AM-89-406

Crystal structure of a Cr^{2+}-bearing pyroxene

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For deposit: Table 3

American Mineralogist, 74, 5-6, 599-603.

#5406 revised version

Supplementary Material for Crystal Structure of a Cr^{2+}-bearing Pyroxene.

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Table 3: Observed and calculated structure factors for Cr-enstatite refined in space group $P2_1/c$. Observed structure factors have been corrected for absorption and extinction, and scaled to the calculated structure factors. Reflections marked with an asterisk are less-thans, and were excluded from the refinements. Refined structural parameters are reported in Table 2 of the paper, the extinction coefficient in Table 1.

CHROMIUM PIGEONITE - SPACE GROUP P2.1/C FACTOR = 1.00

H	OBS	CALC
H 0 0		
0	0	429
1	0*	1
2	21	19
3	2*	5
4	10	4
6	95	94
7	11*	11
8	61	64
9	2*	1
10	73	72
11	7*	5
12	19*	19
H 1 0		
1	6*	4
2	4*	3
3	96	96
4	5*	3
5	50	51
6	7*	2
7	45	46
8	10*	3
9	15	12
10	9*	7
11	19*	10
12	13*	5
H 2 0		
0	14	15
1	5*	1
2	85	85
3	8*	9
4	35	35
5	4*	8
6	8*	7
7	9*	4
8	39	37
9	7*	2
10	16*	11
11	10*	7
12	19*	23
H 3 0		
1	11	10
2	10	8
3	30	29
4	4*	2
5	13	14
6	6*	3
7	15	16
9	8*	10
10	9*	4
11	11*	12
12	10*	2
H 4 0		
0	21	19
1	7*	7
2	48	50
3	7*	4
4	25	25
5	13	13
6	15	16
8	45	42
9	7*	2
10	20	20
11	11*	2
12	19*	20
H 5 0		
1	72	70
3	59	61
4	8*	6
5	30	33
6	5*	3
7	90	89
9	23	23
10	6*	7
H 6 0		
0	158	157
1	8*	6
2	11*	10
3	8*	6
4	34	32
5	4*	5
6	47	46
7	9*	5
8	24	28
10	66	64
H 7 0		
1	17	16
2	15	16
3	9*	11
4	1*	0
5	50	50
6	9*	5
7	22	23
8	9*	4
9	14*	13
10	10*	4
H 8 0		
0	22	20
1	9*	7
2	34	34
3	1*	1
4	6*	8
5	9*	9
6	11*	14
7	6*	1
8	29	29

H	OBS	CALC
H 9 0		
1	12*	12
2	7*	3
3	4*	3
4	11*	5
5	20	16
6	9*	4
H 10 0		
0	22	22
2	18*	19
4	22	19
5	8*	0
6	4*	1
H 11 0		
1	35	37
2	12*	9
3	39	38
5	15*	15
6	8*	5
H 12 0		
0	53	52
1	9*	4
2	4*	8
3	3*	3
H 1 1		
-13	19*	19
-12	3*	2
-11	19*	17
-10	8*	9
-9	7*	1
-8	5*	9
-7	37	37
-6	15	15
-5	3*	4
-4	4*	5
-3	82	83
-1	26	26
0	21	22
1	3*	1
2	5*	5
3	63	63
4	6*	2
6	9*	10
7	43	43
8	5*	2
9	7*	5
10	5*	7
11	15*	8
12	14*	1
H 2 1		
-12	57	53
-11	8*	2
-10	15	12
-9	4*	5
-8	35	36
-7	7*	2
-6	20	20
-5	26	25
-4	46	43
-3	13	12
-2	126	126
-1	14	14
0	61	61
1	20	19
2	72	74
3	10*	9
4	40	38
5	9*	8
6	29	31
7	7*	7
8	49	49
10	27	27
11	1*	0
H 3 1		
-13	13*	14
-12	17*	18
-11	52	55
-9	55	57
-8	14	13
-7	37	37
-6	4*	0
-5	135	135
-4	34	31
-3	114	110
-2	45	44
-1	84	86
0	33	30
1	16	20
2	11	11
3	31	29
4	31	30
5	168	169
6	4*	3
7	3*	3
8	4*	4
9	23	25
10	9*	3
11	39	40
H 4 1		
-12	30	31
-11	10*	6
-10	28	26
-8	15	15
-7	3*	1
-6	6*	3
-5	9*	5
-4	5*	6
-3	26	25
-2	53	52
-1	17	18
0	63	64
1	21	19

