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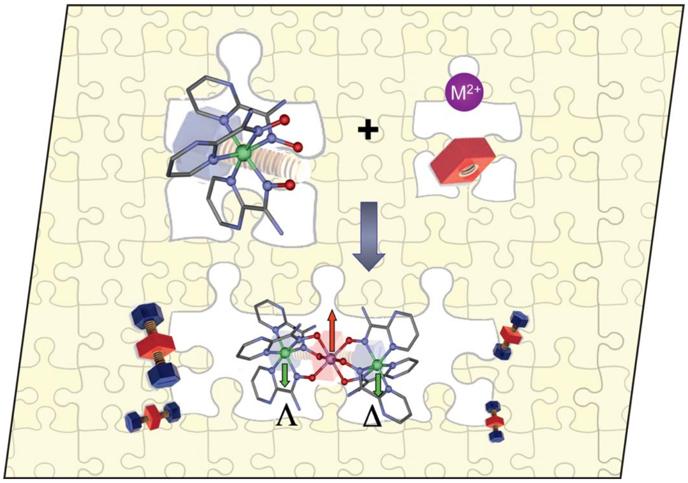
COVER PICTURE

The cover picture shows how oximate-bridged heterometallic trinuclear $Ni^{II}M^{III}Ni^{II}$ complexes can easily be constructed from the assembly of the "in situ" generated *fac*-O_3 $[Ni(HL)_3]^-$ (H_2L = pyrimidine-2-carboxamide-oxime) metalloligand (blue screw) with either M^{2+} ions (M^{2+} = Mn and Fe), which are oxidized during the course of the reaction, or Tb^{3+} ions (red nut). The nickel(II) ions in these centrosymmmetric trinuclear complexes exhibit opposite propeller-like chirality (the blue screws turn on the red nut in opposite directions). The red and green arrows are the spins of the M^{3+} and Ni^{2+} ions, and they are antiparalell, which indicates that the interaction is antiferromagnetic in nature. Details are discussed in the article by E. Colacio et al. on p. 5225 ff.



CONTENTS

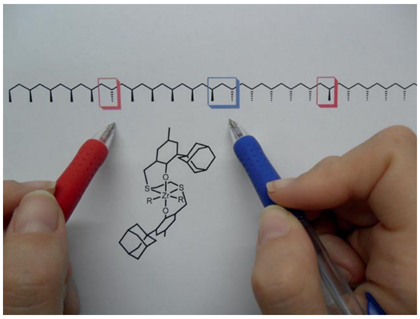
SHORT COMMUNICATION

Polymerization Catalysts

A. Cohen, I. Goldberg, V. Venditto, M. Kol* 5219–5223

Oscillating Non-Metallocenes – from Stereoblock-Isotactic Polypropylene to Isotactic Polypropylene via Zirconium and Hafnium Dithiodiphenolate Catalysts

Keywords: Hafnium / Zirconium / Fluxionality / Ligand design / Isotactic polypropylene



Zr and Hf complexes of an {OSSO} ligand bearing bulky phenolates oscillate between two C_2-symmetric conformations. Controlling the relative rates of monomer insertion and catalyst flip affects the polypropylene microstructure, making it stereoblock-isotactic or isotactic, as demonstrated by catalyst signatures on the polymer backbone.

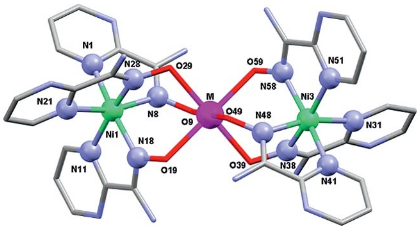
FULL PAPERS

Oximato-Bridged Bimetallic Complexes

C. Kalogridis, M. A. Palacios, A. Rodríguez-Diéguez, A. J. Mota, D. Choquesillo-Lazarte, E. K. Brechin, E. Colacio* 5225–5232

