

role in determining the blocking temperature of the magnetic moment. The synthesis of high-spin molecules has been considered as one possible route to the preparation of molecular-based ferromagnets.

Three new inorganic-organic compounds of formulae  $[\text{Mn}(\text{AcAc})_2(\text{py})_2]_2(\text{ClO}_4)_2$ ,  $[\text{Mn}(\text{AcAc})_3]$  and  $[\text{Mn}(\text{acacen})_2](\text{ClO}_4)$ , were  $\text{AcAc}$  = acetylacetonato,  $\text{acacenH}_2$  =  $\text{N,N}'$ -ethylenebis(acetylacetonato) imine and  $\text{py}$  = pyridine. They might be viewed as new precursors for the design of single molecule or single chain magnets.

[1] Solari E., Latronico M., Blech P., Floriani C., *Inorg. Chem.*, 1996, **35**, 4526. [2] Marvaud V., Decroix C., Scullier A., Tuyéras F., Guyard-Duhayon C., Vaissermann J., Marrot J., Gonnet F., Verdagner M., *Chem. Eur. J.*, 2003, **9**, 1692-1705.

**Keywords:** molecular magnetism, crystal engineering, coordination complexes

#### P.07.11.1

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#### Synthesis and Characterization by Diffraction of X-rays of a new Hybrid Compound Based on Tin

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Organic-inorganic hybrid materials have attracted a great deal of attention during the past few decades because of their ionic, electrical, magnetic and optical properties [1-3]. Only one crystal structure of an arylammonium hexachlorostannate(IV) compound has been reported previously [4]. In this study we present a new organic-inorganic hybrid compound with the formula  $(\text{R-NH}_3)_2\text{SnX}_6$ , it promises both the superior carrier mobility of inorganic semiconductors and the processability of organic materials.

The title compound,  $(\text{C}_7\text{H}_8\text{NO}_2)_2(\text{SnF}_6)$ , crystallized in the  $\text{C}2/c$  space group of the monoclinic system, was prepared from aminobenzoic acid and tin(II) fluoride in hydrofluoric acid. The structure can be described by alternating layers of  $\text{SnF}_6^{2-}$  and  $\text{C}_7\text{H}_8\text{NO}_2^+$  ions along the  $a$  axis. The cations and anions are linked to each other through strong hydrogen bonds, formed by all H atoms covalently bonded to the N and O atoms. This three-dimensional complex network of hydrogen bonds reinforces the cohesion of the ionic structure.

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**Keywords:** hybrid compound, X-ray, single crystal

#### P.07.11.2

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#### X-ray Structural Study of $\sigma$ -borane and Dihydridoborate Ruthenium Complexes

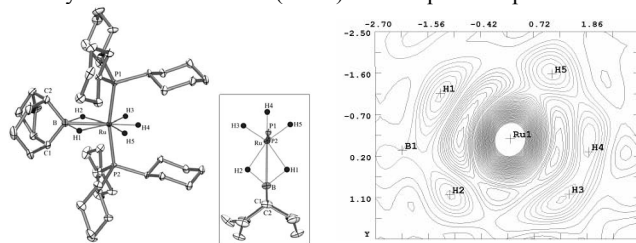
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In this work, we present 3 X-ray structures of a new family of  $\sigma$ -borane and dihydridoborate complexes. Two  $\sigma$ -borane and one dihydridoborate complexes have been produced: respectively  $\text{RuH}_2(\eta^2\text{-HBpin})(\eta^2\text{-H}_2)(\text{PCY}_3)_2$  (2Bpin) and  $\text{RuH}_2(\eta^2\text{-HBcat})(\eta^2\text{-H}_2)(\text{PCY}_3)_2$  (2Bcat), and  $\text{RuH}[(\mu\text{-H})_2\text{BBN}](\eta^2\text{-H}_2)(\text{PCY}_3)_2$  (2BBN).

The formulation of each complex has been ascertained by an X-ray structural study. Each experiment was carried out at 100 °K, in order to prevent as much as possible dihydrogen rotation, and to help the localisation of all the hydrogen atoms around the ruthenium. These complexes have been studied as well by NMR spectroscopy and by DFT/B3LYP calculations.

In the case of 2-BBN, the highly delocalized electronic density precluded any good location in the region of the equatorial plane *trans* to the dihydridoborate, and the hydride positions should be considered as artefacts. To solve this problem, our X-ray structural study has been completed by calculating Fourier differences map of the electronic

density observed at small  $\theta$  ( $< 18^\circ$ ) in the equatorial plane.



**Keywords:** low temperature, hydride structures, Fourier maps

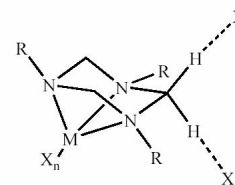
#### P.07.11.3

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#### C-H...X Intermolecular Interaction in Crystals of Triazacyclohexane Complexes

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The ring C-H bonds in the triazacyclohexane of transition metal complexes tend to engage in C-H...X (X = Cl, F, O) dominating the intermolecular interaction [1]. These interactions lead to low solubility of many complexes. The comparative analysis of many neutral and cationic complexes is presented.



[1] Köhn R.D., Kampe P., Kociok-Köhn G., *Eur. J. Inorg. Chem.*, 2005, in press.

**Keywords:** hydrogen bonding, transition metal complexes, triazacyclohexane

#### P.07.11.4

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#### Chirality Inversion Process in Cobaloxime Complex Crystals by Photoirradiation

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It was found that the racemic crystal of (1-cyanoethyl)-(piperidine)cobaloxime complex was transformed to a chiral one on exposure to visible light with retention of the single crystal form [1]. Although the crystal showed the optical rotation after photoirradiation, the molecule in the crystal was racemized. Recently we found that the chirality of the molecule was inverted to the opposite configuration when the crystal was irradiated with visible light.

The first example is the crystal of ((S)-1-ethoxycarbonylethyl)((S)-cyclohexylamine)cobaloxime. The (S)-1-ethoxycarbonylethyl group of the complex was inverted to the opposite configuration. The R:S ratio of the chiral group was changed from 0:100 to 76:24. The second example is the crystal of ((S)-chlorocyanomethyl)(pyridine)cobaloxime. The R:S ratio was changed from 0:100 to 80:20. The third one, which did not show the chirality inversion, is ((R)-tert-butoxycarbonylethyl)(phenylethylamine)cobaloxime. The R:S ratio of the chiral group became from 100:0 to 60:40 and was not changed to 50:50.

Such chirality changes were well explained by the cavity shape of the chiral group in the original crystals.

[1] a) Osano Y.T., et al., *Nature*, 1991, **352** 510; b) Nemoto T., et al., *Bull Chem Soc. Jpn.*, 1999, **72**, 1971.

**Keywords:** chirality, crystalline state reactions, photoreaction