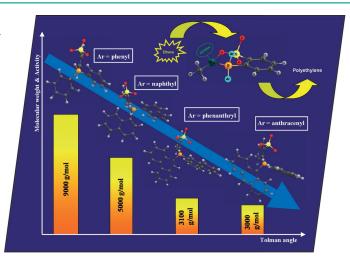


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Other ChemPubSoc Europe journals are Chemistry – A European Journal, ChemBioChem, ChemPhysChem, ChemMedChem, ChemSusChem and ChemCatChem.

COVER PICTURE

The cover picture shows the influence of the structure of a sulfonated phosphane on the performance of the Pd-based catalysts employed in this study. These complexes catalyze ethene polymerization without the need of activation, yielding linear polyethene. The introduction of steric hindrance in the catalyst scaffold results in lower molecular weights and lower activities. Details are discussed in the article by J. M. Claverie et al. on p. 4595ff.



SHORT COMMUNICATIONS

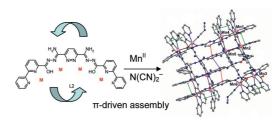
Polymetallic Architectures

K. V. Shuvaev, L. N. Dawe, L. K. Thompson* 4583-4586



A Mn^{II}₁₂ Supramolecular Array with Four Independent Spin-Coupled Subunits

Keywords: Ligand design / Polytopic ligands / Self-assembly / Grid structure / Supramolecular chemistry / Manganese / Copper



The tetratopic pyridazine ligand L2 forms the incomplete Mn^{II}_{12} partial grid $[Mn_{12}-(L2-2H)_6(L-H)_2\{N(CN)_2\}_2](NO_3)_8(H_2O)_{24},$ containing two isolated $\mu\text{-}O\text{-}bridged$ $[2\times2]$ square and two isolated $\mu\text{-}O\text{-}bridged$ dinu-

clear subunits. Multiple π contacts contribute to the assembly via the bipy ends, and the columnar stacked pyridazines. Antiferromagnetic exchange occurs through the μ -O bridges.

(Fluoroalkoxy)aluminates

Y. Li, H. Y. Yeong, E. Herdtweck, B. Voit, F. E. Kühn* 4587–4590

Synthesis, Characterization and Application of Nitrile-Ligated Zinc(II) Complexes Incorporating (Fluoroalkoxy)aluminates

Keywords: Aluminium / Zinc / Nitrile complexes / Polymerization / Anions, weakly coordinating



Nitrile-ligated Zn^{II} complexes with two Albased weakly coordinating anions (WCAs) have been prepared and characterized. The X-ray crystal structure proves the non-coordinating nature of the anions. Synthesis of the compounds is straightforward and high yielding. An application is the room-temperature polymerization of isobutylene resulting in polyisobutylene with high *exo* double bond content.

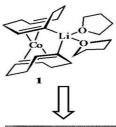
Functional Nanomaterials

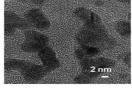
J. Khanderi, J. J. Schneider* 4591-4594



A Single-Source Co/Li/O Organometallic Precursor for Nanocrystalline LiCoO₂ – Synthesis, Formation Pathway, and Electrochemical Performance

Keywords: Nanoparticles / Electrochemistry / Cobalt / Lithium / Single-source precursors





The single-source organometallic precursor, [bis(η -1,5-cyclooctadiene)cobaltlithium], containing Li, Co, and O in the exact 1:1:2 atomic ratio, allows synthesis of electrochemically active nanocrystalline LiCoO₂ at moderate temperatures.

FULL PAPERS

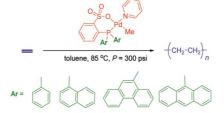
Ethene Polymerization

L. Piche, J.-C. Daigle, R. Poli, J. P. Claverie* 4595–4601



Investigation of Steric and Electronic Factors of (Arylsulfonyl)phosphane-Palladium Catalysts in Ethene Polymerization

Keywords: Phosphane ligands / Palladium / Polymerization



Bulky sulfonated arylphosphane ligands were prepared and used to generate (arylsulfonyl)phosphane-palladium complexes. These complexes catalyze ethene polymerization yielding linear polyethene. The relationship between the catalysts' structures and their activity was discussed.



