

templating effects. The *cnm* ligand has also been shown to be conducive in the formation of transition metal and lanthanoid clusters which are of interest in the area of single molecule magnets.

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Keywords: lanthanide coordination, bimetallics, magnetic materials

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Synthesis and characterization of mixed metal ($\text{UO}_2^{2+}/\text{TM}^{2+}$) inorganic/organic framework materials

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Inorganic materials containing UO_2^{2+} comprise a structurally diverse catalog of compounds wherein layered architectures are most commonly observed. The dimensionality of these structures is typically governed by the terminal nature of the uranyl oxo atoms and the propensity for structure propagation to occur almost exclusively in two dimensions. As a result, three-dimensional structures are not only less frequently observed but also a challenge to obtain synthetically. Within purely inorganic systems, researchers have used templates or, alternatively, incorporated main group or transition metal cations to achieve higher dimensional frameworks. These strategies, in addition to flexible organic linkers, have also been applied to hybrid inorganic-organic systems. Presented here is a series of novel, three-dimensional, mixed metal uranium(VI)/transition metal(II) inorganic-organic hybrid materials. A representative example includes the framework structure of $(\text{UO}_2)_2(\text{O}_3\text{PCH}_2\text{CO}_2)_2\text{Cu}(\text{H}_2\text{O})_3$, monoclinic, $P2_1/c$, $a = 7.6358(3)$, $b = 19.2962(3)$, $c = 11.2401(8)$, $\beta = 100.4990(10)$. This compound exhibits coordination of copper through the nominally terminal uranyl oxygen atoms and illustrates how the addition of transition metal cations can influence the dimensionality, overall topology and luminescent behavior of hexavalent uranium containing architectures.

Keywords: framework structures, uranium(VI), hydrothermal synthesis

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A nine-coordinated Zr^{IV} complex obtained from a novel supramolecular proton transfer compound

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In this research, a novel supramolecular proton transfer compound was synthesized from the reaction between pyridine-2,6-dicarboxylic acid, $\text{C}_7\text{H}_5\text{NO}_4$, and propane-1,3-diamine, $\text{C}_3\text{H}_{10}\text{N}_2$. According to the crystal structure, the resulting compound formulated as $2(\text{C}_3\text{H}_{12}\text{N}_2)^{2+}(\text{C}_7\text{H}_3\text{NO}_4)^{2-}(\text{C}_7\text{H}_{4.5}\text{NO}_4)^{1.5-}(\text{C}_7\text{H}_{3.5}\text{NO}_4)^{0.5-}(\text{C}_7\text{H}_5\text{NO}_4) \cdot 5\text{H}_2\text{O}$. This compound crystallizes in the triclinic system and contains two molecules per unit cell. The unit cell dimensions are $a=7.8355(4)\text{\AA}$, $b=13.5296(6)\text{\AA}$, $c=20.8930(6)\text{\AA}$, $\alpha=106.558(1)^\circ$, $\beta=90.603(1)^\circ$, and $\gamma=106.662(1)^\circ$. The final *R* value was 0.0427 for 9245 reflections. In anionic fragment, one of fourth hydrogen atoms of hydroxy groups is disordered. In cationic fragment, two carbon and nitrogen atoms, are disordered on two position with occupancies 0.88/0.12. Anion molecules form two independent hydrogen bonded zigzag-type chains. The hydrogen bonds as type $\text{O-H}\cdots\text{O}$, $\text{N-H}\cdots\text{O}$, and $\text{N-H}\cdots\text{N}$ play a role in the construction of supramolecular framework. Interactions between cationic and anionic fragments consist of ion-pairing, hydrogen bonds and π - π stacking. The reaction of the proton transfer compound with ZrCl_4 was carried out. This complex formulated as $(\text{C}_3\text{H}_{12}\text{N}_2)[\text{Zr}(\text{C}_7\text{H}_3\text{NO}_4)_3] \cdot 4\text{H}_2\text{O}$. The Zr^{IV} complex crystallizes in the space group $P2_1/c$ of the monoclinic system with four molecules per unit cell. The unit cell dimensions are $a=10.0246(6)\text{\AA}$, $b=17.1883(10)\text{\AA}$, $c=17.8643(10)\text{\AA}$, and $\beta=97.2970(10)^\circ$. The metal ion is ninecoordinated by three pyridine-2,6-dicarboxylate as tridentate ligand. The Zr^{IV} atom is located in the center of a distorted tricapped trigonal prism arrangement. The crystal-packing diagram indicates the layered structure for this complex. This complex arises from ion pairing and the extensive hydrogen bonding.

Keywords: zirconium, supramolecular compounds, crystal structures

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Binuclear Sn(VI) complex obtained from benzene-1,3-diaminium bis(hydrogen pyridine-2,6-carboxylate)

