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The structure of triclinic chloritoid and chloritoid polymorphism

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Abstract

The crystal structure of triclinic chloritoid from Chibougamau, Quebec, [$a = 9.46(1)$, $b = 5.50(1)$, $c = 9.15(1)$Å, $\alpha = 97.05(2)$, $\beta = 101.56(2)$, and $\gamma = 90.10(2)°$; $Z = 4$] was solved using symbolic addition methods, and refined in space group $C\bar{1}$ to $R = 0.080$ ($R_w = 0.060$). The triclinic structure is topologically very similar to that of its monoclinic polymorph. Substitution of Fe^{3+} for Al and Mg for Fe^{2+} occurs in the same two sites in the trioctahedral layer, M(1A) and M(1B) respectively, as in the monoclinic polymorph, and the observed average M–O bond distances for these sites (1.948 and 2.155Å) are in good agreement with those calculated using the refined occupancies of these sites. Other average bond distances in the structure are: M(2A)–O = 1.907, M(2B1)–O = 1.906, M(2B2)–O = 1.906 (octahedral sites occupied by aluminum), and T–O = 1.638Å (tetrahedral site occupied by silicon). Because the structures are so similar, interlayer hydrogen bonding is assumed to occur in the same way as it does in the monoclinic structure, although no hydrogen positions were determined for triclinic chloritoid. The monoclinic and triclinic structures cannot be strictly considered polytypes because there are significant differences between the observed monoclinic atomic coordinates and those calculated from the triclinic atomic coordinates.

Introduction

Two polymorphs of chloritoid, ideally $FeAl_2SiO_5(OH)_2$, are known to occur, one triclinic and the other monoclinic. The monoclinic chloritoid crystal structure has been solved (Harrison and Brindley, 1957) and refined (Hanscom, 1975).

Halferdahl (1961) published an X-ray powder pattern for triclinic chloritoid, and showed that the unit cells of the two chloritoid polymorphs appear to be related so that twinning on a unit-cell scale of the triclinic chloritoid structure can result in a monoclinic structure. Thus, the polymorphism of chloritoid gives all appearances of polytypism with the contents of two unit cells of triclinic chloritoid stacking in the direction of the *c* axis to give the monoclinic structure.

Close association of monoclinic and triclinic chloritoid is frequently described in the literature, and specimens of chloritoid giving X-ray powder patterns characteristic of both structure types have been reported (Halferdahl, 1961).

This paper describes the triclinic chloritoid crystal structure, and the relationship between the two chloritoid structure types.

Occurrence

Several specimens of chloritoid from the Siderite Hill showing, Chibougamau, Quebec, were provided by Dr. L. B. Halferdahl. This locality is a shear zone in a meta-anorthosite near Towle Lake, and about two miles east-southeast of the Chibougamau townsite. The chloritoid occurs as 1 to 2 mm grains in an extremely fine-grained groundmass of sericite and chlorite with minor quartz and carbonate. The geology of the Chibougamau Lake area and the Siderite Hill showing is described in detail by Allard (1960).

Chloritoid from this locality has been analyzed (Halferdahl, 1961, p. 61, #101), and the optical properties have been determined (Halferdahl, 1961, p. 88, Table 20, #12). The observed density is 3.58(2) g cm^{-3}. The crystal used for data collection is a triangular basal cleavage fragment with a computed crystal volume of 1.59 × 10^{-3} mm^3.

