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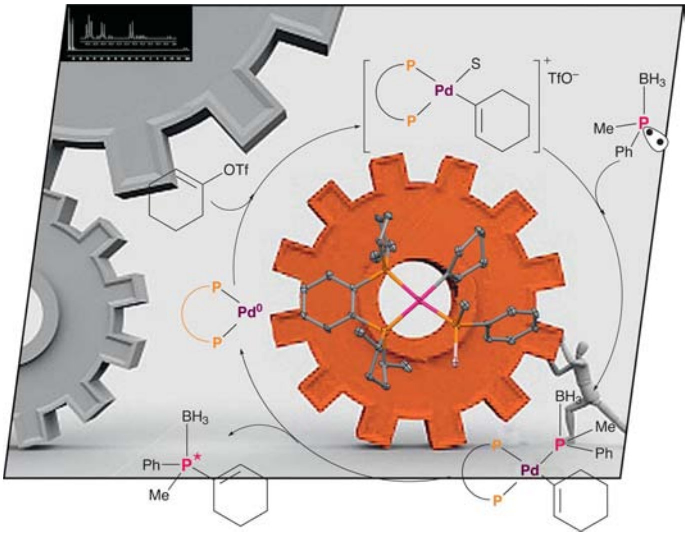
COVER PICTURE

The cover picture shows the catalytic cycle of the Pd-catalysed asymmetric phosphination involving an achiral alkenyl triflate and a racemic boron phosphide. A mechanistic study illustrated by the gears in the background allowed us to identify each main intermediate of this catalytic cycle. To proceed, tools such as ^{31}P NMR spectroscopy and X-ray crystallography were used. Details are discussed in the article by A.-C. Gaumont et al. on p. 2489ff.



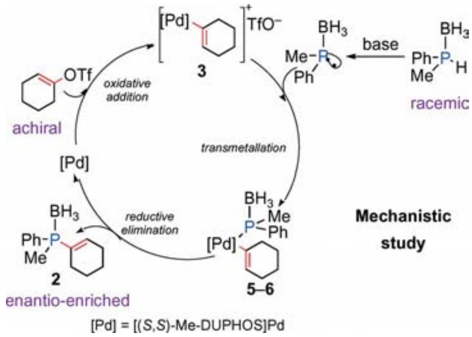
FULL PAPERS

Asymmetric Phosphination

D. Julienne, O. Delacroix, J.-F. Lohier, J. S. de Oliveira-Santos, A.-C. Gaumont* 2489–2498

Mechanistic Insights into the Palladium-Catalysed Asymmetric Phosphination of Cyclohexenyl Triflate

Keywords: Organophosphorus chemistry / Homogeneous catalysis / Phosphane ligands / Palladium / C–P coupling / Cross-coupling



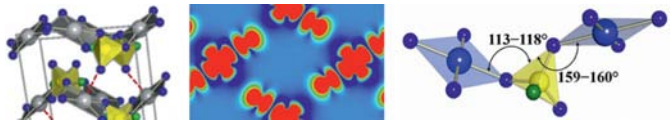
Preliminary mechanistic investigations on the asymmetric C–P cross-coupling reaction between secondary (methyl)phenylphosphane–borane and cyclohexenyl triflate is reported. The individual steps as well as the structure of the main intermediates involved in the catalytic cycle have been determined. A kinetic resolution process was proposed to explain the enantioselection observed.

Magnetism of Silver(II) Salt

P. J. Malinowski, M. Derzsi, Z. Mazej, Z. Jagličić, P. J. Leszczyński, T. Michałowski, W. Grochala* ... 2499–2507

Silver(II) Fluorosulfate: A Thermally Fragile Ferromagnetic Derivative of Divalent Silver in an Oxa-Ligand Environment

Keywords: Silver / Oxidation / Density functional calculations / Fluorosulfate



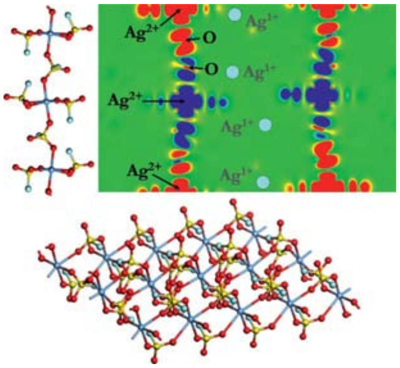
$Ag(SO_3F)_2$ exhibits a puckered sheet structure and it shows 2D ferromagnetism below 25 K; DFT methods predict it to be a magnetic semiconductor with the band gap at the Fermi level of approximately 1.05 eV. Magnetic superexchange take place through the OO moiety of the structural O–S–O bridge while omitting the sulfur atom, similarly as for related $AgSO_4$.

