# Dingdaohengite-(Ce) from the Bayan Obo REE-Nb-Fe Mine, China: Both a true polymorph of perrierite-(Ce) and a titanic analog at the C1 site of chevkinite subgroup

JINSHA XU,<sup>1,\*</sup> GUAMING YANG,<sup>2</sup> GUOWU LI,<sup>3</sup> ZHILAN WU,<sup>4</sup> AND GANFU SHEN<sup>1</sup>

<sup>1</sup>Chengdu Institute of Geology and Mineral Resources, 610082 Chengdu, China
 <sup>2</sup>China University of Geosciences (Wuhan), 430071 Wuhan, China
 <sup>3</sup>China University of Geosciences (Beijing), 100083 Beijing, China
 <sup>4</sup>Technologic Managerial Department, Bayan Obo Iron Mine, 014080 Baotou, China

## ABSTRACT

Dingdaohengite-(Ce), ideally Ce<sub>4</sub>Fe<sup>2+</sup>Ti<sub>2</sub>Ti<sub>2</sub>(Si<sub>2</sub>O<sub>7</sub>)<sub>2</sub>O<sub>8</sub>, is a new member of the chevkinite group minerals from the world-famous Bayan Obo REE-Nb-Fe Mine near Baotou city, Inner Mongolian Autonomous Region, North China. It occurs in the magnesian skarn in the excontact of granite within dolomitic marble. Most individual crystals vary from 0.2 to 1.0 cm in length. Associated minerals are diopside, tremolite, richterite, allanite-(Ce), magnetite, ilmenite, spinel, titanite, pyrochlore, F-rich phlogopite, fluorapatite, quartz, and fluorite, etc. Dingdaohengite-(Ce) is probably of bimetasomatic origin among Ca-Mg-carbonate rock and/or carbonatite, and REE-, F-rich postmagmatic hydrothermal solutions. The mineral is black and becoming brown black in thin fragments. It is translucent to opaque with a submetallic-metallic luster, and a brown streak. It is brittle with conchoidal fracture. No cleavage or parting is observed. Its hardness is VHN<sub>25g</sub> 606.0–717.4 kg/mm<sup>2</sup> (Mohs hardness near 5.9). The measured density is 4.83(7) g/cm<sup>3</sup> and the calculated density is 4.88(0) g/cm<sup>3</sup>. Its reflectance values (for  $\lambda = 589$  nm) are 11.4–12.5%. It is biaxial negative. The strongest six X-ray diffraction lines in the powder pattern [*d* in Å (*I*) (*hkl*)] are 2.7524(100)(T21), 2.7263(98)(313), 3.1978(68)(212), 2.5460(54)(304), 2.8702(52)(020), and 3.1622(46)(312).

An electron-microprobe analysis on the crystal used to collect X-ray intensity data for crystalstructure refinement gives SiO<sub>2</sub> 19.29, TiO<sub>2</sub> 18.26, Al<sub>2</sub>O<sub>3</sub> 0.04, FeO 8.49, Fe<sub>2</sub>O<sub>3</sub> 1.67, ThO<sub>2</sub> 0.16, MgO 1.32, CaO 2.17, Nb<sub>2</sub>O<sub>5</sub> 0.47, Ta<sub>2</sub>O<sub>5</sub> 0.00, La<sub>2</sub>O<sub>3</sub> 19.53, Ce<sub>2</sub>O<sub>3</sub> 28.08, Nd<sub>2</sub>O<sub>3</sub> n.d., Y<sub>2</sub>O<sub>3</sub> 0.00, Na<sub>2</sub>O 0.00, sum 99.48 wt%; the Fe<sup>3+</sup>/Fe<sup>2+</sup> ratio was converted by Mössbauer spectroscopy. The empirical formula is  $(Ce_{2.13}La_{1.49}Ca_{0.48}Th_{0.01})_{\Sigma \pm 11}Fe^{2+}(Ti_{0.88}Fe^{2+}_{0.47}Mg_{0.41}Fe^{3+}_{0.26}Al_{0.01})_{\Sigma \pm 0.3}(Ti_{1.96}Nb_{0.04})_{\Sigma \pm 0.0}(Si_2O_7)_2O_8$ , based on 22 O atoms with prevalence of Ti in the C1 site of the structure. Dingdaohengite-(Ce) is monoclinic, *a* = 13.4656(15) Å, *b* = 5.7356(6) Å, *c* = 11.0977(12) Å,  $\beta$  = 100.636(2)°, *V* = 842.39(46) Å<sup>3</sup>, and *Z* = 2.