Unit cell and space group

Like monoclinic chloritoid, the triclinic structure possesses strong pseudo-hexagonal symmetry. For

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h=-2 k=-6

1	58.0	50.5
2	18.1	15.4
3	4.7	1.9**

h= 0 k=-6

1	65.8	63.8
2	47.5	45.6
3	24.0	22.0

h= 2 k=-6

1	36.0	35.8
2	43.0	39.4

h=-5 k=-5

1	25.3	22.2
2	30.8	23.4
3	19.8	17.5
4	16.6	11.7
5	37.5	31.1

h=-3 k=-5

1	31.9	32.8
2	59.7	60.3
3	66.6	68.1
4	35.2	34.3
5	68.8	72.0
6	40.0	42.8

h=-1 k=-5

1	4.5	2.2**
2	23.0	20.6
3	36.3	37.1
4	28.2	26.2
5	10.9	12.2
6	4.8	0.8**
7	25.3	20.8

h= 1 k=-5

1	36.1	36.8
2	30.2	30.8
3	15.2	15.0
4	42.1	45.7
5	9.8	6.5
6	4.7	3.7**

h= 3 k=-5

1	53.5	53.0
2	74.1	75.9
3	31.3	30.8
4	70.0	71.0
5	46.2	48.1

h= 5 k=-5

1	8.7	1.0
2	34.9	34.0
3	27.2	22.2

h=-8 k=-4

2	33.5	26.8
3	37.5	31.8

h=-6 k=-4

1	46.6	41.2
2	23.0	22.5
3	31.9	33.1
4	56.5	56.3
5	19.9	19.4
6	49.2	55.8
7	49.5	53.8

h=-4 k=-4

1	17.1	17.2
2	55.5	54.7
3	54.4	53.8
4	35.5	33.4
5	63.6	65.3
6	35.9	33.4
7	49.0	49.2
8	10.7	9.2

h=-2 k=-4

1	10.0	10.4
2	14.8	15.3
3	44.9	47.7
4	15.9	18.4
5	40.4	43.6
6	16.2	18.5
7	4.7	1.3**
8	4.8	2.0**

h= 0 k=-4

1	71.4	71.0
2	102.6	108.8
3	31.1	31.0
4	38.9	41.8
5	55.5	59.5
6	90.4	97.5
7	18.2	20.0
8	68.1	76.5

h= 2 k=-4

1	9.9	6.7
2	21.2	16.4
3	50.5	51.2
4	14.0	5.5
5	10.2	5.5
6	26.7	25.1
7	4.6	4.6**

h= 4 k=-4

1	4.8	10.4**
2	27.4	28.0
3	20.1	18.9
4	14.7	20.7
5	87.3	93.8
6	46.1	50.2

h= 6 k=-4

1	19.2	16.6
2	62.8	61.9
3	21.1	19.2
4	47.2	44.1

h=-9 k=-3

1	66.0	59.9
2	70.3	62.5
3	48.9	42.7
4	30.9	26.5

h=-7 k=-3

1	17.4	14.7
2	27.9	24.9
3	4.6	2.4**
4	37.0	33.1
5	24.4	23.7
6	10.8	12.5
7	11.6	3.8

h=-5 k=-3

1	20.0	14.6
2	7.9	8.2
3	11.0	10.8
4	51.4	49.9
5	15.9	16.8
6	25.3	26.5
7	27.4	28.5
8	15.2	14.0

h=-3 k=-3

1	133.7	125.8
2	102.0	96.3
3	43.5	40.5
4	86.5	90.6
5	23.7	21.4
6	27.7	30.9
7	45.5	50.5
8	65.7	69.4
9	12.5	17.2

h=-1 k=-3

1	20.0	20.9
2	17.4	15.1
3	53.6	55.5
4	26.2	26.7
5	4.1	1.3**
6	19.0	16.6
7	21.2	24.2
8	36.4	38.5
9	21.9	21.3

h= 1 k=-3

1	3.7	5.9**
2	20.3	21.8
3	42.6	51.3
4	22.5	23.7
5	17.4	18.2
6	28.4	31.1
7	20.8	26.8
8	4.7	5.6**
9	19.7	25.4

h= 3 k=-3

1	96.1	99.6
2	48.9	49.3
3	81.2	81.9
4	27.6	26.8
5	31.1	28.9
6	40.6	37.0
7	81.7	77.4
8	18.3	18.3

h= 5 k=-3

1	14.0	16.5
2	38.9	41.1
3	25.9	26.4
4	10.1	9.5
5	13.2	11.2
6	11.8	11.3
7	34.3	33.0

