

s13.m35.p24 **The First Example of Hetero-Tetranuclear (VO)₂Gd₂ Compound Assembled via an Amide-Imine Polydentate Ligand. Synthesis and Crystal Structure of [VOLGd(hfac)₂CH₃OH]₂·CH₃OH·(CH₃)₂CO.** Jean-Pierre Costes^a, Sergiu Shova^{b,c}, Yurii Simonov^c, ^aLaboratoire de Chimie de Coordination du CNRS, 205 route de Narbonne, F-31077 Toulouse Cedex, France, ^bDepartment of Chemistry Moldova State University, A.Mateevici str. 60. 2009 Chisinau, Moldova, ^cInstitute of Applied Physics, Academy of Sciences of Moldova, Academiei str. 3. 2028 Chisinau, Moldova. E-mail: simonov.xray@phys.asm.md

Keywords: Complexes of d,f-elements; Cluster; Magnetic properties

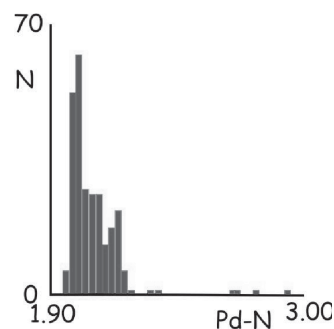
The interest in heteronuclear lanthanide 4f-3d coordination compounds, which are intensively studied due to their specific magnetic properties has been focused mainly on the Gd^{III} (S=7/2) derivatives and S=1/2 species such as copper(II) or vanadyl(II). Consistently, in the great majority of Cu-Gd or VO-Gd complexes studied so far, the intramolecular interaction between the gadolinium ion and the 1/2 spins has been found ferromagnetic, but a few examples of complexes showing an antiferromagnetic behavior do exist. On the other hand the most frequently used ligands are polydentate Schiff base involving various diamino chains. Herein we present the structure and magnetic properties of the novel tetranuclear cluster [VOLGd(hfac)₂CH₃OH]₂·CH₃OH·(CH₃)₂CO (**1**), where H₃L is an (O₃N₂) amide-imine type poly-functional ligand: 1-(2-hydroxybenzamido)-2-(2-hydroxybenzilideneamino)-2-methylpropane; hfac - hexafluoroacetylacetone. According to the X-ray single-crystal studies in **1** two neutral [VOLGd(hfac)₂·CH₃OH] entities are linked via two amide oxygen atoms of the polydentate ligand L³⁻ resulting into the centrosymmetric tetranuclear cyclic structure, where Cu^{II} and Gd^{III} are arrayed alternately. The V atom is located in the inner N₂O₂ cavity of the ligand and has a square-pyramidal geometry, with the oxygen atom in apical position; it is displaced from the mean equatorial coordination plane (0.626 Å) towards the oxygen atom. The Gd^{III} ion is eight-coordinate and GdO₂V core are not planar, the dihedral angle between Gd(1)O(1)O(2) and VO(1)O(2) is equal to 43°. The Gd···V separation constitutes 3.525 Å in dinuclear part and - 6.280 Å in tetranuclear complex. Two solvent methanol molecules are H-bonded with tetranuclear complex as donor of proton via VO²⁺ oxygen atom and as acceptor - via coordinated methanol molecule.

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s13.m35.p25 **Study on Pd-pyrazol bond.** Xavier Solans, Department of Crystallography, University of Barcelona, Spain. E-mail: xavier@geo.ub.es

Keywords: Crystal chemistry; Palladium complexes; Pyrazol

A study on the Pd-pyrazol bond has been carried out from the 94 structures found in the Cambridge structure data base (CCDC) [1] and 14 unpublished structures. In 41 structures the Pd is linked to only one pyrazol, in 61 to two pyrazolyl ligands and in 5 structures the Pd is linked to three pyrazol. The Pd-N bond length alters from 1.964 to 2.925 Å. The mean value is 2.081(7) Å. The different parameters which define the value of this bond length will be discussed in the poster.



[1] F. H. Allen, V. J. Hoy, *Encyclopaedia of Computational Chemistry*, VCH-Wiley, 1, 155-167, 1998