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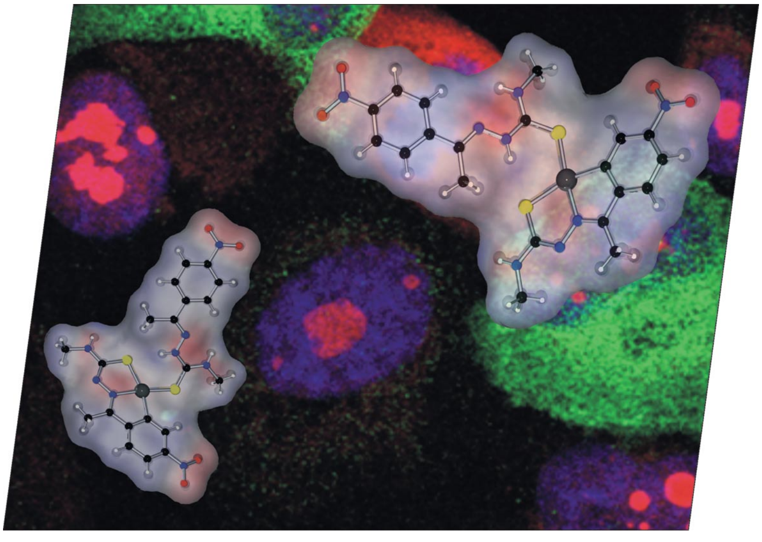
The EUChemSoc Societies have taken the significant step into the future by merging their traditional journals, to form two leading chemistry journals, the *European Journal of Inorganic Chemistry* and the *European Journal of Organic Chemistry.* Three further EUChemSoc Societies (Austria, Czech Republic and Sweden) are Associates of the two journals.

COVER PICTURE

The cover picture shows the crystal structure of a novel intermediate in the *p*-nitroacetophenone 4-methylthiosemicarbazone platination, [PtL1(L1H$_2$)], with potential application as an antitumoral drug. The complex is above an NCI-H460 cell culture background labelled to discriminate between live and dead cells by confocal microscopy. Details are discussed in the Short Communication by A. G. Quiroga et al. on p. 1183ff.



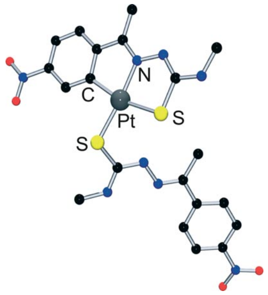
SHORT COMMUNICATIONS

Cytotoxic Pd and Pt Complexes

A. G. Quiroga,* L. Cubo,
P. J. S. Miguel, V. Moneo, A. Carnero,
C. Navarro-Ranninger 1183–1187

Isolation of an Intermediate in the Platination of *p*-Nitroacetophenone 4-Methylthiosemicarbazone: Potential Application as an Antitumor Drug

Keywords: Platinum / Palladium / Thiosemicarbazones / Antitumor drugs / C–M bonds



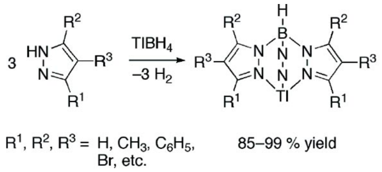
An investigation of the formation and reactivity of Pd and Pt thiosemicarbazone complexes (TSCN) has revealed an unstudied intermediate derived from *p*-nitroacetophenone. The complexes have been characterized and tested against tumor cell lines.

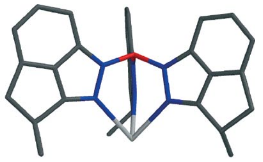
Thallium Scorpionate Synthesis

M. Kitamura,* Y. Takenaka, T. Okuno,
R. Holl, B. Wünsch 1188–1192

A New, Efficient and Direct Preparation of TlTp and Related Complexes with $TlBH_4$

Keywords: N ligands / Tripodal ligands / Thallium / Nitrogen heterocycles





$TlTp^{4Bo3MeCpenta}$

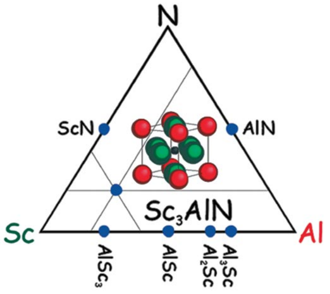
A practical and safe procedure for $TlBH_4$ synthesis by using TlOAc has been established. This success has led to a direct approach to the preparation and characterization of TlTp-related complexes that are key intermediates for various metal–Tp complexes. The method has successfully been applied to the efficient synthesis of $TlTp^{4Bo3MeCpenta}$ from a new and hard-to-obtain chiral pyrazole.

Synthesis of Inverse Perovskites

C. Höglund,* J. Birch, M. Beckers,
B. Alling, Z. Czigány, A. Mücklich,
L. Hultman 1193–1195

Sc_3AlN – A New Perovskite

Keywords: Crystal growth / Density functional theory / Electron microscopy / Perovskite nitride phases / Thin films



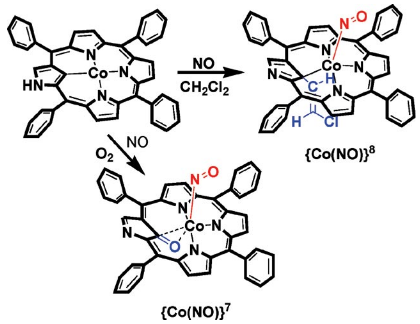
Inverse-perovskite Sc_3AlN is presented as the first ternary phase of the system. Stoichiometric $Sc_3AlN(111)$ films were synthesized on MgO substrates by magnetron sputter epitaxy as shown by elastic recoil detection, X-ray diffraction, and electron microscopy. A unit-cell parameter of 4.40 Å is obtained by measurement and quantum chemistry calculation. Enthalpy comparisons show that Sc_3AlN is thermodynamically stable with respect to its binaries.