h= 7 k=-3

1	21.0	18.7
2	35.8	40.7
3	23.5	20.5
4	4.7	5.4**
5	23.9	19.8

h= 9 k=-3

0	54.7	57.2
1	21.4	22.9

h=-10 k=-2

2	23.5	13.4*
3	60.6	51.4

h=-8 k=-2

1	20.5	16.5
2	35.3	29.9
3	13.2	6.7
4	30.6	26.7
5	38.3	36.6
6	15.0	13.4
7	8.7	5.1

h=-6 k=-2

1	65.1	55.6
2	172.9	177.7
3	26.7	22.5
4	85.2	88.6
5	81.3	88.1
6	61.9	68.3
7	5.0	9.0**
8	60.2	71.4*
9	5.1	2.7**

h=-4 k=-2

1	10.4	4.6
2	24.9	23.8
3	60.6	62.2
4	31.1	28.5
5	16.7	18.1
6	4.7	11.5**
7	28.9	29.3
8	15.7	15.4
9	31.5	33.7

h=-2 k=-2

1	[illegible]4.0	64.1
2	[illegible]1.9	50.1
3	26.2	25.5
4	3.8	1.0**
5	66.2	82.1*
6	85.0	103.8*
7	83.5	99.1*
8	10.1	11.6
9	13.0	17.5
10	9.9	12.8

h= 0 k=-2

1	107.2	105.2
2	156.7	156.6
3	96.3	95.9
4	138.1	145.1
5	87.9	90.3
6	46.5	48.2
7	16.0	19.3
8	70.6	71.0
9	5.2	7.3**

h= 2 k=-2

1	101.3	106.0
2	68.3	70.4
3	92.6	94.4
4	78.0	78.7
5	58.3	60.1
6	38.2	35.1
7	14.4	10.5
8	12.5	12.7
9	23.3	26.0

h= 4 k=-2

1	45.4	46.1
2	15.5	19.3
3	50.4	52.8
4	7.4	3.[illegible]
5	4.5	5.5**
6	4.4	3.0**
7	27.4	31.6
8	5.0	4.4**

h= 6 k=-2

0	145.0	153.7
1	43.0	44.2
2	78.4	77.2
3	87.0	84.1
4	85.9	85.6
5	10.1	5.0
6	66.4	62.9

h= 8 k=-2

0	4.5	2.6**
1	32.5	33.5
2	29.7	28.6
3	4.8	3.1**
4	16.1	12.4

h=-9 k=-1

1	51.9	44.7
2	28.2	22.2
3	31.0	28.0
4	60.7	61.3
5	16.9	13.7
6	51.3	57.6
7	51.2	56.4

h=-7 k=-1

1	17.5	11.0
2	14.1	15.3
3	17.6	12.0
4	50.1	46.9
5	16.2	12.0
6	12.2	15.8
7	31.0	29.7
8	8.5	3.0

h=-5 k=-1

1	10.5	7.2
2	32.8	28.0
3	60.6	59.8
4	23.0	22.6
5	36.1	39.7
6	4.5	8.0**
7	8.5	8.4
8	11.7	7.8
9	24.1	30.0

h=-3 k=-1

1	26.7	28.3
2	19.7	21.6
3	80.2	87.1
4	36.3	36.6
5	92.6	101.2
6	100.1	106.3
7	89.1	90.4
8	26.7	29.8
9	76.7	80.6
10	18.5	21.0

h=-1 k=-1

1	6.9	5.8
2	25.3	25.8
3	69.4	74.8
4	3.7	5.0**
5	9.4	10.7
6	42.3	43.3
7	8.9	11.1
8	33.0	35.9
9	21.8	27.6
10	19.7	19.1

h= 1 k=-1

1	13.1	13.0
2	71.2	74.9
3	29.7	34.0
4	56.6	57.6
5	22.1	23.2
6	6.4	1.8**
7	7.4	7.5**
8	22.2	28.6
9	5.0	1.0**

