

STRUCTURAL REINVESTIGATION OF BENTORITE

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Bentorite, with idealized formula $\text{Ca}_6\text{Cr}_2(\text{SO}_4)_3(\text{OH})_{12}\cdot 26\text{H}_2\text{O}$, a Cr-analogue of ettringite, was accepted as valid mineral species by IMA in 1980. However, its crystal structure was never investigated. The only report on this mineral (GROSS, 1980) states that the powder diffraction pattern of bentorite was satisfactorily indexed from the analogy with ettringite $\text{Ca}_6\text{Al}_2(\text{SO}_4)_3(\text{OH})_{12}\cdot 26\text{H}_2\text{O}$. Therefore, the most probable unit cell is hexagonal *P6/mmc* with parameters $a = 22.35 \text{ \AA}$ and $c = 21.41 \text{ \AA}$.

New bentorite crystals with dark violet colour were found in late low-temperature veins of spurrite rocks associated with ettringite and calcite. The rock specimen was found in pyrometamorphic rocks belonging to the Hatrum Complex and collected in Arad Stone quarry in the Negev Desert, Israel. The main rock-forming minerals are spurrite, shulamitite-sharyginite, brownmillerite, ye'elimitite and mineral of fluorapatite-fluorellestadite series. Baryte, gibbsite, hydrocalumite and sphalerite are accessory minerals.

A careful re-examination of single crystals from the Arad Stone quarry, was done using X-ray single crystal diffraction (SCXRD) on room and low temperature conditions (-100 °C). Bentorite is isostructural with ettringite. It crystallizes in the space group *P31c* and have unit cell parameters $a = 11.1825(8) \text{ \AA}$, $c = 21.5475(13) \text{ \AA}$. Crystal structure was refined up to $R = 4.3\%$ starting from atomic coordinates of ettringite (MOORE & TAYLOR, 1970). The refined chemical composition of our crystal $\text{Ca}_6(\text{Cr}_{1.681}\text{Al}_{0.319})(\text{SO}_4)_3(\text{OH})_{12}\cdot 26(\text{H}_2\text{O})$, matches the chemical analysis of bentorite reported by GROSS (1980).

Moreover, a stepwise substitution of Al^{3+} by Cr^{3+} , was found in ettringite crystals from Ma'ale Adummim in Palestinian Autonomy. This hexagonal prismatic crystals show distinct colour zoning from dark violet over pale rose to transparent. For the purpose of SCXRD investigation, they were cut in three parts, or rather three zones along c-axis. Full crystal structure refinements of all three crystals (zones) resulted in different chemical compositions. The colourless basis of the crystal has average chemical formula $\text{Ca}_6(\text{Al}_{1.602}\text{Cr}_{0.398})(\text{SO}_4)_3(\text{OH})_{12}\cdot 26(\text{H}_2\text{O})$ with 20% Cr^{3+} and 80% Al. Intermediate part has 32% Cr + 68% Al or $(\text{Al}_{1.355}\text{Cr}_{0.645})$. Finally the top of the crystal has $\approx 60\%$ Cr and 40% Al and average chemical formula $\text{Ca}_6(\text{Al}_{0.821}\text{Cr}_{1.179})(\text{SO}_4)_3(\text{OH})_{12}\cdot 26(\text{H}_2\text{O})$.

The substitution of Al^{3+} in ettringite by Cr^{3+} could have important implication in wastewater treatment technology. Thus, formation and temperature stability of Cr^{3+} - bearing ettringite were investigated by WIECZOREK-CIUROWA et al. (2001).

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GROSS, S. (1980): Isr. J. Earth Sci. 29, 81-84.

MOORE, A.E., TAYLOR, H.F.W. (1970): Acta Crystallogr. B26, 386-393.

WIECZOREK-CIUROWA, K., FELA, K., KOZAK, A.J. (2001): J. Therm. Anal. Calorim. 65, 655-660.