H	OBS	CALC
H 4 1		
2	39	36
3	25	25
4	7*	6
6	7*	3
7	11*	13
8	25	26
9	13*	0
10	36	35
11	8*	3
H 5 1		
-12	14*	1
-11	24	20
-10	13*	3
-9	4*	7
-8	8*	12
-7	30	30
-6	27	27
-5	14	13
-4	6*	6
-3	54	56
-2	4*	6
-1	26	28
0	30	30
1	19	18
3	43	44
4	5*	8
5	10*	12
6	10*	15
7	40	39
8	12*	3
9	9*	9
10	8*	10
11	13*	7
H 6 1		
-10	12*	8
-9	15*	5
-8	7*	1
-7	19	20
-6	11*	12
-5	8*	5
-4	8*	12
-3	15	15
-2	3*	4
-1	7*	7
0	26	27
1	16	17
2	5*	1
3	10*	12
4	12*	3
5	7*	6
6	10*	14
7	6*	10
8	12*	7
10	8*	6
H 7 1		
-11	5*	6
-10	21	19
-9	7*	7
-8	12*	3
-7	21	21
-5	26	27
-4	13*	15
-3	41	41
-2	11*	9
-1	12*	5
0	8*	10
1	19	22
2	10*	7
3	38	39
4	17	15
5	19	18
6	9*	0
7	21	18
8	2*	8
H 8 1		
-10	5*	1
-9	8*	14
-8	33	33
-7	9*	11
-6	14*	18
-5	22	21
-4	37	39
-3	17	19
-2	92	93
0	27	28
1	7*	6
2	63	60
3	15	15
4	40	43
5	17*	14
6	31	29
7	13*	12
8	40	38
H 9 1		
-9	27	28
-8	19*	9
-7	25	25
-6	8*	11
-5	65	64
-4	4*	4
-3	22	22
-2	9*	9
-1	34	35
0	8*	8
1	20	19
2	6*	5
3	11*	7
5	79	80
6	11*	7
7	9*	1
H 10 1		
-8	10*	4
-7	13*	18

H	OBS	CALC
H 10 1		
-6	18*	17
-5	14*	7
-4	17*	18
-2	13*	5
-1	11*	0
0	50	48
1	15*	9
3	9*	5
4	11*	14
6	20*	23
H 11 1		
-5	9*	11
-3	24	26
-2	14*	7
-1	12*	6
0	6*	3
1	10*	4
2	8*	2
3	16*	23
4	10*	9
5	11*	10
H 12 1		
-2	15*	4
-1	15*	0
0	17*	14
2	11*	2
H 0 2		
-13	23	23
-12	16*	17
-11	16	11
-10	63	62
-9	9*	1
-8	39	39
-7	65	67
-6	91	92
-5	21	21
-4	98	99
-3	5*	1
-2	44	40
-1	22	22
0	153	153
1	69	67
2	90	87
3	36	35
4	80	82
5	19	20
6	36	35
7	25	24
8	8*	2
9	18	19
10	90	90
11	7*	3
H 1 2		
-13	30	29
-12	13*	14
-11	5*	4
-10	20	20
-9	23	23
-8	7*	2
-7	91	91
-6	5*	3
-5	12	14
-4	27	26
-2	3*	1
-1	7*	8
0	4*	2
1	50	48
2	6*	5
3	65	66
4	27	26
5	57	55
6	3*	4
7	43	43
8	16*	14
9	8*	12
10	9*	15
H 2 2		
-12	27	27
-11	14*	14
-10	20	20
-9	21	22
-8	35	34
-6	56	58
-5	20	20
-4	5*	1
-3	28	28
-2	19	22
-1	8*	8
0	31	29
1	4*	3
2	76	74
3	20	20
4	3*	6
5	15	17
6	6*	9
7	12*	13
8	43	41
9	13*	5
H 3 2		
-12	8*	3
-11	8*	2
-10	3*	6
-9	8*	3
-8	8*	4
-7	12*	10
-6	8*	7
-5	18	18
-4	11	10
-3	21	20
-2	17	16
-1	8*	4
0	16	15
1	28	28

