3	5	3	59.08	1.01	60.53	12.95
-1	5	3	60.55	0.38	59.94	7.97
1	5	3	31.77	0.08	32.01	8.77
3	5	3	13.28	0.50	12.46	15.34
-6	6	3	23.16	1.08	23.90	33.83
-4	6	3	74.97	2.48	75.77	20.18
-2	6	3	81.25	0.72	79.50	12.31
0	6	3	41.17	0.27	42.48	10.22
2	6	3	61.56	1.25	59.83	13.91
4	6	3	5.03	0.56	2.70	23.37
6	6	3	16.94	0.66	18.20	38.61
-5	7	3	7.39	0.44	8.89	29.33
-3	7	3	20.44	0.42	21.44	18.57
-1	7	3	38.32	0.61	38.13	13.59
1	7	3	12.17	0.21	12.15	14.38
3	7	3	15.49	0.70	15.35	20.96
5	7	3	7.36	0.81	7.29	33.31
-4	8	3	9.46	0.41	9.54	26.73
-2	8	3	20.78	0.36	20.96	18.86
0	8	3	11.34	0.21	11.07	16.77
2	8	3	8.31	0.49	8.91	20.46
4	8	3	18.10	0.78	18.75	29.92
-3	9	3	15.45	0.32	15.22	26.05
-1	9	3	32.59	0.45	31.49	21.07
1	9	3	34.96	0.14	33.84	21.87
3	9	3	50.95	1.33	51.23	28.45
-4	10	3	15.49	1.02	16.74	35.16
-2	10	3	22.21	0.17	22.40	27.29
0	10	3	21.87	0.19	22.91	25.20
-3	11	3	25.99	0.16	27.14	35.41
-1	11	3	37.09	0.59	35.84	30.43
1	11	3	23.71	0.48	22.48	31.23
-2	12	3	29.09	0.15	30.41	37.58
0	12	3	28.74	0.14	30.54	35.49
2	12	3	16.29	0.32	16.38	39.18
-6	0	4	7.21	0.44	6.08	26.01
-4	0	4	27.77	0.11	28.19	12.63
-2	0	4	89.17	0.22	89.89	5.02
0	0	4	53.41	1.02	63.05	3.20
2	0	4	152.91	0.70	151.95	7.15
4	0	4	104.67	0.75	102.68	16.88
-7	1	4	18.17	0.51	19.88	35.10
-5	1	4	37.63	0.10	37.78	18.83
-3	1	4	43.10	0.32	42.12	8.34
-1	1	4	22.88	0.08	22.04	3.62
3	1	4	3.60	0.58	1.52	11.53
5	1	4	5.70	0.49	5.98	24.14
-6	2	4	19.28	0.21	19.47	26.94
-4	2	4	40.12	0.44	40.90	13.56
-2	2	4	25.76	0.22	23.11	5.96
0	2	4	10.66	0.20	11.99	4.13
2	2	4	3.97	0.43	1.40	8.09
4	2	4	12.07	0.81	11.04	17.81
6	2	4	19.72	0.22	19.65	33.32

-7	3	4	44.42	0.14	46.48	36.97
-5	3	4	42.08	0.64	41.71	20.70
-3	3	4	43.68	0.88	42.55	10.21
-1	3	4	63.09	0.10	62.65	5.49
1	3	4	15.85	0.12	12.63	6.56
3	3	4	29.09	0.67	27.96	13.40
5	3	4	26.68	0.60	25.84	26.02
-6	4	4	13.58	0.23	13.74	29.75
-4	4	4	5.80	0.81	5.40	16.37
-2	4	4	18.13	0.15	18.20	8.77
0	4	4	36.21	0.06	36.92	6.94
2	4	4	21.33	0.26	20.07	10.89
-5	5	4	19.66	0.47	21.56	24.44
-3	5	4	23.52	0.26	23.94	13.95
-1	5	4	5.81	0.35	5.15	9.24
1	5	4	22.32	0.55	22.21	10.30
3	5	4	11.54	0.40	10.71	17.14
-4	6	4	34.08	1.26	34.17	21.05
-2	6	4	22.82	0.13	22.38	13.45
0	6	4	76.55	0.13	76.55	11.62
2	6	4	114.25	1.94	111.24	15.57
4	6	4	57.52	1.37	58.41	25.30
-5	7	4	34.51	1.17	36.21	30.06
-3	7	4	28.30	0.53	29.39	19.57
-1	7	4	8.86	0.26	8.29	14.85
1	7	4	10.04	0.32	9.39	15.92
5	7	4	6.39	0.87	6.93	35.37
-4	8	4	17.04	0.44	16.33	27.60
-2	8	4	22.24	0.14	21.59	20.00
0	8	4	6.80	0.55	6.04	18.17
2	8	4	5.65	0.92	4.38	22.12
4	8	4	9.67	0.34	8.95	31.85
-5	9	4	29.97	1.09	31.04	37.55
-3	9	4	21.90	0.21	21.94	27.06
-1	9	4	19.35	0.33	17.40	22.34
1	9	4	5.27	0.52	5.17	23.40
3	9	4	22.81	0.54	23.57	30.24
-4	10	4	10.50	0.31	10.38	36.02
-2	10	4	11.63	0.28	12.30	28.42
0	10	4	13.40	0.31	14.09	26.60
2	10	4	12.97	0.85	12.72	30.55
-1	11	4	10.57	0.36	9.39	31.70
1	11	4	12.52	0.24	10.77	32.76
-2	12	4	15.97	0.62	16.40	38.72
0	12	4	26.74	0.41	27.09	36.89
-6	0	5	25.47	0.23	24.91	27.01
-4	0	5	61.43	0.15	60.63	13.89
-2	0	5	16.37	0.11	12.59	6.56
0	0	5	75.87	1.14	75.57	5.00
2	0	5	54.14	0.47	53.24	9.21
4	0	5	69.36	0.54	68.17	19.21
6	0	5	41.51	0.33	42.39	34.98
-7	1	5	15.87	0.61	15.83	35.97
-5	1	5	8.03	0.72	7.36	19.96
-3	1	5	11.19	0.18	10.23	9.74
-1	1	5	12.10	0.10	10.57	5.29
1	1	5	11.66	0.24	9.75	6.62
3	1	5	8.00	0.49	8.47	13.72
5	1	5	18.39	0.36	18.26	26.61
-4	2	5	11.32	0.20	10.10	14.83

