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# Orthorhombic Jahn-Teller distortion and Si-OH in mozartite, $CaMn^{3+}O[SiO_3OH]$: A single-crystal X-ray, FTIR, and structure modeling study

DANIEL NYFELER,[1] CHRISTINA HOFFMANN,[1] THOMAS ARMBRUSTER,[1] MARTIN KUNZ,[2] AND
EUGEN LIBOWITZKY[3]

[1]Laboratorium für chemische und mineralogische Kristallographie, Universität Bern, Freiestrasse 3, CH-3012 Bern, Switzerland
[2]High Pressure Group, European Synchrotron Radiation Facility, BP 220, Avenue des Martyrs, F-38043 Grenoble, Cedex, France
[3]Institut für Mineralogie und Kristallographie, Universität Wien-Geozentrum, Althanstrasse 14, A-1090 Wien, Austria

## ABSTRACT

The structure of mozartite, $CaMn^{3+}O[SiO_3OH]$, was refined in space group $P2_12_12_1$ from X-ray single-crystal data collected at 100 K ($R$ = 2.45%, $R_w$ = 2.62%), 300 K ($R$ = 2.60%, $R_w$ = 2.68%), and 500 K ($R$ = 2.79%, $R_w$ = 2.81%). The $Mn^{3+}O_6$ octahedron shows approximately orthorhombic geometry, which is explained by a combination of a tetragonally compressed Jahn-Teller effect with lattice-induced stress. Comparison with isostructural vuagnatite, $CaAl(OH)SiO_4$, which shows no distortions due to electronic effects, indicates that the distorted octahedral geometry in mozartite causes shifts in valence sums of the O atoms that are hydrogen bonded. As a result, the OH group in mozartite is located at the isolated $SiO_4$ apex and is not linked to the octahedron as reported for isostructural minerals. Isostructural minerals of the adelite group with tetrahedral $As^{5+}$ and $V^{5+}$ exhibit a different Jahn-Teller distortion with tetragonally elongated geometry for octahedral $Cu^{2+}O_6$.

The $O\text{-}H \cdots O$ distance of $<2.5$ Å in mozartite is one of the shortest hydrogen bonded $O \cdots O$ distances in minerals and leads to a diffuse FTIR absorption peak (stretching mode) polarized parallel to $b$ between 1300 and 1700 $cm^{-1}$.