Heterometallic Oximato-Bridged Linear Trinuclear $Ni^{II}-M^{III}-Ni^{II}$ (M^{III} = Mn, Fe, Tb) Complexes Constructed with the *fac*-O_3 $[Ni(HL)_3]^-$ Metalloligand (H_2L = pyrimidine-2-carboxamide oxime): A Theoretical and Experimental Magneto-Structural Study

Keywords: Magnetic properties / Heterometallic complexes / Manganese / Iron / Lanthanides / Oximate / Density functional calculations



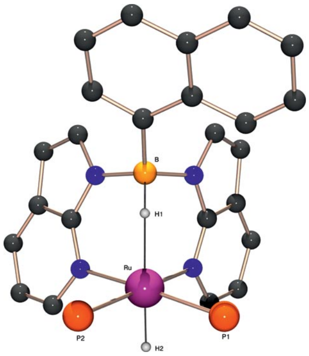
Three oximato-bridged linear heterobimetallic complexes [NiMNi] (M = Mn^{3+}, Fe^{3+}, Tb^{3+}) have been prepared using $[Ni(HL)]^-$ (H_2L = pyrimidine-2-carboxamide oxime). The size of the antiferromagnetic interactions in the Mn^{3+} and Fe^{3+} complexes has been supported by DFT calculations and justified on based on structural parameters, e.g. the Ni–N–O–M torsional angle and the distortion from the OC-6 octahedral to the TPR-6 trigonal prismatic geometry.

Azaindole-Based Scorpionates

N. Tsoureas, R. F. Hope, M. F. Haddow, G. R. Owen* 5233–5241

Important Steric Effects Resulting from the Additional Substituent at Boron within Scorpionate Complexes Containing κ^3-*NNH* Coordination Modes

Keywords: N ligands / Ruthenium / Steric hindrance / Boron / Hydrides



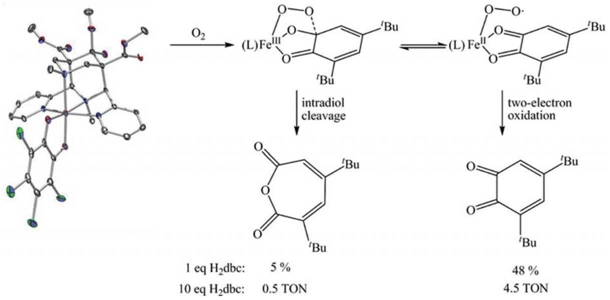
The synthesis of a number of ruthenium hydride complexes containing azaindole-based scorpionate ligands is reported herein. The scorpionate ligands bind to the metal centre with κ^3-*NNH* coordination modes. The strong borohydride···metal interaction pulls the additional substituent at the boron atom towards the bulky triphenylphosphane ligands.

Biomimetic Catechol Oxidation

P. Comba,* H. Wadepohl, S. Wunderlich **5242–5249**

Oxidation versus Dioxygenation of Catechol: The Iron–Bispidine System

Keywords: Biomimetic catalysis / Oxidation / Environmental chemistry / Coordination chemistry / Iron complexes / Density functional calculations



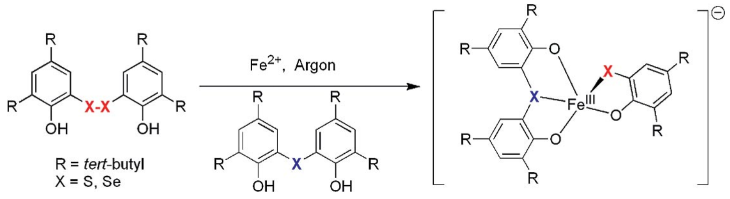
The iron–bispidine-catalyzed oxidation and dioxygenation of 3,5-di-*tert*-butylcatecholate (dbc^{2-}) by [Fe^{II}(**L**)X_2]$^{n+}$ and air (O_2) was studied experimentally and supported by a crystal structure determination and by a DFT-based analysis. The [Fe^{II}(**L**)X_2]$^{n+}$/O_2/dbc^{2-} system catalyzes the intradiol cleavage of dbc^{2-} but only with relatively low activity; most of the substrate is oxidized in a two-electron oxidation to give the benzoquinone (dbq) product.