-2	2	5	19.61	0.10	21.05	7.49
0	2	5	12.74	0.13	12.61	5.93
2	2	5	38.20	0.53	37.10	10.15
4	2	5	19.34	0.16	19.51	20.14
6	2	5	23.08	0.33	23.74	35.92
-7	3	5	19.50	0.37	20.39	37.84
-5	3	5	38.21	0.70	38.12	21.84
-3	3	5	79.49	1.48	77.93	11.61
-1	3	5	144.23	0.75	147.51	7.16
1	3	5	113.94	1.92	120.41	8.49
3	3	5	6.08	0.82	6.49	15.60
5	3	5	15.01	0.52	15.99	28.48
-6	4	5	21.05	0.42	21.77	30.75
-4	4	5	11.48	0.62	11.03	17.64
-2	4	5	6.60	0.29	5.49	10.30
0	4	5	22.10	0.09	21.40	8.74
2	4	5	6.86	0.48	7.44	12.96
4	4	5	41.02	1.11	40.63	22.95
6	4	5	22.34	0.17	22.85	38.72
-5	5	5	11.98	0.51	11.75	25.58
-3	5	5	5.15	0.73	3.45	15.35
3	5	5	14.79	0.43	15.12	19.34
5	5	5	24.79	0.74	24.19	32.22
-6	6	5	31.66	0.68	32.78	35.43
-4	6	5	19.80	0.29	19.75	22.32
-2	6	5	4.34	0.56	3.23	14.98
0	6	5	31.20	0.09	30.80	13.42
2	6	5	12.86	0.24	11.38	17.64
4	6	5	67.69	2.02	67.23	27.63
-3	7	5	10.90	0.55	10.95	20.97
-1	7	5	25.48	0.42	24.64	16.52
1	7	5	8.79	1.19	7.53	17.85
5	7	5	5.63	0.84	4.91	37.84
-4	8	5	15.22	0.71	15.99	28.87
-2	8	5	15.75	0.21	15.49	21.53
0	8	5	11.55	0.24	10.19	19.97
2	8	5	6.40	0.67	4.90	24.19
4	8	5	20.60	0.69	21.55	34.18
-5	9	5	18.14	0.41	19.55	38.68
-3	9	5	39.07	0.66	39.05	28.46
-1	9	5	86.36	1.19	83.95	24.01
1	9	5	53.65	0.62	53.99	25.34
-4	10	5	7.73	0.39	6.25	37.29
0	10	5	5.29	0.85	4.53	28.39
2	10	5	19.10	0.65	19.10	32.61
-3	11	5	6.40	0.54	5.93	37.81
-1	11	5	7.09	0.69	6.80	33.37
1	11	5	6.08	0.49	4.91	34.69
0	12	5	20.55	0.27	21.36	38.69
-6	0	6	54.53	0.25	54.55	28.41
-4	0	6	115.11	0.57	112.54	15.56
-2	0	6	117.62	0.11	120.71	8.49
0	0	6	54.63	0.60	58.29	7.20
2	0	6	17.01	0.13	17.49	11.68
4	0	6	35.14	0.26	33.78	21.94
6	0	6	42.84	0.32	43.09	37.98
-5	1	6	9.96	0.27	10.11	21.50
-3	1	6	11.67	0.22	11.32	11.54
-1	1	6	3.22	0.48	4.09	7.35
1	1	6	25.34	0.53	28.03	8.95

