

100 mm) IP detector; the 2 θ accessed range is 0 – 36°. The behaviour of the unit cell parameters as a function of pressure and the bulk modulus values were derived by processing the powder patterns. The ab-initio MD simulations, performed on the basis of the experimental cell parameters, provided the atomistic structural interpretation of the response of gismondine to compression.

Gismondine cell parameters regularly decrease and the P-induced modifications are reversible upon decompression. The bulk modulus calculated on the basis of the experiment performed with silicon oil is $K_0 = 63.8(2)$ GPa. The bulk modulus derived for the three data sets collected on LiABW using different P-transmitting media are $K_0 = 68(2)$, 64.8(8) and 60(5) GPa for silicon oil, alcohol-water and pentane-isopentane, respectively.

Keywords: zeolites, high-pressure diffraction, molecular dynamics simulations

P.10.06.3

Acta Cryst. (2005). A61, C381

The Crystal Structure of Chabasite-K

Polina Gavrilenco^a, Olga Yakubovich^a, Werner Massa^b, Igor Pekov^a,
^aGeological department, MSU, Russia. ^bPhilipp-Universität, Marburg, Germany. E-mail: polinka_gav@mail.ru

The chabasite group contains four minerals: chabasite-Ca, chabasite-Na, chabasite-K, and chabasite-Sr. The crystal structure of the K representative in this group has not been investigated before.

The good isometric crystals of chabasite-K were found in late hydrothermalites of Khibiny alkaline massif, Kola Peninsula, Russia. The average result of electron-microprobe analyses is: Na₂O 2.62, K₂O 7.22, CaO 4.61, SrO 1.44, BaO 0.04, Al₂O₃ 18.75, SiO₂ 46.41, H₂O 19.35, total 100.44 wt.%. The crystal structure of chabasite-K (K_{1.33}Na_{1.02}Ca_{0.84})[Al₄Si₈O₂₄] \cdot 12.17H₂O, hexagonal, space group $R\bar{3}c$, $a = 13.831(3)$, $c = 15.023(5)$ Å, $V = 2489.3(1)$ Å³, $Z = 3$, has been determined using a pseudomerohedrally twinned crystal [Enraf Nonius CAD4, MoK α , graphite monochromator, twin ratio 0.535(1) : 0.465(1), $wR_2 = 0.1177$ for all 6265 unique reflection, $R = 0.047$ for 4745 observed reflection with $I > 1.96\sigma(I)$]. Because of a high mobility of cations within the big framework cavities the experimental data were received at low temperature $T = 193$ K.

It has been established that K-bearing chabasite contains five independent sites of cations within the large cavities of Si,Al tetrahedral framework. Eight sites for water molecules were found in the structure. We compared the atoms' distribution in the framework cavities with similar data for chabasites of different composition and origin. Basing on the crystal chemical, mineralogical and geochemical data for zeolites of alkaline formation we assume that the number of cations in the chabasite-K from low-temperature hydrothermalites could be the result of a natural ion-exchange process.

Keywords: zeolite, chabasite-K, crystal structure

P.10.06.4

Acta Cryst. (2005). A61, C381

Crystallochemistry of Natural Zeolites from "Tuful de Dej" (Romania)

Lucia Robu, I.N. Robu *Geological Institute of Romania, Caransebes str. 1, 012271- Bucuresti, Romania.* E-mail: inrobu@yahoo.com

In Romania, natural zeolites occur in different geological environments (magmatic, crystalline and sedimentary), but the largest spreading is known in the sedimentary formations of the Transylvanian Basin, hosted by the Badenian volcanic tuffs ("Tuful de Dej").

The X-Ray investigations in two different zones of the Transylvanian Basin (the Dej-Bistrita Nasaud and Cluj Napoca Zones) have emphasized (i) a large variation of the zeolitic species, (ii) common and different species (iii) some differences between those two zones: a relative mineralogical homogeneity in the Dej-Bistrita Nasaud (*ferrierite*, *mordenite*, *epistilbite*, *thomsonite*, *natrolite*, *scolecite*, *faujasite*) and more variations in the Cluj Napoca One (*thomsonite*, *faujasite*, *scolecite*, *mesolite*, *heulandite*, *mordenite*, *epistilbite*, *gonnardite*, *ferrierite*, *clinoptilolite*, *chabazite*, *natrolite*).

