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# Takéuchiite, a new oxyborate mineral from Långban, Sweden

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**Abstract**

Takéuchiite, $Mg_{1.59}Mn^{2+}_{0.42}Mn^{3+}_{0.78}Fe^{3+}_{0.19}Ti^{4+}_{0.01}BO_5$, occurs as acicular crystals in granular dolomite and calcite from the Långban mine, Värmland, Sweden. It is orthorhombic, space group *Pnnm* or *Pnn*2 with $a = 27.50(1)$, $b = 12.614(2)$, $c = 6.046(1)$Å, $V = 2097$Å$^3$, $Z = 24$. The strongest lines in the X-ray diffraction pattern ($d$, in Å; intensity; *hkl*) are: 1.511, 100, 004; 2.60, 90, 640; 5.20, 85, 320; 2.035, 80, 850 (and 922, 10 02) and 3.02, 65, 002. Takéuchiite is black and opaque with metallic luster and brown streak and has a hardness of 6. The calculated density is 3.93 g/cm$^3$. Morphologically, takéuchiite forms long prismatic crystals with dominant form {320}.

## Introduction

This new mineral was first identified in a high-resolution electron microscope during an extensive investigation of synthetic and natural oxyborates of the pinakiolite family (Bovin *et al.*, 1980a; Bovin and O'Keeffe, 1980). The electron diffraction pattern and electron micrographs showed that it was a new species, and we take pleasure in naming it takéuchiite in honor of Professor Yoshio Takéuchi of the University of Tokyo. He predicted (Takéuchi, 1978) the existence of a compound with the structure found for the new mineral (Bovin *et al.*, 1980b), and he has also made a major contribution to the understanding of the pinakiolite family of minerals by solving the structures of orthopinakiolite (Takéuchi *et al.*, 1978) and ludwigite (Takéuchi *et al.*, 1950). The new mineral and the name have been approved by the Commission on New Minerals and Mineral Names, IMA. The holotype is deposited in the mineral collection of the Smithsonian Institution (catalog #138548). A piece of that specimen will also be deposited in the Swedish Museum of Natural History (Naturhistoriska Riksmuseet) in Stockholm, Sweden.

## Occurrence

Takéuchiite was found in a Långban specimen labeled orthopinakiolite (catalog #138548) from the Smithsonian Institution. Studies in a high-resolution electron microscope showed that all dark crystals in that specimen were takéuchiite and not orthopinakiolite. The paragenesis is the same as for orthopinakiolite. The crystals are imbedded in a coarse-grained dolomite which also contains a considerable amount of calcite (not mentioned in earlier descriptions of pinakiolite and orthopinakiolite specimens). To find out if the new mineral also occurred with orthopinakiolite, the specimen used by Takéuchi *et al.* (1978) from the Swedish Museum of Natural History (catalog #R332376) was carefully investigated in the electron microscope, but no crystals of takéuchiite were found in it. Specimens of pinakiolite (Smithsonian #B12313 and Naturhistoriska Riksmuseet #R31527) were investigated also and likewise no takéuchiite was found. The morphology of takéuchiite, orthopinakiolite, and ludwigite (not reported from Långban) are very similar; it is therefore possible that other specimens labeled orthopinakiolite from Långban could be takéuchiite.

## Crystallography

Single crystals of the new mineral were studied by Weissenberg X-ray techniques. These showed that takéuchiite has space group *Pnnm* or *Pnn*2. Electron diffraction patterns recorded along the shortest axis (Fig. 1) revealed the same lattice parameters as X-ray diffraction, but showed in thick crystals the appearance of forbidden (in X-ray) reflections caused by dynamical scattering. The lattice parameters obtained from the single-crystal studies were refined by least-squares calculations of powder-diffraction data

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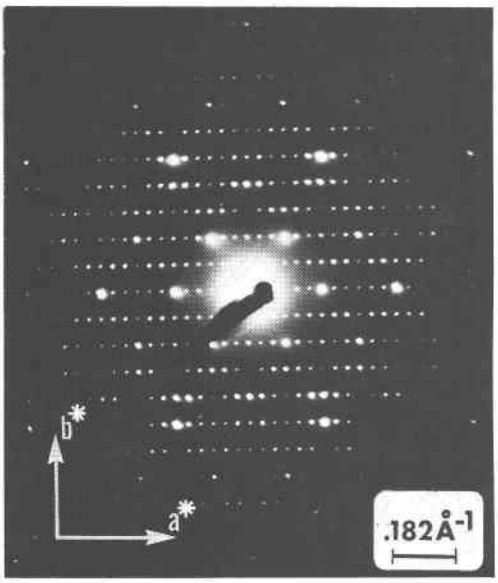


Fig. 1. Electron diffraction pattern recorded with the electron beam parallel to the *c* axis of a crystal of takéuchiite.

obtained with a Guinier-Hägg focussing camera using Cu$K\alpha$ radiation and with KCl ($a$ = 6.2929Å) as an internal standard. All the lines could be indexed with the orthorhombic cell: $a$ = 27.50(1), $b$ = 12.614(2) and $c$ = 6.046(1)Å. The powder-diffraction data of takéuchiite are listed in Table 1.

