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.

References:

Keywords: carnallite, pseudo-carnallite, blue halite

P10.05.32

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

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Crystals of carnallite (K(MgCl)(6H2O)) and pseudo-carnallite (K(Al2MgCl14H4O)) 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=9.5568(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 Pnma (ITC No. 52) which was also determined for the carnallite group in 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...).

References:

Keywords: carnallite, pseudo-carnallite, blue halite

P10.05.34

Peculiar site preferences of B and Ga in MgAl2O4 spinel solid solutions

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Single crystals of MgAl2O4, B2O3 and MgAl2O4GaxOa 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 MgAl2O4 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
of Mg or Al between the tetrahedral and octahedral sites is almost constant against Ga content in the MgAl\textsubscript{2}Ga\textsubscript{3}O\textsubscript{8} solid solution. A compositional variable of the Ga/(Mg+Ga) ratio in the octahedral site is not influenced by the occupancy of Al. The occupancy of Al is independent of the occupancy of Ga, though it depends on the occupancy of Mg according to thermal history. The local Al-O bond length in the tetrahedral site is 0.15 Å longer than the expected bond length. The nature that Al in spinel structure occupies mainly the octahedral site arises from the character of Al itself.

Keywords: spinel, crystal structure, NMR spectroscopy

P10.05.35

Soft synthesis and crystallographic characterization of calcium magnesium mixed carbonates

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It seems to be generally accepted that smithsonite, magnesite, siderite, as well as mixed carbonates like dolomite (MgCaCO\textsubscript{3}) or huntite (Mg\textsubscript{2}Ca\textsubscript{2}CO\textsubscript{3}) have been formed in the nature under hydrothermal conditions. Rao et al. developed a general soft synthesis procedure for obtaining anhydrous carbonates by precipitation from solution at normal pressure. They had success in the synthesis of smithsonite and siderite, but failed in the magnesite synthesis. This finding questions that the hydrothermal synthesis were the only way of genesis of some of these minerals in nature. The scope of this work is to apply the Rao et al. method to the synthesis of double carbonates of general formula Mg\textsubscript{x}Ca\textsubscript{1-x}CO\textsubscript{3}. The compounds obtained have been characterized by X-ray fluorescence, atomic absorption analysis, TG and X-ray powder diffraction. The results obtained clearly demonstrate that anhydrous double calcium magnesium carbonate minerals can be obtained by soft synthesis for x composition ranging from 0 to 0.7. Hydroxysalts instead of anhydrous salts are obtained for larger values of x. The crystallographic parameters of the anhydrous compounds have been calculated and it has been shown that the volume of the cell accomplishes with the Vegard law.

Keywords: alkaline-earth double carbonates, lattice parameters

P10.05.36

Synchrotron X-ray diffraction studies of two olivines from the comet Wild 2

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Introduction and Experimental Methods: We have analyzed a collection of the Comet Wild 2coma grains returned by the NASA Stardust Mission. This is the first solid sample return mission since Apollo 17. The purpose of the diffraction experiment is to permit the structure refinement of olivine including site occupancies. In addition to the intrinsic importance of the olivine structures for revealing the thermal history of Wild 2 materials, we wish to test reports that olivine recovered after hypervelocity capture in silica aerogel has undergone a basic structural change due to capture heating [Foster N.J. et al. (2007) MAPS 42, A51]. The diffraction equipment placed at beam line BL4B1 of the Photon Factory, KEK was developed for microdiffraction studies of materials. [Ohsumi K. et al. (1991) J. Appl. Cryst., 24, 344 & (1995) Rev. Sci. Instr., 66(2), 1448]. This equipment has been successfully applied to various extraterrestrial materials [Ivanov A. V. et al. (2000) Amer. Min. 85, 1082]. Two Laue patterns of the samples (C2054,0,35,4 and C2067,1,111,4) were taken on an IP after 90 and 120 minutes exposures respectively. Structure refinements and Results: All Laue spots of both patterns are indexed by the traditional cell parameters of olivine. Structure refinements were carried out by a least-squares method minimizing the residual factor(R) based on the integrated intensities of Laue spots. The results of the several cycles of least-squares refinements including site occupancies of both samples lead the chemical formula as (Mg\textsubscript{0.83}Fe\textsubscript{0.16})\textsubscript{2}Si\textsubscript{0.00}O\textsubscript{4} for C2054 and (Mg\textsubscript{0.85}Fe\textsubscript{0.29})SiO\textsubscript{4} for C2067. Success of the refinement assuming the traditional cell parameters implies that the cell parameters of Wild 2 olivine cannot be significantly different from its typical values.

Keywords: synchrotron X-ray diffraction, microcrystallography, mineralogy and crystallography using X-ray diffrac