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A bimetallic Rb/Cr oxalate polymer (compound II) has been synthesized under hydrothermal conditions with selected starting salts and then investigated structurally at low temperature. Several discrepancies have been found with the reported room-temperature diaqua (µ-oxalato) chromium III rubidium (compound I)[1]. Indeed, the structures of the two compounds I and II are completely different, due probably to the synthetic conditions. According to the authors, the compound I crystallizes in space group C2/m and has a layered structure with the Cr, Rb atoms and one oxygen from water molecule lying on special positions. Moreover, the unique oxalate ligand forms a bridge between metal centers. The Cr atom is coordinated to 2 bidentate-chelating oxalates and 2 aqua ligands in a trans-conformation and any water molecule has been found around the 8-coordinated Rb atom. At 100K, the compound II shows a new atomic arrangement, which represents a novel structure type with interesting structural features. First, in the more distorted octahedra $CrO_4(H_2O)_{22}$ all ligands are in a cis-conformation while the alkali metal is surrounded by seven O atoms from oxalate groups, completed with two H₂O molecules which are bridging the Cr and Rb metals in chains of one edge-shared polyhedra, running along [100] direction. The two independent ligands play several roles, as bridging the metal atoms in the two other directions or interacting with the H₂O molecules, as medium or strong H-bonds, in order to build an extended three-dimensional network. Moreover, from the connection of the all different units in the 3D framework, two kinds of channels appear and run respectively along the [100] and [010] directions, with rhombic and rectangular section. It is noteworthy to underline that one of the two organic ligands offers an interesting and unusual conformation mode, since it displays simultaneously the conventional chelating mode i.e the μ_2 - η^4 coordination and the rather scarce μ_2 - η^3 chelating mode, involving two O atoms of the same carboxylate function. The diaqua dioxalate rubidium chromium(II) investigated at low temperature, exhibits distinct structural differences if compared with the reported previously double alkali and transition metal oxalates which have all layered structures [2][3]. This result can be related to the parameters governing the single crystal synthesis.

[1]Kolitsh, U.; *Acta Cryst.*, 2004, C60, n° 3, m129- m133).
[2] Gleizs, A.; Maury, F.; Galy, J., Inorg. Chem., 1980, 19, 2074.
[3]. Schwendtner, K.; Kolitsh, U. Acta Cryst., 2004, E60, m659-m661

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Polymorphism of Silicates of Anhydrous Cement as Treasury for the Most Advanced Concretes. <u>Frederic Dunstetter</u>^a, Mireille Courtial^{a,b}, Marie-

25th European Crystallographic Meeting, ECM 25, İstanbul, 2009 *Acta Cryst.* (2009). A**65**, s 185 Noelle de Noirfontaine^a. ^aLSI, Ecole Polytechnique, F-91128 Palaiseau, France. ^bUniversite d'Artois, F-62408 Bethune, France. E-mail: <u>dunste@wanadoo.fr</u>

Anhydrous cement is a mixture of the so-called clinker –an artificial rock made in cement kiln – and various additives. Clinker contains at least four major phases. Two calcium silicates Ca_3SiO_5 (50 to 70 wt % of clinker; 7 polymorphs) and Ca_2SiO_4 (15 to 30 wt %; 5 polymorphs), and two calcium aluminates (5 to 20 wt %). The crystallographic structure of six of the seven polymorphs of Ca_3SiO_5 are known nowadays, among them three were determined in the last eight years [1-3]. The structure of the five polymorphs of Ca_2SiO_4 is known since the 80's [4,5] but an important effort is still in progress in order to understand the complex twin and microstructural features [6].

During the subsequent hydration of cement, in order to produce concrete, the phases of clinker dissolve and various hydrated species precipitate and constitute the "glue" of the final material. Since the initial compounds disappear during hydration, only a very low effort was dedicated to the study of physicochemical properties of the anhydrous phases.

The situation is now very different, for the new high performance concretes developed since the 90's contain less and less water in the initial mixture. Then, more and more (0% to 40 vol %) anhydrous clinker now remains in this type of concrete. An important component of the very high strength (200 to 800 MPa, to be compared to 30 MPa for the ordinary concrete) is due to the very high Young modulus of the four phases of clinker (130 GPa) compared to all the other phases (20 to 30 GPa for the hydrates and 70 GPa for silica).

Therefore, the last decade has seen a renewal of the study of all basic physicochemical properties of the phases of clinker.

Within this context, we present here the actual status of the crystallographic knowledge of polymorphism of the two silicates Ca_2SiO_4 .

[1] F. Dunstetter et al. Cem. Concr. Res. 36 2006 39-53. [2] V.K. Peterson et al. J. Am. Ceram. Soc. 87 1625-1634 2004. [3] A.G. De la Torre et al, Cem. Concr. Res. 38 2008 1261-1269. [4] W.G. Mumme et al. N. Jb. Miner. Abh 169 35-68 1995. [5] H. Saalfeld et al. Z. Kristallogr 155 65-73 1981. [6] K. Fukuda et al. J. Am. Ceram. Soc. 91 4093-4100 2008.

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Structure of Metastable ScBO₃ Phases. <u>Elena</u> <u>Kudrenko^a</u>, Vladimir Morozov^b, Ivan Shmyt'ko^a, Gennadi Strukov^a, Tatjana Fursova^a. ^aInstitute of Solid State Physics Russian Academy of Sciences, Chernogolovka, Moscow distr. 142432, Russia. ^bMoscow State University, Department of Chemistry, Moscow, 119899, Russia. E-mail: <u>lenak@issp.ac.ru</u>

New metastable phases have been found during the annealing of the amorphous ScBO₃ sample at the different temperatures. The analysis of X-ray powder diffraction