The crystal structure of takéuchiite is closely related to the other members of the pinakiolite family (Bovin *et al.*, 1980b). As can be seen from Table 2, *b* and *c* are almost identical to those of the ludwigite and orthopinakiolite.

Table 1. Powder diffraction data for takéuchiite. Intensities visually estimated

| $I/I_0$ | d(obs) | d(calc) | h k l | $I/I_0$ | d(obs) | d(calc) | h k l |
|---|---|---|---|---|---|---|---|
| 5 | 6.07 | 6.05 | 0 0 1 | 5 | 2.007 | 2.008 | 10 1 2 |
| 5 | 5.92 | 5.90 | 1 0 1 | | | 2.010 | 1 0 3 |
| 20 | 5.74 | 5.73 | 2 2 0 | 30 | 1.997 | 1.998 | 8 3 2 |
| 10 | 5.35 | 5.35 | 1 1 1 | 5 | 1.960 | 1.961 | 10 4 1 |
| 85 | 5.20 | 5.20 | 3 2 0 | 45 | 1.939 | 1.941 | 3 6 1 |
| 65 | 3.02 | 3.02 | 0 0 2 | 50 | 1.915 | 1.915 | 1 2 3 |
| 40 | 2.76 | 2.76 | 6 3 1 | 25 | 1.646 | 1.647 | 5 6 2 |
| 70 | 2.73 | 2.73 | 0 2 2 | 60 | 1.582 | 1.581 | 7 7 1 |
| 90 | 2.60 | 2.60 | 6 4 0 | 20 | 1.562 | 1.562 | 9 3 3 |
| 60 | 2.526 | 2.523 | 6 0 2 | 40 | 1.537 | 1.537 | 4 8 0 |
| 10 | 2.458 | 2.459 | 7 4 0 | 30 | 1.523 | 1.523 | 1 8 1 |
| 5 | 2.356 | 2.354 | 7 1 2 | 100 | 1.511 | 1.511 | 0 0 4 |
| 45 | 2.238 | 2.239 | 7 2 2 | 60 | 1.471 | 1.470 | 0 2 4 |
| 70 | 2.209 | 2.210 | 6 5 0 | 55 | 1.380 | 1.381 | 9 7 2 |
| 10 | 2.075 | 2.076 | 6 5 1 | 60 | 1.305 | 1.305 | 5 7 3 |
| | | 2.034 | 8 5 0 | | | | |
| 80 | 2.035 | 2.034 | 9 2 2 | | | | |
| | | 2.034 | 10 0 2 | | | | |

Table 2. Crystal data for pinakiolite-related minerals

| Mineral | a | b | c | β | S.G. |
|---|---|---|---|---|---|
| Pinakiolite | 21.79 | 5.977 | 5.341 | 95.83 | *C2/m* |
| Hulsite | 10.695 | 3.102 | 5.431 | 94.21 | *P2/m* |
| Ludwigite | 9.14 | 12.45 | 3.05 | | *Pbam* |
| Vonsenite | 9.73 | 12.35 | 3.05 | | *Pbam* |
| Orthopinakiolite | 18.375 | 12.591 | 6.068 | | *Pnnm* |
| Takéuchiite | 27.50 | 12.614 | 6.046 | | *Pnnm* |

## Morphology

Takéuchiite occurs as acicular, isolated crystals (Fig. 2). The dominant form is {320} as can be seen in a cross section of the crystal in Figure 3. The crystal faces are sometimes striated in the *c*-axis direction due to alternating growth of other forms together with {320}. The indices of the other forms have not been determined. Some crystals have terminated


Fig. 2. Photograph of two takéuchiite crystals imbedded in dolomite/calcite.

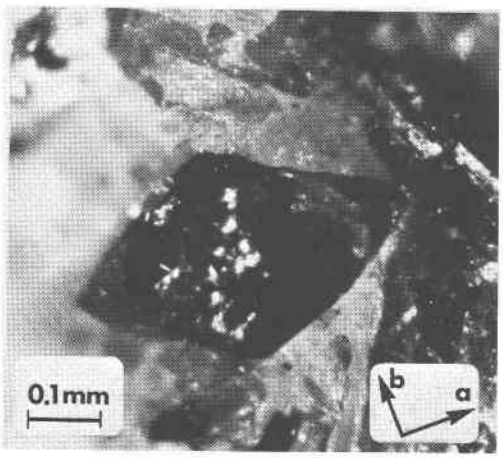


Fig. 3. Photograph showing the cross section of a takéuchiite crystal.

ends with crystal faces not parallel to the *c* axis. Such faces are very small and have not been indexed. The crystals can be up to 10 mm long and 0.5 mm thick. Fracture is uneven.

