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Structure Refinement of Kochsándorite, A Basic Double-Carbonate Mineral. István E. Sajó. *Chemical Research Centre of the Hungarian Academy of Sciences. Budapest, Hungary.*
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Kochsándorite, $CaAl_2(CO_3)_2(OH)_4 \cdot H_2O$, a recently discovered mineral species [1] of the dundasite group crystallizes in *Pnma* space group. Of this mineral group dundasite is the only member for which the structure is known [2]. In the lack of proper sized crystals the structure of the other members of the group (dresserite, strontiodresserite, kochsándorite) was not determined, however they are supposed to be isostructural with dundasite [1].
High quality powder diffraction data of kochsándorite were collected in a focusing mirror – capillary geometry instrumental setup using Cu Kα radiation. Initial atomic coordinates were taken from the dundasite structure and geometrical constraints were used for bond lengths during refinement. The resulting structure exhibits partial similarity with the members of dawsonite group. The nature and origin of this similarity is discussed.

[1] Sajó I.E., Szakáll S, *Can. Min*., **2007**, 45, 479. [2] Cocco G., Fanfani L., Nunzi A. & Zanazzi P.F., *Mineral. Mag*. **1972**, 38, 564.

Keywords: rietveld refinement; powder diffraction; mineral structure

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New High Temperature Phases of the Type M(Py)$_n$Cl$_2$. Edith Alig[a], Lothar Fink[a], Tuncay Yeşilkaynak[b], Nevzat Külcü[b]. [a]*Institute Inorganic and Analytical Chemistry, Goethe-University Frankfurt, Germany.* [b]*Mersin University, Faculty of Arts and Sciences, Department of Chemistry, Mersin-Turkey.*
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Several compounds of the type $[M(II)(Py)_n]Cl_2$ with (M= Ni, Cu; $2 < n < 4$) were synthesized. Thermal decomposition led to various high temperature phases with different pyridine contents. For the copper compound $[Cu(C_5H_5N)_2]Cl_2$ [1] a new phase, $[Cu(C_5H_5N)]Cl_2$, was observed at temperatures above 170°C. At 230°C, ongoing decomposition resulted in another phase with less amount of pyridine. Above 270°C a mixture of different copper phases occurred, after that at 330°C Cu_2OCl_2 and, finally, CuO was observed (T > 430°C). For the nickel compound, $[Ni(C_5H_5N)_4]Cl_2$, [2] the thermal treatment resulted in the pyridine complex $[Ni(C_5H_5N)_2]Cl_2$ at 130°C and another phase, $[Ni(C_5H_5N)]Cl_2$, at temperatures above 190°C. At 310°C $NiCl_2$ was present while NiO was the stable phase above 490°C. Structural characterisation of the nickel and copper phases will be reported.

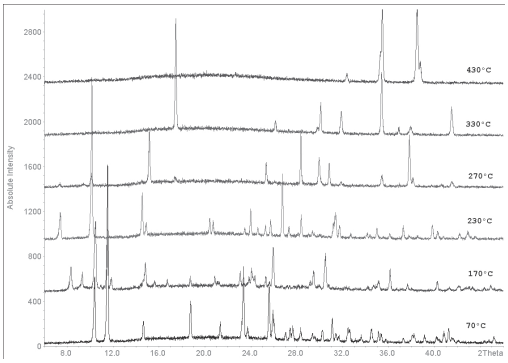

Fig.1: Thermal decomposition of $[Cu(Py)_2]Cl_2$

[1] B. Morosin, **1975**, *Acta Crystallogr.*, Sect. B. Struct. Crystallogr. Cryst. Chem., 31, 632 [2] G.J. Long, P.J. Clarke, **1978**, *Inorg. Chem.*,17,1394.

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Refinement of TLS Matrices from Powder Diffraction Data: Application to Naphthalene. Ivan Halasz[a], Robert E. Dinnebier[a]. [a]*Max-Planck Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany.*
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Analysis of thermal motion of molecules in crystals with the assumption of a rigid body can be approached in two ways: (1) TLS matrices can be refined from the independently refined ADPs of each atom and (2) ADP parameters can be *a priori* constrained to conform to the rigid body assumption. In the latter case the translational (T), librational (L) and the correlation (S) matrices contain the refineable parameters and the ADPs are than calculated from them [1,2]. The approach (2) is, regarding the number of required parameters, a compromise between the usual practice with powder diffraction data which is to describe the thermal motion of all atoms by a common isotropic Debye-Waller factor and an independent anisotropic refinement of each atom customary with single crystal data sets. The flexible macro scripting language of TOPAS [3] has been used to implement the refinement of TLS matrices from the approach (2) for powder diffraction data and has been applied to crystalline naphthalene for data collected between 293 K and 343 K. The refinement of elements of TLS matrices is performed in the Cartesian coordinate system followed by calculation of each atom's ADPs in the crystal coordinate system. Results are compared to previous studies [4,5] on thermal motion in crystalline naphthalene and the feasibility of this approach for routinely collected laboratory powder diffraction data is estimated. The macro scripts are readily applied to other molecular compounds for which the results of refinement of TLS matrices are also presented.