

depicted above holds also for the $m=15$ (P) and the $m=18$ (C) polysomes.

[1] Capitani G.C., Mellini M., *Am. Mineral.*, 2004, **89**, 147. [2] Mellini M., Viti C., *Am. Mineral.*, 1994, **79**, 1194.

Keywords: antigorite, structure, polysomatism

P.10.05.10

Acta Cryst. (2005). A61, C378

Two kinds of Superstructures of (Ge, Si) Wollastonite

Fumito Nishi^a, Yoshio Matsumoto^b, Ritsuro Miyawaki^c, Yasuhiro Kudoh^d, ^aSaitama Institute of Technology, Fusaiji 1690, Okabe, Saitama, JAPAN. ^bTohoku University, Sendai, Miyagi, JAPAN. ^cDept. of Geology and Paleontology, Shinjuku Branch of National Science Museum, Shinjuku, Tokyo, JAPAN. ^dInstitute of Mineralogy, Petrology and Economic Geology, Faculty of Science, Tohoku University, Sendai 980-8578, Miyagi, Japan. E-mail: nishi@sit.ac.jp

Two kinds of superstructures of wollastonite whose compositions were Ca(Ge_{0.55}, Si_{0.45})O₃ and Ca(Ge_{0.65}, Si_{0.35})O₃ were synthesized. The former is called 0.55Wo and the latter 0.65Wo in this abstract. The lattice constants of 0.55Wo and 0.65Wo are: (angstrom, degree) $a=2X8.016(4)$, $2X8.038(5)$, $b=7.421(1)$, $7.451(1)$, $c=7.157(2)$, $7.194(1)$, $\alpha=90.08(2)$, $89.93(1)$, $\beta=94.86(2)$, $94.85(2)$, $\gamma=103.44(2)$, $103.34(1)$, respectively. Though both of them are twice as large as the basic structure of wollastonite, those structures are different. Basically, 0.55Wo has the two units of the basic-wollastonite along a-axis and has no other partial structures in it. The largest difference between the basic wollastonite and 0.55Wo is the fact that the basic wollastonite has an inversion center but 0.55Wo has not it. Therefore, the basic wollastonite includes only 15 independent atoms but 0.55Wo includes the 60 atoms in the unit cell. The final R-value was 6% after the structure refinement of 0.55Wo. 0.65Wo has the two units of the basic-wollastonite along a-axis, too. However, the X-ray diffraction pattern of 0.65Wo was largely different from that of 0.55Wo and it showed the extinction rule of the pseudo-C lattice. The structure model having the stacking of the basic-wollastonite unit with $b/2$ displacement were tried and the R-value was 9% after the structure refinement.

Keywords: structure analysis, superstructure, wollastonite

P.10.05.11

Acta Cryst. (2005). A61, C378

Light-Induced Degradation Dynamics in Realgar (As₄S₄)

Atsushi Kyono^a, Mitsuyoshi Kimata^a, Tanao Hattai^b, ^aDivision of Earth Evolution Sciences, University of Tsukuba, Japan. ^bJRCAS, Tsukuba, Japan. E-mail: kyono@arsia.geo.tsukuba.ac.jp

Light-induced degradation in realgar (As₄S₄) has been studied by means of four-circle XRD and XPS. Because of the alteration of realgar exposed to light, the a lattice parameter and $c \sin\beta$ value increase linearly, which leads to a continuous increase of the unit cell volume. Nevertheless, no correlation exists between the continuous increase of the unit cell volume and the bond distance variations in As₄S₄ molecules. The most pronounced change was observed in the distance between centroids in As₄S₄ cage. The spread of As₄S₄ intermolecular distances increases continuously from 5.642 Å to 5.665 Å, which directly affects the unit cell volume expansion of realgar. In addition, the O1s peak increases rapidly after light exposure. The result substantiates the reaction proposed by Bindi et al. [1]. That is, realgar is transformed into pararealgar if oxygen exists and produces As₄S₅ molecule. The additional S atom at As₄S₄ molecule contributes to anisotropic expansion for the a and c axes because the direction for the additional S atom points toward [4-14] in the unit cell. Furthermore, an S atom in the As₄S₅ molecule is released from one of equivalent As-S-As linkages in As₄S₅; it turns itself into the As₄S₄ molecular of pararealgar. The free S atom is re-attached to another As₄S₄ (realgar type) molecule, and reproduces an As₄S₅ molecule. The reproduced As₄S₅ molecule turns itself into the As₄S₄ molecular of pararealgar again. This cycle that realgar is indirectly transformed into pararealgar via As₄S₅ molecule is repeated during light exposure.

