FA2-MS16-P01

Extended symbols for coordination polyhedra after Parthé (1990). Rudolf Allmann[a], Roland Hinek[b]. [a]*Im Grund 5, D 35043 Marburg,* [b]*FIZ Karlsruhe, D 76344 Eggenstein-Leopoldshafen.*

In his book Parthé (1990) has defined short symbols for coordination polyhedra. We use these symbols to describe the coordination polyhedra in the Inorganic Crystal Structure Database ICSD. As not all polyhedra occurring in ICSD are described by Parthé, we extended his nomenclature. The following letters are used:

l: coplanar or collinear, n: non-coplanar or non-collinear,
p: prism, ap: antiprism, y: pyramid, by: bipyramid,
t: tetrahedron, o: octahedron, cb: cube, i: icosahedron;
tt: truncated tetrahedron, dh: pentagon-dodecahedron
co: cuboctahedron, aoc: anticuboctahedron; rd: rhombic dodecahedron, bds: bisdisphenoid, tds: trisdisphenoid
FK: Frank-Kasper polyhedra (for more than 12 neighbors),
c: for an additional capped face (equatorial),
c': capped polar face of prisms or antiprisms
(outside): if the central atom is outside of the polyhedron

For the different coordination numbers the following symbols result:

2: 2l, 2n; **3**: 3l, 3n
4: 4l, 4n, 4t, 4y (central atom at the centre of the base)
5: 5l, 5n, 5y, 5by
6: 6l, 6n, 6o, 6p, 6y, 6by and 6ap (deformed octahedra)
7: 7y, 7by, 6o1c (= 6ap1c), 6p1c;
8: 8cb, 8ap, 8bds, 8by, 6p2c, 6p2c'
9: 6p3c (= 8ap1c'), 8p1c'
10: 10p, 10ap, 8p2c', 8ap2c', 7y3c';
11: 6p3c2c', 10p1c', 10ap1c'
12: 12co, 12aco, 12i, 12p, 10p2c', 10ap2c', 12tt, 12tds, 6p6c
13: 12p1c', 12ap1c', 13FK;
14: 14FK (= 12ap2c'), 12p2c', 14rd;
15: 15FK, 10p5c; **16**: 16FK (=12tt4c); **17:** 10p5c2c';
18: 12p6c; **20**: 12p6c2c', 20dh
Also other improvements in ICSD will be reported.

Ref: E. Parthé (1990), Elements of inorganic structural chemistry, K.Sutter Parthé Publisher, Petit-Lancy, Switzerland
Also in: J. Lima-de-Faria (1994), Structural mineralogy, Kluwer Academic Publishers, Dordrecht, Netherlands

FA2-MS16-P02

Elastic properties and thermal expansion of acetylsalicylic acid. Johannes D. Bauer, Eiken Haussühl, Björn Winkler. *Institut für Geowissenschaften, Goethe-Universität Frankfurt am Main, Germany.*
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Acetylsalicylic acid form I (Aspirin®, ASA) crystallizes in the monoclinic space group $P2_1/c$. The crystal structure is composed of centrosymmetric dimers, in which the molecules are linked by two hydrogen bonds [1]. Up to now only incomplete elastic stiffness tensors have been determined by experimental and computational techniques [2]. Single crystals of optical quality with volumes up to about 30 cm^3 were grown from ethanolic solution by lowering of the temperature in the range between about 300 and 290 K. The complete elastic stiffness tensor was determined experimentally for the first time by different ultrasonic methods (plane parallel plate ultrasonic technique and resonant ultrasound spectroscopy) on oriented macroscopic samples. The thermal expansion was measured with a commercial dilatometer.
The thermal expansion of ASA is anisotropic, the minimum of the longitudinal effect is parallel to the direction [010], the effects perpendicular to this direction are larger by a factor of two. The anisotropy of the elastic stiffness is less pronounced, the maximum of the longitudinal effect (approx. 14 GPa) is observed in the direction of the hydrogen bonds linking the centrosymmetric ASA-dimers in the crystal structure.
The experimentally obtained elastic stiffness coefficients are discussed with respect to the results of force field and density functional theory (DFT) calculations.

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[1] Wheatley, P.J., *J. Chem. Soc.*, 1964, Part 4,6036. [2] Kim, Y., Machida, T., Taga, T., Osaki, K., *Chem. Pharm. Bull.* 1985, 33(7), 2641.

Keywords: elastic properties, crystal structure - physical property relationships, Acetylsalicylic acid

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Metal insulator transitions in $RE_{1-x}M_xTiO_3$: evidence for charge order stabilizing an insulating phase. A.C. Komarek[a], M. Reuther[a], T. Lorenz[a], A. Cousson[b], F. Bourrée[b], D. Trots[c,d], C. Baeths[c,d], and W. Morgenroth[c] , and M. Braden[a]. [a]*II. Physik. Institut, Univ. zu Köln, Germany,* [b]*Laboratoire Léon Brillouin, Saclay, France,* [c]*Hasylab, DESY, Hamburg, Germany,* [d]*Materials Science, TU Darmstadt, Germany.*
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By doping $LaTiO_3$ and $YTiO_3$ with Sr and Ca, respectively, one may suppress the Mott insulating state of the parent compound similar to the well-known phase diagram of high-T_c superconducting cuprates. However, whereas only a few percent of Sr content imply metallic properties in $La_{1-x}Sr_xTiO_3$, the analogous materials $Y_{1-x}Ca_xTiO_3$ stay insulating up to rather high Ca concentrations of about 35%. Comprehensive neutron and x-ray diffraction studies combined with characterization of the macroscopic properties allow us to explain the enhanced stability of the insulating phase in $Y_{1-x}Ca_xTiO_3$. At intermediate Ca content we find a clear evidence for charge ordering. The insulating phase exhibits a structural phase transition associated with a splitting of the Ti-site. TiO_6 octahedrons with large and small volume present a 3-dimensional checker-board type ordering, which via empirical relations indicates ordering of the Ti valence states. The charge-ordered phase in the perovskite titanates is further stabilized by replacing Y through a smaller rare earth shifting the critical concentration of the metal-insulator transition close to x=0.5.

Keywords: metal-insulator transitions, transition metal-rare earth oxides, X-ray and neutron diffraction