Mixed-Valent Silver Compounds

T. Michałowski, P. J. Malinowski, M. Derzsi, Z. Mazej, Z. Jagličić, P. J. Leszczyński, W. Grochala* 2508–2516

$Ag_3(SO_3F)_4$: A Rare Example of a Mixed-Valent Ag^{II}/Ag^{I} Compound Showing 1D Antiferromagnetism

Keywords: Silver / Mixed-valent compounds / Density functional calculations / Fluorosulfate



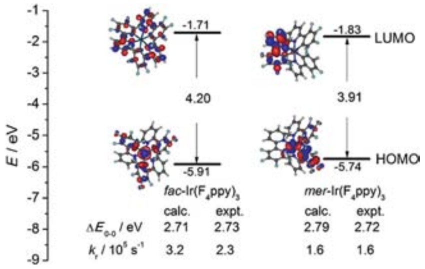
Dark brown monoclinic $Ag_3(SO_3F)_4$ shows 1D antiferromagnetism with an anomalously large superexchange coupling constant of −7.5 meV per pair of paramagnetic Ag^{II} cations (for the spin density see the figure). One-dimensional $[Ag^{II}SO_3F]^+$ chains, linked through fluorosulfate anions into $[Ag^{II}(SO_3F)_3]^-$ sheets, constitute characteristic structural features responsible for magnetic behaviour.

Computation of Ir Phosphorescence

X. Li, B. Minaev, H. Ågren,* H. Tian* 2517–2524

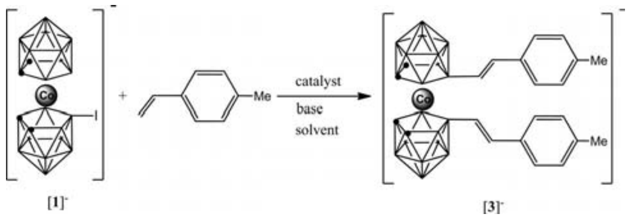
Theoretical Study of Phosphorescence of Iridium Complexes with Fluorine-Substituted Phenylpyridine Ligands

Keywords: Iridium / Fluorine / Organic light-emitting diodes / Phosphorescence / Density functional calculations



The phosphorescence of iridium complexes with $F_n$ppy (ppy = phenylpyridine) ligands was studied by linear and quadratic response theory. The 0–0 transition energy and the radiative rate constant were well predicted, thus proving the usefulness of quantum chemical calculations in aiding experiments.

B–H Activation



The applicability of Heck reaction on metallacarboranes induced cascade B–C_{vinyl} coupling that produces multiple B–C_{vinyl} bonds starting from a single B–I bond.

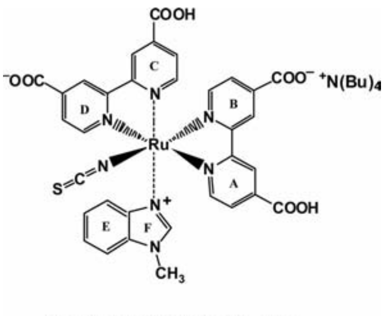
P. Farrεs, D. Olid-Britos, C. Viñas, F. Teixidor* **2525–2532**

Unprecedented B–H Activation Through Pd-Catalysed B–C_{vinyl} Bond Coupling on Borane Systems

Keywords: Cobalt / Palladium / Heck reaction / Cross-coupling / B–C coupling

Dye-Sensitized Solar Cells

The dye-sensitized solar cell (DSC) N719 thermal degradation products $[Ru(LH)_2(NCS)$(4-*tert*-butylpyridine)][$N(Bu)_4$] (**1**) and $[Ru(LH)_2(NCS)$(1-methylbenzimidazole)][$N(Bu)_4$] (**2**) were synthesized from $[Ru(LH)_2(NCS)_2][N(Bu)_4]_2$ (N719) and characterized by ESI-MS and NMR spectroscopy. DSCs prepared with **1** and **2** have efficiencies lower than N719 cells.