Iridium Catalysis

A number of acetylacetonato(phosphane)-iridium complexes have been prepared by addition of phosphane to the iridium complex [Ir(acac)(η^2 -coe)₂] (1). The readily prepared complexes are active and selective catalyst precursors for the intramolecular cyclization of 4-pentynoic and 5-hexynoic acids to give the corresponding exocyclic lactones.

$$\begin{array}{c} \text{O} & \frac{\text{Ir}(\text{acac})(\eta^2\text{-coe})_2 + }{\text{phosphane}} \\ \text{OH} & \frac{\text{r.t.}}{} \end{array}$$

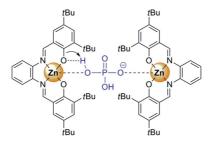
M. J. Geier, C. M. Vogels, A. Decken, S. A. Westcott* 4602–4610

Acetylacetonato(phosphane)iridium Complexes: Synthesis and Catalytic Activity in the Cyclization of Alkynoic Acids

Keywords: Iridium / Phosphane ligands / Cyclization / Lactones

Phosphate Activation

Dihydrogen phosphate provokes an anionspecific reaction with Zn(salphen) chromophores leading to protonated ligand structures. The demetalation process was investigated by NMR, MS and UV/Vis techniques. Kinetic studies suggest that the initial stage of the reaction comprises a phosphate-bridged dimetallic Zn(salphen) complex in which dihydrogen phosphate is activated for proton transfer.



Proton acceptor

Lewis acid activator

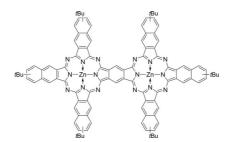
Dimetallic Activation of Dihydrogen Phosphate by Zn(salphen) Chromophores



Keywords: Anions / Chromophores / N,O ligands / Salen / Zinc

Near-Infrared Dyes

A new stable near-infrared dye with strong absorption at $\lambda = 965 \text{ nm} - \text{a}$ dinuclear naphthalocyanine analogue – was synthesized in a good yield.



S. G. Makarov,* O. N. Suvorova, G. Schnurpfeil, D. Wöhrle* ... 4617–4621

Synthesis of a Dinuclear Naphthalocyanine Analogue with Absorption in the NIR

Keywords: Fused-ring systems / Phthalocyanines / Naphthalocyanines / Zinc / NIR absorption / Dyes/Pigments

Rhenium(I) and technetium(I) carbonyl halide complexes of ligands derived from 4,5-diazafluoren-9-one (df) and 1,10-phenanthroline-5,6-dione (phen) derivatives of benzoic and 2-hydroxybenzoic acid hydraz-

ides have been prepared. The metal centres (Re^I and Tc^I) are coordinated through the nitrogen imine atoms to give a five-membered chelate ring, and the hydrazone group stands uncoordinated.

Re(I) and Tc(I) Carbonyl Complexes

P. Barbazán, A. Hagenbach,

E. Oehlke, U. Abram,* R. Carballo,

S. Rodríguez-Hermida,

E. M. Vázquez-López* 4622-4630

Tricarbonyl Rhenium(I) and Technetium(I) Complexes with Hydrazones Derived from 4,5-Diazafluoren-9-one and 1,10-Phenanthroline-5,6-dione

Keywords: Rhenium / Technetium / Carbonyl ligands / Hydrazone ligands

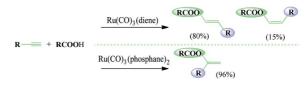
CONTENTS

Ru-Catalyzed Hydrocarboxylation

S. T. Tan, W. Y. Fan* 4631-4635

Ligand-Controlled Regio- and Stereoselective Addition of Carboxylic Acids Onto Terminal Alkynes Catalyzed by Carbonylruthenium(0) Complexes

Keywords: Alkynes / Carboxylic acids / Ruthenium / Ligand effects / Hydrocarboxylation



Product selectivity is a major problem in transition metal-catalyzed hydrocarboxylation reactions. In this paper we report the ability of Ru(CO)₃L₂ (where L is a 2 e⁻ donor) to catalyze the addition of various

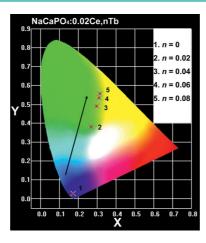
carboxylic acids onto terminal alkynes. A direct relationship between the regioselectivity of the product and the electronic property of the catalysis metal centre was observed.

