100 mm) IP detector; the 2θ 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 modula 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

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The Crystal Structure of Chabasite-K

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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: Na_2O 2.62, K_2O 7.22, CaO 4.61, SrO 1.44, BaO 0.04, Al_2O_3 18.75, SiO_2 46.41, H_2O 19.35, total 100.44 wt.%. The crystal structure of chabasite-K $(K_{1.33}Na_{1.02}Ca_{0.84})[Al_4Si_8O_{24}]\cdot 12.17H_2O$, hexagonal, space group $R\bar{3}c$, a=13.831(3), c=15.023(5)Å, V=2489.3(1) $Å^3$, Z =3, has been determined using a pseudomerohedrically 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

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

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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 Transivanian 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 Fe $^{3+}$ and K are presented too, emphasizing some possible substitutions between Al - Fe^{3+} 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

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Open-framework Germanates by Organic Templating

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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 (B_2Ge) 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.

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Keywords: zeolites, open-frameworks, germanates

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

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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 mesoprous 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

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Hydrothermal Crystallization and Characterization of R^{+3}: $AlPO_4$ Zeolites, where R=Ce, Pr and Nd

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Zeolites are the most important technological materials made up of framework of aluminosilicates, aluminophosphates, vanadophosphates, silicoaluminophosphates and so on. In the recent years the interest is being extended greatly from the molecular sieves to selective catalysis, gas adsorption, nanoparticle hosts, atmospheric ecosystems, etc. These aluminophosphate molecular sieve zeolites have uni-, two-, and three-dimensional channels which are obtained hydrothermally in the presence of organic amines as structure directing agents. VPI-5 is an important aluminophosphate molecular sieve with 18 tetrahedral rings and free diameter of 12.1 Å. In this paper, the authors discuss the synthesis of R^{+3}: aluminophosphate, where R=Ce, Pr and Nd. The addition of R^{+3} into the aluminophosphate framework not only enhances the stability of the framework, but also enlarges the pore diameter, which helps in the sieving of large molecules. Further, the efficiency of the catalytic activity can be elevated. The materials obtained have been subjected to a systematic characterization using Powder XRD, IR, SEM, BET and Positron Annihilation Life time measurements. The preliminary investigation shows that the following results: FTIR spectra show that the R^{+3} is inserted into the $AlPO_4$ pores. Cell volume has increased considerably with the insertion of R+3 elements into zeolites framework. Consequently the surface area decreased. Positron annihilation lifetime spectroscopy data show that micro void content increases as the surface area decreases.

Keywords: $AlPO_4$ zeolites, hydrothermal crystallization, rare earth elements

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Gallium Substitution in Alumosilicate Halide Sodalites

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In the $Na_8[AlSiO_4]_6X_2$ sodalite system (X = Cl, Br, I) the aluminium atoms were partially substituted with gallium progressively. The synthesised products represented the new composition $Na_8[Al_{1-y}Ga_ySiO_4]_6X_2$ ($0 \leq y \leq 1$). Gallium concentrations for different compositions were calculated using X-ray powder data Rietveld refinements and ^{29}Si MAS NMR spectroscopy. The lattice parameters increased [1, 2] linearly from $[AlSiO_4]_6$ to $[GaSiO_4]_6$ framework matrix. The Al/Ga-O distance was found as an average magnitude [2], which increases with increasing gallium concentration while the Si-O distance remained almost constant at 162.8 pm ($\sigma \sim 2$), 163.4 pm ($\sigma \sim 3$) and 162.6 ($\sigma \sim 2$) for the chloride, bromide and iodide sodalite, respectively. The increasing average tilt of the framework Al/GaO_4 and SiO_4 tetrahedra led to Na-O and Na-X distances shortening as a consequence of increasing gallium content in the trivalent site of the framework. The degree of framework oxygen *s*-hybridisation was observed linearly correlated to average T-O distances. In the XRD patterns no clear hints for domain formation of aluminium and gallium enriched parts in the crystals were observed. However, the ^{29}Si MAS NMR spectra showed clearly a non statistical distribution of the different $Si-(OT^1_4)$ surroundings for bromide and iodide sodalites ($y \sim 0.30 - 0.70$). In the chloride sodalite series, aluminium and gallium were observed statistically distributed throughout the crystals.