$[Ru(LH)_2(NCS)(MBI)][N(Bu)_4]$ (**2**)

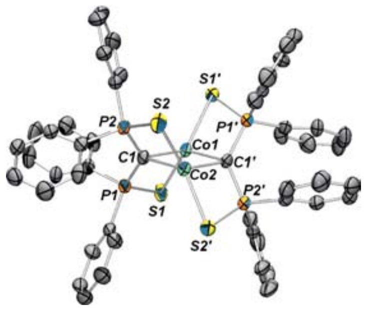
P. T. Nguyen, B. X. T. Lam, A. R. Andersen, P. E. Hansen, T. Lund* **2533–2539**

Photovoltaic Performance and Characteristics of Dye-Sensitized Solar Cells Prepared with the N719 Thermal Degradation Products $[Ru(LH)_2(NCS)$(4-*tert*-butylpyridine)][$N(Bu)_4$] and $[Ru(LH)_2(NCS)$(1-methylbenzimidazole)][$N(Bu)_4$]

Keywords: Solar cells / Dyes / Electrochemistry / Sensitizers

Nature of M–C Bonds

Reactions of geminal dianions derived from bis(dimethylthiophosphinoyl)methane and tetraisopropyl methylenediphosphonate with $CoCl_2$ yield dinuclear Co^{II} complexes featuring a Co_2C_2 square core.



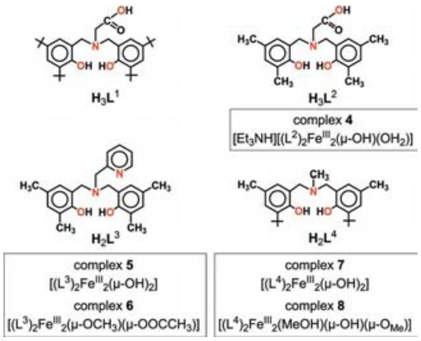
H. Heuclin, T. Cantat, X. F. Le Goff, P. Le Floch, N. Mezailles* **2540–2546**

Coordination Behavior of the S–C–S Monoanion and O–C–O and S–C–S Dianions toward Co^{II}

Keywords: Cobalt / Anions / Pincer ligands / Density functional calculations

Diiron(III) Complexes

A magneto-structural correlation of asymmetrically dibridged (hydroxo, methoxo, acetato) diferric(III) complexes with similar compounds of the literature is attempted.



T. Weyhermüller, R. Wagner, P. Chaudhuri* **2547–2557**

Asymmetrically Dibridged Diiron(III) Complexes with Aminebis(phenoxide)-Based Ligands for a Magnetostructural Study

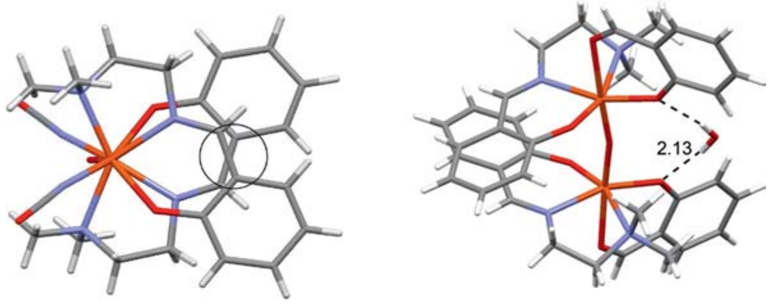
Keywords: Transition metals / Iron / Magnetic properties / N,O ligands / Through-bond interactions

Fe–O–Fe Bridging Angle

R. Biswas, M. G. B. Drew, C. Estarellas, A. Frontera,* A. Ghosh* 2558–2566

Synthesis and Crystal Structures of μ-Oxido- and μ-Hydroxido-Bridged Dinuclear Iron(III) Complexes with an N_2O Donor Ligand – A Theoretical Study on the Influence of Weak Forces on the Fe–O–Fe Bridging Angle

Keywords: Iron / Schiff bases / N,N,O ligands / Crystal structures / Density functional calculations



