

# SYNTHESIS AND STRUCTURE OF TRIS [HEXAAQUACOBALT] BIS [TRIHYDROGEN [ [(2,4,6-TRIMETHYLBENZENE-1,3,5-TRIYL) TRIMETHANEDIYL]TRIS(PHOSPHONATE)]] UNDECAHYDRATE

*Piotr Garczarek<sup>1</sup>, Jan Janczak<sup>2</sup> and Jerzy Zoń<sup>1\*</sup>*

<sup>1</sup>*Department of Medicinal Chemistry and Microbiology, Faculty of Chemistry, Wrocław University of Technology, Wybrzeże Wyspiańskiego 27, 57-300 Wrocław, Poland*

<sup>2</sup>*Institute of Low Temperatures and Structure Research, Polish Academy of Science, 2 Okólna St., PO Box 1410, 50-950 Wrocław, Poland*

Synthesis of phosphonic acids with their perspective application in metal phosphonate synthesis has been a field of interest in our laboratory.<sup>1,2,3</sup> Special attention has been given to phosphonic acids based on rigid aromatic scaffold possessing limited conformational freedom.<sup>4,5</sup> 2,4,6-Trimethylbenzenetriyl-1,3,5-tris(methylphosphonic acid) seems especially interesting due to steric hindrance caused by methyl groups which control conformational flexibility of the methylphosphonic groups.

Herein we report synthesis and structure of product resulting from reaction of cobalt (II) acetate and 2,4,6-trimethylbenzenetriyl-1,3,5-tris(methylphosphonic acid). Ligand was synthesized using slightly modified previously reported method.<sup>6</sup> Reaction was carried out in room temperature *via* slow solvent evaporation method. Water was used as solvent.

Tris [hexaaquacobalt] bis [trihydrogen [ [(2,4,6-trimethylbenzene-1,3,5-triyl) trimethanediyl]tris(phosphonate)]] undecahydrate (**1**) crystallizes in  $P\bar{1}$  space group of the triclinic crystal system. Asymmetric unit consists of one phosphonic acid residue, one and a half hexaaquacobalt cation and five and a half water molecules. One of the metal ions occupies a special position in the inversion center (0,0,0).<sup>7</sup> Ligand molecule is triply deprotonated – each phosphonic group is in singly deprotonated state.<sup>8</sup> Structure of the salt is held together by number of hydrogen bonds.

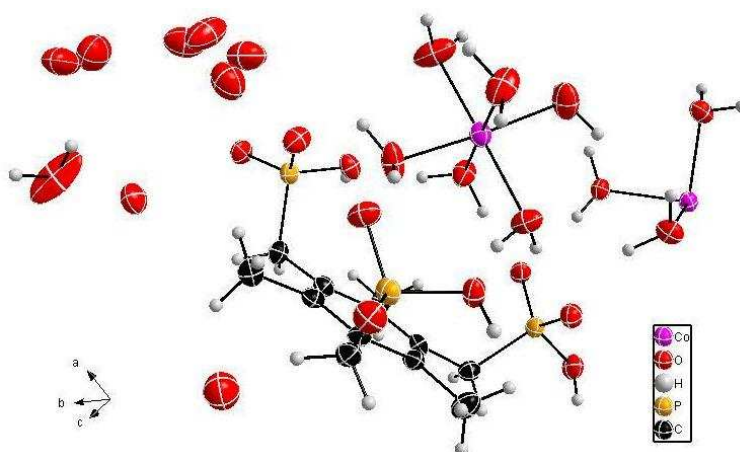


Figure 1. Asymmetric unit of **1**.  
(thermal ellipsoids at 50% probability level)

Reference:

1. Zoń J., Garczarek P., Białek M., „Synthesis of Phosphonic Acids and Their Esters as Possible Substrates for Reticular Chemistry” in *Metal Phosphonate Chemistry. From Synthesis to Applications*, Clearfield A., Demadis K. (Eds), RSC, Cambridge, 2011, pp 170-191; ISBN: 9788184973564.
2. Kong D., Zoń J., McBee J., Clearfield A., *Inorg. Chem.*, **45**, 977 (2006).
3. Zoń J., Videnova-Adrabińska V., Janczak J., Wilk M., Samoć A., Gancarz R., Samoć M., *CrystEngComm*, **13**, 3474 (2011).
4. Konar S., Zoń J., Prosvirin A.V., Dunbar K.R., Clearfield A., *Inorg. Chem.*, **46**, 5229 (2007).
5. Zoń J., Kong D., Gagnon K., Perry H., Holliness L., Clearfield A., *Dalton Trans.*, **39**, 11008 (2010).
6. Murugavel R., Singh M.P., *New. J. Chem.*, **34**, 1846 (2010).
7. Wilk M., Janczak J., Videnova-Adrabińska V., *Acta Cryst.* **C67**, m9 (2011).
8. Fu R.-B., Wu X.-T., Hu S.-M., Zhang J.-J., Fu Z.-Y., Du W.-X., *Polyhedron* **22**, 2739 (2003).