Melcherite, trigonal $\text{Ba}_2\text{Na}_2\text{Mg}[\text{Nb}_6\text{O}_{19}] \cdot 6\text{H}_2\text{O}$, the second natural hexaniobate, from Cajati, São Paulo, Brazil: Description and crystal structure

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ABSTRACT

Melcherite (IMA2015-018), ideally $\text{Ba}_2\text{Na}_2\text{Mg}[\text{Nb}_6\text{O}_{19}] \cdot 6\text{H}_2\text{O}$, occurs as a vug mineral in the carbonatite of the Jacupiranga mine, Cajati county, São Paulo state, Brazil, associated with dolomite, calcite, magnetite, pyrrhotite, tochilinite, ‘pyrochlore’ and fluorapatite. This is also the type locality for zirkelite, quintinite, menezesite and pauloabibite. The mineral forms irregular, tabular crystals up to 200 µm in maximum dimension. Melcherite is transparent and displays a vitreous lustre; it is beige with a white streak. It is non-fluorescent. The mineral displays perfect cleavage on $\{001\}$. Chemical composition varies from $\text{Ba}_2\text{Na}_2\text{Mg}[\text{Nb}_6\text{O}_{19}] \cdot 6\text{H}_2\text{O}$ to ($\text{BaK})(\text{NaCa})\text{Mg}[\text{Nb}_6\text{O}_{19}] \cdot 6\text{H}_2\text{O}$. Empirical formulae for the first and the second compositions are: $(\text{Ba} 1.75\text{K} 0.19)\Sigma 1.94(\text{Na}1.80\text{Ca}0.19)\Sigma 1.99(\text{Mg}0.96\text{Mn}0.02\text{Al}0.02)\Sigma 1.00\text{Nb}6.02\text{O}19.00\cdot 6\text{H}_2\text{O}$ and $(\text{Ba}0.99\text{K}1.00)\Sigma 1.99(\text{Na}1.02\text{Ca}0.96)\Sigma 1.98(\text{Mg}0.95\text{Mn}0.05)\Sigma 1.00\text{Nb}6.02\text{O}19.00\cdot 6\text{H}_2\text{O}$, respectively. Data for a single crystal with the second composition are: trigonal, $R3\bar{1}$, $a = 9.0117(6)$ Å, $c = 23.3986(16)$ Å, $V = 1645.64(19)$ Å$^3$ and $Z = 3$. Calculated density for this formula is 3.733 g/cm$^3$, and the calculated mean refractive index is 1.924. Melcherite is a hexaniobate that has structural layers parallel to the xy plane that stack along the c axis with simultaneous 1/3 [110] displacement so as to produce an $R$ lattice. The melcherite structure is built by layers of $[(\text{Ba,K})(\text{O,H}_2\text{O})_6]\text{polyhedra and the [Nb}_6\text{O}_{19}]^8\text{−super-octahedron (Lindqvist anion) interconnected by [(Na,Ca)O}_6]\text{polyhedra. Cations of Mg}^{2+}$ are bonded to six water molecules each and are not associated with Lindqvist oxygen ions. The mineral is named in honour of Geraldo Conrado Melcher (1924–2011), a pioneer in Jacupiranga carbonatite studies.

KEYWORDS: melcherite, new mineral, hexaniobate, crystal structure, chemical composition, Jacupiranga mine, Cajati, Brazil.

Introduction

**MELCHERITE** is the second natural hexaniobate. The first described was peterandresenite (Friis *et al.*, 2014) and hansesmarkite was recently discovered (Friis *et al.*, 2017). Polyoxometalates of niobium are dominated by the Lindqvist hexaniobate ion, ($\text{Nb}_6\text{O}_{19})^8\text{−}$, and its synthesis and stability requires alkaline conditions. The crystal structure of these compounds was first described by Lindqvist (1953). Hexaniobates are negatively charged clusters of six mutually edge-sharing NbO$_6$ octahedra forming a super-octahedron (Nyman, 2011).
Possible polyoxoniobate applications include their use as reagents in the break-down of nerve agents and in the development of filter media protection against chemical warfare agents (Kinnan et al., 2014). Polyoxometalates have also been investigated in coordination chemistry, leading to the development of hybrid organometallic hexametalate complexes (Abramov et al., 2016), and the synthesis of new polyoxoniobates coordinated to copper complexes (Wang et al., 2008).