The crystal structure of dingdaohengite-(Ce) was refined with space groups  $P2_1/a$  and C2/m. Pseudo-extinction was found, i.e., reflections with h + k = 2n are systematically strong, while those with h + k = 2n + 1 are weak, which show that the true space group of dingdaohengite-(Ce) is  $P2_1/a$  (pseudo-C2/m).

**Keywords:** Dingdaohengite-(Ce),  $P2_1/a$  (pseudo-C2/m) space group, chevkinite subgroup, new mineral, Bayan Obo, China

# INTRODUCTION

Chevkinite is not only a name given to a mineral species; it is also a group and subgroup name for the REE (or Sr)-Fe (or Zr)-Ti silicate minerals. As a mineral species from Urals, Russia, it was named after General-Major Konstatin Vladimirovich Tschevkin (Chevkin) (1802–1875), Chief of Staff of the Russian Mining Engineers Corps., by a German mineralogist Rose as early as 1839 (Vlasov et al. 1964). About 150 years later, it had been redefined as chevkinite-(Ce) by Nickel and Mandarino (1987). The chevkinite group can be divided into two subgroups according to the  $\beta$  angle: the chevkinite subgroup with  $\beta \approx 100^{\circ}$ and the perrierite subgroup with  $\beta \approx 113^{\circ}$ . Chevkinite-(Ce), polyakovite-(Ce) (Popov et al. 2001), and maoniupingite-(Ce) (Shen et al. 2005) should fit into the chevkinite subgroup. Strontiochevkinite, which has been described by Haggerty and Mariano (1983), is isostructural with perrierite-(Ce) but not with chevkinite-(Ce) (Toraya 1993; Miyawaki et al. 2002). It is noteworthy that the actual space groups of chevkinite group minerals and its synthetic materials are under discussion in the past 50 years, and a natural member with space group  $P2_1/a$  in this mineral subgroup has not been found.

Fortunately, we found such a mineral, which is isostructural with chevkinite-(Ce), space group  $P2_1/a$  with Ti dominant at the

<sup>\*</sup> E-mail: xujinsha117@yahoo.com.cn

*C*1 site of the structure in 2004. It is obvious that this mineral should be regarded as a new mineral. The new mineral is named dingdaohengite-(Ce) after Ding Daoheng (1899–1955), who made the first discovery of the world-famous Bayan Obo REE-Nb-Fe ore deposit in 1927 and to indicate that Ce is the dominant cation of rare-earth elements of the mineral.

Although the mineral has been investigated systematically in the late twentieth century (Peng and Pan 1964; Zhang and Tao 1986; Institute of Geochemistry 1988; Zhang et al. 1998), its space group was predicated as C2/m because of technological limitations and was misdefined as chevkinite-(Ce).

The new mineral and its name have been approved by the International Mineralogical Association Commission on New Minerals and Mineral Names (IMA 2003-017). Holotype material is deposited at the Geological Museum of China, Beijing, China.

