o.m12.p5 **The influence of metal coordination on ligand geometry: The structures of 2-(diphenylphosphino) acetophenone and bis(2-(diphenylphosphino) acetophenone)palladium(II)triflate.** M. H. Johansson, C. Andersson, A. Oskarsson. *Inorganic Chemistry 1, Chemical Centre, Lund University, P.O. Box 124, S-221 00 Lund, Sweden.*
Keywords: half-normal probability plots, palladium(II), synchrotron radiation.

The Pd-compound was prepared by treating tetrakisacetonitrile-palladium-bistriflate with 2-(diphenylphosphino)acetophenone in CH_2Cl_2 for 4 hours at room temperature. The solvent was evaporated giving an orange oil. The compound was crystallized from hexane giving orange prisms.

The Pd-compound crystallizes in the orthorhombic space group $P2_12_12_1$ with cell dimensions a= 11.867(2), b=18.162(4), c=19.603(4) A, V=4224.9(15) A^3 and Z=4. The organic ligand crystallizes in the monoclinic space group $P2_1/c$ with cell dimensions a=11.050(2), b=16.052(3), c=9.7082(19) A, β=109.58(3)°, V=1622.4(6) A^3 and Z=4. The total number of unique reflections collected is 13131 for the Pd- compound ($\theta \leq 31.7°$) using MoKα radiation. The organic compound diffracts poorly and data collected at the home source was not of acceptable quality. The data was collected at the synchrotron, Max laboratory in Lund, Sweden (5640 unique reflections, $\theta \leq 41.1°$, λ=0.852 A). Both structures were solved by direct methods and the final R-values are 0.043 (Pd-stucture) and 0.059 (organic structure).

Two chelating ligands bind to palladium via phosphorus and oxygen in a psuedo square-planar *cis*-configuration. The Pd-O distances are 2.060(3) and 2.096(2) A and the Pd-P distances are both 2.229(1) A. The geometry of the two ligands in the metal complex show only small differences, but is significantly different from that of the free ligand. The largest differences are seen in the angles around phosphorus and the angles around the carbon with the keto oxygen.

o.m12.p6 **Synthesis and Structure of a New Binuclear Complex [BaCo $(C_3H_2O_4)_2$ $(H_2O)_4$].** A. Djeghri [a], F. Balegroune [a], A. Guehria-Laidoudi [a], L. Toupet [b], P. Briard [c]. [a]*Laboratoire de Cristallographie Appliquée, Institut de Chimie, USTHB, BP 32, El-Alia, 16111 Bab-Ezzouar, Alger, Algérie.* [b]*Groupe Matière Condensée et Matériaux, Université de Rennes I, Avenue du Général Leclerc, 35042 Rennes Cedex, France.* [c]*Laboratoire de Chimie Structurale et Inorganique Moléculaire, Université de Rennes I, Avenue du Général Leclerc, 35042 Rennes Cedex, France.*
Keyword: malonate, DRX, polymeric structure.

In alkaline-earth metals complex series, malonic acid is known as bonding preferentially to the larger members like calcium and barium, exhibiting great coordination ability [(1,2)].

A new malonate complex containing barium and cobalt have been prepared in order to investigate possible discriminate between two different metals of approximatively the same radius.

The bis-malonato tetra-aqua barium (II) cobalt (II) was obtained as single crystals from a solution in the system cobalt-barium-malonic acid, with controlled conditions of pH, heating and storage.

It crystallizes in the orthorhombic system, space group Pccn with: a = 18.974 (4) Å, b = 6.783 (3) Å, c = 9.394 (2) Å, V = 1209.8 (6) $Å^3$, Z = 4. The asymmetric unit contains one cobalt, one barium, one malonate group and two water molecules.

The final R and wR values are 0.029 and 0.039. The structure is built up from $[BaCo(C_3H_2O_4)_2(H_2O)_4]$ molecules forming a polymeric framework.

Owing to its position on a symmetry center, the cobalt is four-coordinated in an octahedral polyhedron. The oxygens around it are contributed by three malonate groups. Two of these are chelating one barium and one cobalt in "malonate mode" [(2)] involving in each case the two oxygens of the two carboxylate functions. The two another malonate groups have a coordination slightly different: by one function, they were monodentate, bridging two cobalts according to the sequence [Co-O4-C3-O3-Co] and by their second function, they were bidentate and hence bridges one cobalt and one barium.

The barium, which lies on a crystallographic two-fold axis, is eight-coordinated. The coordination sites are occupied by four oxygens from malonate groups and four oxugens from water molecules. The coordination polyhedron around the barium may be described as a slightly distorted square antiprism.

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