The mineral is named in honour of Geraldo Conrado Melcher (1924–2011). He was professor at the Department of Mining Engineering at the Polytechnic School, University of São Paulo and was also a pioneer in Jacupiranga carbonatite studies (Melcher, 1966).

Both the description and name were approved by the Commission on New Minerals, Nomenclature and Classification (CNMNC) of the International Mineralogical Association (IMA2015-018). Type material is deposited in the Museu de Geociências, Instituto de Geociências, Universidade de São Paulo, Rua do Lago, 562, 05508-080 – São Paulo, SP, Brazil. Specimen number: DR982. Part of the cotype sample has been deposited at the University of Arizona Mineral Museum, RRUFF Project (deposition no. R130752).

### Occurrence

The mineral occurs in the carbonatite of the Jacupiranga mine (24°43′47″S, 48°06′37″W), Cajati County, São Paulo, Brazil (Menezes Filho and Martins, 1984). For general information about this carbonatite see Menezes Filho et al. (2015). This is also the type locality for zirkelite (Hussak and Prior, 1895), quintinite (Chao and Gault, 1997), menezesite (Atencio et al., 2008) and pauloabibite (Menezes Filho et al., 2015). Although the joint occurrence of menezesite, pauloabibite and melcherite has not been observed, these minerals may be related genetically. Pauloabibite is trigonal NaNbO₃, isostructural with ilmenite (Menezes Filho et al., 2015). The synthetic analogue of pauloabibite was reported by Kinomura et al. (1984) and Kumata et al. (1990) from a two-step synthesis method, involving the preparation of Na₈Nb₆O₁₉·1₃H₂O (a hexaniobate) followed by hydrothermal reaction with NaOH in a silver-lined vessel at 250°C. Menezesite is a heteropolyoxoniobate, cubic ([Ba,K]₁₂□₅,Mg)₂Zr₄(BaNb₁₂O₄₂)·1₂H₂O (Atencio et al., 2008). According to Nyman et al. (2002), the heteropolyanions of W, Mo and V are formed simply by acidification of solutions of their oxoanions. Under similar conditions, these oxoanion precursors are not available for Nb, and Nb-oxo chemistry is dominated by formation of the Lindquist ion [Nb₆O₁₉]⁸⁻ (present in melcherite). However, heteropolyniobate (present in menezesite) formation is favoured in hydrothermal reactions of aqueous, alkaline precursor mixtures. A competing phase to the formation of polyoxoniobates in hydrothermal aqueous reactions involving Nb and an alkali hydroxide is NaNbO₃, avoided by using short reaction times (i.e. 24 hours or less) (Nyman et al., 2002). So melcherite could have originally formed under acid conditions, and afterwards, under basic conditions, menezesite and pauloabibite could have formed.

Quintinite, menezesite, pauloabibite and melcherite occur in the so-called ‘intermediate
zone’, characterized by a high dolomite and slightly anomalous ‘pyrochlore’ content. Associated minerals are dolomite, calcite, magnetite, pyrrhotite, tochilinite, ‘pyrochlore’, pyrite and fluorapatite. Melcherite formed as a carbonatite vug mineral.

Habit and physical properties

Melcherite forms irregular, tabular crystals up to 200 µm in maximum dimension (Fig. 1). The mineral is transparent and displays a vitreous lustre; it is beige and the streak is white. It is non-fluorescent under both short (254 nm) and long wavelength (366 nm) ultraviolet radiation. The mineral displays perfect cleavage on {001}. Fracture was not determined. Twinning and parting were not observed. The Mohs hardness and density were not measured due to the paucity of material but the calculated density is 3.733 g/cm³ [based on the empirical formula (Ba0.99K1.00)Σ1.99(Na1.02Ca0.96Σ1.98(Mg0.95Mn0.05Σ1.00Nb6.02O19.00·6H2O)]. Refractive indices were not measured due to paucity of material. The mean refractive index is estimated as 1.924 using the Gladstone-Dale relationship (Mandarino, 1981).

