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Very strong ferromagnetic interaction in a new asymmetrical binuclear μ-methoxo-bridged Mn(III) complex

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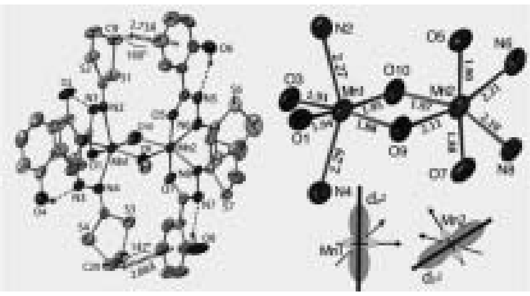
Manganese complexes can act as paramagnetic building blocks for Single Molecule Magnets (SMM) and also for multidimensional expanded structures.[1] The magnetic behavior of a variety of such compounds has been explored during the last decades with the aim of designing SMM or Single Chain Magnets.[2,3] The choice of binuclear transition metal building blocks with different exchange coupling patterns creates a number of exciting possibilities in this area.[4] In this communication, we present the preparation, crystal structure analysis and a detailed magnetic study of exchange interaction between manganese centers of the dinuclear $Mn(III)_2(\mu\text{-}OMe)_2(HL)_4$*.[5]
The new binuclear Mn(III) complex described here presents one of the strongest intramolecular ferromagnetic interaction ($J=19.7\ cm^{-1}$). This strong interaction is supported by DFT calculations which also confirm the negative sign of the $D_{S=4}$ parameter. Such binuclear complexes with very strong ferromagnetic interaction and axial magnetic anisotropy are excellent candidates to be incorporated into polymeric and/or supramolecular networks that could present interesting magnetic properties, if one achieves correctly designed interactions.[2]



ORTEP view of the new binuclear complex (left) showing specific intramolecular hydrogen bonds. Partial view of the molecular core (right) with an indication of the relative orientation of Jahn-Teller elongated (dz^2) axes around both Mn(III) atoms.
** H_2L=2-salicyloylhydrazono-1,3-dithiolane.*

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New Compounds of L-Alanine with Inorganic Materials

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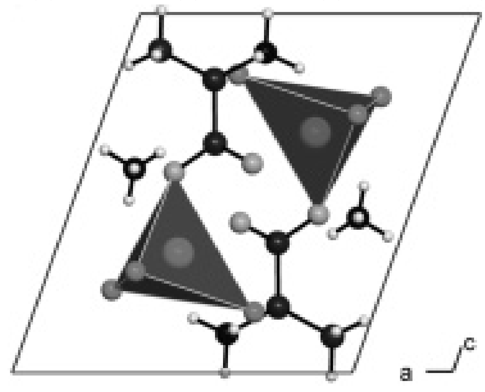
Keywords: alanine, crystal structure, amino-acid coordination compounds

We have investigated materials containing alanine and inorganic compounds. Alanine - as all amino acids - is amphoteric, it can act as an cation, as an anion or as a zwitter-on, i.e., an overall neutral group. Consequently, alanine can combine with anions, cations or overall neutral chemical constituents. Thus, the existence of a large number of compounds of alanine with inorganic materials is conceivable.
A search of the crystallographic data banks (i.e., CSD, PC-PDF) revealed over 200 alanine compounds. However, in most of these substances alanine is combined with other organic molecules. Only 48 compounds of alanine and inor-ganic materials were found, e.g., Co^{III} L-Alaninate$_3$.H_2O [1].
We attempted the syntheses of several new members of this group. Although racemic alanine compounds can form non-centrosymmetrical crystals (as it is the case for DL-Alanin itself [2], as well as for the non-chiral amino acid glycine and its salts, e.g. [3]), most of these compounds are centro-symmetrical. Thus, we have used L-alanine exclusively in order to ensure non-centrosymmetry. Recently, we have found three new species, the crystal structures of whichare discussed in the presentation.
Crystal data (in Å and °):
Alanine alaninium triiodide, s.g. $P2_12_12_1$
a = 8.366(2), b = 8.912(2), c = 41.889(8)
Alanine $SrCl_2\beta 3H_2O$, s.g. $P2_1$
a = 8.540(2), b = 7.167(1), c = 8.769(2), β = 95.02(3)
Alanine NH_4 Zn Cl_3, s.g. $P2_1$ (see figure below)
a = 7.944(2), b = 7.567(2), c = 8.903(2), β = 109.65(3)



Crystal structure of Alanine NH_4 Zn Cl_3. Note the polarity of the structure (necessary because of the alanine molecule) is expressed also by the ammonium ions.

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