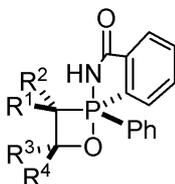


agree with a mechanism that involves a [2+2] cycloaddition to give a 1,2-oxaphosphetane intermediate. Those compounds are in general highly thermally labile species and only a small number of these intermediates have been isolated and structurally characterized through X-ray diffraction studies.

Here we report the full structural study of five novel spiro-1,2-oxaphosphetanes, including its electron density topological features [3]. The five oxaphosphetanes reported here present a distorted TBP structure with the oxygen and nitrogen atoms in the apical positions. The presence of the bidentate ligand ortho-benzamide contributes to stabilize the 1,2-oxaphosphetane ring.



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**Keywords:** oxaphosphetane, Wittig reaction, organophosphorus compounds

#### FA4-MS33-P22

#### Synthesis and Crystal Structure of aqua[N,N'-bis(3-methoxysalicylidene)-propane-1,2-diaminato]-methanolanomanganese(III) perchlorate. Buket Safak,

Hulya Kara *Department of Physics, Balikesir University, Balikesir, Turkey*  
E-mail: [buketsafak@bau.edu.tr](mailto:buketsafak@bau.edu.tr)

The title compound, a hydrogen-bonded pseudo-dimer,  $\text{Mn}(\text{C}_{19}\text{H}_{18}\text{N}_2\text{O}_4)(\text{CH}_3\text{O})(\text{H}_2\text{O})\text{ClO}_4$  (I), has been structurally characterized. The compound I crystallizes in monoclinic space group P2(1)/c with  $a = 13.359$ ,  $b = 13.338$ ,  $c = 14.185$  Å,  $\beta = 118.09^\circ$ . In complex (I), the molecule comprises a manganese(III) centre coordinated by the nearly planar Schiff-base ligand [the angle between the least-squares planes of the aromatic rings of the ligands is  $9.15^\circ$ ] with Mn–O<sub>phenol</sub> bond lengths of 1.870(4) Å and 1.869(4) Å, together with Mn–N<sub>imin</sub> bond lengths of 1.974(4) and 1.990(5) Å. The coordination sphere of the manganese centre is completed by a methanol molecule [Mn–O<sub>metoh</sub> 2.296(5) Å] and a water molecule [Mn–O<sub>water</sub> 2.208(3) Å]. The central Mn<sup>III</sup> ion adopts an elongated octahedral coordination geometry, with the displacement of the Mn<sup>III</sup> ion from the O1/N1/N2/O2 least-squares plane is 0.035(2) Å. In the crystal structure of (I), adjacent molecules are linked by hydrogen bonds [O5<sup>1</sup>–O1<sup>1</sup> = 2.969 Å, O5<sup>1</sup>–O2<sup>1</sup> = 2.916 Å, O5<sup>1</sup>–O3<sup>1</sup> = 2.898 Å and O5<sup>1</sup>–O4<sup>1</sup> = 2.883 Å; symmetry code, (i)  $[-x+1, -y+1, -z]$ , to form hydrogen-bonded pseudo-dimers, with additional face-to-face  $\pi$ - $\pi$  stacking interactions between the benzene groups (C6<sup>1</sup>–C10 = 3.697 Å and C5<sup>1</sup>–C11 = 3.950 Å); symmetry code, (i)  $[-x+1, -y+1, -z]$ . Moreover, hydrogen bonds [O6–O10A<sup>ii</sup> = 2.871 Å] (ii)  $[x+1, y, z]$  are formed between the axial methanol ligand and the perchlorate ion.

**Keywords:** crystal structure analysis, supramolecular chemistry, molecular magnets

#### FA4-MS33-P24

**Structure and optical properties of natural low dimensional semiconductors.** David G. Billing, Robert S. Black, *Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, PO Wits 2050, Johannesburg, South Africa*  
E-mail: [Dave.Billing@wits.ac.za](mailto:Dave.Billing@wits.ac.za)

Inorganic-organic nanocomposite materials have been studied extensively in recent years because of the variety of interesting and useful properties associated with this family of compounds. The layered hybrids specifically the 2D  $(\text{RNH}_3)_2\text{MX}_4$  and  $(\text{NH}_3\text{RNH}_3)_2\text{MX}_4$  series, have shown good semiconduction, photoconductivity, photoluminescent and electroluminescent behaviour due to their inherent quantum well nature [1]. The quantum confinement of excitons in the 2D layers enhances the optoelectronic properties of the structure due to the enhanced binding energy. The nanocomposite method of synthesis is a bottom-up approach which produces multiple quantum well structures with predefined well thicknesses which is advantageous over the traditional MBE growth techniques which limits thickness. The manipulation of the barrier (insulator) layer is done by using various organic amine cations which enables adjustment of the well (interlayer) spacing and also has the ability to induce inorganic bond length, and bond angle distortions. Previously published results suggest [2-3] that the well (interlayer) X<sup>-</sup>X contacts play a large role in the shifting of the band gap at these short distances. A study of  $(\text{X-C}_n\text{H}_{2n}\text{NH}_3)_2\text{PbX}_4$  (where  $n = 2-6$  and X = halogen; OH) as a function of chain length and terminal halogen substitution gives insight into these interactions [4-5]. Optical experiments performed suggest the resultant photoluminescence emissions do not only change with the inorganic well (interlayer) spacing, but also has a strong conduction band mixing related to the (I<sup>-</sup>X) interactions. These interactions give rise to intense sharp, but split emission lines, which are not necessarily just related to Pb(6p)  $\rightarrow$  Pb(6s) emissions [69].

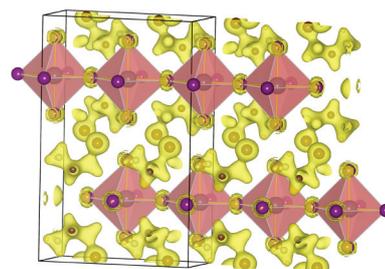


Fig. Charge density plot of  $(\text{BrC}_2\text{H}_4\text{NH}_3)_2\text{PbI}_4$

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**Keywords:** Natural quantum wells, Inorganic-organic hybrids, Photoluminescence, Nanocomposites