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Alkali and Alkaline-Earth Metal Aquacomplexes with the Bridging Ligand Xylenediyl-4-Bis(Phenylphosphinate): Analysis by Powder X-Ray Diffraction and Production of Structural Models by 3D Printing

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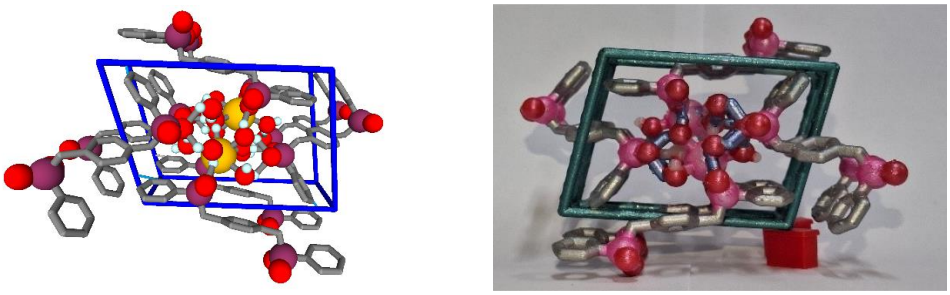
Crystallization of alkali and alkali-earth metals with the bridging ligand xylenediyl-4-bis(phenylphosphinate) ($XBPP^{2-}$, $O_2PPhC_6H_4PhPO_2^{2-}$) form different crystal structures of coordination polymers. Using different conditions—20–25 °C without humidity control, 4–6 °C with 20% relative humidity; 50 °C without humidity control; 50 °C at 22% humidity, 50 °C at 45% humidity—crystals $[Na_2(XBPP)(H_2O)_8]\cdot H_2O$ **1**, $[K_2\{(HXBPP\}_2(H_2O)_4]$ **2**, $[Ca_2(XBPP)(H_2O)_4]\cdot 3H_2O$ **3**, $[Ca_2(XBPP)(H_2O)_5]\cdot 3H_2O$ **4**, $[Sr(H_2O)_5](XBPP)\cdot H_2O$ **5**, $[Sr_2(XBPP)_2(H_2O)_6]\cdot H2O$ **6**, $[Ba(XBPP)(H_2O)_4]$ **7** and $[Ba(XBPP)(H_2O)_3]$ **8** formed and their crystal structures were determined by single crystal X-ray diffraction. In these crystal structures, the $XBPP^{2-}$ ligand binds directly to the metals, forming coordination polymers, except in the case of **5** where it acts as a counter-ion, and the water molecules form complex hydrogen bonding nets. The compounds have different structural arrangements, depending on the metal and the interactions between the water molecules. The crystal structures obtained have very complicated crystalline unit cells. To better present these cells, 3D molecular models were printed using a resin printer. Figure 1 shows the unit of **7** as from Diamond [1] (a) and the painted 3D printed resin model (b).

Powder X-ray analysis was used to check for crystalline purity of crystalline samples [2]. The samples of the single crystals were ground and subjected to powder X-ray diffraction analysis. The diffractograms show that all the samples contain additional crystalline phases in addition to the crystalline phase of the single crystal.



(a) (b)

Figure 1. Model of **7** using Diamond (a), e painted 3D printed model of **7** (b).

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