## **BACKGROUND INFORMATION**

Natural chevkinite subgroup minerals are usually highly metamict. Thus, the synthetic materials and annealed natural chevkinite subgroup mineral samples have mainly been used to analyze their structure. In this case, there were five different views on their possible space groups: (1) space group C2/m, based on the P(uvw) map and an analog to the structure of perrierite-(Ce) (Gottardi 1960; Peng and Pan 1964; Sokolova et al. 2004); (2) space group  $P2_1/a$ , based on the structural refinement for synthetic Mg-chevkinite-(Ce) and Co-chevkinite-(Ce) (Calvo and Faggiani 1974); (3) the space group for the natural material is C2/m, and the synthetic material is  $P2_1/a$  (Yang et al. 1991); (4) space group is pseudo-C2/m or  $P2_1/a$ , based on the structure determination for rengeite (Miyawaki et al. 2002); and (5) space group can be in both C2/m and  $P2_1/a$  depending on their differences in chemical composition and the order or disorder arrangement of cation in the structure (Yang et al. 2002). However, a natural mineral with space-group  $P2_1/a$  of chevkinite subgroup has not been found until dingdaohengite-(Ce) was discovered. The idealized crystal-chemical formula for chevkinite group can be written as  $A_4^{3+}B^{2+}C_2^{3+}Ti_2^{4+}(Si_2O_7)_2O_8$ , where A = REE, Th, Ca, Sr, Na, and K are in tenfold coordination;  $B = Fe^{2+}$ , Mg, Mn, and Ca are in sixfold coordination; C = Ti,  $\text{Fe}^{3+}$ ,  $\text{Fe}^{2+}$ , and Mg are in sixfold coordination (Ito and Arem 1971). It was assumed that the Ti-cation is ordered in the crystal structure. The distribution of Ti is partially ordered among C1, C(2A), and C(2B) sites in the structure of synthetic chevkinite (Calvo and Faggiani 1974). The formula can be expressed as  $A_4^{3+}B^{2+}C1_2C(2A)C(2B)(Si_2O_7)_2O_8$ , where  $A = Nd^{3+}$ ;  $B = Mg^{2+}$  or  $Co^{2+}$ ; C[C1 + C(2A) + C(2B)] =Ti<sup>4+</sup>, Mg<sup>2+</sup>, or Co<sup>2+</sup>. A natural member with Ti dominant at the C1 site of the chevkinite subgroup has not been discovered until dingdaohengite-(Ce) was found. Although perrierite-(Ce) also has Ti dominant at the C1 site, it is inappropriate to define perrierite-(Ce) as a polymorph (Peng and Pan 1964; Ito and Arem 1971) or a dimorph of chevkinite-(Ce) (Zhang et al. 1998; Mandarino 1999) because their  $\beta$  angles are different.

#### **O**CCURRENCE AND ORIGIN OF THE MINERAL

The Bayan Obo REE-Nb-Fe ore deposit is situated in Inner Mongolian Autonomous Region of North China, about 130 km north of Baotou City. It is the world's largest known rare-earth mine and an important new minerals locality (over 10 new minerals have been discovered) in China. Dingdaohengite-(Ce) occurs in a magnesian skarn in the eastern part of the mine, which is mainly found in the exocontact of granite within dolomitic marble, and less important in the endocontact of granite.

It is associated with diopside, tremolite, richterite, F-rich phlogopite (more accurately), it should be considered as an independent mineral species (Xu and Shen 2005), humite, chlinohumite, chondrodite, allanite-(Ce), magnetite, ilmentite, spinel, titanite, pyrochlore, fluorapatite, fluorellestadite(?), calcite, dolomite, pyrite, quartz, fluorite, and zircon. Subject to the traditional theory, dingdaohengite-(Ce) was perhaps a product of bimetasomatism among Ca-Mg-carbonate rock and/or carbonatite, and REE-, F-rich postmagmatic hydrothermal solutions. A detailed geological description of the mine and a full description of the corresponding mineral assemblages can be found in the work of the Institute of Geochemistry, China (1998).

# **APPEARANCE, PHYSICAL, AND OPTICAL PROPERTIES**

Dingdaohengite-(Ce) occurs as euhedral to subhedral short prismatic or thick tabular (//001) crystals. The main crystal forms of an ideal crystal are  $\{100\}$ ,  $\{001\}$ ,  $\{201\}$ ,  $\{1\overline{10}\}$ ,  $\{110\}$ ,  $\{1\overline{11}\}$ ,  $\{111\}$ ,  $\{20\overline{1}\}$ , and  $\{1\overline{10}\}$ , etc. (Zhang and Tao 1986). These forms are practically identical to those of chevkinite group minerals. Most individual crystals are 0.2–1.0 cm in length with the largest crystal exceeding 1.5 cm.

Dingdaohengite-(Ce) is black and becoming brown black in thin fragments. It is translucent to opaque with a submetallicmetallic luster, and a brown streak. It is brittle with conchoidal fracture. No cleavage or parting is observed. It does not fluorescence in either long- or short-wave ultraviolet light. The mineral is not magnetic. It is moderately electromagmatic. The density, measured by hydrostatic weighing in distilled water, is 4.83(7) g/cm<sup>3</sup> (mean of two determinations) and the calculated density is 4.88(0) g/cm<sup>3</sup>. Dingdaohengite-(Ce) shows a Mohs hardness of 5.9, and micro-indentation tests gave a mean of 650.3 kg/mm<sup>2</sup> with range of 606.0–717.4 kg/mm<sup>2</sup> (VNH load 25 g).