Mineral chemistry

Melcherite crystals were embedded in epoxy resin and polished. In the back-scattered electron images, we can see that the crystals are zoned (Fig. 2). The chemical analyses (Table 1) were done by means of a Cameca SX100 electron microprobe (wavelength dispersive spectroscopy mode, 15 kV, 10 nA and 20 µm beam diameter). H2O was inferred from the crystal structure determination. H2O was initially assumed by difference prior to the matrix correction (PAP) and then calculated by stoichiometry post matrix correction due to software limitations. Analyses from the brighter areas of the melcherite crystal (Fig. 2 back-scattered electron image) have the following composition: (Ba1.75K0.19)Σ1.94(Na1.80Ca0.19)Σ1.99(Mg0.96Mn0.02Al0.02)Σ1.00Nb6.02O19.00·6H2O (mean of four analytical points). Those from the darker areas correspond to (Ba0.99K1.00)Σ1.99(Na1.02Ca0.96Σ1.98(Mg0.95Mn0.05)Σ1.00Nb6.02O19.00·6H2O (mean of eight analytical points). The enrichment in Ba is coupled to the enrichment in Na and depletion of K and Ca. The analyses were obtained in points of several shades of grey observed in back-scattered electron
images distributed in different crystals. These analyses were ordered by ascending Ba atoms per formula unit, numbered from 1 to 25, and served as the basis for the construction of the graph in Fig. 3.

Chemical composition varies from Ba₂Na₂Mg[Nb₆O₁₉]·₆H₂O to (BaK)(NaCa)Mg[Nb₆O₁₉]·₆H₂O. Coupled heterovalent substitutions at two sites are verified. As discussed by Hatert and Burke (2008), where a heterovalent substitution occurs at a given crystallographic site, the charge balance can also be maintained by coupling this substitution to another heterovalent substitution at a different site. At the Ba site, the atom Ba²⁺ is replaced progressively by K⁺, and to maintain charge balance, the atom Na⁺ is replaced progressively by Ca²⁺ at the Na site. The substitution mechanism is Ba²⁺ + K⁺ ↔ Na⁺ + Ca²⁺. The boundary site occupancies between the two members of the series is (BaK)(NaCa)Mg[Nb₆O₁₉]·₆H₂O. We could imagine a solid-solution series from Ba₂Na₂Mg[Nb₆O₁₉]·₆H₂O to K₂Ca₂Mg[Nb₆O₁₉]·₆H₂O, with two mineral species, but the composition varies only from the first end-member to the intermediate member. As no analyses correspond to predominant K and Ca, only one mineral species is defined.

The formula BaCa₂Mg[Nb₆O₁₉]·₆H₂O (Andrade et al., 2015) is incorrect because Na was not identified. The change in formula was previously approved executively by CNMNC IMA Newsletter No. 29 (Hålenius et al., 2016): “Soon after the approval of the new mineral melcherite (IMA No. 2015-018; see CNMNC Newsletter 25), the authors of the proposal have communicated results of subsequent analytical work on this mineral, which verifies essential contents of sodium. The new data were examined carefully by the CNMNC officers and were found reliable. The revised simplified formula, Ba₂Na₂Mg[Nb₆O₁₉]·₆H₂O, has been approved executively.” A fragment of the darker part was extracted from the polished section for crystal structure determination.

**Crystal structure determination**

Powder X-ray diffraction data (XRD) were obtained using a Siemens D5000 diffractometer equipped with a Göbel mirror and a position-sensitive detector using CuKα radiation and 40 kV and 40 mA at the Instituto de Geociências of the Universidade de São Paulo (Table 2). Unit-cell parameters refined from the powder data are as follows: trigonal, space group: R₃, a = 9.022(2) Å, c = 23.410(6) Å, V = 1650.2(8) Å³ and Z = 3.
### Table 2. Powder X-ray diffraction data for melcherite.

