08.2-10 JAHN-TELLER-EFFECT AND CRYSTAL STRUCTURE IN THE SOLUTION-FUROSCISSON PRODUCTS (II). \( \text{NaN}_2\text{MnF}_6 \) AND \( \text{NaN}_2\text{MnP}_4 \cdot z\text{H}_2\text{O} \). W. Masse and R. E. Schmidt, Sonderforschungsbereich 127 (Kodansallstruktur und Chemische Sindung) und Fachbereich Chemie der Universität Marburg, Hans-Meerwein-Str., D-3550 Marburg, Germany

Single crystals of \( \text{NaN}_2\text{MnF}_6 \) and the novel hydrate \( \text{NaN}_2\text{MnP}_4 \cdot z\text{H}_2\text{O} \) have been grown from aqueous hydrofluoric acid solutions of MnF\(_2\) and NaF. The crystal structures were determined from 4-circle diffractometer X-ray data.

\( \text{NaN}_2\text{MnP}_4 \cdot z\text{H}_2\text{O} \). Space group \( C2/c \).

\( a = 7.719 \text{ Å} \)
\( b = 5.236 \text{ Å} \)
\( c = 10.862 \text{ Å} \)

\( \beta = 108.99^\circ \)

\( R_w = 2.3\% \) for 1679 reflections.

The crystal structure consists of kinked trans-chains of \( [\text{MnP}_4\text{F}_6]^{2-} \) octahedra interconnected by coordinated Na-ions. The pronunciation lengthening of the axial Mn-F bond (\( d(\text{Mn-F})_{\text{ax}} = 2.109(1) \text{ Å} \)) is partly due to the Jahn-Teller-effect of the \( d^3 \)-high spin configuration of Mn\(^{3+}\).

\( \text{NaN}_2\text{MnP}_4 \cdot z\text{H}_2\text{O} \). Space group \( C2/c \).

\( a = 16.361 \text{ Å} \)
\( b = 6.676 \text{ Å} \)
\( c = 11.303 \text{ Å} \)

\( \beta = 108.99^\circ \)

\( R_w = 2.3\% \) for 1679 reflections.

The crystal structure is partially due to the Jahn-Teller-effect of the \( d^3 \)-high spin configuration of Mn\(^{3+}\).

08.2-11 STRUCTURAL STUDIES OF THORTVEITITE-LIKE \( \text{Mn}_2\text{P}_2\text{O}_7 \)

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The crystal structure of \( \text{Mn}_2\text{P}_2\text{O}_7 \) is reported to be isostructural with thortveitite, \( \text{Sc}_2\text{Y}_2\text{Si}_2\text{O}_7 \). It was recently refined in space group \( C2/c \) (I. C. C. and R. E. Schmidt, Sonderforschungsbereich 127 (Kodansallstruktur und Chemische Sindung) und Fachbereich Chemie der Universität Marburg, Hans-Meerwein-Str., D-3550 Marburg, Germany). The crystal structure consists of kinked trans-chains of \( [\text{MnP}_4\text{F}_6]^{2-} \) octahedra interconnected by coordinated Na-ions. The structure is partially due to the Jahn-Teller-effect of the \( d^3 \)-high spin configuration of Mn\(^{3+}\).