In reflected light, dingdaodengite-(Ce) is grayish yellow and shows weak anisotropy and bireflectance. Pleochroism is observed with different gray tones. Its reflectance values are given in Table 1.

In transmitted light, dingdaohengite-(Ce) is strongly pleochroic,  $\mathbf{X} =$  yellowish or brownish and  $\mathbf{Z} =$  brown black. It is biaxial negative, with large  $2V (\approx 60^\circ)$ , and  $n_\alpha = 1.978 \pm 0.005$ ,  $n_\gamma = 2.010 \pm 0.005$  (white light) (Zhang and Tao 1986) ( $n_\beta$  has not

| R <sub>min</sub> (%)  | R <sub>max</sub> (%) | λ (nm) |  |  |  |  |
|---|----------------------|--------|--|--|--|--|
| 10.1  | 10.4                 | 400    |  |  |  |  |
| 10.4  | 10.9                 | 420    |  |  |  |  |
| 10.7  | 10.8                 | 440    |  |  |  |  |
| 10.7  | 11.0                 | 460    |  |  |  |  |
| 11.0  | 11.8                 | 470    |  |  |  |  |
| 11.2  | 11.8                 | 480    |  |  |  |  |
| 11.4  | 11.8                 | 500    |  |  |  |  |
| 11.6  | 12.1                 | 560    |  |  |  |  |
| 11.6  | 11.9                 | 580    |  |  |  |  |
| 11.4  | 12.5                 | 589    |  |  |  |  |
| 11.0  | 11.8                 | 600    |  |  |  |  |
| 10.6  | 11.7                 | 620    |  |  |  |  |
| 10.6  | 11.6                 | 640    |  |  |  |  |
| 10.6  | 11.8                 | 650    |  |  |  |  |
| Note: CiC uses used on the standard in sim Analyzaw Chan Jianui |                      |        |  |  |  |  |

Note: SiC was used as the standard in air; Analyzer: Shen Jiagui.

been determined). The dispersion is r > v. Twinning can sometimes be observed. The optical orientation is  $\mathbf{Y} = \mathbf{b}$ ,  $c \wedge r \approx 4^{\circ}$ . A Gladstone-Dale calculation gives a compatibility index of 0.025, which is rated as excellent (Mandarino 1981).

The differential thermal analysis curve of dingdaohengite-(Ce) reveals no distinct changes between 330 and 1200 °C (Fig. 1).

## Spectroscopic characterization

The infrared spectrum of dingdaohengite-(Ce) between 300 and 3800 cm<sup>-1</sup> was recorded using a PECo. 938 G-4 infrared spectrometer. The spectrum of the mineral is shown in Figure 2.

Mössbauer spectrum from dingdaohengite-(Ce) (Fig. 3) has been obtained at room temperature. The spectrum consists of three quadruple doublets: two for Fe<sup>2+</sup> and one for Fe<sup>3+</sup>. Mössbauer parameters and Fe<sup>3+</sup>/ $\Sigma$ Fe ratios of the mineral are given in Table 2.

#### **CHEMICAL COMPOSITION**

Chemical analyses were carried out with a JCXA-733 electron microprobe, operating in wavelength-dispersive mode with excitation voltage of 15–25 kV, specimen current 20 nA, and a 1–2  $\mu$ m beam diameter. The following standards were used: synth-CaSiO<sub>3</sub> (Si, Ca), K-feldspar (Al), ilmenite (Ti), synth-ThO<sub>2</sub> (Th), "titanomagnetite" (Fe), forsterite (Mg), synth-Nb<sub>2</sub>O<sub>5</sub> (Nb), La-bearing glass (La), and Ce-bearing glass (Ce). The mean of five analyses from the crystal used to collect X-ray intensity data for crystal-structure refinement, with ranges and standards employed are given in Table 3. It is discovered that dingdaohengite-(Ce) is characterized by Ti and Fe enrichment in the chevkinite subgroup minerals.

