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Description and crystal structure of turtmannite, a new mineral with a 68 Å period related to mcgovernite

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ABSTRACT

Jacobsite-rich Fe-Mn ores of probable Dogger age fill paleokarst pockets in the Triassic marbles of the Barrhorn Unit under Pipjigletscher in the Turtmanntal, Valais, Switzerland. These ores and embedding rocks underwent Tertiary metamorphism under upper greenschist facies conditions. Some of these jacobsite ores contain minor amounts of a yellow micaceous mineral, which appears to be a new Mn-Mg silicate-vanadate-arsenate that was named "turtmannite" with respect to the type locality. Turtmannite flakes up to 200 μm in length occur parallel to the main schistosity, or fill thin discordant veinlets. Turtmannite is rhombohedral $R\bar{3}c$, with $a_H = 8.259(2)$ and $c_H = 204.3(3)$ Å in the hexagonal setting. The corresponding primitive rhombohedral cell has $a_R = 68.31$ and $\alpha_R = 6.92°$. HRTEM images indicate that turtmannite is perfectly ordered along **c**.

The structure of turtmannite has been solved to a final *R*1 of 12.4% on a Siemens Smart CCD diffractometer with Mo*K*α X-radiation, and a detector to sample distance extended to 12 cm. The structure consists of 84 oxygen layers stacked along **c**, with twelve close-packed layers followed by two non-close-packed layers. This sequence is repeated six times. The structure contains eight symmetrically distinct cation layers. Three different occupational variants have been recognized leading to the following hypothetical end-member formulae and approximate abundances:

I	$^{[IV]}Mn_{1.5}{}^{[IV]}Mg_3{}^{[VI]}(Mn,Mg)_{21}[(V,As)O_4]_3[SiO_4]_3O_5(OH)_{20}$,	50%
II	$^{[IV]}Mn_{1.5}{}^{[VI]}(Mn,Mg)_{21}[(V,As)O_4]_3[SiO_4]_3[AsO_3](OH)_{21}$	33%
III	$^{[IV]}Mn_{1.5}{}^{[VI]}(Mn,Mg)_{21}[(V,As)O_4]_3[SiO_4]_2[SiO_3OH](OH)_{25}$	16%

The simplified chemical formula for turtmannite can be written as:

$$(Mn,Mg)_{22.5}Mg_{3-3x}[(V,As)O_4]_3[SiO_4]_3[AsO_3]_xO_{5-5x}(OH)_{20+x}.$$

The unit cell of turtmannite is similar to those of mcgovernite, a Mn-Mg-Zn arsenate from Sterling Hill, New Jersey, and an unnamed "mcgovernite-like" Mn-Mg arsenate from the Kombat Mine, Namibia. The crystal structure of turtmannite is close to the model predicted for mcgovernite by Moore and Araki (1978).