White-Light LEDs

N. Guo, Y. H. Song, H. P. You,* G. Jia, M. Yang, K. Liu, Y. H. Zheng, Y. J. Huang, H. J. Zhang* 4636–4642

Optical Properties and Energy Transfer of NaCaPO₄:Ce³⁺,Tb³⁺ Phosphors for Potential Application in Light-Emitting Diodes

Keywords: Terbium / Cerium / Phosphors / Luminescence / Energy transfer



The developed phosphors can generate lights from blue to green and eventually to the yellow-greenish region under the excitation of UV radiation by appropriately tuning the activator content. The phosphors have the advantages of appropriate emission efficiency and relatively low price, thus indicating that they have potential application as a UV-convertible phosphor for white-light LEDs.

Ruthenium Complexes

S. Stagni,* A. Palazzi, P. Brulatti, M. Salmi, S. Muzzioli, S. Zacchini, M. Marcaccio,* F. Paolucci 4643–4657

5-(2-Thienyl)tetrazolates as Ligands for Ru^{II}-Polypyridyl Complexes: Synthesis, Electrochemistry and Photophysical Properties

Keywords: Ruthenium / N ligands / Polypyridyl complexes / Thiophenes / Electrophilic addition / Cyclic voltammetry



The synthesis, structural study and investigation of the redox and photophysical properties of new mono- and dinuclear [Ru(tpy)(bpy)]-type (tpy = 2,2':6',2"-terpyridine, bpy = 2,2'-bipyridyl) complexes



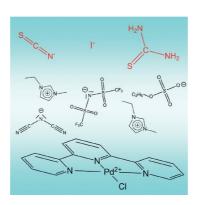
that contain (thienyl)tetrazolates, are reported. Regioselective electrophilic additions were performed on all derivatives to allow modification of their structural and electronic features.

Ligand Substitutions in ILs

S. Kern, P. Illner, S. Begel, R. van Eldik* 4658–4666

Mechanistic Studies on Fast Ligand-Substitution Reactions of a Very Labile Pd^{II} Complex in Several Ionic Liquids

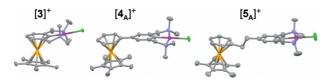
Keywords: Kinetics / Reaction mechanisms / Ionic liquids / Palladium / Ligand substitution



Kinetic study on the influence of ionic liquids on ligand-substitution reactions of a very labile Pd^{II} complex. Ionic liquids are far from being innocent reaction media!



Ruthenium-to-Platinum Interactions



A series of heterobimetallic Ru,Pt complexes is presented in which a $[Ru(C_5R_5)]^+$ fragment (R = H or Me) is η^6 -coordinated to a phenyl ring, and a Pt center is simultaneously η^1 -coordinated to an NCN-

pincer ligand. Depending on the connectivity between both organometallic fragments, very strong to very weak ruthenium-to-platinum interactions are experimentally observed.

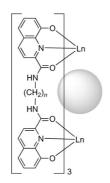
S. Bonnet, M. A. Siegler, J. H. van Lenthe, M. Lutz, A. L. Spek, G. van Koten, R. J. M. Klein Gebbink* 4667–4677

Ruthenium-to-Platinum Interactions in η^6, η^1 NCN-Pincer Arene Heterobimetallic Complexes: An Experimental and Theoretical Study

Keywords: Heterometallic complexes / Ruthenium / Platinum / Density functional calculations / Arenes

Lanthanide Helicates

Two 2-amido-8-hydroxyquinolines that are bridged through amide linkages by diamines are appropriate ligands for the self-assembly of dinuclear triple-stranded lanthanide(III) helicates. The formation of the coordination compounds might be supported by appropriate templates.

