that these different magnetic structures have been found by the authors to be related with the values of certain topological invariants [2]. It seems that the above approach could serve also for the description of the symmetry groups of all the other aperiodic structures, like e.g. the modulated nonmagnetic structures, quasicrystals (nonmagnetic and magnetic) etc.

[1] J. Warczewski, P. Gusin, T. Śliwińska, G. Urban, J. Krok-Kowalski, *Central European Journal of Physics*, 5(3) **2007** 377-384. [2] P. Gusin, and J. Warczewski, *Journal of Magnetism and Magnetic Materials*, 281/2-3 **2004** 178-187.

Keywords: magnetic ordering; magnetic crystal structures; symmetry of structures

FA4-MS01-O4

Giant Unit Cell Structures in the System Al-Cu-Ta. Thomas Weber[a], Julia Dshemuchadse[a], Matthias Conrad[b], Bernd Harbrecht[b], Walter Steurer[a]. [a]*Laboratory of Crystallography, ETH Zurich, Switzerland.* [b]*Fachbereich Chemie, Philipps-Universität Marburg, Germany.*
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Three cluster-based structures of unprecedented complexity have been observed in the system Al-Cu-Ta [1, 2]: *cF*432-$Al_{69}Ta_{39}$ (AT-19), a = 19.153 Å, V = 7,026 Å^3, *cF*(5,928-x)-$Al_{56.6}Cu_{3.9}Ta_{39.5}$, x = 33 (ACT-45), a = 45.376 Å, V = 93,428 Å^3 and *cF*(23,256-x)- $Al_{55.4}Cu_{5.4}Ta_{39.1}$, x = 98 (ACT-71), a = 71.490 Å, V = 365,372 Å^3. The space group is $F\ 3m$ in all three cases. Despite the complexity of the structures, usage of cutting edge X-ray diffraction technology allowed to collect high quality diffraction data suitable for precise structure determination. There are two complementary approaches to the understanding of the structures. First, the crystals can be seen as cluster-based compounds. The common fundamental building unit is a triple-shell $Al_{102}Ta_{57}$ fullerene cluster with a diameter of about 13.5 Å. In the case of AT-19 the fullerenes form a distorted *fcc* packing, where the empty spaces are filled by Friauf or CN15 Frank-Kasper polyhedra. ACT-45 and ACT-71 host super clusters built of four or ten fullerenes, respectively, *i.e.* fragments of the AT-19 structure. The super clusters are separated by extended blocks, which are related to Laves phases. An alternative approach to the understanding of the structures is describing them as modulated structures. The common basic structure is a 6.5 Å sized cubic Laves phase. AT-19, ACT-45 and ACT-71 are 3-fold, 7-fold and 11-fold commensurate super structures, respectively. The lattice of the basic structure can clearly be identified in the diffraction pattern, however, many satellite reflections show intensities, which are comparable or even stronger than main intensities. An interesting and quite exceptional aspect of the structures investigated in this work is that they show self-templating properties: when shifting the along a main axis projected structure by 1/4 unit translation it is found that densely filled regions are systematically superimposed to loosely filled regions and *vice versa*.

[1] Weber, T., Dshemuchadse, J., Kobas, M., Conrad, M., Harbrecht, B., Steurer, W, *Acta Cryst. B*, accepted for publication. [2] Conrad, M., Harbrecht, B., Weber, T., Jung, D.Y., Steurer, W., *Acta Cryst B*, accepted for publication.

Keywords: Al-Cu-Ta; metallic clusters; modulated structures

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$K_4CoMo_3O_{12}$ at Low Temperatures: Phase Transitions and Modulated Structures. J. M. Engel[a], H. Ehrenberg[b]. [a]*Institut für Werkstoffwissenschaft, Technische Universität Dresden, Helmholtzstrasse 7, D-01069, Dresden.* [b]*Institute for Complex Materials, IFW Dresden, Helmholtzstrasse 20, D-01069 Dresden, Germany.*
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$K_4CoMo_3O_{12}$ shows a large variety of different polymorphic modifications from a high-temperature phase till several high-pressure phases [1]. Consequently low-temperature single-crystal experiments on α-$K_4Co(MoO_4)_3$ at 200, 150 and 101K were performed. All data were collected with a Xcalibur system from Oxford-Diffraction equipped with a Sapphire2 detector using ω- and φ-scans. The cooling was performed with a cryo system also from Oxford-Diffraction.
The structural changes at low temperatures were indicated by additional reflections detected in the projection of the reciprocal space. In the case of the data at 200K the superstructure reflections bisect the a*-axis. However in the data at 150K and 101K occur satellite reflections with modulation vectors close to q = 1/2 a* + 1/3 b* + 1/3 c*. The refinement of the q-vector leads to q = 0.501 a* + 0.350 b* + 0.318 c* at 150K and to q = 0.501 a* + 0.343 b*+ 0.328 c* at 101K, respectively. Therefore we are dealing here with incommensurately modulated structures.
The first low-temperature modification at 200K has also the space group P-1 with four formula units per unit cell and the lattice dimensions a = 15.3637(6), b = 9.8492(4), c = 10.0014(4) Å as well as α = 92.819(3), β = 106.588(4) and γ = 105.772(3)°. The significant alteration in the structure is a fractional change of the coordination of Co from six to five.
Ignoring the superstructure reflections from the data of 150K and 101K, the average structures exhibit again exclusively six-fold coordinated Co atoms.

We will present the results of the data analysis and compare the structures with each other.

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