In the light of 22 atoms of oxygen per formula unit and Ti occupancy at the C1 site from the structural analysis, the empirical formula of dingdaohengite-(Ce) calculated is  $(Ce_{2.13}La_{1.49}Ca_{0.48}Th_{0.01})_{\Sigma 4.11}Fe^{2+}(Ti_{0.88}Fe^{2+}_{0.47}Mg_{0.41}Fe^{2+}_{0.26}Al_{0.01})_{\Sigma 2.03}(Ti_{1.96}Nb_{0.04})_{\Sigma 2.00}Si_4O_{22}$ , the simplified formula is (Ce,  $La)_4Fe^{2+}(Ti, Fe^{2+}, Mg, Fe^{3+})_2Ti_2Si_4O_{22}$ , ideally  $Ce_4Fe^{2+}Ti_2Ti_2Si_4O_{22}$ . To the authors' knowledge this is the first time that a naturally occurring dingdaohengite-(Ce) with Ti dominant at the C1 site of the structure in the chevkinite subgroup has been described

 
 TABLE 2.
 Mössbauer parameter for dingdaohengite-(Ce) at room temperature (Analyzer: Huang Hongbo)



**FIGURE 1.** Differential thermal curve of dingdaohengite-(Ce). Analyzer: Yuan Zuanru.

and reported.

Dingdaohengite-(Ce) does not dissolve in aqua regia, HCl, and HNO<sub>3</sub>. It does however dissolve slowly in  $H_2SO_4$  and  $H_3PO_4$ .

# X-RAY CRYSTALLOGRAPHY AND CRYSTAL-STRUCTURE DETERMINATION

Dingdaohengite-(Ce) is poor in uranium and thorium; it is non-metamict and crystalline in nature. The X-ray powder diffraction data were obtained using a DMX/IIA-type diffractometer with Ni-filtered CuK $\alpha$  radiation. The indexed powder pattern and refined cell dimensions are given in Table 4. From the unit-cell parameters, the axial ratios of the mineral are *a:b:c* = 2.35:1.00:1.93.

The structure of dingdaohengite-(Ce) was refined, using the SHELXTL/PC (Bruker AXS, Inc.) with space group  $P2_1/a$  and C2/m separately, based on 2372 reflections. Their results show that both models have an excellent *R* factor:  $R_1 = 0.027$  with  $P2_1/a$  and  $R_1 = 0.021$  with C2/m. To distinguish between the two space groups,  $P2_1/a$  and C2/m, the distribution of diffraction intensities of dingdaohengite-(Ce) were investigated. Pseudo-extinction was found, i.e., reflections with h + k = 2n condition are systematically

TABLE 3. Dingdaohengite-(Ce): Microprobe analysis\* and formula

|                                  | 5 5     |             |      |
|----------------------------------|---------|-------------|------|
| Const.                           | wt%     | Range       | apfu |
| SiO <sub>2</sub>                 | 19.29   | 18.91-19.63 | 4.00 |
| $AI_2O_3$                        | 0.04    | 0.00-0.09   | 0.01 |
| TiO <sub>2</sub>                 | 18.26   | 17.80-18.64 | 2.84 |
| ThO₂                             | 0.16    | 0.02-0.33   | 0.01 |
| FeO <sub>total</sub>             | (10.00) | 9.92-10.22  |      |
| Fe <sub>2</sub> O <sub>3</sub> † | 1.67    |             | 0.26 |
| FeO†                             | 8.49    |             | 1.47 |
| MgO                              | 1.32    | 1.23-1.42   | 0.41 |
| CaO                              | 2.17    | 1.86-2.37   | 0.48 |
| Ta₂O₅                            | 0.00    |             | 0.00 |
| Nb <sub>2</sub> O <sub>5</sub>   | 0.47    | 0.18-0.56   | 0.04 |
| $La_2O_3$                        | 19.53   | 19.31-19.98 | 1.49 |
| Ce <sub>2</sub> O <sub>3</sub>   | 28.08   | 26.06-28.52 | 2.13 |
| $Nd_2O_3$                        | n.d.    |             |      |
| $Y_2O_3$                         | 0.00    |             | 0.00 |
| Na₂O                             | 0.00    |             | 0.00 |
| Total                            | 99.48   |             |      |

Note: Type of microprobe: JCXA-733 (WDS); 15–25 Kv; 2.0  $\times$  10<sup>-8</sup> A; Beam: 1–2  $\mu m.$ 

\* Mean value of 5 analyses of the refined crystal.

 $\dagger$  Conversion by Fe  $^{3+}/Fe^{2+}$  radio from Mössbauer spectroscopy. Analyzer: Chen Zhenyu.