h= 3 k=-1

0	25.2	36.6*
1	15.0	15.0
2	86.2	80.3
3	41.8	36.4
4	99.0	91.1
5	112.1	103.6
6	109.3	101.5
7	27.5	27.0
8	85.5	76.9
9	24.8	25.5

h= 5 k=-1

0	20.8	22.5
1	20.0	20.7
2	65.9	61.9
3	6.0	0.7**
4	4.5	10.2**
5	31.5	26.9
6	13.2	13.2
7	37.3	33.0

h= 7 k=-1

0	6.6	6.1**
1	47.4	45.[illegible]
2	25.5	28.5
3	35.2	29.3
4	30.5	24.1
5	12.1	9.7
6	15.1	3.8*

h= 9 k=-1

0	20.0	18.0
1	57.4	53.3
2	24.7	21.5
3	45.3	42.3

h=-10 k= 0

1	17.3	15.2
2	25.5	19.7
3	19.3	12.4
4	29.5	23.1
5	29.4	24.1

h=-8 k= 0

1	56.5	48.9
2	34.7	31.2
3	5.7	2.6**
4	31.5	29.0
5	35.2	34.1
6	36.0	35.8
7	86.2	90.8
8	38.9	43.8

h=-6 k= 0

1	145.7	124.7*
2	102.1	89.4*
3	50.6	51.3
4	76.8	82.8
5	24.1	20.9
6	27.6	33.6
7	37.9	45.6
8	65.6	71.0
9	11.0	18.1

h=-4 k= 0

1	94.5	80.9*
2	74.4	71.2
3	91.9	92.6
4	80.9	84.9
5	70.1	75.9
6	51.1	53.5
7	26.5	33.2
8	25.3	25.9
9	4.7	6.3**
10	12.2	15.9

h=-2 k= 0

1	6.8	6.2
2	22.4	20.9
3	77.9	81.9
4	21.7	20.3
5	29.9	35.0
6	32.2	37.1
7	20.0	20.3
8	13.5	14.4
9	15.4	19.7
10	5.0	3.6**

h= 0 k= 0

3	108.7	101.3
4	6.4	9.4**
5	5.2	11.6**
6	110.2	106.4
7	8.2	18.2**
8	110.4	107.5
9	13.1	20.9**
10	107.6	92.9*

h= 2 k= 0

0	33.2	27.8
1	42.4	37.6
2	61.0	46.3*
3	50.4	46.9
4	13.8	12.0
5	19.1	17.6
6	17.2	15.6
7	43.7	40.9
8	19.3	22.8
9	24.6	22.8

h= 4 k= 0

0	33.5	26.7
1	40.8	24.0*
2	32.3	30.4
3	63.9	60.9
4	105.6	92.5*
5	132.0	116.3*
6	38.2	35.7
7	22.6	19.6
8	9.9	10.7

h= 6 k= 0

0	118.0	116.4
1	41.3	40.6
2	85.9	86.0
3	31.2	31.3
4	22.2	17.1
5	41.9	34.7
6	86.4	73.2*
7	24.0	19.9

h= 8 k= 0

0	49.4	47.7
1	52.2	49.8
2	39.4	38.4
3	67.2	60.9
4	27.0	24.8
5	17.6	13.2

h=10 k= 0

0	21.1	9.5*
1	34.6	30.9

h=-9 k= 1

1	22.9	30.3
2	47.7	59.3*
3	59.7	72.0*
4	29.1	30.9
5	66.2	77.5*
6	38.3	43.6

h=-7 k= 1

1	10.5	9.7
2	10.0	17.7
3	41.1	43.2
4	26.7	21.0
5	26.9	28.8
6	17.8	15.6
7	16.8	14.3
8	5.2	8.9**

h=-5 k= 1

1	20.8	24.8
2	11.9	13.6
3	36.0	43.1
4	33.1	38.9
5	9.6	10.1
6	4.5	2.8**
7	17.4	21.8
8	35.7	38.1
9	6.9	3.3**