## Physical properties

Takéuchiite is black with metallic luster at crystal faces. The opacity precluded measurements of reliable optical parameters. Its streak is brown. The hardness (Mohs) is approximately 6, the same as for orthopinakiolite. The calculated density is 3.93 g/cm$^3$. Takéuchiite shows no fluorescence in ultraviolet radiation and is not ferromagnetic. Crystals are fairly stable in an electron beam accelerated at 100 kV.

## Chemistry

Crystals of takéuchiite were chemically analyzed with the Cameca MS46 electron microprobe of the Arizona State University microprobe laboratory, utilizing an operating voltage of 15 kV (10 kV for light elements) and a beam current of 45 nA (or 150 nA for light elements). The standards used were rhodonite for Mn, Springwater olivine for Mg, Fe, Si, and sphene for Ca and Ti. In determining boron, pinakiolite was used as standard, and it was found that, within experimental error, the content of boron is the same for pinakiolite and takéuchiite. A wavelength-dispersive scan indicated no other elements with atomic number greater than nine. Calcium and silicon were found in trace amount only. The mean value of 12 analysis points of four different crystals is presented in Table 3 and is compared with published analyses for pinakiolite and orthopinakiolite. No investigation was performed to determine the oxidation state of iron, but judging from orthopinakiolite (Takéuchi *et al.*, 1978) iron should be trivalent. Takéuchiite is intermediate in composition between orthopinakiolite and pinakiolite, as might be expected from structural considerations (Bovin *et al.*, 1980b).

Table 3. Chemical analyses of elemental percentages for takéuchiite, pinakiolite, and orthopinakiolite. Standard deviations for the last digit are given within brackets for takéuchiite

| Elements | Mineral | | |
|---|---|---|---|
| | Pinakiolite* | Orthopinakiolite** | Takéuchiite |
| Mg | 20.7 | 16.7 | 18.6(3) |
| Mn | 32.0 | 34.4 | 31.7(5) |
| Al | 0.7 | — | — |
| Fe | 0.6 | 5.8 | 5.2(1) |
| Ti | 0.1 | | 0.3 |
| B | 5.4 | | ~5.4 |
| O | 39.8 | | (38.8)*** |

*"theoretical" formula of Moore and Araki (1974)
**Takéuchi (1978)
***by difference

The ideal formula of minerals of the pinakiolite family is $M_3BO_5$, where M represents octahedrally-coordinated ions of total charge +7. Accordingly, we have used the analysis reported to Table 3 to calculate the atomic composition, based on three octahedral cations: $Mg_{1.59}Mn^{2+}_{0.42}Mn^{3+}_{0.78}Fe^{3+}_{0.19}Ti^{4+}_{0.01}BO_5$. The elemental composition in weight percent according to this formula is Mg 18.7, Mn 31.9, Fe 5.1, Ti 0.3, B 5.2, O 38.7, in close agreement with that observed. The percentage figures computed from the ideal structure can differ from the experimentally determined ones because crystals of takéuchiite as well as those of pinakiolite and orthopinakiolite contain a

Table 4. Chemical formula for $M_3BO_5$ minerals related to pinakiolite

| Mineral & Reference | Structural Formula |
|---|---|
| Pinakiolite<br>Moore & Araki (1974) | $Mg_{1.68}Mn^{2+}_{0.09}Mn^{3+}(Al^{3+},Fe^{3+},Mn^{4+})_{0.11}BO_5$ |
| Hulsite<br>Konnert *et al.* (1976) | $Mg_{0.64}Fe^{2+}_{1.46}Fe^{3+}_{0.67}Sn^{4+}_{0.20}BO_5$ |
| Ludwigite<br>Takéuchi *et al.* (1950) | $(Mg,Fe^{2+})_2Fe^{3+}BO_5$ |
| Vonsenite<br>Takéuchi (1956) | $Mg_{0.75}Fe^{2+}_{1.25}Fe^{3+}BO_5$ |
| Orthopinakiolite<br>Takéuchi *et al.* (1978) | $Mg_{1.42}Mn^{2+}_{0.43}Mn^{3+}_{0.88}Fe^{3+}_{0.22}BO_5$ |
| Takéuchiite<br>this work | $Mg_{1.59}Mn^{2+}_{0.42}Mn^{3+}_{0.78}Fe^{3+}_{0.19}Ti^{4+}_{0.01}BO_5$ |

considerable number of structural defects (Bovin *et al.*, 1980a). The structural defects are very likely associated with local deviations from the ideal stoichiometry. The chemical formula of takéuchiite is compared to the formula of the other known members of the pinakiolite family in Table 4. Takéuchiite is insoluble in concentrated HCl, $HNO_3$, and $H_2SO_4$.

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