## P.10.02.9

**Ternary Phases in the Yb-Zn-Al System**

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The facility of ytterbium to form compounds with zinc (eight phases in the Yb-Zn system) and the presence of $YbAl_2$ with intermediate valence in the Yb-Al system have led to the study of the ternary Yb-Zn-Al system with the aim of finding compounds with possible interesting magnetic properties.

The alloys were prepared by melting the elements and annealing at 600-750°C. All samples were examined by optical and microprobe analysis and the crystal structure was determined by X-ray powder and single crystal methods.

Thirteen phases were identified. Six of them correspond to phases already present in the Yb-Zn or Yb-Al system [1], where the third element substitutes the Zn or Al atoms, more or less extensively, maintaining the same structure. Examples are $YbZn_{0.88}Al_{1.12}$ ($MgCu_2$-type) and $Yb_3Zn_{4.48}Al_{6.16}$ ($La_3Al_{11}$-type). Six ternary compounds crystallize with other known structure types. Examples are YbZnAl ($MgNi_2$-type) with all mixed Zn/Al occupations of the Ni sites and $Yb_8Zn_{48.5}Al_{17.5}$ isotypic with $Yb_8Cu_{17}Al_{49}$ [1], with partial ordering of the Zn atoms. A new hexagonal structure is observed for $YbZn_{7.3}Al_{0.5}$, by taking nine $CaCu_5$ cells and substituting some of the Yb atoms (28.9%) with mixed Zn/Al pairs. This substitution mechanism, known for a long time, is found also in $YbZn_{7.8}Al_{0.4}$ and $YbZn_{9.2}Al_{1.3}$ with structures derived from the $U_2Zn_{17}$ and $SmZn_{11}$ types, respectively.

[1] *CRYSTMET, Structure and Powder Database for Metals*, 2004.
**Keywords: crystal chemistry and structure, intermetallic compounds, ternary alloys**

## P.10.02.10

**An Unconventional Look at Sulfides and Selenides: Anion-centred Polyhedra**

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Lower sulfides of palladium, $Pd_4S$, $Pd_3S$, and $Pd_{16}S_7$, resemble alloys with "clathrated" S atoms and a very complex metal framework. In terms of anion-centred polyhedra, however, $Pd_4S$ consists of corner-connected $SPd_8$ bisdisphenoids (CN=8), $Pd_3S$ of corner-connected complex CN=6 polyhedra whereas $Pd_{16}S_7$ contains clusters of tetrahedrally arranged trigonal prisms $SPd_6$, interconnected by flattened $SPd_4$ tetrahedra. Edge- and corner-sharing $SM_4$ tetrahedra in various arrangements form the structures of PdS, PdSe and PtS. Clusters of tetrahedra as well as 4- and 6-petal rosettes of tall CN=5 coordination prisms $SM_5$ are in the structure of $Rh_{17}S_{15}$ and $Ni_{10}Pd_7S_{15}$; the same six-petal rosettes, interconnected by tetrahedra, form the structure of pentlandite $Co_9S_8$. Surprisingly simple structures formed by anion-centred polyhedra are found in tetrahedrite, $Ag_2S$, $Cu_2Se_2$, and also $Bi_2S_3$, $Cu_2S$ and talnakhite.

The anion-centred configurations depend on the cation:anion ratio (metal-rich sulfides have higher CN) and on the type of cation. Especially Cu and Ag form typical anion-based polyhedra. Uniformity and small number of configurations suggest that the directional bonds of an anion may be equally important as those of the cation present. It means that an insight deeper than the usual anion-packing considerations might be necessary. Cation-lined interspaces between the anion-centred polyhedra and the contracted polyhedron edges with metal-metal bonds are of special interest.

**Keywords: coordination and inorganic compounds, sulfides, selenides**

## P.10.02.11

**The Term Systematics**

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Every science is represented by its terms. Systemic terms are used in all sciences and other terms in concrete sciences. The term sequence is used in all sciences.The sequence s < f < d < p elements is the basis of chemical compounds, mineral systematics.

Many terms represent different sequences in chemistry, crystallography. These are series: homologous, linear, polytypic, heteropolytypic, pseudopolytypic, polysomic, modular, plesiotypic, meroplesiotypic, space modulated; series of: mixed layer structures (s.), syntactic s., fragment s, transmineral s., symbiotic s., sonar s., super space s., long period s., chemical twin s., topological s., related s., topology related s., gray isomorphic s., partial isotypic s., intergrowth at the level of unit cell s., crystallographic shear s., multystory s., O, OD, MDO s., superstructures, cluster substructures, matrix combinations, sminal structure types, structure type spectra, ordered isomorphs, 0-3 dimensional isomorphs, 0-3 dimensional elements, details, domains, V-D domains, as trees of polymorph structure types, as trees of symmetry groups, as Belov classes, subclasses, as planar static waves, as concentration waves, as elastic waves, as standing waves, as homologous structure type classes, as refrain series of merons, as series of supramolecular syntons.

The term systematics (a branch of systematics) allows finding and solving discrepancies between mineral species and external form terms, revealing relationship, difference, synonymy, constructing sceletal part of science.

**Keywords: systematics, term, science**

## P.10.02.12

**Alkaline Earth Aluminates/Gallates and Perovskites: Two Sides of the Same Coin**

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The crystal chemistry of alkaline earth oxoaluminates and gallates covers a large variety of different structure types. However, most of the compounds are based on $[AlO_4]$- or $[GaO_4]$-tetrahedra with various degrees of connectivities. The structures of the materials are similar to those observed in silicates (which have been studied in much more detail) and can be classified using the same concepts proposed by Liebau [1].

However, many of the alkaline earth rich compounds can be related to the perovskite structure type as well. For example, the "cyclo-gallate" $Sr_3Ga_2O_6$ containing isolated six-membered $[Ga_6O_{18}]$-rings can be alternatively regarded as an example for a defect $ABO_3$-perovskite with 12.5% vacancies in the A-substructure and 25% oxygen vacancies: $(Sr_{7/8}\square_{1/8})(Ga_{3/4}Sr_{1/4})(O_{3/4}\square_{1/4})_3$.

This new concept has been successfully applied to about ten recently determined crystal structures of oxoaluminates/gallates. Using the classical description based on the connectivity of the tetrahedra, the crystal structures look quite different. The "perovskite-approach" offers an elegant way to relate these structures in a simple way.

[1] Liebau F., *Structural Chemistry of Silicates*, Springer, 1985.
**Keywords: crystal chemistry of inorganic compounds, structural relationships, aluminum compounds**

## P.10.02.13

**Order-Disorder Phenomena in Nitridosilicates and Nitridophosphates**

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Among numerous (oxo-)nitridosilicates synthesized in the past years, some compounds exhibit interesting order-disorder phenomena. Whereas the ordered structure of $Ho_2[Si_4N_6C]$ [1] can be derived from the highly symmetrical framework nitridosilicate $BaYb[Si_4N_7]$ [2] by "chemical twinning", the same $N^{[4]}(SiN_{3/2})_4$ (X = N, C) building

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