3	1	6	29.94	0.36	29.69	16.32
5	1	6	10.16	0.35	9.69	29.47
-6	2	6	11.37	0.40	11.94	29.35
-2	2	6	28.92	0.20	29.60	9.43
0	2	6	14.74	0.19	17.27	8.13
2	2	6	62.08	1.28	62.72	12.61
4	2	6	25.18	0.34	24.74	22.87
6	2	6	5.26	0.61	5.19	38.91
-7	3	6	19.95	0.26	20.04	39.11
-3	3	6	28.02	0.61	27.01	13.41
-1	3	6	51.28	0.48	53.58	9.23
1	3	6	111.92	2.98	125.94	10.82
3	3	6	68.40	1.51	68.34	18.19
5	3	6	16.31	0.59	16.02	31.34
-4	4	6	11.53	0.22	10.91	19.31
-2	4	6	6.07	0.33	5.02	12.23
0	4	6	43.29	0.21	43.93	10.94
2	4	6	23.44	0.50	24.00	15.42
4	4	6	18.38	0.46	17.91	25.68
-5	5	6	13.11	0.46	13.40	27.11
-3	5	6	24.56	0.41	24.30	17.15
-1	5	6	4.30	0.68	3.28	12.97
1	5	6	18.00	0.67	19.02	14.56
3	5	6	15.07	0.48	15.50	21.94
-6	6	6	30.47	0.64	30.53	36.83
-4	6	6	86.69	2.12	86.35	23.99
-2	6	6	99.08	0.42	97.55	16.91
4	6	6	24.31	0.72	23.22	30.36
-5	7	6	7.41	0.41	7.48	32.73
-1	7	6	5.47	0.44	5.62	18.59
1	7	6	19.11	0.56	20.39	20.18
3	7	6	29.60	0.82	29.47	27.55
-2	8	6	6.25	0.46	6.89	23.46
0	8	6	40.28	0.30	39.75	22.17
2	8	6	32.99	0.64	32.63	26.65
4	8	6	22.40	0.35	21.42	36.91
-3	9	6	11.15	0.28	11.07	30.26
-1	9	6	23.14	0.14	23.32	26.07
1	9	6	59.40	2.04	65.12	27.67
3	9	6	47.04	0.93	47.13	35.04
-4	10	6	8.38	0.96	8.30	38.96
2	10	6	19.13	0.33	18.82	35.08
-1	11	6	10.99	0.48	10.62	35.43
-6	0	7	18.30	0.23	19.05	30.21
-4	0	7	15.72	0.23	14.38	17.63
-2	0	7	124.30	0.49	126.57	10.82
0	0	7	62.40	0.70	66.86	9.79
2	0	7	12.81	0.24	12.18	14.54
4	0	7	16.35	0.18	14.28	25.07
-5	1	7	5.30	0.77	5.26	23.43
-3	1	7	10.82	0.38	10.52	13.74
-1	1	7	26.78	0.33	31.71	9.82
1	1	7	23.11	0.32	27.35	11.68
5	1	7	9.55	0.32	9.95	32.73
-2	2	7	57.38	0.09	57.24	11.76
0	2	7	32.61	0.08	33.30	10.73
2	2	7	11.02	0.20	11.31	15.48
-5	3	7	56.66	0.74	56.48	25.30
-3	3	7	4.43	0.60	4.94	15.61
-1	3	7	14.74	0.25	17.69	11.69



