The structure is based on a framework built up by connecting [001] double chains of octahedra; wide [001] channels in the framework are occupied by a single chain of face-sharing octahedra [M(1) site] and by the Si-tetrahedra.
By putting 2.88 Si + 0.02 P in the T sites, the cell with a = 12.02(3), b = 20.22(3), c = 4.732(2)Å (s.g. Pmcn) contains four f.u. with composition
$[(Mg_{0.49}Ti_{0.19}Fe_{0.01}\square_{0.31})(Al_{0.71}Mg_{0.25}\square_{0.04})_2$

$(Al_{0.95}\square_{0.05})_4][Si(Si_{0.94}P_{0.01}\square_{0.05})_2O_{15.04}(OH)_{2.96}]B$
in agreement with electron- and ion-microprobe analyses. Only one hydrogen atom has been found in the difference Fourier. The further two hydrogens required by the chemical formula are disordered over more than two oxygens; their presence is confirmed by calculations of the charge distribution.
Smaller Al-free tetrahedra and lower contents of high-charge cations in the face-sharing octahedra under compression, are proposed to be the crystallochemical basis for the formation of magnesiodumortierite under the Dora-Maira metamorphic conditions.
The following general formula for the minerals of the dumortierite group is proposed

$$\{M'(M'')_2(M''')_4O_{18-x-y}(OH)_x\}T'_{3-x}T''_yB$$

where: M' = Al, Mg, Ti, Fe, RE(?) [M(1) site]; M'' = Al, Mg [M(4) site]; M''' = Al [M(2) and M(3) sites]; T'= Si, Al, P [T(1) and T(2) sites]; T'' = Sb occurs in holtite (Hoskins, Mumme and Pryce, 1989, Min. Mag., 53, 457-463) and forms a pyramidal group with three oxygen atoms [T(1) and T(2) sites]. In all sites, particulary in M(1), vacances can occur.

PS-08.01.31 STRUCTURAL MODEL AND POLYTYPISM IN TUNGUSITE.

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Tungusite is a light green hydrous silicate of Ca and Fe reported from different localities of the Siberian Platform and described the first time by V.I. Kudriashova (1966, Dokl. Akad. Nauk SSSR, 171, 1167-1170).
On the basis of X-ray (powder patterns) and electron diffraction studies (selected area and oblique texture patterns) and of comparison with the crystal structures of reyerite (Merlino, 1989, Min. Mag., 52, 247-256) and gyrolite (Merlino, 1989, Min. Mag., 52, 377-387) new data on tungusite have been obtained.
No single crystals suitable for X-ray structural studies have been found and the electron diffraction shows a widespread stacking disorder along the c* axis. The most ordered sample shows a metrically monoclinic C-centred cell, with a = 9.66, b = a√3, c = 21.86 Å, α ≈ 100, ß = 90, γ = 90°. By analogy with gyrolite, the structural model is based on a triclinic ($P\bar{1}$) cell with a ≈ b = 9.66, c = 21.86 Å, α ≈ 98.6, ß = 90, γ = 120°. The proposed model maintains the $S_1OS_2X\bar{S}_2\bar{O}S_1$ sequence of tetrahedral (S), octahedral (O) and complex (X) sheets reported in gyrolite by Merlino; it differs from this structure pratically only for the contents of the complex sheet X. While in gyrolite the X sheet contains only one Na and two Ca octahedra plus water molecules, in tungusite this sheet is completely filled by nine octahedra. The following ideal crystallochemical formula is derived for tungusite:

$$(Ca_{14}M_9^{2+})[T_8O_{20}(OH)_6][T'_8O_{20}(OH)_8]_2,$$

where M is mainly a bivalent with minor monovalent and trivalent cation ($Fe^{2+} \approx 6$, $Na^{+} \approx 2$, $Fe^{3+} \approx 1$, in our samples); T and T' are mainly Si with, in our samples, a maximum of 2Al which should stay in T' (S_2 sheet). This type of substitutions in M requires that some OH are replaced by H_2O. Some of our samples ("white tungusite") show clearly a composition which is intermediate between tungusite and gyrolite.
With reference to the C-centred cell, possible polytypes can be derived by shifts only along the b axis (±1/9, ±2/9, ±4/9; monoclinic cells) and along a axis as well (±1/3, ±1/2, ±1/6; triclinic cells). The shifts are referred to the O sheets with respect to the S_1 and S_2 sheets.

PS-08.01.32 CRYSTAL STRUCTURE OF $Sr(ReO_4)_2.H_2O$

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The existence of strontium perrhenate monohydrate was mentioned for the first time by Smith & Maxwell (J. Am. Chem. Soc., 1951, 73, 658-660) and proven by means of X-ray powder and TGA analysis by Wassilopulos (Über Polinare Oxide des 4 and 7 wertigen Technetium mit Erdaklalien. Karlsruhe. Kernf. Inst. Radiochem., 1965, S. 67)

Our STA analysis of fresh $Sr(ReO_4)_2.2H_2O$ prepared according to Smith & Maxwell (1951) supported the existence of the monohydrate in the temperature range of 66 - 155°C. Complete powder data were evaluated (PDF 42-682; Macicek). We managed to grow single crystals of $Sr(ReO_4)_2.H_2O$ from absolute CH_3OH. Crystal data: M_r = 606.03, orthorhombic, Pbca (61), a = 11.594(2), b = 12.304(1), c = 23.885(4)Å, V = 3407 $Å^3$, Z = 16, D_x = 4.73 $g.cm^{-3}$, R = 0.042 for 2151 reflections with $I > 2\sigma(I)$.

Coordination polyhedron of Sr(1) consists of nine oxygen atoms from eight ReO_4 tetrahedra and one water molecule at 2.548(16) - 2.686(15)Å. Sr(2) is coordinated to eight oxygen atoms from seven ReO_4 groups and the second H_2O molecule [2.507(15) - 2.614(20)Å]. Sr(1) atom participates in seven double [Sr...Sr 6.175(3) - 6.530(3)Å] and one single Sr-T-Sr [Sr...Sr 6.818(3)Å] bridges, while Sr(2) forms six double [Sr...Sr 6.325(3) - 6.558(3)Å] and three single [Sr...Sr 6.632(3) - 6.818(3)Å] bridges. The ReO_4 tetrahedra have irregular geometry with Re-O distances and [O-Re-O] angles within 1.702(15)-1.742(15)Å and [106.7(8)-111.8(7)°]. Three of the ReO_4 groups are linked to four Sr ions, and the fourth one only to three. The non-coordinated oxygen from $Re(4)O_4$ has three closest neighbours: O(22) at 3.233(22)Å, O(23) at 3.282(23)Å and O(13) at 3.368(22)Å.

PS-08.01.33 STRUCTURES OF CALCIUM AND LEAD PERRHENATE UREA HYDRATES.

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Preliminary investigation of the system $M(ReO_4)_2$-Urea-H_2O, M = large divalent cations, indicate formation of 1:1:1 addition compounds. Single crystals of lead and calcium species have been studied on an Enraf-Nonius CAD4/SDP44 diffractometric system.