S–S/Se–Se Bond Reactivity

T. Kanti Paine, D. Sheet, T. Weyhermüller, P. Chaudhuri* **5250–5257**

Iron(II)-Mediated Reductive Cleavage of Disulfide and Diselenide Bonds: Iron(III) Complexes of Mixed *O,X,O* and *O,X* (X = S, Se) Donor Ligands

Keywords: Disulfide / Diselenide / Cleavage reactions / Thiophenolate / Selenophenolate / Iron



The disulfide and diselenide bonds of 2,2′-diheterobis(4,6-di-*tert*-butylphenol) are reductively cleaved by an iron(II) salt in the presence of *O,X,O* donor ligands resulting in the formation of mixed ligand five coordinate iron(III) complexes.

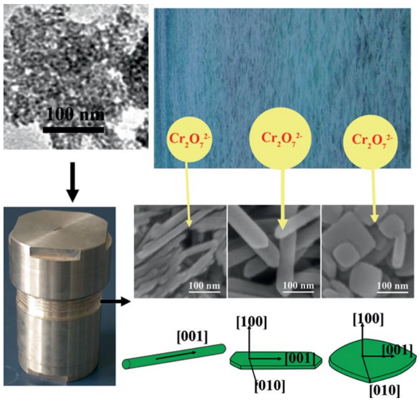
γ-AlOOH Nanomaterials

L. Zhang, X. Jiao,* D. Chen,* M. Jiao **5258–5264**

γ-AlOOH Nanomaterials with Regular Shapes: Hydrothermal Fabrication and $Cr_2O_7^{2-}$ Adsorption

Keywords: γ-AlOOH / Nanostructures / Hydrothermal synthesis / Adsorption

Well-defined boehmite (γ-AlOOH) nanorods, nanobelts and nanoplates were prepared by hydrothermal treatment of γ-AlOOH nanoparticles. The nanomaterials with different shapes exhibited different adsorption capabilities for $Cr_2O_7^{2-}$ in aqueous solution, and the nanobelts showed an adsorption of up to 95.5%.



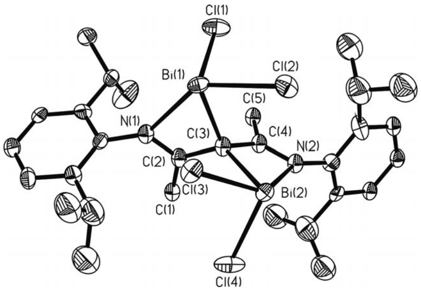
Organobismuth(III) Complexes

Y. Li, H. Zhu,* G. Tan, T. Zhu, J. Zhang **5265–5272**

The (β-Diketiminato)bismuth(III) Complex [LBiCl(μ-Cl)]$_2$ {L = HC[(CMe)(NAr)]$_2$, Ar = 2,6-iPr$_2$C$_6$H$_3$} and Its Derivatives: The Presence of Versatile Ligand Ligation Modes

Keywords: β-Diketiminato ligands / Bismuth / Isomerization / Ligation modes / N ligands

The reaction of $BiCl_3$ and LLi {L = HC[(CMe)(NAr)]$_2$, Ar = 2,6-iPr$_2$C$_6$H$_3$} under various conditions afforded a series of complexes, which revealed the complexity of the system and showed versatile L ligation modes at the metal atom.