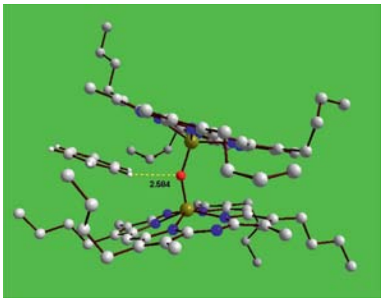
Two new dinuclear Fe^{III} complexes with a tridentate N,N,O donor ligand have been synthesized and characterized. One has an unsupported oxido bridge with a small Fe–O–Fe angle, and the other has a hydroxido bridge supported by a formato ligand. A theoretical study has been performed to study the influence of weak interactions on the small Fe–O–Fe angle in the oxido-bridged complex.

Porphyrinoids

P. A. Stuzhin,* A. Ul-Haq, S. E. Nefedov, R. S. Kumeev, O. I. Koifman ... 2567–2578

Synthesis and Study of the Binuclear μ-Oxodiiron(III) Complexes of 5-Monoaza- and 5,15-Diaza-Substituted β-Octaalkylporphyrins

Keywords: Porphyrinoids / Dimerisation / Iron / Bridging ligands



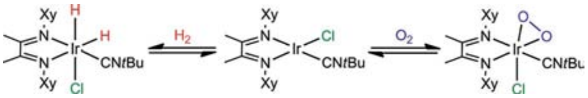
The μ-oxo bridge in β-alkylsubstituted μ-oxodiiron(III) complexes of *meso*-monoaza- and *meso*-diazaporphyrins is accessible for H-bonding interaction with solvent molecules. This very likely determines the lower stability of these species in acidic medium compared with the derivatives of *meso*- or β-phenylated porphyrins.

Peroxido Complexes

A. Penner, T. Braun* 2579–2587

Rhodium and Iridium Complexes with α-Diketimine Ligands: Oxidative Addition of H_2 and O_2

Keywords: Rhodium / Iridium / Diimines / Hydrido complexes / Peroxido ligands



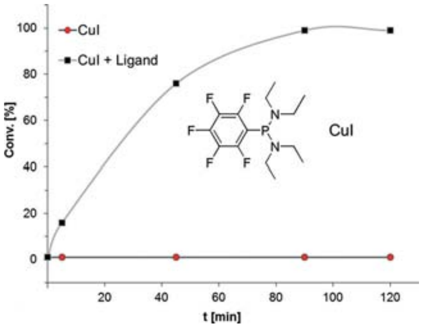
Unique rhodium(I) and iridium(I) α-diketimine compounds were synthesized starting from $[M(\mu\text{-}Cl)(coe)_2]_2$ (M = Rh, Ir, coe = cyclooctene). Treatment with H_2 or O_2 led to the formation of an Ir^{III} dihydrido complex as well as Rh^{III} and Ir^{III} peroxido complexes. The reactions with H_2 and O_2 are reversible.

Push–Pull Phosphanes

A. Orthaber, M. Fuchs, F. Belaj, G. N. Rechberger, C. O. Kappe, R. Pietschnig* 2588–2596

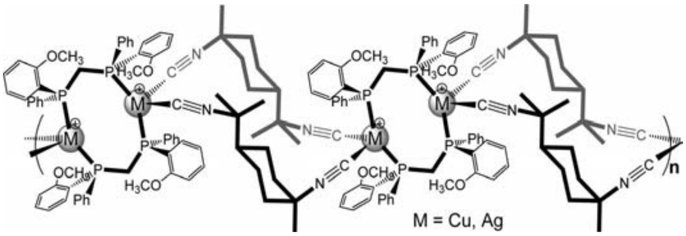
Bis(diethylamino)(pentafluorophenyl)phosphane – a Push–Pull Phosphane Available for Coordination

Keywords: Phosphorus / Fluorinated ligands / Homogeneous catalysis / Click chemistry



Unlike their previously reported congeners, "push–pull"-substituted (amino)(fluoroaryl)phosphanes have been made available for reactions at phosphorus including coordination to metal centers, which was employed for catalyzing C–C coupling and "click" reactions.

