

tetrahedra and the very rare triarsenate groups  $As_3O_{10}$  which together serve as building units to form an intersecting tunnel structure with the  $Cs^+$  cations located at the intersections of tunnels. Crystals of  $Cs(GaOH)_2H(AsO_4)_2$  were grown by a high-temperature, high-pressure hydrothermal method. It crystallizes in the monoclinic space group  $P2_1/c$  with  $a=4.6479(4)$ ,  $b=6.051(1)$ ,  $c=16.457(2)$  Å,  $\beta=92.99(1)^\circ$ ,  $V=462.2(1)$  Å<sup>3</sup>,  $Z=2$ ,  $R=0.045$  for 929 independent reflections with  $I > 2.5 \sigma(I)$ . The structure contains infinite chains of  $GaO_6$  octahedra sharing trains edges. These chains are connected by arsenate groups to form layers in the  $ab$ -plane. The layers are linked by  $Cs^+$  cations and hydrogen bonding.

**PS08.00.27 RIETVELD REFINEMENT OF  $Na_2CaMg(PO_4)_2$ ,  $NH_4Al_3(SO_4)_2(OH)_6$ .** J. Maixner, H. Hejdrová, Central Laboratories, Institute of Chemical Technology, Technická 5, 166 28 Praha 6, Czech Republic

The structure analysis of  $Na_2CaMg(PO_4)_2$  and  $NH_4Al_3(SO_4)_2(OH)_6$  has been made by means of X-ray powder diffraction using Rietveld method.

The first compound is known as the mineral brianite(1) and it is structurally isomorphous with the mineral merwinite  $Ca_2CaMg(SiO_4)_2$  (2). The other compound is structurally isomorphous with  $KAl_3(SO_4)_2(OH)_6$  (3). None of these compounds has got an entry in ICSD or PDF-2 databases. Therefore, we have refined the structures of these minerals and prepared powder cards for them. The initial cell parameters were evaluated with TREOR 90(4) and the framework atom positions with temperature factors were taken from the literature. The theoretical powder patterns were calculated and their comparison with measured data undoubtedly confirmed isomorphism of solved structures.

The X-ray data were collected on DRON-UM-1 powder diffractometer with  $CuK\alpha$  radiation ( $7-120^\circ 2\theta$  range,  $0.02^\circ$  step size, 5 seconds per step). The Howard's version DBWS 4.1(5) was used for the Rietveld refinement. The table 1. summarises final cell parameters and R factors for both structures.

Table 1.: Final cell parameters and R factors for both structures.

a(Å)	b(Å)	c(Å)	$\beta$ (°)	V(Å <sup>3</sup> )	$R_w$ %
13.385(6)	5.204(1)	9.119(1)	90.78(2)	635.1(5)	8.12
7.007(1)	7.007(1)	17.616(1)	120.0	749.3(1)	10.55

- (1) L. Fuchs et al., *Geochim. Cosmoch. Acta* **31**, 1711 (1967)
- (2) P. B. Moore & T. Araki, *Am. Mineralogist*, **57**, 1355 (1972)
- (3) S. Manchetti, *Neus Jahrbuch fur Mineralogie*, 406 (1976)
- (4) P. E. Werner, *Z. Krist.*, **120**, 375 (1964)
- (5) D. L. Bish & S. A. Howard, *J. Appl. Cryst.*, **21**, 86 (1988)

**PS08.00.28 QUANTITATIVE RELATIONS AMONG CRYSTAL STRUCTURES ZEOLITES OF NATROLITE - EDINGTONITE GROUP.** Malinovsky Y., Institute of Crystallography of Russian Academy of Sciences, Leninskii pr.59., Moscow, 117333, Russia; Burzlaff H., Rothammel W., Institut für - Angevandte Physik der Universität Erlangen- Nurnberg, Bismarckstr. 10, D-91054, Erlangen, Germany.