Chemically, they include Al, Si, Na and Ca in their crystalline

network but Fe³⁺ and K are presented too, emphasizing some possible substitutions between Al - Fe³⁺ and Na - K.

Chemical homogeneity emphasized by zeolites from the Dej Bistrita-Nasaud Zone and some obvious differences remarked in the Cluj Napoca Zone have determined the similar zeolitic minerals and zeolitic mineral assemblages in the Dej-Bistrita Nasaud Zone and more differences in the Cluj Napoca Zone.

Keywords: zeolites, chemistry, X-ray

P.10.06.5

Acta Cryst. (2005). A61, C381

Open-framework Germanates by Organic Templating

Xiaodong Zou, Liqiu Tang, Yafeng Li, Tony Conradsson, *Structural Chemistry, Stockholm University, SE-106 91 Stockholm, Sweden.* E-mail: zou@struc.su.se

Templated germanates have recently drawn great interests due to their remarkably abundant crystal chemistry. The structure diversity of germanates is associated with the ability of germanium to form oxygen polyhedra with four, five and six coordinations.

Recently, a number of new zeolite topologies was discovered in germanates and silicogermanates (ASV, IWR, IWW, UOZ). The major impact of incorporating germanium into zeolite structures is that the T-O-T angles can be much smaller for Ge (~130°) than for Si (~145°). The smaller T-O-T angles are needed for framework structures with 3- and 4-rings, and thus very open frameworks with low framework densities.

We present several germanates with novel zeolite topologies, including a pure germanate FOS-5 (BEC) and a borogermanate SU-16^[1] (SOS). The building units are double 4-rings (D4R) in FOS-5 and two edge-sharing 3-rings (B₂Ge) in SU-16.

We also summarize several novel germanates and silicogermanates with extra-large rings, formed by one or two types of clusters. Two of them are SU-12^[2] and SU-14. Both SU-12 and SU-14 are built from the same (Ge, Si)₇ clusters and contain 24-ring channels. Due to the different connections of the (Ge, Si)₇ clusters, the 3D structures of SU-12 and SU-14 are different, and as well as their 3D intersecting channels.

[1] Li Y.F., Zou X.D., *Angew. Chem. Int. Ed.*, 2005, **44**, early view. [2] Tang L.Q., Dadachov M.S., Zou X.D., *Chem. Mater.*, 2005, in press.

Keywords: zeolites, open-frameworks, germanates

P.10.06.6

Acta Cryst. (2005). A61, C381

Synthesis and Characterization of Highly Dispersed Tungsten Oxide into SBA Molecular Sieve

Ching-Yuan Cheng, Kuan-Jiuh Lin, *Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan.* E-mail: d9051010@mail.nchu.edu.tw

Incorporation of transition metals such as Ti, V, Cr into the framework of the molecular sieves is a general method for introducing catalytic sites into mesoporous materials. Numerous attempts have been made to prepared transition metal-substituted mesoporous materials for making them into effective catalysts which are available of treating large molecules. Tungsten-containing mesoporous materials have attracted much attention in past years. Several groups have tried to synthesized mesoporous tungsten oxide materials or incorporated tungsten into mesoporous materials. However, the oligomer species formed as framework-skeleton synthesized are still a problem for all transition-metal doped mesoporous materials. Herein, the new tungsten SBA molecular sieve using highly dispersed method was showed the attractive performance in direct catalytic conversion. The $p6mm$ hexagonal structure of WSBA molecular sieve was showed on powder diffraction patterns. TEM and BET measurement show WSBA with narrowed distribution pore size and rigid structure after the reaction. The high dispersion of tungsten oxide into molecular skeleton was confirmed by UV and Raman spectrum.

Keywords: tungsten, high dispersion, mesoporous materials