1	3	7	32.28	0.18	37.11	13.55
3	3	7	60.55	1.21	60.84	21.19
5	3	7	40.52	1.04	39.53	34.60
-4	4	7	25.91	0.15	26.31	21.37
-2	4	7	24.35	0.11	24.70	14.57
0	4	7	55.62	0.12	56.06	13.54
2	4	7	21.97	0.64	22.61	18.29
4	4	7	10.14	0.88	9.68	28.81
-3	5	7	15.90	0.35	16.06	19.35
-1	5	7	29.76	0.24	34.09	15.44
1	5	7	29.34	0.12	32.70	17.30
5	5	7	5.16	0.73	4.63	38.35
-6	6	7	16.69	0.66	17.45	38.64
-4	6	7	26.26	0.62	24.96	26.05
-2	6	7	66.71	0.09	65.40	19.25
0	6	7	66.27	0.21	65.93	18.22
2	6	7	13.63	0.46	13.27	22.97
-5	7	7	11.23	0.28	11.73	34.66
-1	7	7	15.69	0.18	18.04	21.05
1	7	7	7.08	0.69	7.51	22.91
-4	8	7	5.88	0.60	7.45	32.60
-2	8	7	11.58	0.32	12.31	25.80
0	8	7	26.36	0.13	26.06	24.77
-1	9	7	15.25	0.35	19.18	28.54
1	9	7	21.80	0.15	21.81	30.40
3	9	7	31.56	0.33	31.70	38.04
-2	10	7	27.66	0.15	27.83	34.22
0	10	7	23.89	0.24	24.19	33.19
2	10	7	12.97	1.02	13.57	37.94
-1	11	7	23.81	0.15	26.18	37.90
-2	0	8	35.75	0.28	36.94	13.56
0	0	8	65.33	0.23	70.90	12.79
2	0	8	63.98	1.09	68.11	17.81
4	0	8	38.75	0.71	36.52	28.60
-5	1	8	20.17	0.16	20.03	25.77
-3	1	8	34.51	0.19	34.06	16.34
-1	1	8	18.46	0.18	20.29	12.69
-6	2	8	21.51	0.28	21.36	33.35
-4	2	8	20.53	0.23	20.39	21.03
-2	2	8	33.78	0.14	34.87	14.49
0	2	8	5.93	0.32	4.99	13.73
2	2	8	25.22	0.58	26.95	18.74
-5	3	8	68.51	0.56	67.86	27.64
-3	3	8	66.41	0.22	66.17	18.21
-1	3	8	8.84	0.68	8.49	14.56
5	3	8	6.34	0.48	5.03	38.27
-4	4	8	31.34	0.58	31.07	23.84
-2	4	8	13.63	0.34	14.07	17.30
0	4	8	12.75	0.39	12.20	16.54
2	4	8	10.09	0.25	11.18	21.55
4	4	8	18.40	0.42	17.81	32.34
-5	5	8	13.87	0.22	14.13	31.38
-3	5	8	24.05	0.13	24.48	21.95
-1	5	8	4.41	0.73	4.11	18.30
1	5	8	5.85	0.41	6.25	20.43
3	5	8	5.62	0.69	5.81	28.33
-4	6	8	16.98	0.37	17.71	28.52
-2	6	8	31.74	0.12	31.30	21.98
0	6	8	58.70	0.23	58.01	21.22
2	6	8	32.83	1.18	35.12	26.23

4	6	8	41.37	0.95	38.77	37.02
-5	7	8	15.26	0.76	15.67	37.00
-3	7	8	24.27	0.32	24.04	27.57
-1	7	8	22.78	0.13	24.07	23.92
-4	8	8	32.54	0.44	32.04	35.07
-2	8	8	20.69	0.16	20.05	28.53
-3	9	8	36.68	0.50	36.38	35.06
-1	9	8	11.84	0.41	11.16	31.40
-2	10	8	9.23	0.59	9.39	36.95
0	10	8	6.26	0.49	5.61	36.19
-6	0	9	48.79	0.22	48.72	35.01
-4	0	9	14.28	0.19	13.23	22.96
0	0	9	29.80	0.10	30.56	16.19
2	0	9	5.69	0.51	4.77	21.47
4	0	9	16.71	0.26	15.84	32.53
-5	1	9	16.52	0.41	16.27	28.50
-1	1	9	6.70	0.32	7.86	15.95
3	1	9	6.78	0.38	6.67	26.51
-6	2	9	21.66	0.55	21.83	35.95
-2	2	9	22.60	0.14	23.57	17.62
0	2	9	5.01	0.51	4.84	17.13
2	2	9	11.25	0.56	12.17	22.41
-5	3	9	26.46	0.15	25.88	30.37
-3	3	9	60.76	0.21	61.05	21.21
-1	3	9	66.29	0.52	67.99	17.82
1	3	9	68.30	0.09	66.37	20.21
3	3	9	46.94	1.37	47.14	28.38
-6	4	9	11.95	0.27	12.12	38.76
-4	4	9	12.21	0.56	11.98	26.71
0	4	9	22.11	0.13	21.68	19.93
2	4	9	6.89	0.38	8.04	25.21
4	4	9	7.46	0.42	7.22	36.27
-5	5	9	17.46	0.40	16.54	34.12
-3	5	9	11.90	0.51	10.89	24.95
1	5	9	4.89	0.79	3.32	23.96
3	5	9	10.68	0.31	11.08	32.13
-4	6	9	13.85	0.46	12.76	31.39
-2	6	9	11.87	0.23	11.05	25.11
2	6	9	6.58	0.59	6.97	29.89
-3	7	9	4.50	0.71	4.76	30.57
-1	7	9	7.85	0.53	8.45	27.18
-2	8	9	12.51	0.24	13.12	31.66
0	8	9	24.33	0.31	22.86	31.16
-3	9	9	41.06	0.19	40.96	38.05
-1	9	9	37.29	0.13	37.08	34.67
1	9	9	39.28	0.35	37.29	37.06
-4	0	10	36.96	0.12	35.55	26.23
-2	0	10	58.86	0.80	65.36	20.22
0	0	10	50.81	0.13	48.32	19.99
2	0	10	11.44	0.43	12.88	25.53
-1	1	10	7.91	0.34	8.52	19.62
1	1	10	13.01	0.49	13.44	22.27
3	1	10	13.85	0.48	16.25	30.71
-4	2	10	6.11	0.69	5.87	27.16
-2	2	10	15.76	0.49	18.28	21.16
0	2	10	11.07	0.21	10.67	20.92
2	2	10	13.18	0.21	12.70	26.47
4	2	10	9.55	0.32	9.70	37.79
-1	3	10	5.37	0.84	4.51	21.49
1	3	10	13.08	0.30	11.49	24.14