h=-3 k= 1

1	88.8	106.5*
2	135.8	156.2*
3	88.7	96.7
4	131.1	146.9*
5	84.2	88.2
6	47.1	49.1
7	11.5	18.3
8	70.0	70.5
9	5.8	6.5**

h=-1 k= 1

0	12.1	13.0
1	7.7	9.8
2	64.0	71.1
3	25.0	27.6
4	27.1	30.7
5	31.3	32.7
6	16.3	15.7
7	18.0	17.9
8	31.5	38.5
9	17.4	20.4

h= 1 k= 1

0	29.2	28.1
1	34.6	33.5
2	52.4	49.6
3	70.7	66.9
4	14.4	5.3
5	11.5	1.5
6	17.7	16.7
7	38.6	36.0
8	4.8	2.9**
9	14.5	15.4

h= 3 k= 1

0	85.8	92.3
1	146.1	154.2
2	99.1	98.3
3	146.3	142.4
4	105.5	96.6
5	60.2	54.8
6	15.5	9.6
7	78.7	67.1*
8	7.4	7.7**

h= 5 k= 1

0	3.8	10.0**
1	49.5	52.3
2	30.2	30.4
3	4.3	4.5**
4	34.7	32.7
5	13.3	4.2
6	23.7	17.4
7	42.8	39.3

h= 7 k= 1

0	35.8	29.8
1	35.9	30.7
2	46.0	45.0
3	13.2	9.7
4	10.9	0.9
5	5.0	4.4**

h= 9 k= 1

0	73.9	73.3
1	36.7	38.3
2	59.7	66.6
3	51.1	53.0

h=-10 k= 2

1	31.4	26.2
2	31.3	32.8

h=-8 k= 2

1	8.8	1.4
2	20.1	24.8
3	34.8	39.4
4	20.6	26.5

5	21.7	26.6
6	4.8	1.9**

h=-6 k= 2

1	60.0	72.3*
2	92.4	109.8*
3	27.5	28.3
4	37.8	40.6
5	55.3	62.2
6	89.4	97.5
7	21.8	20.5
8	73.7	78.5

h=-4 k= 2

0	32.8	32.7
1	9.2	6.2
2	21.9	27.0
3	39.0	49.3*
4	14.2	15.3
5	4.3	1.5**
6	34.9	38.7
7	12.5	14.9
8	20.8	21.6
9	26.6	31.8

h=-2 k= 2

0	22.6	21.5
1	11.6	11.4
2	61.0	62.6
3	6.2	7.0**
4	52.0	55.5
5	106.2	111.0
6	97.0	94.6
7	40.0	43.9
8	11.0	5.2
9	12.2	11.6

h= 0 k= 2

0	30.3	35.9
1	13.7	15.2
2	83.6	82.4
3	39.3	35.1
4	98.5	91.8
5	117.5	106.5*
6	114.0	97.8*
7	32.1	29.4
8	90.5	77.0*
9	24.0	23.5

h= 2 k= 2

0	53.1	53.8
1	108.2	105.4
2	78.5	75.3
3	94.5	87.7
4	62.6	59.5
5	54.4	49.5

6	14.0	11.5
7	8.6	4.8**
8	10.6	6.4

h= 4 k= 2

0	5.3	0.9**
1	49.6	46.4
2	39.4	36.5
3	25.2	19.7
4	20.6	17.4
5	12.7	6.6
6	20.6	10.3*
7	30.7	28.6

h= 6 k= 2

0	75.7	82.4
1	33.3	38.3
2	35.3	36.4
3	44.6	42.2
4	102.1	103.9
5	32.3	27.4
6	80.8	78.4

h= 8 k= 2

0	12.7	10.7
1	45.2	43.0
2	4.8	3.5**
3	9.9	7.5

h=-9 k= 3

1	60.0	64.0
2	41.5	45.4
3	21.3	23.0

h=-7 k= 3

0	7.3	9.8**
1	32.1	35.8
2	23.4	21.5
3	14.6	15.3
4	33.8	35.7
5	4.7	5.0**
6	14.7	10.5