The comparative quantitative evaluation of crystal structure similarity degree was applied to small group of zeolite minerals. A procedure of quantitative evaluation is based on the concept of mapping [1]. A derived structure (2) is called to be related to a basic one (1) if it can be mapped by a pair of matrices (A,S). A is a non-singular  $3 \times 3$  matrix, S is a  $(3 \times 1)$  column matrix.  $M=(A,S)$  is called the mapping of the relationship. The special computer program was created [2]. The type of symmetry relationship among more than 10 structures of natrolite-edingtonite-scolecite-thomsonite-kalbarsite series was shown. There is a strong specific influence of cation type on the tetrahedral network. The influence

of different cations (in row H-Na-K-Rb-Ca-Ba) on other atomic positions in the structure is quantitatively estimated. The role of water molecules was discussed.

[1] Burzlaff H., Rothammel W., On Quantitative - Relations among Crystal Structures, *Acta Cryst. A* **48** (1992), pp.483-490.

[2] Malinovsky Yu.A., Burzlaff H., Rothammel W., Structure of Lovozerite Type - a Quantitative Investigation, *Acta Cryst. B* **49** (1992), pp.158-164

**PS08.00.29 STRUCTURES OF  $SrSiO_3$  AND  $SrGeO_3$ .** Fumito Nishi, Saitama Institute of Technology, Fusaiji 1690, Okabe-machi, Ohsato-gun, Saitama-ken, Japan

I succeeded in synthesizing  $SrSiO_3$  and  $SrGeO_3$  single crystals. The space group is  $C2/c$  and the crystal data are:  $a=12.305(4)$ ,  $12.533(3)$  Å;  $b=7.129(2)$ ,  $7.262(1)$  Å;  $c=10.861(2)$ ,  $11.259(3)$  Å;  $\beta=111.60(2)$ ,  $111.30(2)^\circ$  for  $SrSiO_3$  and  $SrGeO_3$ , respectively. Hilmer (1962) studied the crystal structure of  $SrGeO_3$  by Weissenberg method and Nadezhina, Pobedinskaya, Ilyukhin, Nikishina and Belov (1977) studied it by four-circle diffractometer. According to my results, it may be said that Hilmer's crystal is same polymorph as mine but he misunderstood its unit cell. On the contrary, it is certain that Nadezhina's one is another polymorph having  $SrGeO_3$  contents. I can summarize: (1) Both structures include the layers comprised by  $SiO_4$  or  $GeO_4$  three-membered rings and the layers comprised by  $SrO_8$  polyhedra. (2) They are piled up along  $c$  direction alternately. (3) In viewpoint of the polytypic consideration, my crystals are classified into the 6-layer group which are studied by Yamanaka and Mori (1981).

Hilmer, W. *Kristallografiya* **7**, 704 (1962).

Nadezhina, T. N., Pobedinskaya, E. A., Ilyukhin, V. V., Nikishina, N. N. & Belov, N. V. *Dokl. Akad. Nauk SSSR*, **233**, 1086 (1977).

Yamanaka, T. and Mori, H. *Acta Cryst.* **B37**, 1010 (1981).

**PS08.00.30 CHARACTERIZATION OF  $UO_{2+2}$  EXCHANGE Y-ZEOLITE.** M.T. Olguín, S. Bulbulian, Instituto Nacional de Investigaciones Nucleares A.P. 18-1027, C.P. 11801 México D.F, México; J. Duque, R. Pomés, Centro Nacional de Investigaciones Científicas Apdo 6990 La Habana Cuba; M.E. Villafuerte-Castrejón, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, A. P. 70-360, México D.F. 04510 México; P. Bosch, Universidad Autónoma Metropolitana-Iztapalapa, A.P. 35-532 México D.F. 09340, México

The present study involves the incorporation of uranyl ion into Y-zeolite. The  $Na^+ - UO_{2+2}$  exchange in the framework was measured by neutron activation analyses. The X-Ray diffraction patterns of the materials have been studied in order to understand the behavior of uranyl ions in the zeolite and in order to present the unknown crystal data.

The Y-zeolite framework distort in response to the cation present in the structure. Hence the position of the  $UO_{2+2}$  in the structure was inferred from powder X-Ray diffraction data.