3	3	10	41.23	0.65	45.44	32.58
-4	4	10	21.84	0.27	21.97	29.97
0	4	10	6.45	0.39	6.17	23.73
2	4	10	5.21	0.79	5.14	29.28
-5	5	10	10.53	0.41	8.38	37.25
-3	5	10	6.51	0.65	6.12	28.35
1	5	10	4.54	0.57	3.32	27.89
3	5	10	9.58	0.60	12.07	36.32
-4	6	10	38.44	0.56	37.13	34.65
-2	6	10	30.57	0.18	33.59	28.64
0	6	10	48.73	0.29	45.12	28.41
2	6	10	9.51	0.68	10.20	33.96
-1	7	10	6.13	0.49	7.07	30.85
1	7	10	16.83	0.41	16.92	33.50
-2	8	10	5.05	0.64	3.16	35.19
-1	9	10	8.09	0.34	6.96	38.33
-4	0	11	8.30	0.34	8.53	29.89
-2	0	11	11.49	0.23	10.89	24.15
0	0	11	52.58	0.22	48.86	24.19
2	0	11	52.82	0.32	51.26	30.00
-3	1	11	4.89	0.63	3.89	26.54
-1	1	11	11.00	0.44	10.82	23.68
1	1	11	14.45	0.39	12.83	26.60
3	1	11	7.16	0.54	6.76	35.30
-2	2	11	4.86	0.51	4.76	25.09
0	2	11	15.97	0.17	15.33	25.12
2	2	11	27.74	0.14	26.52	30.93
-5	3	11	39.93	0.47	36.96	37.04
-3	3	11	44.87	0.14	44.72	28.41
-1	3	11	9.70	0.51	10.54	25.55
1	3	11	14.25	0.28	14.08	28.47
3	3	11	7.50	0.41	6.09	37.17
-2	4	11	15.39	0.19	16.37	27.90
0	4	11	24.64	0.15	22.86	27.93
2	4	11	15.75	0.39	15.48	33.74
-3	5	11	6.43	0.41	5.24	32.15
-1	5	11	16.94	0.22	15.76	29.30
1	5	11	16.78	0.19	15.11	32.22
-4	6	11	6.47	0.46	5.43	38.32
-2	6	11	15.09	0.21	14.05	32.57
0	6	11	47.32	0.13	42.66	32.61
2	6	11	31.91	0.17	30.98	38.42
-3	7	11	4.84	0.58	2.18	37.77
1	7	11	7.89	0.37	7.33	37.83
0	8	11	10.14	0.31	11.02	39.16
-4	0	12	10.94	0.33	10.92	33.96
-2	0	12	12.93	0.37	12.79	28.48
0	0	12	27.61	0.13	23.00	28.78
2	0	12	43.09	0.12	39.57	34.86
-3	1	12	10.00	0.27	11.55	30.73
-1	1	12	16.95	0.19	15.18	28.14
1	1	12	5.88	0.53	4.97	31.33
-4	2	12	14.27	0.22	13.98	34.90
-2	2	12	27.07	0.13	25.32	29.42
0	2	12	11.69	0.32	10.73	29.72
2	2	12	6.84	0.80	5.55	35.80
-3	3	12	40.75	0.29	44.23	32.61
-1	3	12	54.23	0.20	50.70	30.02
1	3	12	11.27	0.54	11.39	33.20
-4	4	12	6.71	0.65	6.72	37.70

-2	4	12	11.57	0.27	11.23	32.23
0	4	12	21.20	0.15	18.74	32.53
2	4	12	7.08	0.73	5.62	38.60
-1	5	12	12.41	0.28	11.12	33.76
0	6	12	8.76	0.62	6.26	37.21
-4	0	13	29.83	0.34	30.63	38.43
-2	0	13	12.32	0.23	10.65	33.21
0	0	13	19.85	0.17	18.71	33.78
-3	1	13	6.20	0.68	6.55	35.33
-1	1	13	6.35	0.59	5.59	33.01
1	1	13	13.30	0.24	11.90	36.46
-2	2	13	15.21	0.31	14.16	34.15
0	2	13	12.24	0.28	10.08	34.72
-3	3	13	9.23	0.53	6.44	37.20
-1	3	13	44.05	0.12	39.13	34.88
1	3	13	39.31	0.19	35.07	38.33
-2	4	13	5.93	0.91	5.05	36.96
-2	0	14	37.72	0.27	33.92	38.35
0	0	14	20.27	0.27	16.90	39.18

