

MS36-P15**Synthesis, structural and characterization of three barium aromatic coordination polymers displaying a hydrogen-bonded layer structures**

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Coordination polymer materials have been demonstrated to have excellent properties and potential applications such as catalysis, magnetic, optical materials, gas adsorption, anti-bacterial agents, antitumor drugs, and so on [1-2].

Our research interest has been focused on a systematic study of coordination polymers based *s*-block alkaline-earth metal ions and organic diacids [3]. In this paper, we reported the synthesis and characterization of three Ba coordination polymers from 1,2-benzene--dicarboxylic acid [Ba(H₂O)(OOC-C₆H₄-COOH)₂], 2,2'-biphenyldicarboxylic acid [Ba(OOC-(C₆H₄)₂-COO)(H₂O)₄] 0.25 H₂O and 1,4-butanedicarboxylic acid (adipic acid) [Ba(OO-(CH₂)₄-COO)]. The three compounds crystallise in space groups P2₁/c, P₄ and P-4b2 respectively.

The structure of the first complex is built up from polymeric aquabis(hydrogeno-*o*-phthalate)barium(II) units. Each barium(II) binds to ten O-donors atoms, eight of which belong to six symmetry-related [HBDC] ligands and the remaining two to two water molecules. Thus, the coordination geometry around the Ba(II) atom can be best described as a distorted bicapped square antiprism. In such a way, the complex units are assembled into a two-dimensional infinite layer structure parallel to the (001) plane. The inorganic barium-oxygen layers are generated from Ba₂O₂₀ units which share faces and edges with neighbours to form chains along the [010] and [100] directions, respectively.

For complex [Ba(OOC-(C₆H₄)₂-COO)(H₂O)₄] 0.25 H₂O, the Ba (II) ions are ten-coordinated with three carboxylate oxygen atoms and with seven oxygen water molecules. Therefore, the coordination geometry around Ba(II) ions can be described as distorted bicapped dodecahedra. Its coordination architecture is built up from two-dimensional inorganic sub-networks made from face-sharing ten-coordinated Ba(II) polyhedra connected by the 2,2' diphenate linkers. Strong hydrogen bonds involving all the coordinated water molecules and the O atoms of the carboxylate groups lead to the formation of a three-dimensional network.

In the last complex, the asymmetric unit consists of one Ba(II) cation lying on -4 axis and one half dicarboxylate ligand. The barium is eight-coordinated by eight oxygen atoms belonging to eight equivalent dicarboxylate ligands. The coordination geometry around the Ba(II) can be best described as a distorted bicapped trigonal prism. The adipate ligands are tetradentate with syn/anti conformation. The structure is built up from chains of isolated polyhedra BaO₈ running parallel to [100] axis which are further connected through bridging dicarboxylate anions and separated by an infinite array of alkyl chains into 3D structure.

References:

- [1] Tranchemontagne, D. J., Mendoza-Cortés, J. L., O'Keeffe, M. & Yaghi, O. M. (2009). *Chem. Soc. Rev.*, 38, 1257-1283.
- [2] Yan, Y., Yang, S.H., Blake, A. J. & Schröder M. (2014). *Acc. Chem. Res.*, 47, 296-307.
- [3] Djehni, S., Balegroune, F., Guehria-Laidoudi, A., Dahaoui, S. & Lecomte, C. (2007). *Acta Cryst.*, C63, m91-m93.

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