| \(d_{\text{obs}}(\text{Å})\) | \(I_{\text{obs}}\) | \(d_{\text{calc}}(\text{Å})\) | \(I_{\text{calc}}\) | \(h\) | \(k\) | \(l\) |
|------------------|-------------|------------------|-------------|---|---|---|
| 11.337           | 6           | 11.705           | 0           | 0 | 0 | 2  |
| 7.805            | 100         | 7.803            | 46          | 0 | 0 | 3  |
| 7.410            | 14          | 7.411            | 100         | 1 | 0 | 1  |
| 6.505            | 7           | 6.499            | 34          | 0 | 1 | 2  |
| 5.906            | 6           | 5.852            | 0           | 0 | 0 | 4  |
| 4.508            | 10          | 4.511            | 1           | 1 | 1 | 0  |
| 3.904            | 22          |                  |             |   |   |     |
|                  |             | 3.905            | 13          | 2 | 1 | 3  |
|                  |             | 3.905            | 3           | 1 | 1 | 3  |
|                  |             | 3.902            | 16          | 0 | 0 | 6  |
| 3.852            | 21          | 3.853            | 33          | 0 | 2 | 1  |
| 3.250            | 33          | 3.249            | 37          | 0 | 2 | 4  |
| 3.074            | 9           | 3.075            | 9           | 1 | 0 | 7  |
| 3.000            |             | 14              | 2           | 0 | 5 |     |
| 2.952            | 13          |                  |             |   |   |     |
|                  |             | 2.951            | 10          | 1 | 1 | 6  |
|                  |             | 2.951            | 1           | 2 | 1 | 6  |
|                  |             | 2.930            | 4           | 2 | 1 | 1  |
|                  |             | 2.930            | 2           | 3 | 1 | 1  |
| 2.861            | 8           |                  |             |   |   |     |
|                  |             | 2.863            | 35          | 1 | 3 | 2  |
|                  |             | 2.863            | 4           | 1 | 2 | 2  |
| 2.740            | 8           | 2.740            | 13          | 0 | 1 | 8  |
| 2.637            | 8           | 2.637            | 27          | 2 | 1 | 4  |
|                  |             | 2.637            | 5           | 3 | 1 | 4  |
|                  |             | 2.604            | 3           | 3 | 0 | 0  |
|                  |             | 2.601            | 1           | 0 | 0 | 9  |
|                  |             | 2.541            | 1           | 0 | 2 | 7  |
|                  |             | 2.498            | 4           | 1 | 3 | 5  |
|                  |             | 2.471            | 4           | 3 | 0 | 3  |
|                  |             | 2.471            | 2           | 0 | 3 | 3  |
|                  |             | 2.342            | 4           | 2 | 0 | 8  |
|                  |             | 2.253            | 1           | 2 | 1 | 9  |
| 2.243            | 6           | 2.243            | 7           | 1 | 0 | 10 |
| 2.214            |             | 22              | 1           | 9 | 2 | 7  |
| 2.167            |             | 21              | 3           | 2 | 2 | 3  |
| 2.166            | 30          | 2.166            | 32          | 3 | 0 | 6  |
| 2.166            |             | 1              | 0           | 3 | 6 |     |
| 2.158            | 12          | 2.158            | 1           | 1 | 3 | 1  |
| 2.158            |             | 1              | 1           | 4 | 1 | 4  |
| 2.131            |             | 2              | 1           | 4 | 1 | 2  |
| 2.078            | 4           | 2.079            | 1           | 1 | 2 | 8  |
| 2.053            | 5           | 2.053            | 0           | 1 | 0 | 11 |
| 2.053            |             | 0              | 0           | 1 | 11 |
| 2.034            | 4           | 2.032            | 2           | 1 | 4 | 4  |
| 2.008            |             | 3              | 0           | 2 | 10 |
| 1.967            |             | 5              | 3           | 1 | 5  |
| 1.953            |             | 5              | 2           | 2 | 6  |
| 1.869            |             | 1              | 2           | 0 | 11 |
| 1.840            |             | 2              | 3           | 0 | 9  |
| 1.840            |             | 1              | 0           | 3 | 9  |
| 1.836            | 4           | 1.835            | 1           | 3 | 1 | 10 |
| 1.819            |             | 3              | 1           | 3 | 7  |
| 1.791            |             | 2              | 2           | 1 | 12 |

(continued)

The strongest reflections are given in bold.

### Table 3. Structure refinement results for melcherite.

| Ideal chemical formula | Ba\(_2\)Na\(_2\)Mg[\(\text{Nb}_6\text{O}_{19}\)]·6\(\text{H}_2\text{O}\) |
|------------------------|--------------------------------------------------|
| Crystal size (mm)      | 0.07 × 0.05 × 0.05                               |
| Space group            | \(R\bar{3}\)                                      |
| \(a (\text{Å})\)       | 9.0117(6)                                        |
| \(c (\text{Å})\)       | 23.3986(16)                                     |
| \(V (\text{Å}^3)\)     | 1645.64(19)                                     |
| \(Z\)                  | 3                                               |
| \(\rho_{\text{cal}} (g/cm^3)\) | 3.748                                      |
| \(\lambda (\text{Å})\) | 0.71073                                         |
| \(\mu (\text{mm}^{-1})\) | 5.46                                          |
| \(2\theta_{\text{max.}}\) for data collection(°) | ≤66.38                                  |
| No. of reflections collected | 5316                                         |
| No. of independent reflections | 1403                                     |
| No. of reflections with \(I > 2\sigma(I)\) | 1319                                    |
| No. of parameters refined | 65                                           |
| \(R_{\text{int}}\)     | 0.022                                           |
| Final \(R\) factors [\(I > 2\sigma(I)\)] | \(R_1 = 0.017, wR_2 = 0.042\)                    |
| Final \(R\) factors (all data) | \(R_1 = 0.019, wR_2 = 0.041\)                |
| Goodness-of-fit        | 1.13                                            |
| Largest diff. peak and hole | 1.30 and −1.59 e Å\(^{-3}\)                  |