H	OBS	CALC
H 3 2		
2	3*	0
3	7*	4
4	14	14
5	6*	1
6	7*	3
7	6*	6
8	3*	9
10	9*	5
H 4 2		
-12	16*	19
-11	12*	4
-10	12*	11
-9	12*	10
-8	26	26
-7	6*	3
-6	8*	9
-5	24	23
-4	8*	3
-3	12	13
-2	54	51
-1	9*	9
0	29	29
1	26	26
2	43	41
3	9*	6
4	14	16
5	3*	2
6	5*	2
7	9*	2
8	20	24
9	6*	4
10	10*	8
H 5 2		
-11	6*	9
-10	13*	19
-9	9*	5
-8	7*	14
-7	85	85
-6	22	22
-5	10*	6
-4	11*	10
-3	57	58
-2	6*	7
-1	30	30
0	46	47
1	35	31
2	8*	8
3	93	95
5	18	18
6	7*	11
7	42	42
8	6*	6
9	21	19
10	11*	7
H 6 2		
-11	15*	12
-10	36	33
-8	19	19
-7	33	33
-6	71	73
-5	8*	9
-4	56	57
-3	22	22
-2	46	46
0	111	112
1	17	17
2	50	51
3	37	37
4	37	36
5	5*	6
6	17	21
7	13*	5
8	10*	7
9	7*	13
H 7 2		
-11	14*	8
-9	18*	19
-8	6*	8
-7	27	26
-5	39	42
-4	4*	1
-3	4*	6
-2	17	16
-1	10*	9
0	3*	4
1	19	20
2	8*	12
3	17	17
4	3*	0
5	40	40
7	6*	11
H 8 2		
-10	5*	3
-9	11*	12
-8	24	24
-6	24	25
-5	3*	6
-4	8*	7
-3	8*	6
-2	24	23
-1	14	11
0	12*	15
1	12*	10
2	30	31
3	7*	4
4	16*	11
5	7*	8
7	6*	1
8	19*	20
H 9 2		
-8	11*	14
-7	10*	3
-6	7*	1

H	OBS	CALC
H 9 2		
-5	13*	15
-4	7*	2
-3	8*	4
-2	12*	13
-1	8*	11
1	18*	15
2	9*	0
3	13*	3
4	6*	3
5	18*	19
7	5*	3
H 10 2		
-8	5*	8
-7	13*	9
-6	9*	2
-5	21	18
-4	10*	12
-3	4*	8
-2	18*	19
-1	9*	7
0	31	32
1	9*	8
2	15*	20
3	14*	0
4	3*	3
5	8*	0
H 11 2		
-6	15*	16
-4	14*	11
-3	38	36
-2	8*	7
-1	16*	14
0	26	26
1	22	21
2	14*	11
3	61	64
H 12 2		
-2	32	29
-1	15*	1
H 1 3		
-13	19*	6
-12	7*	2
-11	10*	14
-10	22	23
-9	7*	8
-7	36	33
-6	8*	9
-5	24	24
-4	23	25
-3	47	46
-2	12	10
-1	37	37
0	30	30
1	11*	4
2	2*	2
3	37	39
4	8*	7
6	14	15
7	28	27
8	6*	2
9	10*	7
H 2 3		
-13	9*	2
-12	35	34
-11	12*	13
-10	5*	5
-9	34	33
-8	41	43
-7	20	19
-6	7*	2
-5	30	31
-4	6*	5
-3	19	18
-2	117	118
-1	24	24
0	16	16
1	17	17
2	32	31
4	21	22
5	31	30
6	13*	16
7	11*	3
8	41	43
9	7*	5
H 3 3		
-13	7*	1
-12	36	37
-11	34	35
-10	7*	9
-9	74	74
-8	39	39
-7	16	17
-6	22	22
-5	68	68
-4	6*	7
-3	39	38
-2	75	77
-1	96	95
0	23	22
1	81	79
2	22	23
3	30	32
4	10*	11
5	84	84
6	22	23
7	34	35
8	29	31
9	31	30
H 4 3		
-12	16*	18
-11	6*	1

H	OBS	CALC
H 4 3		
-10	11*	8
-9	19	19
-8	21	22
-7	26	26
-6	17	17
-5	6*	8
-4	19	20
-3	9*	3
-2	74	73
-1	4*	3
0	45	45
1	9*	5
2	8*	4
3	14	14
4	8*	9
5	12*	15
6	7*	2
8	19	15
9	9*	1
H 5 3		
-11	17*	15
-10	22	21
-9	23	22
-8	13*	11
-7	21	21
-6	6*	4
-5	15	16
-4	23	23
3	49	50
-2	19	19
-1	37	37
0	18	18
1	9*	6
3	33	31
4	13*	13
5	13*	17
6	14*	15
7	18	18
H 6 3		
-11	13*	8
-10	16*	15
-9	4*	8
-8	2*	5
-6	9*	10
-4	13*	12
-3	17	18
-2	13	13
-1	6*	5
0	6*	8
2	8*	7
3	8*	7
4	14*	16
5	10*	2
6	9*	10
7	4*	0
H 7 3		
-10	10*	9
-9	17*	15
-8	7*	1
-7	29	29
-6	8*	9
-5	20	18
-3	7*	7
-2	11*	14
0	24	24
3	19	21
4	18*	6
5	27	28
6	10*	8
7	23	24
H 8 3		
-10	11*	3
-9	23	22
-8	37	35
-7	13*	5
-6	21	23
-5	34	35
-4	7*	1
-3	10*	11
-2	71	70
-1	21	20
0	14*	11
1	23	23
2	41	43
3	16*	5
4	7*	7
5	22	23
6	17*	19
H 9 3		
-9	51	50
-8	22	22
-7	27	25
-5	27	26
-4	9*	3
-3	23	24
-2	41	42
-1	41	41
0	11*	2
1	20	19
2	12*	6
3	23	21
5	58	58
H 10 3		
-7	16*	15
-6	9*	5
-5	4*	1
-4	23	24
-3	18	19
-2	8*	5
-1	13*	11
0	27	27
1	9*	5
2	3*	1