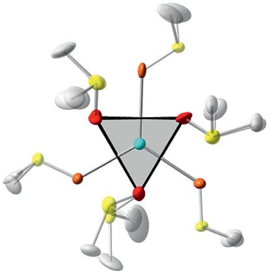
CONTENTS

Structure Elucidation

N. Torapava,* D. Lundberg,
I. Persson **5273–5278**

A Coordination Chemistry Study of Solvated Thorium(IV) Ions in Two Oxygen-Donor Solvents

Keywords: Actinides / Radiochemistry / Thorium / Coordination modes / Structure elucidation / Solvent effects / EXAFS spectroscopy



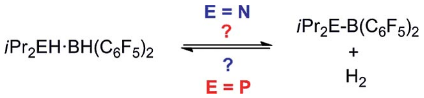
The structures of the dimethyl sulfoxide and *N*,*N*′-dimethylpropyleneurea solvated thorium(IV) ions have been determined in solution by using extended X-ray absorption fine structure (EXAFS), and that of solid oxoniumbis[nonakis(κ*O*-dimethyl sulfoxide)thorium(IV)]trifluoromethanesulfonate dihydrate has been determined by single-crystal X-ray diffraction and EXAFS.

Aminoborane Chemistry

A. P. M. Robertson, G. R. Whittell,
A. Staubitz, K. Lee, A. J. Lough,
I. Manners* **5279–5287**

Experimental and Theoretical Studies of the Potential Interconversion of the Amine–Borane *i*Pr$_2$NH·BH(C$_6$F$_5$)$_2$ and the Aminoborane *i*Pr$_2$N=B(C$_6$F$_5$)$_2$ Involving Hydrogen Loss and Uptake

Keywords: Main group elements / Amines / Boranes / Dehydrogenation / Hydrogenation



$$i\mathrm{Pr_2EH{\cdot}BH(C_6F_5)_2} \underset{\substack{?\\ E\,=\,P}}{\overset{\substack{E\,=\,N\\ ?}}{\rightleftharpoons}} i\mathrm{Pr_2E\text{-}B(C_6F_5)_2} + \mathrm{H_2}$$

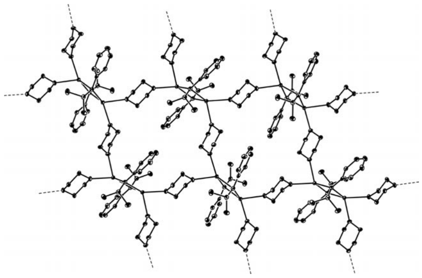
Interconversion between the amine–borane adduct *i*Pr$_2$NH·BH(C$_6$F$_5$)$_2$ and the related aminoborane *i*Pr$_2$N=B(C$_6$F$_5$)$_2$ via hydrogen loss/uptake has been studied. Fundamental differences in reactivity from the analogous phosphane–borane/phosphanylborane system have been rationalised by DFT calculations.

Sodium and Potassium Anilides

C. Glock, H. Görls,
M. Westerhausen* **5288–5298**

Electronic, Steric, and Ligand Influence on the Solid-State Structures of Substituted Sodium and Potassium Anilides

Keywords: Sodium / Potassium / Amides / Anilides / Metalation / Transamination reactions



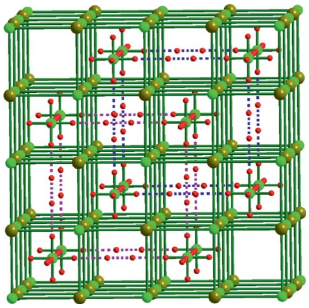
Substituted sodium and potassium anilides can be prepared by the metalation and transamination of anilines. The solid-state structures of the products strongly depend on the softness of the metal, the Lewis basic coligands (denticity, donor strength, bulkiness), and the steric demand of the *N*-bound substituent, which lead to dimers, layer structures (see picture), and 3D networks.

Heterometallic Frameworks

Y. Xu, Y.-X. Che, F.-Y. Cheng,
J.-M. Zheng* **5299–5304**

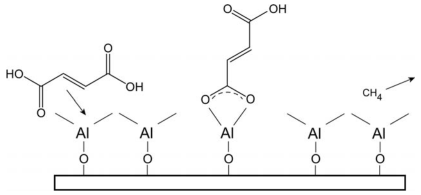
Synthesis, Structures, and Adsorption Properties of Two New La^{III}–Mg^{II} Heterometallic Polymers

Keywords: Metal–organic frameworks / Adsorption / Hysteresis / Heterometallic frameworks / Magnesium / Lanthanum



Two new 3D La^{III}–Mg^{II} heterometallic frameworks are reported. Interestingly, twofold 3D supramolecular hydrogen-bonding networks in **1** interpenetrate with the metal-only NaCl-like net of the packing structure, which forms a threefold interpenetrated topology. The hydrogen adsorption properties of the two polymers have been investigated.