FIGURE 2. Infrared absorption spectrum of dingdaohengite-(Ce). Analyzer: Wu Zhiwei.

**TABLE 4.** X-ray powder diffraction data for dingdaohengite-(Ce)

|       |               |                |     |       | -             | -          |     |
|-------|---------------|----------------|-----|-------|---------------|------------|-----|
| Ī     | $d_{\rm obs}$ | $d_{\rm calc}$ | hkl | 1     | $d_{\rm obs}$ | $d_{calc}$ | hkl |
| 36 38 | 5.4612        | 5.4598         | 002 | 54 28 | 2.5460        | 2.5397     | 304 |
| 34 31 | 4.8902        | 4.8803         | 111 | 29 28 | 2.2395        | 2.2430     | 601 |
| 35 39 | 4.6154        | 4.6088         | 111 | 25 26 | 2.1704        | 2.1753     | 421 |
| 68 46 | 3.6421        | 3.6567         | 112 | 38 24 | 1.9783        | 1.9767     | 024 |
| 39 35 | 3.4890        | 3.4796         | 311 | 24 21 | 1.9649        | 1.9667     | 115 |
| 52    | 3.3424        | 3.3407         | 401 | 19    | 1.8697        | 1.8669     | 513 |
| 100   | 3.1978        | 3.2105         | 212 | 19    | 1.7259        | 1.7237     | 711 |
| 98    | 3.1622        | 3.1605         | 312 |       | 1.6364        | 1.6369     | 714 |
|       | 3.0946        | 3.1011         | 113 |       | 1.5073        | 1.5077     | 802 |
|       | 3.0199        | 3.0155         | 401 |       | 1.4696        | 1.4701     | 900 |
|       | 2.8702        | 2.8661         | 020 |       | 1.3427        | 1.3431     | 341 |
|       | 2.7524        | 2.7391         | 121 |       | 1.2739        | 1.2734     | 144 |
|       | 2.7263        | 2.7277         | 313 |       |               |            |     |

Notes: The experimental conditions were CuK $\alpha$  radiation; 30 kV; 30 mA; 4 °2 $\theta$ /min.; Ni-filter; DMX/II A-type diffractometer. The *d*-values were calculated from refined unit-cell parameters: *a* = 13.4656(15) Å, *b* = 5.7356(6) Å, *c* = 11.0977(12) Å,  $\beta$  = 100.636(2)°; Analyzers: Lei Xingrong and Yu Jishun.



**FIGURE 3.** Room-temperature Mössbauer spectrum for dingdaohengite-(Ce). Analyzer: Huang Hongbo.

TABLE 5. Comparison of the structural data for dingdaohengite-(Ce) with other related minerals

| Mineral               | Dingdaohengite<br>-(Ce) |                    | Maoniu- Pingite<br>-(Ce) | Chevkinite<br>-(Ce) | Polyakovite<br>-(Ce) | Synthetic Mg-<br>chevkinite-(Nd) | Perrierite-(Ce) |
|-----------------------|-------------------------|--------------------|--------------------------|---------------------|----------------------|----------------------------------|-----------------|
|                       | This study              | Previous study     |                          |                     |                      |                                  |                 |
| a (Å)                 | 13.4656(15)             | 13.70              | 13.385(2)                | 13.395(5)           | 13.398(1)            | 13.395(5)                        | 13.61 ± 0.02    |
| b (Å)                 | 5.7356(6)               | 5.82               | 5.742(1)                 | 5.745(2)            | 5.6974(5)            | 5.745(2)                         | 5.62            |
| c (Å)                 | 11.0977(12)             | 11.20              | 11.059(2)                | 11.086(3)           | 11.042(1)            | 11.086(3)                        | 11.67 ± 0.01    |
| Space group           | P21/a                   | C2/m               | C2/m                     | C2/m                | C2/m                 | C2/m                             | C2/m(?)         |
| β (°)                 | 100.636(2)              | 100.50             | 100.60(1)                | 100.65(3)           | 100.539(2)           | 100.65(3)                        | 113.50          |
| R*                    | 0.026                   | _                  | 0.024                    | _                   | 0.046                | _                                | _               |
| Locality              | China                   | China              | China                    | U.S.A.              | Russia               | Synthetic                        | Italy           |
| Ref.                  | The authors             | Pen and Pan (1964) | Shen et al. (2005)       | ICDD42-1394         | Popov et al. (2001)  | ICDD42-1394                      | Gottardi (1960) |
| * $R = $ final $R$ in | dex from the str        | ucture refinement. |                          |                     |                      |                                  |                 |