CHROMIUM PIGEONITE - SPACE GROUP P2.1/C FACTOR = 1.00

H	OBS	CALC
H 10 3		
3	17*	13
H 11 3		
-5	8*	0
-4	10*	9
-3	8*	11
-1	16*	16
0	10*	9
1	13*	10
H 0 4		
-13	27	26
-12	19	12
-11	27	28
-10	31	32
-9	12*	8
-8	5*	4
-7	59	58
-6	56	57
-5	17	17
-4	108	107
-3	76	76
-2	25	25
-1	29	28
0	59	60
1	7*	8
2	35	36
3	73	73
4	58	57
5	23	26
6	40	41
7	11*	9
8	14*	15
H 1 4		
-13	17*	16
-12	8*	3
-11	14*	11
-10	10*	9
-9	20	18
-8	16	14
-7	45	45
-6	27	28
-5	12*	7
-4	33	36
-3	34	33
-2	45	45
0	33	35
1	12*	12
2	16	16
3	57	57
5	18	19
6	5*	7
7	18*	14
8	10*	2
H 2 4		
-13	16*	16
-12	20	21
-11	12*	12
-10	10*	4
-9	8*	10
-8	13*	12
-7	6*	9
-6	19	19
-5	49	50
-4	12*	11
-3	4*	1
-2	36	36
-1	2*	1
0	10*	7
1	39	40
2	28	28
3	9*	10
4	17	17
5	7*	9
6	1*	4
7	12*	6
8	19*	24
H 3 4		
-12	14*	11
-9	6*	6
-8	4*	1
-7	9*	2
-6	20	18
-5	7*	2
-4	6*	2
-3	5*	3
-2	7*	11
-1	5*	5
0	10*	7
1	8*	4
2	14	15
3	7*	2
4	9*	8
H 4 4		
-12	23	23
-11	7*	6
-10	15*	12
-9	24	26
-7	14	14
-6	14	14
-5	20	21
-3	14	16
-2	28	29
-1	7*	8
0	21	22
1	7*	3
2	23	23
3	7*	1
4	9*	11
5	27	29
6	15*	5
7	5*	6
H 5 4		
-11	20	21
-10	28	28
-9	16*	18
-8	10*	8
-7	49	48
-6	18	19
-5	15	13
-4	45	45
-3	47	47
-2	7*	5
-1	9*	10
0	32	32
1	7*	2
2	13*	9
3	72	71
4	26	25
5	12*	4
6	17*	20
7	19*	20
H 6 4		
-11	23	20
-10	26	24
-9	4*	11
H 6 4		
-8	9*	1
-7	46	46
-6	34	35
-5	20	20
-4	64	67
-3	35	35
-2	21	20
-1	9*	9
0	46	47
1	12*	8
2	18	18
3	55	52
4	35	37
6	27	31
H 7 4		
-10	7*	5
-9	23	21
-8	18	17
-7	17*	17
-6	12*	11
-5	17	16
-4	3*	9
-3	5*	7
-2	22	23
-1	17	15
1	20	19
2	15*	14
3	28	27
4	14*	4
5	26	27
H 8 4		
-9	14*	10
-8	7*	2
-6	9*	15
-5	21	22
-4	19	18
-3	12*	11
-2	14*	15
-1	7*	5
0	7*	5
1	17*	15
2	23	23
3	6*	10
4	16*	16
H 9 4		
-8	8*	5
-7	8*	8
-6	12*	12
-5	14*	14
-3	14*	7
-2	10*	6
-1	13*	2
0	8*	1
1	8*	8
2	12*	10
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