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[2] Murshed M. M., Gesing Th. M., *Z. Kristallogr.*, 2005, **Suppl**. **22**, 27.

Keywords: sodalite, gallium, substitution

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Na/K and Na/Li Substituted Aluminosilicate Nitrate Cancrinites

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Cancrinites are the original class of microporous materials with so called ε-cages of sixring and fourring formed by TO_4-units (here T = Al, Si) and thereby including larger channels through the structures. We report here on synthesis and characterisation of the new forms of Na/K, Na/Li substituted cancrinites. The sodium form $Na_{6+x}[Al_6Si_6O_{24}](NO_3)_x(H_2O)_y$ (TG => $x \approx 1$, $y \approx 3$) was directly prepared by soft chemical methods [1]. This form has been used as mother compound together with $LiNO_3$ and KNO_3 solutions under synthesis conditions obtaining the appropriate Li and K form. The lattice parameter (Tab. 1) show increased values with increasing cation size. This is explained by a decrease of the tilt angle of rigid TO_4-unit as defined here and supported by results of Rietveld refinements of X-ray powder data and infrared investigations.

Table 1: Lattice parameter of the different cancrinite forms

Cancrinite form	a /pm	c /pm	V /10^6pm^3
Na/Li	1246.76(5)	501.92(3)	675.66(7)
Na	1265.89(2)	518.15(1)	719.08(3)
Na/K	1303.56(5)	535.65(2)	788.27(7)

[1] Buhl J.-Ch., Stief F., Fechtelkord M., Gesing Th.M., Taphorn U., Taake C., *J. Alloys Compd.*, 2000, **305**, 93.

Keywords: cancrinite, substitution, synthesis

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The Crystal Structure of Sacrofanite, the 74 Å Phase of the Cancrinite Group

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Sacrofanite, a = 12.903(2), c = 74.284(8) Å, space group $P\bar{6}2c$, is the largest member known to date of the cancrinite group, displaying a 28 layer stacking sequence along the *c* axis. The members of this group share some structural features with zeolites, their structural cages hosting extra-framework ions as well as H_2O molecules. The crystal structure of sacrofanite has been modeled on the basis of HRTEM images collected by means of a JEOL 4000EX microscope and processed with the program CRISP. The obtained model has been successfully refined *vs*. synchrotron radiation data (collected at the X-ray Diffraction Beamline at the Elettra facility, Trieste, Italy) up to R = 0.083 for 2426 reflections, with a resolution of 0.96 Å. The layer stacking sequence has Zhdanov symbol |12(8)21|12(8)21|, and corresponds to ABCABACACABACBACBACABABACABC..., where A, B and C stand for the positions of the six-member rings in each layer. The topological symmetry is $P6_3/mmc$; however the ordering of Si and Al in the tetrahedral sites reduces the symmetry to $P\bar{6}2c$. The resulting framework is formed by two sequences of four cancrinite cages and two sodalite cages along 0, 0, *z*, whereas sequences of one losod, one cancrinite, one losod, two sodalite, one liottite, and two sodalite cages develop along both ⅓, ⅔, *z* and ⅔, ⅓, *z*. These cages host extra-framework cations and anions, as well as water molecules. The crystal chemical formula of sacrofanite, as obtained from the refinement, is $(Na,K)_{98}Ca_{20}(Si_{84}Al_{84}O_{336})(SO_4)_{26}Cl_2{\cdot}8H_2O$.

Keywords: crystal structure, HRTEM, synchrotron radiation

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$BaZn_2(AsO_4)_2{\cdot}H_2O$: A Framework Structure Related to Feldspar

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