TABLE 6. Predominant elements in the non-silicate part of the structure, space group, and  $\beta$  angle of some chevkinite group minerals

|                     |    |    |                  | 1                | , 1   | 5 17  | 1 3         |       | 5 1                    |
|---------------------|----|----|------------------|------------------|-------|-------|-------------|-------|------------------------|
| Mineral             | A1 | A2 | В                | C1               | C(2A) | C(2B) | Space group | β°    | C = C1 + C(2A) + C(2B) |
| Chevkinite-(Ce)     | Ce | Ce | Fe <sup>2+</sup> | Fe <sup>3+</sup> | Ti    | Ti    | C2/m        | 100±  | Ti                     |
| Maonuipingite-(Ce)  | Ce | Ce | Fe <sup>3+</sup> | Fe <sup>3+</sup> | Ti    | Ti    | C2/m        | 100±  | Ti                     |
| Polyakovite-(Ce)    | Ce | Ce | Mg               | Cr <sup>3+</sup> | Ti    | Ti    | C2/m        | 100±  | Ti                     |
| Perrierite-(Ce)     | Ce | Ce | Fe <sup>2+</sup> | Ti               | Ti    | Ti    | P21/a       | 114±  | Ti                     |
| Dingdaohengite-(Ce) | Ce | Ce | Fe <sup>2+</sup> | Ti               | Ti    | Ti    | P21/a       | 100.6 | Ti                     |

strong, while those with h + k = 2n + 1 are weak. By neglecting systematically weak (h + k = 2n + 1) reflections, the space group of dingdaohengite-(Ce) "becomes" C2/m. Although the space groups  $P2_1/a$  and C2/m have the same lattice parameters, the repetition of symmetry unit with respect to the (010) mirror is a double in the C2/m model compared with the  $P2_1/a$  model. Therefore dingdaohengite-(Ce) should be regarded as having a superstructure with  $P2_1/a$  (pseudo C2/m) symmetry.

Incidentally, we have found a natural chevkinite-(Ce) specimen from Panzhihua in Sichuan Province, China. X-ray singlecrystal diffraction experiment and structure determination of the specimen revealed that its space group is C2/m, and we did not find any weak reflections violating the *C* cell in the diffraction data. A more extensive account of Panzhihua chevkinite-(Ce) will be reported separately. Sokolova et al. (2004) have reported that the space group of both annealed and unannealed chevkinite-(Ce) s from Mongolian Altay is C2/m after crystal structure refinement. Therefore, the chevkinite group minerals might have the  $P2_1/a$  as well as the C2/m space groups. In other words, both  $P2_1/a$ and C2/m are their true space groups. The discovery and study of this new mineral—dingdaohengite-(Ce) represents a significant step forward in the discussion of the true space group symmetry of the chevkinite group.

As described by Li et al. (2005), the structure of natural non-metamict Ti- and Fe<sup>2+</sup>-rich chevkinite-(Ce), or dingdaohengite-(Ce) is made up of two sheets: one is a sheet of Si<sub>2</sub>O<sub>7</sub> groups of Si-tetrahedra and *C*-octahedra, and the other is a sheet of octahedral. Both sheets are parallel to the **a-b** plane. The two sheets alternate along the **c**-axis and form a three-dimensional framework. The rare earth ions lie between the disilicate groups and the sheets of octahedra.

## **RELATIONSHIP TO OTHER SIMILAR SPECIES**

A comparison of the structural data for dingdaohengite-(Ce) and other similar mineral species are given in Table 5. The predominant elements in the non-silicate part of the structure, space group, and  $\beta$  angle of some chevkinite group minerals are listed in Table 6.

As dingdaohengite-(Ce) is a new member of the chevkinite subgroup, it shows a distinct chemical composition and unit cell with  $\beta \approx 100^{\circ}$  compared with other members of the subgroup. It is a dimorph or a polymorph of perrierite-(Ce) with Ti dominant at the *C*1 site (corresponded to the *M*2 site of Sokolova et al. 2004) of the structure.

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