END

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+           XLS - Least-squares crystal structure refinement           +
+                                                                 +
+           SHELXTL PLUS - Release 4.11/V                             +
+ Copyright 1990 Siemens Analytical X-ray Instr., Inc. All rights reserved. +
+ License: Geological Sciences University of Illinois, Stephen Guggenheim +
+                                                                 +
+           RANO started at 09:54:48 on 23-Jun-92                     +
+++++

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TITL RANCOURT BIOTITE HEAT TREATED (RANO) IN C2/M
CELL 0.71073  5.3099  9.185  10.093  90.00 100.069  90.00
ZERR  1.00  0.0005  0.001  0.002  0.00  0.01  0.00
LATT  7
SYMM -X, Y, -Z
SFAC A1  7.061625  0.797640  7.172649  11.666479  0.556002  200.176666 =
      1.668019  27.350302  1.416414  0.167  0.232  978.7  2.27
SFAC M1  8.283765  4.405341  2.261523  13.374294  3.813178  0.537183 =
      1.132520  80.185349  1.721814  0.159  0.392  1627.6  1.60
SFAC M2  8.283765  4.405341  2.261523  13.374294  3.813178  0.537183 =
      1.132520  80.185349  1.721814  0.159  0.392  1627.6  1.60
SFAC T1  5.040259  3.147538  0.858992  80.787247  3.329262  1.128188 =
      1.344917  31.146509  1.297733  0.068  0.066  284.6  1.17
SFAC O-1  4.191600  12.857300  1.639690  4.172360  1.526730  47.017900 =
      -20.307000 -0.014040  21.941200  0.008  0.006  30.48  0.66
SFAC OH,F 4.321104  11.077127  1.914772  3.651860  1.403507  39.875435 =
      -20.567442 -0.012152  22.198444  0.011  0.008  41.2  0.66
UNIT 2.0 2.0 4.0 8.0 22.0 4.0

```

V = 484.67 F(000) = 468.00 MU = 3.06 MM-1

```

L.S. 4
FVAR  6.32219
A      1  10.00000  10.50000  10.00000  10.25000  0.03072  0.02910 =
      0.03852  10.00000  0.00650  10.00000
M1     2  10.00000  10.00000  10.50000  10.25000  0.01436  0.01320 =
      0.02755  10.00000  0.00582  10.00000
M2     3  10.00000  0.34202  10.50000  10.50000  0.00856  0.01314 =
      0.02162  10.00000  0.00221  10.00000
T      4  0.07342  0.16738  0.22318  11.00000  0.00814  0.00776 =
      0.01767  0.00007  0.00253 -0.00004
O1     5  0.03098  10.00000  0.16605  10.50000  0.02821  0.01073 =
      0.02115  10.00000  0.00310  10.00000
O2     5  0.31550  0.23798  0.16450  11.00000  0.01640  0.02454 =
      0.02425 -0.00171  0.00483 -0.00533
O3     5  0.12945  0.16940  0.38964  11.00000  0.00983  0.01138 =
      0.01718  0.00060  0.00228  0.00073
OH     6  0.13587  10.50000  0.40095  10.50000  0.01387  0.01225 =
      0.02292  10.00000  0.00416  10.00000
END

```

3.26 SECONDS CPU TIME 873 PAGE FAULTS

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RESIDUALS BEFORE CYCLE 1 FOR RANCOURT BIOTITE HEAT TREATED (RANO) IN
R = 0.0392 RW = 0.0392 RG = WR = 0.0467 RM = 0.0467
N = 634 NP = 53 MAX(NP) = 800 Total NP = 53 S = Goof = 1.8810
UNIT WEIGHTS

```

CYCLE 1

ESD SHIFT/ESD

CORRELATION MATRIX ELEMENTS GREATER THAN 0.5

0.

22.35 SECONDS CPU TIME 78 PAGE FAULTS

RESIDUALS BEFORE CYCLE 2 FOR RAN COURT BIOTITE HEAT TREATED (RANO) IN

R = 0.0392 RW = 0.0392 RG = WR = 0.0467 RM = 0.0467  
N = 634 NP = 53 MAX(NP) = 800 Total NP = 53 S = Goof = 1.8810

UNIT WEIGHTS

CYCLE 2

ESD SHIFT/ESD

CORRELATION MATRIX ELEMENTS GREATER THAN 0.5

0.