Weighting scheme: \(w = 1/[\sigma^2(F_{o}^2) + (0.0146P)^2 + 5.6144P]\), where \(P = \max(0,F_{o})^2 + (2F_{o}F_{c})/3\).
A single-crystal X-ray study was carried-out using a Bruker APEX II CCD diffractometer with graphite-monochromated MoKα (λ = 0.71073 Å) radiation and gave the following data: trigonal, space group: R3, a = 9.0117(6) Å, c = 23.3986(16) Å, V = 1645.64(19) Å³ and Z = 3. The X-ray absorption correction was applied to intensity data using the program SADABS from Bruker.
Fig. 4. Crystal structure of melcherite. (Ba,K) = yellow; (Na,Ca) = pink; Mg = green; Nb = blue; O = red and OW = grey.

Fig. 5. Lindquist polyanions $[\text{Nb}_6\text{O}_{19}]^{8-}$ stacking sequence in the crystal structure of melcherite.
The SHELXL-97 package (Sheldrick, 2008) was used for the direct methods structure solution and its subsequent refinement. The Ba and Na sites were refined assuming full but joint occupation by Ba/K and Na/Ca respectively, which yielded occupancy values close to those indicated by the empirical formula based on the electron microprobe analysis. A final difference-Fourier synthesis

Table 6. Selected interatomic bond lengths (Å) and octahedral distortion indices for melcherite (Ba$_2$Na$_2$MgNb$_6$O$_{19}$·6H$_2$O), peterandresenite (Mn$_4$Nb$_6$O$_{19}$·14H$_2$O) and hansemarkite (Ca$_2$Mn$_2$Nb$_6$O$_{19}$·20H$_2$O).

|                 | Melcherite (This work) | Peterandresenite (Friis et al., 2014) | Hansemarkite (Friis et al., 2017) |
|-----------------|------------------------|---------------------------------------|-----------------------------------|
| Nb–O1           | 2.0154(13)             | 2.3982(1)                            | 2.3990(6)                         |
| Nb–O1           | 2.0161(13)             | 1.7685(8)                            | 1.780(1)                          |
| Nb–O2           | 1.7906(14)             | 1.9767(8)                            | 1.962(1)                          |
| Nb–O3           | 1.9691(13)             | 1.9799(6)                            | 1.973(1)                          |
| (Nb–O)          | 1.9731(13)             | 2.0080(6)                            | 2.020(1)                          |
| Nb–O4           | 2.3678(2)              | 2.0290(8)                            | 2.034(1)                          |
| (Nb–O)          | 2.022                  | 2.027                                | 2.028                             |
| OV*             | 10.513                 | 10.506                               | 10.723                            |
| OAV             | 113.650                | 132.281                              | 119.622                           |
| OQE             | 1.040                  | 1.046                                | 1.042                             |
| Mg–OW5          | 2.0602(16)             | 2.3679(1)                            | 2.3576(6)                         |
| (Mg–OW)         | 2.060                  | 1.9716(8)                            | 1.977(1)                          |
| OV              | 11.603                 | 2.0208(8)                            | 1.766(1)                          |
| OAV             | 12.285                 | 2.0208(8)                            | 1.982(1)                          |
| OQE             | 1.003                  | 1.777(1)                             | 2.019(1)                          |
| (Na,Ca)–O2      | 2.3501(15)             | 2.021                                | 2.021                             |
| (Na,Ca)–O1      | 2.4476(15)             | 110.055                              | 108.276                           |
| OAV             | 15.689                 | 1.039                                | 1.039                             |
| OAV             | 354.100                | 1.039                                | 1.039                             |
| OQE             | 1.113                  | 2.0645                               | 2.3764(6)                         |
| Mn1–O2          | 2.0645                 | 2.0645                               | 2.3764(6)                         |
| Mn1–O2          | 2.220                  | 2.220                                | 2.033(1)                          |
| Mn1–O6          | 2.3250                 | 2.3250                               | 2.100(1)                          |
| Mn1–O6          | 2.253(2)               | 2.253(2)                             | 1.785(1)                          |
| (Mn1–O)         | 2.208                  | 2.208                                | 2.023                             |
| OV              | 13.518                 | 13.518                               | 10.691                            |
| OAV             | 146.530                | 146.530                              | 121.348                           |
| OQE             | 1.044                  | 1.044                                | 1.044                             |
| Mn2–O7          | 2.088(1)               | 2.088(1)                             | 2.230(1)                          |
| Mn2–O9          | 2.106(2)               | 2.106(2)                             | 2.230(1)                          |
| Mn2–O10         | 2.237(1)               | 2.237(1)                             | 2.230(1)                          |
| Mn2–O10         | 2.240(1)               | 2.240(1)                             | 2.230(1)                          |
| Mn2–O11         | 2.240(1)               | 2.240(1)                             | 2.230(1)                          |
| Mn2–O11         | 2.191                  | 2.191                                | 2.178                             |
| OV              | 13.992                 | 13.992                               | 13.417                            |
| OAV             | 4.489                  | 4.489                                | 104.704                           |
| OQE             | 1.003                  | 1.003                                | 1.030                             |

