

## **A NEW SALT-INCLUSION SULPHATE PHASE FROM A BURNING COAL DUMP: CRYSTAL-STRUCTURAL, CHEMICAL AND RAMAN-SPECTROSCOPIC CHARACTERISATION**

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A previously unknown salt-inclusion compound has been found on the burning coal dump of the Anna mine near Alsdorf, Aachen, North Rhine-Westphalia, Germany [1,2]. The compound forms small yellowish green to pale greenish sprays composed of acicular, transparent crystals with pointed terminations. The length of the crystals does not exceed approximately 0.4 mm. The phase is accompanied by clairite (NH<sub>4</sub>-Fe-sulphate), tschermigite (alum-type NH<sub>4</sub>-Al-sulphate), rostitite/khademite (NH<sub>4</sub>-Al-OH/F-sulphate), boussingaultite/mohrite (NH<sub>4</sub>-Al/Fe-sulphates) and others.

Semiquantitative chemical analyses of the crystals by SEM-EDS showed the presence of Na, minor K, Fe, minor Al, S and Cl. Single-crystal laser-Raman spectra demonstrated the presence of considerable amounts of NH<sub>4</sub>, and also indicated variable NH<sub>4</sub>/K ratios.

The crystal structure of the new phase was solved and refined from single-crystal X-ray diffraction data (Mo-K $\alpha$ , CCD area detector, 293 K, crystal size 0.02 x 0.02 x 0.36 mm). Crystal data: *I*4<sub>1</sub>/*acd* (no. 142), *a* = 18.259(3), *c* = 11.557(2) Å, *V* = 3853.0(11) Å<sup>3</sup>, and *Z* = 16, *R*(*F*) = 4.5 %. The derived chemical formula is (NH<sub>4</sub>,K)<sub>4</sub>(Fe,Al)<sub>2</sub>(OH)<sub>2</sub>(SO<sub>4</sub>)<sub>4</sub>·NaCl, in agreement with approximate elemental ratios calculated from the SEM-EDS spectra, the association with other NH<sub>4</sub>-Fe/Al-phases and with bond-valence calculations. The refined NH<sub>4</sub>/K ratio is about 0.89:0.11, and the Fe/Al ratio about 0.88:0.12.

The unusual crystal structure of the new phase is based on spiralling chains parallel to [001] of corner-sharing distorted (Fe,Al)O<sub>6</sub>-octahedra (<(Fe,Al)-O> = 1.99 Å), decorated by SO<sub>4</sub> tetrahedra. Channels parallel to [001] contain alternating Na and Cl atoms, i.e., linear ...Na-Cl-Na-Cl... chains which could also be described as chains of distorted NaO<sub>4</sub>Cl<sub>2</sub> octahedra linked by their Cl corners. The Na-Cl bond length equals 2.89 Å. The nine-coordinated (NH<sub>4</sub>,K) site (range NH<sub>4</sub>-(O,Cl) = 2.90-3.52 Å) occupies a void in the resulting framework.

The novel structure type will be discussed and compared to those of other natural and synthetic representatives of the rare class of salt-inclusion compounds.

The material containing the new phase was kindly supplied by Mr Frank de Wit, Netherlands.

- [1] Blaß, G. & Strehler, H. (1993): Mineralien-Welt 4 (4), 35-42. (in German)
- [2] Blaß, G. & Graf, H.-W. (1996): Mineralien-Welt 7 (2), 55-64. (in German)
- [3] Sindern, S., Warnsloh, J. M., Witzke, T., Havenith, V., Neef, R. & Etoundi, Y. (2005): Eur. J. Mineral. 17, Beih. 1, 130.