22.31 SECONDS CPU TIME 1 PAGE FAULTS

RESIDUALS BEFORE CYCLE 3 FOR RAN COURT BIOTITE HEAT TREATED (RANO) IN

R = 0.0392 RW = 0.0392 RG = WR = 0.0467 RM = 0.0467  
N = 634 NP = 53 MAX(NP) = 800 Total NP = 53 S = Goof = 1.8810

UNIT WEIGHTS

CYCLE 3

ESD SHIFT/ESD

CORRELATION MATRIX ELEMENTS GREATER THAN 0.5

0.

22.30 SECONDS CPU TIME 1 PAGE FAULTS

RESIDUALS BEFORE CYCLE 4 FOR RAN COURT BIOTITE HEAT TREATED (RANO) IN

R = 0.0392 RW = 0.0392 RG = WR = 0.0467 RM = 0.0467  
N = 634 NP = 53 MAX(NP) = 800 Total NP = 53 S = Goof = 1.8810

UNIT WEIGHTS

CYCLE 4

ESD SHIFT/ESD

			ESD	SHIFT/ESD
1	OVERALL SCALE	6.32219	0.02284	0.000
2	A U11	0.03072	0.00120	0.000
3	A U22	0.02910	0.00119	0.000
4	A U33	0.03852	0.00132	0.000
5	A U13	0.00650	0.00102	0.000
6	M1 U11	0.01436	0.00085	0.000
7	M1 U22	0.01320	0.00083	0.000
8	M1 U33	0.02755	0.00101	0.000
9	M1 U13	0.00582	0.00074	0.000
10	M2 Y/B	0.34202	0.00014	0.000
11	M2 U11	0.00856	0.00050	0.000
12	M2 U22	0.01314	0.00059	0.000
13	M2 U33	0.02162	0.00061	0.000

CORRELATION MATRIX ELEMENTS GREATER THAN 0.5

0.

22.35 SECONDS CPU TIME 78 PAGE FAULTS

RESIDUALS BEFORE CYCLE 2 FOR RANCOURT BIOTITE HEAT TREATED (RANO) IN

R = 0.0392 RW = 0.0392 RG = wR = 0.0467 RM = 0.0467  
N = 634 NP = 53 MAX(NP) = 800 Total NP = 53 S = Goof = 1.8810  
UNIT WEIGHTS

CYCLE 2

ESD SHIFT/ESD

CORRELATION MATRIX ELEMENTS GREATER THAN 0.5

0.

22.31 SECONDS CPU TIME 1 PAGE FAULTS

RESIDUALS BEFORE CYCLE 3 FOR RANCOURT BIOTITE HEAT TREATED (RANO) IN

R = 0.0392 RW = 0.0392 RG = wR = 0.0467 RM = 0.0467  
N = 634 NP = 53 MAX(NP) = 800 Total NP = 53 S = Goof = 1.8810  
UNIT WEIGHTS

CYCLE 3

ESD SHIFT/ESD

CORRELATION MATRIX ELEMENTS GREATER THAN 0.5

0.

22.30 SECONDS CPU TIME 1 PAGE FAULTS

RESIDUALS BEFORE CYCLE 4 FOR RANCOURT BIOTITE HEAT TREATED (RANO) IN

R = 0.0392 RW = 0.0392 RG = wR = 0.0467 RM = 0.0467  
N = 634 NP = 53 MAX(NP) = 800 Total NP = 53 S = Goof = 1.8810  
UNIT WEIGHTS

CYCLE 4

ESD SHIFT/ESD

			ESD	SHIFT/ESD
1	OVERALL SCALE	6.32219	0.02284	0.000
2	A U11	0.03072	0.00120	0.000
3	A U22	0.02910	0.00119	0.000
4	A U33	0.03852	0.00132	0.000
5	A U13	0.00650	0.00102	0.000
6	M1 U11	0.01436	0.00085	0.000
7	M1 U22	0.01320	0.00083	0.000
8	M1 U33	0.02755	0.00101	0.000
9	M1 U13	0.00582	0.00074	0.000
10	M2 Y/B	0.34202	0.00014	0.000
11	M2 U11	0.00856	0.00050	0.000
12	M2 U22	0.01314	0.00059	0.000
13	M2 U33	0.02162	0.00061	0.000