Chiral Coordination 1D-Polymers



The (*R*,*R*)- and (*S*,*S*)-bis(*o*-anisylphenylphosphanyl)methane and bis(*m*-xylylphosphanyl)methane ligands (dppm*) react with $Cu(BF_4)_2/Cu$ and $Ag(BF_4)$ to form the chiral binuclear complexes, which in turn react with 1,8-diisocyano-*p*-menthane (dmb) to give the first *P*-stereogenic 1D coordination polymers $\{[M_2(dppm^*)_2(dmb)_2](BF_4)_2\}_n$. The isostrutural nature of these new polymers with the parent symmetric dppm-containing polymers was unambiguously demonstrated by using a combination of several structure elucidation methods. All compounds and polymers were also characterized by circular dichroism spectroscopy.

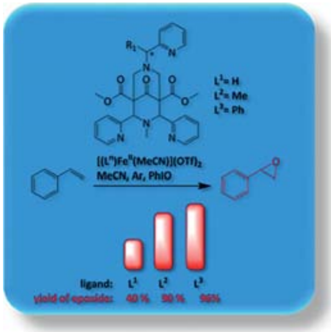
**C. Salomon, D. Fortin, N. Khiri, S. Jugé,*
P. D. Harvey*** **2597–2609**

The First *P*-Stereogenic 1D Coordination Polymers with the Metal Centers in the Backbone

Keywords: Silver / Copper / Phosphane ligands / Chirality / Coordination polymers

Oxidation Catalysis

Both the redox potential and the efficiency of the catalytic oxidation by a biomimetic bispidine-based iron precatalyst are optimized by increasing the ligand rigidity.



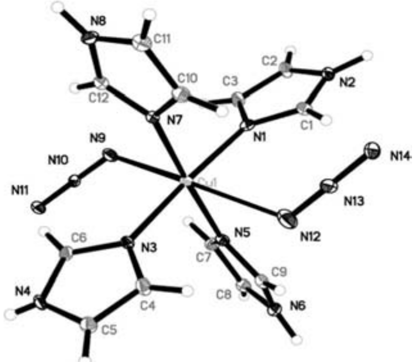
**P. Comba,* H. Wadepohl,
S. Wiesner** **2610–2615**

Optimization of the Efficiency of Oxidation Catalysts Based on Iron Bispidine Complexes

Keywords: Homogeneous catalysis / Oxidation / Iron / Bioinspired catalysis / Rigid ligands

Energetic Compounds

$Cu(IMI)_4(N_3)_2$ (IMI = imidazole) crystallizes in the orthorhombic space group $Pna2_1$. The metal cations are six-coordinate, and are linked to two azido ligands by μ_1-azido bridges and to four imidazole molecules through nitrogen atoms. In addition, this compound has high impact and friction sensitivity and therefore has potential application as an energetic material.



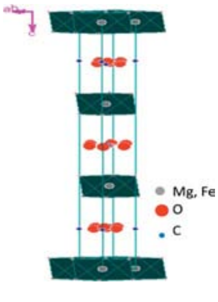
**B.-d. Wu, S.-w. Wang, L. Yang,*
T.-l. Zhang, J.-g. Zhang, Z.-n. Zhou,
K.-b. Yu** **2616–2623**

Preparation, Crystal Structures, Thermal Decomposition and Explosive Properties of Two Novel Energetic Compounds $M(IMI)_4(N_3)_2$ (M = Cu^{II} and Ni^{II}, IMI = Imidazole): The New High–Nitrogen Materials (N > 46%)

Keywords: Copper / Nickel / Azides / Imidazole / Decomposition / Sensitivity

Layered Double Hydroxides

UV/Vis spectrophotometry shows that Mg/Fe LDH crystallizes with a fixed Fe content. The structure of the Mg/Fe–CO_3 LDH was obtained by Rietveld refinement. The ordered Mg/Fe–CO_3 LDH was prepared by cation exchange starting from $Mg(OH)_2$. The UV/Vis absorption spectra show that the LDH composition corresponds to [Mg]/[Fe] = 4.



**G. V. Manohara, S. V. Prasanna,
P. V. Kamath*** **2624–2630**

Structure and Composition of the Layered Double Hydroxides of Mg and Fe: Implications for Anion-Exchange Reactions

Keywords: Ion exchange / UV/Vis spectroscopy / Magnesium / Iron / Hydroxides

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* Author to whom correspondence should be addressed.

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