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The crystal structure of huemulite
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The crystal structures of natural (from the West Sunday Mine, Utah, USA) and synthetic huemulite, Na3Mg(V2O3)24H2O have been solved and refined to R = 0.0313 (for 3535 unique Fo > 4σF reflections) and 0.0246 (for 3672 unique Fo > 4σF reflections), respectively. Huemulite is triclinic, space group P, with Z = 1; unit-cell dimensions of the natural sample are a 9.045(2), b 11.3337(3), c 11.7327(8) Å, α 105.223(7), β 97.383(7), γ 100.790(7)°, V 1120.30(9) Å³, whereas those of the synthetic sample are a 9.0425(2), b 11.3303(2), c 11.7353(8) Å, α 105.222(7), β 97.377(7), γ 100.791(7)°, V 1119.47(8) Å³. The structure consists of decavanadate oxyanions (V10O30)4− linked via an interstitial complex composed of isolated [Mg(H2O)6]3+ octahedra and an [Na(H2O)4]4+ cationic group (defining an infinite zig-zag chain). There are also four isolated H2O groups, two of them positionally disordered. All except 4 H atoms have been located, showing a network of H-bonds that further links the interstitial complex and the structural unit, stabilizing the atomic arrangement. The Lewis acidity of the interstitial complex (0.18) is almost coincident with the upper limit of basicity of the structural unit (0.17), thus showing that the valence-matching principle is maintained in this structure.

It is probable that the X-ray pattern and the unit-cell dimensions informed in the original description of huemulite [1] were measured using a mixture that included fully hydrated and partially dehydrated material.

Huemulite is closely related to a synthetic family of general formula Na3Mg(V2O3)24H2O (M=Mg) [2–3], the main difference (in addition to having ~23 H2O molecules instead of ~24) being that the latter compounds have a unit cell with doubled volume. Unit cell and atomic positions of huemulite are related to those of the synthetic family by the transformation matrix M = [1 0 0 / 0 1 1 / 0 1 -1]. After the transformation, the space group of huemulite becomes P. Some of the symmetry restrictions (inversion centers, cell centering, etc.) present in huemulite are relaxed, with the consequence that fewer atoms are symmetry-related in the synthetic family.


Keywords: mineralogy, vanadium, valence-matching principle

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Structural Investigations of Synthetic Analogues of Murataite
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The crystal structures of Murataite (A = Ni, Mg) [1] and its synthetic analogues, Ni2+AI2Si5O18(H2O)2+ or (AIV5O18)(H2O)2, have been solved and refined to R = 0.0313 (for 3535 unique Fo > 4σF reflections) and 0.0246 (for 3672 unique Fo > 4σF reflections), respectively. Huemulite is triclinic, space group P, with Z = 1; unit-cell dimensions of the natural sample are a 9.045(2), b 11.3337(3), c 11.7327(8) Å, α 105.223(7), β 97.383(7), γ 100.790(7)°, V 1120.30(9) Å³, whereas those of the synthetic sample are a 9.0425(2), b 11.3303(2), c 11.7353(8) Å, α 105.222(7), β 97.377(7), γ 100.791(7)°, V 1119.47(8) Å³. The structure consists of decavanadate oxyanions (V10O30)4− linked via an interstitial complex composed of isolated [Mg(H2O)6]3+ octahedra and an [Na(H2O)4]4+ cationic group (defining an infinite zig-zag chain). There are also four isolated H2O groups, two of them positionally disordered. All except 4 H atoms have been located, showing a network of H-bonds that further links the interstitial complex and the structural unit, stabilizing the atomic arrangement. The Lewis acidity of the interstitial complex (0.18) is almost coincident with the upper limit of basicity of the structural unit (0.17), thus showing that the valence-matching principle is maintained in this structure.

It is probable that the X-ray pattern and the unit-cell dimensions informed in the original description of huemulite [1] were measured using a mixture that included fully hydrated and partially dehydrated material.

Huemulite is closely related to a synthetic family of general formula Na3Mg(V2O3)24H2O (M=Mg) [2–3], the main difference (in addition to having ~23 H2O molecules instead of ~24) being that the latter compounds have a unit cell with doubled volume. Unit cell and atomic positions of huemulite are related to those of the synthetic family by the transformation matrix M = [1 0 0 / 0 1 1 / 0 1 -1]. After the transformation, the space group of huemulite becomes P. Some of the symmetry restrictions (inversion centers, cell centering, etc.) present in huemulite are relaxed, with the consequence that fewer atoms are symmetry-related in the synthetic family.


Keywords: mineralogy, vanadium, valence-matching principle

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