14	M2	U13	0.00221	0.00044	0.000
15	T	X/A	0.07342	0.00020	0.000
16	T	Y/B	0.16738	0.00012	0.000
17	T	Z/C	0.22318	0.00011	0.000
18	T	U11	0.00814	0.00045	0.000
19	T	U22	0.00776	0.00045	0.000
20	T	U33	0.01767	0.00052	0.000
21	T	U23	0.00007	0.00043	0.000
22	T	U13	0.00253	0.00038	0.000
23	T	U12	-0.00004	0.00041	0.000
24	O1	X/A	0.03098	0.00094	0.000
25	O1	Z/C	0.16605	0.00047	0.000
26	O1	U11	0.02821	0.00242	0.000
27	O1	U22	0.01073	0.00189	0.000
28	O1	U33	0.02115	0.00217	0.000
29	O1	U13	0.00310	0.00187	0.000
30	O2	X/A	0.31550	0.00059	0.000
31	O2	Y/B	0.23798	0.00038	0.000
32	O2	Z/C	0.16450	0.00032	-0.001
33	O2	U11	0.01640	0.00146	0.000
34	O2	U22	0.02454	0.00162	0.000
35	O2	U33	0.02425	0.00151	0.000
36	O2	U23	-0.00171	0.00139	0.000
37	O2	U13	0.00483	0.00120	0.000
38	O2	U12	-0.00533	0.00131	0.000
39	O3	X/A	0.12945	0.00052	0.000
40	O3	Y/B	0.16940	0.00032	0.000
41	O3	Z/C	0.38964	0.00029	0.000
42	O3	U11	0.00983	0.00116	0.000
43	O3	U22	0.01138	0.00119	0.000
44	O3	U33	0.01718	0.00128	0.000
45	O3	U23	0.00060	0.00113	0.000
46	O3	U13	0.00228	0.00100	0.000
47	O3	U12	0.00073	0.00106	0.000
48	OH	X/A	0.13587	0.00075	0.000
49	OH	Z/C	0.40095	0.00042	0.000
50	OH	U11	0.01387	0.00176	0.000
51	OH	U22	0.01225	0.00170	0.000
52	OH	U33	0.02292	0.00192	0.000
53	OH	U13	0.00416	0.00148	0.000

CORRELATION MATRIX ELEMENTS GREATER THAN 0.5

0.

22.79 SECONDS CPU TIME 7 PAGE FAULTS

RANCOURT BIOTITE HEAT TREATED (RANO) IN

ATOM	X/A	Y/B	Z/C	K	U11	U22	U33	U23	U13	U12	Ueq
A	0.00000	0.50000	0.00000	0.25000	0.03072	0.02910	0.03852	0.00000	0.00650	0.00000	0.03272
	0.00000	0.00000	0.00000	0.00000	0.00120	0.00119	0.00132	0.00000	0.00102	0.00000	0.00074
M1	0.00000	0.00000	0.50000	0.25000	0.01436	0.01320	0.02755	0.00000	0.00582	0.00000	0.01811



	<i>X</i>	<i>Y</i>	<i>Z</i>		<i>U11</i>	<i>U22</i>	<i>U33</i>	<i>U23</i>	<i>U13</i>	<i>U12</i>	<i>Ueq</i>
	0.00000	0.00000	0.00000	0.00000	0.00085	0.00083	0.00101	0.00000	0.00074	0.00000	0.00054
M2	0.00000	0.34202	0.50000	0.50000	0.00856	0.01314	0.02162	0.00000	0.00221	0.00000	0.01449
	0.00000	0.00014	0.00000	0.00000	0.00050	0.00059	0.00061	0.00000	0.00044	0.00000	0.00034
T	0.07342	0.16738	0.22318	1.00000	0.00814	0.00776	0.01767	0.00007	0.00253	-0.00004	0.01116
	0.00020	0.00012	0.00011	0.00000	0.00045	0.00045	0.00052	0.00043	0.00038	0.00041	0.00028
O1	0.03098	0.00000	0.16605	0.50000	0.02821	0.01073	0.02115	0.00000	0.00310	0.00000	0.02017
	0.00094	0.00000	0.00047	0.00000	0.00242	0.00189	0.00217	0.00000	0.00187	0.00000	0.00130
O2	0.31550	0.23798	0.16450	1.00000	0.01640	0.02454	0.02425	-0.00171	0.00483	-0.00533	0.02158
	0.00059	0.00038	0.00032	0.00000	0.00146	0.00162	0.00151	0.00139	0.00120	0.00131	0.00091
O3	0.12945	0.16940	0.38964	1.00000	0.00983	0.01138	0.01718	0.00060	0.00228	0.00073	0.01281
	0.00052	0.00032	0.00029	0.00000	0.00116	0.00119	0.00128	0.00113	0.00100	0.00106	0.00073
OH	0.13587	0.50000	0.40095	0.50000	0.01387	0.01225	0.02292	0.00000	0.00416	0.00000	0.01623
	0.00075	0.00000	0.00042	0.00000	0.00176	0.00170	0.00192	0.00000	0.00148	0.00000	0.00107

RESIDUALS BEFORE CYCLE 5 FOR RANCOURT BIOTITE HEAT TREATED (RANO) IN  
R = 0.0392 RW = 0.0392 RG = WR = 0.0467 RM = 0.0467  
N = 634 NP = 53 MAX(NP) = 800 Total NP = 53 S = Goof = 1.8810  
UNIT WEIGHTS

6.91 SECONDS CPU TIME 59 PAGE FAULTS

0.45 SECONDS CPU TIME 128 PAGE FAULTS

## 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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