h=-5 k= 3

0	12.1	8.7
1	4.3	6.5**
2	12.5	11.9
3	51.1	56.3
4	15.1	11.9
5	19.7	20.9
6	23.9	23.0
7	10.6	8.7

h=-3 k= 3

0	124.4	126.5
1	101.5	104.1
2	40.0	40.2
3	83.7	88.5
4	27.6	23.5
5	25.2	24.3
6	46.1	44.7
7	79.4	71.6
8	20.4	19.4

h=-1 k= 3

0	32.2	33.3
1	50.0	51.4
2	20.1	23.6
3	41.3	44.8
4	13.2	12.3
5	24.3	22.6
6	6.2	7.8**
7	32.7	33.3
8	26.1	23.5

h= 1 k= 3

0	18.4	12.1
1	23.7	11.7*
2	68.3	66.1
3	19.2	11.6
4	12.7	11.0
5	22.6	19.0
6	20.5	16.5
7	23.8	17.6

h= 3 k= 3

0	107.8	105.8
1	48.9	50.8
2	79.3	81.5
3	28.6	28.1
4	26.0	25.3
5	31.6	27.8
6	91.0	77.2*
7	24.8	20.6

h= 5 k= 3

0	38.4	36.5
1	25.7	23.1
2	39.0	36.4
3	20.6	20.0
4	15.3	11.2
5	4.9	2.2**

h= 7 k= 3

0	16.8	13.9
1	49.2	51.4
2	14.2	11.2
3	4.8	1.5**

h=-8 k= 4

0	29.1	30.4
1	26.4	30.9
2	5.0	5.6**

h=-6 k= 4

0	27.4	29.2
1	52.4	58.3
2	66.4	69.0
3	32.2	36.6
4	68.0	72.0
5	45.9	45.3

h=-4 k= 4

0	36.3	41.8
1	44.2	57.5*
2	32.2	37.6
3	55.1	61.7
4	27.8	30.3
5	58.4	60.6
6	14.0	15.2

h=-2 k= 4

0	11.9	12.3
1	12.6	11.2
2	43.1	40.4
3	37.9	37.7
4	10.6	1.5
5	12.8	1.1*
6	13.9	14.9

h= 0 k= 4

0	152.1	157.5
1	42.2	41.8
2	77.9	76.9
3	87.5	86.1
4	86.9	83.1
5	12.8	4.3
6	67.1	64.1

h= 2 k= 4

0	6.3	6.0**
1	42.9	42.0
2	19.6	20.3
3	20.6	19.7
4	35.2	32.8
5	4.6	3.3**
6	18.1	10.1

h= 4 k= 4

0	6.6	6.3**
1	7.1	8.5**
2	14.0	13.5
3	83.0	75.2
4	72.8	61.3*
5	63.5	54.2

h= 6 k= 4

0	80.8	78.7
1	36.4	33.4
2	68.4	66.0
3	57.2	57.7

h=-5 k= 5

0	8.9	3.5**
1	8.1	9.4**
2	30.9	27.8
3	25.9	20.6

h=-3 k= 5

0	28.2	26.4
1	26.3	23.9
2	58.5	57.1
3	23.9	19.4
4	49.3	49.8

h=-1 k= 5

0	10.9	8.1
1	17.9	15.3
2	30.3	33.7
3	14.9	15.9
4	4.8	2.8**

h= 1 k= 5

0	4.4	2.6**
1	35.8	35.7
2	37.8	36.2
3	14.8	13.8
4	10.7	6.7

h= 3 k= 5

0	16.4	15.3
1	61.8	59.4
2	21.7	19.1
3	45.3	41.6

h= 5 k= 5

0	21.7	16.1
1	37.7	31.2

h=-2 k= 6

0	12.8	8.6

h= 0 k= 6

0	58.2	54.2
1	23.1	22.9