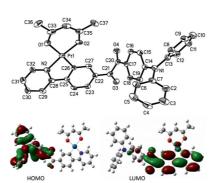


M. Albrecht,* O. Osetska 4678-4682

Ditopic 8-Hydroxyquinoline-2-carboxamides as Ligands for the Formation of Dinuclear Lanthanide(III) Helicates

Keywords: Lanthanides / Self-assembly / Helicates

[(Aryl-ppy)Pt(acac)] complexes have been prepared that show room-temperature phosphorescence at 490–590 nm. The emission colour tuning effect is attributed to either the elevated HOMO energy or the decreased LUMO energy. The luminescent O₂-sensing properties of the complexes in polymer films were studied. A white lightemitting OLED was fabricated with **Pt-3** with a CIE of (0.32, 0.32).



Phosphorescent Complexes

Tuning the Emission Colour of Triphenylamine-Capped Cyclometallated Platinum(II) Complexes and Their Application in Luminescent Oxygen Sensing and Organic Light-Emitting Diodes

Keywords: Phosphorescence / Luminescence / Sensors / Density functional calculations / OLEDs / Platinum

Vanadium-Peptide Interactions

G. Micera, E. Garribba* 4697-4710

Application of DFT Methods in the Study of V^{IV}O²⁺-Peptide Interactions

Keywords: Vanadium / Peptides / EPR spectroscopy / UV/Vis spectroscopy / Density functional calculations



Nine V^{IV}O²⁺ complexes formed by oligopepetides were studied by DFT methods. The geometry, ⁵¹V (A) and ¹⁴N superhyperfine coupling constants (A^N), ¹⁴N nuclear quadrupole coupling constants (C^O), elec-

tron absorption parameters (λ_{max} and ε_{max}), features of the V-N⁻ amide bond, molecular orbital composition, Wiberg bond indices and the spin densities were calculated.

CONTENTS

Metallocenes

I. Greger, G. Kehr, G. Erker* 4711-4715

Zirconocene Functional Group Chemistry: Photochemical [4+4] Cycloaddition of Isoprenyl Sidechains to the Bent Metallocene Framework

Keywords: Metallocenes / Sandwich complexes / Zirconium / Hafnium / Photochemistry / Cycloaddition

The (4-isoprenyl-Cp)₂MCl₂ complexes A (M = Zr, Hf) undergo rapid photochemical [4+4] cycloaddition to give the cyclooctadienylene-bridged ansa-metallocenes B in high yield.

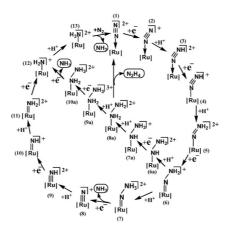
Allen and Senoff's Complex

S. Baskaran, C. Sivasankar* 4716-4719



Functionalization of Dinitrogen Using a Historically Significant Ru Complex: A New Life for an Old Complex

Keywords: Computational chemistry Reaction mechanisms / Nitrogen Ruthenium / Allen and Senoff complex



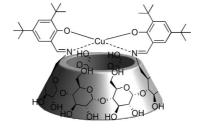
In the Allen and Senoff complex dinitrogen can be converted to ammonia and hydrazine in the presence of copper and LutH+ in water. The calculated thermodynamic barriers reveal that hydrazine formation is more favorable than ammonia formation.

Metallocapped Cyclodextrins

E. Deunf, E. Zaborova, S. Guieu, Y. Blériot, J.-N. Verpeaux, O. Buriez,* M. Sollogoub,* C. Amatore* ... 4720-4727

Synthesis and Electrochemical Study of an Original Copper(II)-Capped Salen-Cyclodextrin Complex

Keywords: Copper / Metalloenzymes / Cyclodextrins / Electrochemistry



A new metallocapped cyclodextrin was synthesized by a regioselective debenzylation reaction that was induced by diisobutylaluminium hydride (DIBAL-H). The electrochemical investigation of this original complex demonstrated that grafting of a copper salen-type complex to a cyclodextrin leads to changes in the reactivity of the intermediary species.

Supporting information on the WWW (see article for access details).

If not otherwise indicated in the article, papers in issue 28 were published online on September 20, 2010

^{*} Author to whom correspondence should be addressed.