$Ca_2Mg(NO_3)_6*12H_2O$ – FIRST RESULTS ON A NEW COMPOUND RETRIEVED FROM CHIMNEY DEPOSITS OF A COMBINED HEAT AND POWER PLANT

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Nitrate minerals containing alkaline earth cations are rather rare. So far only two hydrous natural species have been reported in the literature: nitrocalcite ($Ca(NO_3)_2*4H_2O$, RIBAR et al., 1973) and nitromagnesite ($Mg(NO_3)_2*6H_2O$, SCHEFER & GRUBE, 1995). In the field of technical mineralogy, on the other hand, both phases have attracted much more interest. For example, both compounds are among the most common deterioration agents responsible for salt attack of buildings and monuments. Furthermore, nitromagnesite has been studied intensively as a potential thermal energy storage material (ZALBA et al., 2002). To the best of our knowledge no synthetic or natural hydrous Ca-Mg-nitrate has been reported so far. The results of the present investigation will fill this gap.

Starting point for this study was a routine X-ray powder diffraction phase analysis of a series of samples which were obtained from incrustrations of an exhaust gas chimney of a combined heat and power plant located in Malchow/Germany. Phase analysis using the current version of the PDF-4 database showed the existence of a small amount of anhydrite as well as bassanite. However, the majority of the peaks could not be attributed to any phase or phase mixture contained in the powder diffraction file. A re-examination of the residual under a petrographic microscope revealed that the sample contained a large number of colourless transparent crystals. A single-crystal of good optical quality was further studied by X-ray single-crystal diffraction (performed at 25 °C). The crystal structure could be solved by direct methods and difference Fourier synthesis. Structure solution was also used to establish the chemical composition: $Ca_2Mg(NO_3)_6*12H_2O$. The presence of water as well as nitrate moieties in the structure was confirmed by micro-Raman spectroscopy. Basic crystallographic data of the previously unknown material are as follows: trigonal symmetry, space group *R* -3, a=10.5583(5) Å, c=19.5351(10) Å, V=1885.98(16)Å^3, Z=3, R(|F|)=0.0248 for 744 reflections with $I>2\sigma(I)$. Principal structural building units are columns containing an alternating sequence of $Mg(H_2O)_6$-octahedra and CaX_9 tricapped trigonal prisms. (X:H_2O molecules, O atoms from the nitrate groups). Linkage between the polyhedra of a single column as well as between neighbouring columns is provided by hydrogen bonding. Using the result of the structural investigation a quantitative phase analysis of the incrustrations based on the Rietveld method could be accomplished.

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