*OV = octahedral volume (Å³), OAV = octahedral angle variance (°²), and OQE = octahedral quadratic elongation (Robinson et al. 1971).
allowed the H atom positions of the water molecule to be located, which were then refined with soft restraints of 0.86 Å on the O–H distances and 1.40 Å on the H–H distance, and with $U_{\text{iso}}$ values fixed at $\sim$1.5 times that of the O atom. Refinement of this final model converged to an $R_1$ of 0.017 and the crystal chemical formula obtained is $(\text{Ba}_{1.06}\text{K}_{0.94})$$(\text{Na}_{1.09}\text{Ca}_{0.91})\text{Nb}_6\text{Mg}[\text{O}_{18.98}\text{O(H)}_{0.02}]\Sigma_{19.00}\cdot6\text{H}_2\text{O}$, where a small fraction of the oxygen atoms in the hexaniobate polyanion is assumed to be replaced by OH groups in order to balance the slight positive charge deficiency associated with the Ba/K and Na/Ca sites. Details of the data collection and structure refinement are given in Tables 3 and 4. Selected bond distances and associated bond-valence sum calculations, using the parameters of Brese and O’Keefe (1991), are given in Table 5.

Melcherite is a hexaniobate that has structural layers parallel to the $xy$ plane that stack along the $c$ axis with simultaneous $1/3$ [1 1 0] displacement so as to produce an $R$ lattice. The melcherite structure (Figs 4 and 5) is built by layers of $[(\text{Ba},\text{K})(\text{O},\text{H}_2\text{O})_6]$ polyhedra and the $\text{Nb}_6\text{O}_{19}^{8-}$ super-octahedron (Lindqvist anion) interconnected by $[(\text{Na},\text{Ca})\text{O}_6]$ polyhedra. There is a significant distortion present in the Nb–O octahedron forming the hexaniobate polyanion, as measured by the octahedral angle variance (OAV), $=113.650^\circ$, and quadratic elongation (OQE), $=1.040$ indices (Robinson et al., 1971). The results are comparable to the NbO$_6$ octahedra present in the crystal structure of peterandresenite and hansesmarkite (Table 6). Ba/K is coordinated by six oxygens and three water molecules. Na/Ca is coordinated by six oxygen atoms in a distorted octahedron and the OAV and OQE values are 354.100$^2$ and 1.113, respectively. Mg$^{2+}$ cations are bonded to six water molecules each and are not associated with Lindqvist oxygen ions. The comparison with MnO$_6$ in peterandresenite and hansesmarkite shows that the octahedral coordination of the Mg cation is relatively undistorted, as indicated by the values of OAV $=12.285^2$ and OQE $=1.003$ (Table 6).

The mineral is similar structurally to the synthetic compounds $\text{Cs}_8\text{Na}_2\text{Nb}_6\text{O}_{19}\cdot18\text{H}_2\text{O}$.
and Rb₆(H₂Nb₆O₁₉)·19H₂O, studied by Nyman et al. (2006) (Table 7). They have the same space group as melcherite, R₃. The unit-cell dimensions and arrangement of the Lindqvist ion [Nb₆O₁₉]₈⁻ are very similar. The crystallographic parameters of melcherite are compared with those of the other hexaniobate minerals in Table 8.

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