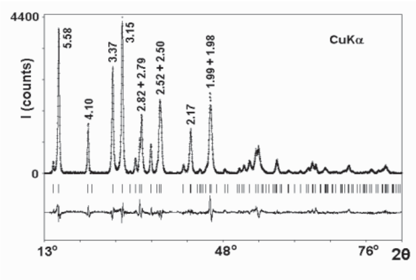
s8.m27.p18 Crystal structure solution of the low and high temperature forms of potassium dawsonite: An intermediate compound in the alkaline hydrolysis of calcium aluminate cements. L. Fernández-Carrasco and J. Rius. *Institut de Ciencia de Materials de Barcelona (CSIC), 08193-Bellaterra, Catalunya, Spain. E-mail: jordi.rius@icmab.es*

Keywords: Dawsonite; X-ray powder diffraction; Ab-initio structure solution

Potassium dawsonite is formed as an intermediate compound during the alkaline hydrolysis in Calcium Aluminate Cements. The crystal structure of potassium dawsonite $KAl(CO_3)(OH)_2$ has been solved with the origin-free modulus sum function [1] from X-ray powder diffraction data and refined with the Rietveld method (Figure). It crystallises in the orthorhombic *Cmcm* space group with unit cells parameters a = 6.3021(3) Å, b = 11.9626(5) Å, c = 5.6456(3) Å and Z = 4. The structure consists of carboaluminate chains, formed by the basic unit $[Al_2(OH)_4(CO_3)_2]^2$ arranged along the c axis -. The carbonate groups are placed in an alternate manner at both sides of the carboaluminate chains. The carboaluminate chains are also held together by the K^+ cations that are located in the middle of three such chains. Finally, the chemical reactions explaining the alkaline hydrolysis process in Calcium Aluminate Cements are postulated [2].



Rietveld refinement of HT- K dawsonite

In order to optimise the synthesis conditions of K-dawsonite, several syntheses at different temperatures and KOH solution concentrations were necessary. In these preliminary syntheses another compound of similar composition but crystallising in the orthorhombic Pmna space group with unit cell parameters a = 8.3312(6) Å, b = 5.6606(4) Å, c = 11.2682(8) Å was also formed. The crystal structure of this low temperature form of K dawsonite has been also solved with the origin-free modulus sum function [1] and is closely related to the high temperature form. Even though it has not been still identified in CAC pastes or mortars, it could be possible to find it in samples with high alkali content.

[1] Rius,J. (1993) *Acta Cryst.* A**49**, 406-409.
[2] Fernandez-Carrasco, L., Puertas, F., Blanco-Varela, M. T., Vazquez,T., Rius,J. (2004) *Cement and Concrete Research* (in the press)

s8.m27.p19 Corrosion Monitoring of Oil Field Equipment Using XRD Phase Analysis. István E. Sajó,[a] Nuri Al-Roba[a,b] Rehab Elalem[b] and Assma Marei[b], [a]*Chemical Research Centre of Hungarian Academy of Science, Budapest, Hungary, and* [b]*Petroleum Research Centre, Tripoli, Libyan Arab Jamahiriya. E-mail: sajo@chemres.hu*

Keywords: Quantitative phase analysis; Full profile fit; Corrosion products

Oil field production equipment is run in highly corrosive environment. Downhole and surface corrosion damage and related expenses can be minimized monitoring the corrosion processes. Solids formed during the corrosion processes can be collected from scales and deposits adhering inner surfaces and filtering recirculated water. A full profile fitting XRD evaluation method was developed (XDB) [1], and applied to identify and quantify the components of oil field related corrosion products. A reference database of corrosion specific phases was compiled to support and facilitate reliable phase quantification. Powder diffraction scans of corrosion samples were taken and evaluated for quantitative phase compositon. The use of this approach is illustrated on a few characteristic examples, representing the major types of corrosion occurring in oil field production environment.

[1] F.Feret, M. Authier-Martin & I. Sajó, *Clays and Clay Minerals*, **45**: 418-427 (1997).