Thin Films of Coordination Polymers



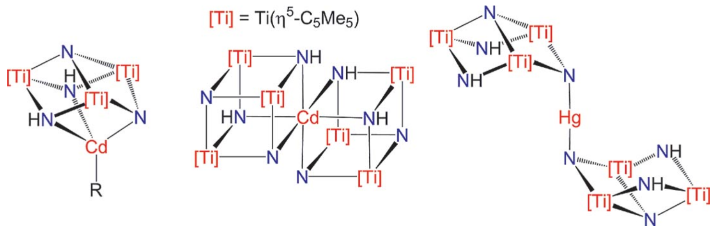
An investigation of the growth of organic–inorganic hybrid materials based on systematic variation of unsaturated linear carboxylic acids and trimethylaluminium was performed by atomic layer deposition (ALD). Self-limiting, temperature-dependent ALD-type growth was found. The surface roughness and topography, and the optical and wetting properties of the resultant films were investigated.

K. B. Klepper,* O. Nilsen, T. Levy, H. Fjellvåg 5305–5312

Atomic Layer Deposition of Organic–Inorganic Hybrid Materials Based on Unsaturated Linear Carboxylic Acids

Keywords: Organic–inorganic hybrid materials / Atomic layer deposition / Carboxylic acids / IR spectroscopy

Cage Compounds



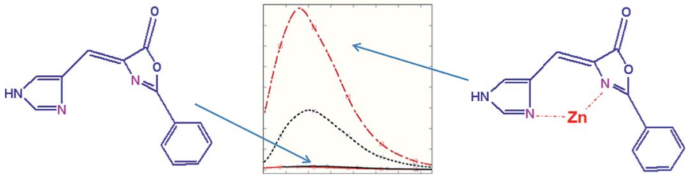
Several nitrido metallocubanes and incomplete cube-type compounds have been prepared from the reaction between [{Ti(η^5-C$_5$Me$_5$)(μ-NH)}$_3$(μ$_3$-N)] (**1**) and cadmium and mercury derivatives.

A. Martín, M. Mena, A. Pérez-Redondo, C. Yélamos* 5313–5321

Cadmium and Mercury Complexes Containing Trinuclear Titanium Imido-Nitrido Metalloligands

Keywords: Cadmium / Cage compounds / Mercury / Nitrides / Titanium

Fluorescent GFP Analogues



A synthetic green fluorescent protein analogue showed Zn^{2+}-induced fluorescence in organic solvents ($\Phi = 0.07$ at r.t. and up to 0.3 at low temperature). The fluorescence mechanism and the solvent effects were investigated by experimental observations and theoretical calculations.

J. Kang, X. Fang, X. Chen, G. Zhao, A. Ren, J. Xu,* W. Yang* 5322–5327

The Zinc-Dependent Fluorescence of a Synthetic GFP-Like Chromophore in Organic Solvents 💻

Keywords: Luminescence / Sensors / Fluorescent sensors / Zinc / Green fluorescent protein analogue / Chromophores / Density functional calculations / Solvent effects

CORRECTION

Keywords: Ruthenium / Scorpionate ligands / Phosphane ligands / N,O ligands

Synthesis and Structural Features of New Ruthenium(II) Complexes Containing the Scorpionate Ligands Tris(pyrazol-1-yl)methanesulfonate (Tpms) and Tris(pyrazol-1-yl)methane (Tpm)

S. Miguel, J. Diez, M. P. Gamasa, M. E. Lastra* 5328

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* Author to whom correspondence should be addressed.

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