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In recent years, our research group have studied and worked on several bi- or trivalent metal complexes with several proton transfer ion pairs containing pyridine-2,6-dicarboxylic acid, pydcH_2 . In resulting complexes, some fragments of ion pairs coordinate to metal ions and some other fragments act as counter ions in the structure. Here we wish to report the molecular structure of the Sn(VI) complex, which obtained from a novel proton transfer compound $(\text{bdaH}_2)(\text{pydcH})_2 \cdot 2\text{H}_2\text{O}$. The proton transfer compound $(\text{bdaH}_2)(\text{pydcH})_2 \cdot 2\text{H}_2\text{O}$, has been prepared from the reaction between benzene-1,3-diamine, *bda*, and pyridine-2,6-dicarboxylic acid, pydcH_2 . The reaction of this adduct with $\text{Sn}(\text{CH}_3)_2\text{Cl}_2$ gives complex with stoichiometry $[\text{Sn}(\text{pydc})(\text{OC}_2\text{H}_5)(\text{CH}_3)_2(\mu\text{-O})]_2$. This complex was characterized by IR, NMR spectroscopy and X-ray crystallography. This complex crystallizes in the monoclinic system, space group $P2_1/c$, with four molecules per unit cell. The unit cell dimensions are $a=11.5924(14)\text{\AA}$, $b=13.2674(17)\text{\AA}$, $c=7.7566(10)\text{\AA}$

with $\beta = 92.602(2)^\circ$. The final R value is 0.0258 for 2795 reflection measured. The X-ray analysis shows that benzene-1,3-diamine fragment in proton transfer compound is not contribute in the molecular structure of complex. The molecular structure consists of two metal fragments linked *via* the central four membered Sn_2O_2 ring. Each of two Sn atoms is coordinated by the chelate $(\text{pydc})^{2-}$ ligand, one bridging oxygen atom of carboxylate group, two terminal methyl group and as well as by one terminal ethoxy group. Therefore, the coordination number is seven for each central atom and distorted pentagonal bipyramid geometry is observed around the tin atoms.

Keywords: crystal structures, supramolecular chemistry, weak interactions

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A structural study of metal complexes of bisphosphonate partial ester derivatives

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The chemistry of metal bisphosphonates (BPs) is a growing area of interest due to the unique properties of these compounds, including chemical and thermal stability and the possibility to manipulate their structure. Metal BPs also exhibit a variety of open frameworks such as layered and microporous structures offering a diversity of practical applications in the areas of ion-exchange, catalysis, and sorption. Clodronate, (dichloromethylene)bisphosphonate, Cl_2MBP , is one of the best-documented BPs since it is effectively used in therapeutics. We have focused on studying the complexing properties of ester derivatives of clodronate with the divalent metal cations [1-3]. We present here the crystal structures and characterization of three novel Cd complexes of phenyl esters and alkyl ester derivatives of Cl_2MBP . The structures of the complex crystals were determined by X-ray single-crystal diffraction. All three compounds are coordination polymers with a layered structure. In the case of the Cd complex of the asymmetrical alkyl ester derivative of Cl_2MBP , the layers are connected into a 3D framework through hydrogen bonds. The Cd^{2+} cations of all compounds are in an octahedral environment. However, these layered architectures are different due to the different metal/ligand ratio and different protonation degree and coordination mode of the BP anions.

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Keywords: bisphosphonate, metal complexes, crystal structures

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High pressure synthesis and analysis of new yellow emission Sr_2ZnS_3 : Eu visible-light driven phosphor

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Yellow emission phosphors, which can be excited by blue light, are actively sought for the applications in the LED based lighting. In this work we report synthesis and crystal structure of the new compound Sr_2ZnS_3 , which demonstrates strong yellow fluorescence when activated with Eu^{2+} . Mn doped Ba_2ZnS_3 material is a well-known important green emission phosphor. Recently, the Eu^{2+} activated compound also attracted much attention as a prospective red phosphor for the LED-based applications. Nevertheless, no successful report on synthesis of Sr_2ZnS_3 could be found in literature although in analogy with Ba_2ZnS_3 such a compound should have a remarkable potential as a host for development of new fluorescent materials. In this work Sr_2ZnS_3 was prepared for the first time from the individual metals sulfides under 5GPa pressure at 1000C. The composition of the material was confirmed by EDS. It has tetragonal unit cell (space group $Pbn2_1$) with $a=16.41\text{Å}$, $b=8.464\text{Å}$ and $c=4.071\text{Å}$. The crystal structure was solved *ab initio* using powder diffraction data. A series of Eu^{2+} activated phosphors was prepared from $\text{Sr}_{1-x}\text{Eu}_x\text{S}$ ($0.01 < x < 0.06$) precursors. In order to achieve homogeneous distribution of the activator, the precursors were synthesized by polymerizable complex method combined with conversion of the intermediate carbonate into sulfide by H_2S . The obtained Sr_2ZnS_3 :Eu materials demonstrated strong yellow emission, which can be excited by the near-UV and visible light, and it makes Sr_2ZnS_3 :Eu sulfide an appealing yellow phosphor for LED-based applications. Currently available samples demonstrate fluorescence intensity of 43% compared to one of the best commercial Ce^{3+} doped yttrium-aluminum garnet (YAG-P46) phosphor. The support of this work by Kakenhi grant 20900106 is acknowledged.

Keywords: phosphors, high-pressure high-temperature synthesis, *ab-initio* powder structure determination

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Designing Zn and Co based 1-D coordination polymers with possible magnetic and electronic properties

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Several coordination polymers composed of Zn and Co as metal ions and various aromatic carboxylates as ligands have been synthesized and their structures determined. Typical structures are composed of 1-D chains in which divalent metal ions (Zn or Co) form a polymeric chain surrounded by carboxylate ligands. In all cases the carboxylate ligands coordinate to two metal ions and as a consequence act as a bridge between them, with the coordination environment being tetrahedral in some structures, or a combination of tetrahedral and octahedral in others. Some examples containing oxygen as an additional bridging atom have also been synthesized. In all the structures, the neighboring chains interact with each other through C-H... π and π ... π interactions. All the structures are