[1] Bindi L., Popova V., Bonazzi P., *Can. Mineral.*, 2003, **41**, 1463.

Keywords: single-crystal XRD, mineral physics, photochemistry

P.10.05.12

Acta Cryst. (2005). A61, C378

A Revision of the Structure and Crystal-Chemistry of the Arrojadite-Group

Roberta Oberti^a, Fernando Cámara^a, Christian Chopin^b, ^aCNR-IGG, Pavia, Italy. ^bLab. de Géologie, ENS-CNRS, Paris, France. E-mail: oberti@crystal.unipv.it

Arrojadite, dickinsonite and sigismundite define a group of phosphates with a very complex structure and crystal-chemistry, which has not been satisfactorily characterized so far. Previous works described the structure in the $C2/c$ space group which implies the presence of half-occupied P1 phosphate groups sharing basal faces and with the apical oxygen atoms pointing in opposite directions, and of partial occupancy at 10 out of the 49 sites in the asymmetric unit. Electron microprobe analyses suffer from severe interference problems due to the coexistence of P, Fe and F.

Single-crystal refinement, Raman spectroscopy and well-controlled *in situ* microchemical analysis of selected samples allowed a better interpretation of the structure and crystal-chemistry of the arrojadite group. The correct space group is Cc , and the lowering in symmetry implies recognition of strong cation ordering among the 21 cationic sites besides the 12 PO₄ groups. The correct number of OH groups pfu is 3 and not 2 (2 OH are bonded to octahedral sites and 1 to a PO₄ group), and a selectivity is shown for F incorporation at one of these sites. The active exchange vectors were identified, and a new nomenclature has been proposed on crystal-chemical basis.

The $C2/c$ derives from the presence in some samples of Cc domains related by a diad along b plus a $1/2$ shift along c . This feature cannot be treated by X-ray structure refinement, and may be related to growth defects occurring during high- T crystallisation (in pegmatites).

Keywords: phosphate crystal-chemistry, mineralogy, crystal-structure

P.10.05.13

Acta Cryst. (2005). A61, C378

Supramolecular Arrangement of Tensioactive Molecules in Interlayer Spaces of Two Organophilic Clays

Sandrine Geiger^{a,b}, H. Othmani^{a,c}, M. Benna-Zayani^c, B. Fraisse^b, M. Trabelsi-Ayadi^c, N. Kbir-Arighuib^d, J.L. Grossiord^d, N.E. Ghermani^{a,b}, ^aLaboratoire de physique pharmaceutique (UMR 8612), Faculté de Pharmacie de Châtenay-Malabry, France. ^bLaboratoire structure, propriétés et modélisation des solides, Ecole Centrale de Paris, France. ^cLaboratoire de Physico-chimie minérale, Département de Chimie, Faculté des Sciences de Bizerte, Tunisie. ^dInstitut National de Recherche Scientifique et Technologique, Hammam Lif, Tunisie. E-mail: sandrine.geiger@cep.u-psud.fr

Studies of mixed systems using clays and tensioactive molecules (TA) are of particular importance in many fields such as medicine, pharmacy and cosmetics. The substitution of the initial cations and intercalation of cationic organic molecules in the interlayer spaces of the clay structure lattice provide new physicochemical properties. The aim of the present study consist in a structural characterisation of two different purified and organophilic clays, mainly made of smectite with a marked montmorillonitic nature, as a function of the inserted TA quantity using high-resolution X-ray powder diffraction. Two different TA are used, the benzyltétradécyltriméthylammonium (BTDMA) and the benzyldodécyltriméthylammonium (BDDMA).

Keywords: organomineral materials, powder X-ray diffraction, supramolecular assemblies

P.10.05.14

Acta Cryst. (2005). A61, C378-C379

Ti-investigation by XPS of Biotite from Metapelites of El Joyazo (Spain)

Ernesto Mesto^a, Fernando Scordari^a, Giuseppe Cruciani^b,