

the ideal size. For the reduction of the structural strain, two H atoms may replace the Mg atom predominantly at the M2 site, giving the vacancy at the M2 site.

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Carnallite and pseudo-carnallite as solid inclusions in blue halite from Klodawa Salt Mine, Poland

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Crystals of carnallite ($\text{KMgCl}_3 \cdot 6\text{H}_2\text{O}$) and pseudo-carnallite ($\text{K}_3\text{Al}_2\text{MgCl}_{11} \cdot 14\text{H}_2\text{O}$) were found in blue halite from Klodawa Salt Mine as colourless solid inclusions [1]. Their structures were determined from X-ray diffraction data collected for the single crystals. Both type of crystals are orthorhombic and have similar lattice parameters. Carnallite I: $a=16.1505(2)$, $b=22.5190(4)$, $c=9.5680(1)$ Å, $V=3479.8(1)$ Å³ and II: $a=16.1440(3)$, $b=22.5128(4)$, $c=9.5672(2)$ Å, $V=3477.2(1)$ Å³. The carnallite structures were refined to $R1=0.0351$ for I, and $R1=0.0413$ for II. Pseudo-carnallite I: $a=16.1446(3)$, $b=22.5206(5)$, $c=9.5535(2)$ Å, $V=3473.5(1)$ Å³ and II: $a=16.1499(3)$, $b=22.5178(5)$, $c=9.5681(2)$ Å, $V=3479.5(1)$ Å³. The pseudo-carnallite structure were refined to $R1=0.0506$ for I, and $R1=0.0445$ for II. The crystal structures belong to the same space group Pnna (ITC No. 52) which was also determined for the carnallite from Wathlingen, Hanover, Germany [2]. In the structure of pseudo-carnallite there is only one type of Mg^{2+} ion in special position (4 d 2..) coordinating 6 water molecules, Mg^{2+} in the general position is substituted by Al^{3+} ion surrounded by 4 water molecules and 2 chloride anions in cis-position. K^+ ions are in the same positions like in carnallite itself. Four chloride anions occupy the general position, one Cl^- is in the special position (4 d 2.), and 2 additional Cl^- ions are in the general position with site occupancy factor of 0.5. Six water molecules are in the general position and two additional in special positions (4 d 2..).

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Keywords: carnallite, pseudo-carnallite, blue halite

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Synthesis and structural studies of the ettringite group of minerals

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The ettringite group of minerals is composed of hydrated calcium sulphate hydroxide minerals that have a common trigonal structure. The group is named after its most common member ettringite, which is itself, a rather uncommon mineral. Ettringite, which has the general formula $\text{Ca}_6\text{X}_2(\text{SO}_4)_3(\text{OH})_{12} \cdot 26\text{H}_2\text{O}$, where $\text{X} = \text{Al, Cr, Fe, Mn, Si}$ and the sulphate group can be substituted by carbonate, nitrate or borate groups, occurs naturally but is also an important industrial mineral. Delayed ettringite formation in cement pastes, mortars and concretes is a major cause of softening and disintegration of cements and concretes and this has major implications for the construction industry. A potential application of ettringite that is currently being investigated, is its use in the removal of metal species from waste effluents in industry. This can be achieved by adding calcium oxide and aluminium sulfate to the waste effluent and mixing to form ettringite. When ettringite is formed in the presence of other metal species, they can be incorporated into the ettringite structure either on the Al^{3+} site, or on the SO_4^{2-} site if they are present as oxyanions. A systematic study of the structural chemistry of Ettringite and its related phases has been undertaken using powder and single-crystal x-ray diffraction and neutron diffraction of both natural and synthetic samples. A detailed analysis of new and existing synthetic analogues of these mineral phases and investigations into potential solid solutions that may exist between different members of the Ettringite group has been carried out. It is my intention to report on the results of this study, with particular emphasis on the synthesis of new analogues and the solid solutions that exist between the different members of the ettringite group.

Keywords: ettringite, solid solutions, structural chemistry

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Peculiar site preferences of B and Ga in MgAl_2O_4 spinel solid solutions

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Single crystals of $\text{MgAl}_{1.8}\text{B}_{0.2}\text{O}_4$ and $\text{MgAl}_{2-x}\text{Ga}_x\text{O}_4$ spinel solid solutions were synthesized under the pressure of 5-11 GPa and the flux method, respectively. The crystal structures of spinel solid solution were refined single crystal X-ray diffraction and ²⁷Al MAS NMR measurements. The site preference of B is peculiar further than that of Al and Mg in MgAl_2O_4 spinel. Small B atom occupies the octahedral site, and hardly occupies tetrahedral site to keep the structure with high symmetry. The distribution of Ga are little affected by a change of the temperature. The degree of order-disorder