N-Confused Porphyrin Complexes

C.-H. Hung,* C.-H. Peng, Y.-L. Shen,
S.-L. Wang, C.-H. Chuang,
H. M. Lee 1196–1199

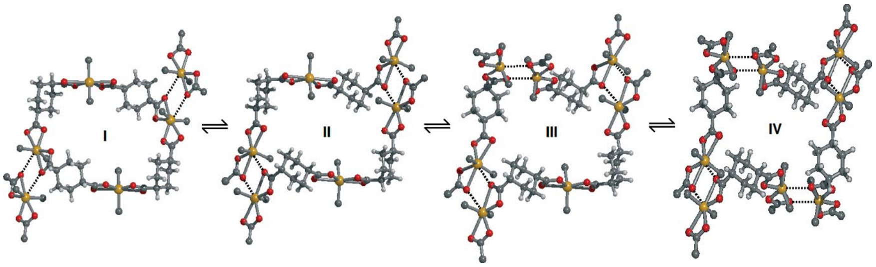
Preparation and Oxygenation of Cobalt N-Confused Porphyrin Nitrosyl Complexes

Keywords: Cobalt / Porphyrinoids / Nitrogen oxides / Oxygenation / X-ray diffraction



The nitrosylation of Co(*H*CTPP) in CH_2Cl_2 generated [Co(CTPPC_2H_2Cl)(NO)], which is a $\{Co(NO)\}^8$ cobalt nitrosyl complex with a chlorovinyl group substituted on the inner carbon atom of the N-confused porphyrin ring. In the presence of oxygen, the oxygenation product [Co(CTPP*O*)(NO)], a $\{Co(NO)\}^7$ cobalt nitrosyl complex, was obtained.

Self-Assembly Dynamics



The self-assembly and ring-chain rearrangement dynamics for a metal-organic tin complex consisting of a cyclotetranuclear and polymeric isomer is analyzed employing a combination of liquid-phase and solid-state techniques.

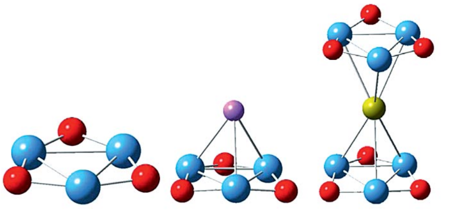
I. F. Hernández-Ahuactzi, J. Cruz-Huerta, V. Barba, H. Höpfl,* L. S. Zamudio-Rivera, H. I. Beltrán 1200–1204

Sequence of Metal-Organic Oligomer-Polymer Exchange Equilibria in Solution: Supramolecular Isomerism, Self-Assembly Dynamics and Carboxylate Shift of Di-*n*-butyltin *cis*-1,4-Cyclohexanedicarboxylate

Keywords: Carboxylate shift / Organotin carboxylate / Self-assembly dynamics / Supramolecular chemistry / Tin

FULL PAPERS

Sandwich-Type Complexes



D_{3h} $Ta_3O_3^-$ ($^1A_1'$) C_{3v} $[Ta_3O_3]Li$ ($^1A_1$) D_{3h} $[Ta_3O_3]Ca[Ta_3O_3]$

Half-sandwich-type C_{3v} $[Ta_3O_3]A$ (A=Li, Na, K) and full-sandwich-type D_{3h} $[Ta_3O_3]B[Ta_3O_3]$ (B=Ca, Sr, Ba) complexes containing $Ta_3O_3^-$ δ and π double aromatic ligands were investigated at the DFT level. These ligands may form the basis for a new branch of coordination chemistry.

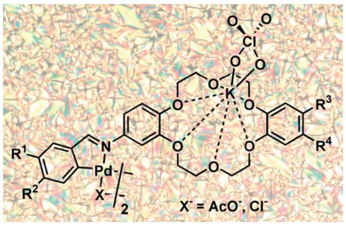
S.-D. Li,* C.-Q. Miao, J.-C. Guo 1205–1209

$[Ta_3O_3]A$ (A = Li, Na, K) and $[Ta_3O_3]B[Ta_3O_3]$ (B = Ca, Sr, Ba): Sandwich-Type Complexes Containing $Ta_3O_3^-$ δ and π Double Aromatic Ligands

Keywords: Sandwich-type complexes / Aromatic Ligands / Geometrical structure / Electronic structure / Density functional theory

Mesomorphic Palladium Complexes

Mesomorphic *ortho*-palladated $[Pd(\mu\text{-}X)L]_2$ (X^- = CH_3COO^-, Cl^-) complexes with unusual imines containing substituted dibenzo-18-crown-6-ethers (HL) show a preference for smectic C phases and form stable Langmuir films at the air–water interface. Complexation with potassium perchlorate produces a significant increase in the mesophase range and stability.



S. Coco,* C. Cordovilla, P. Espinet,* J.-L. Gallani, D. Guillon, B. Donnio 1210–1218

Supramolecular Aggregates in Fluid Phases: Mesomorphic *ortho*-Palladated Complexes with Substituted Crown Ethers and Their Potassium Adducts

Keywords: Crown ethers / Palladium / Liquid crystals / Langmuir films

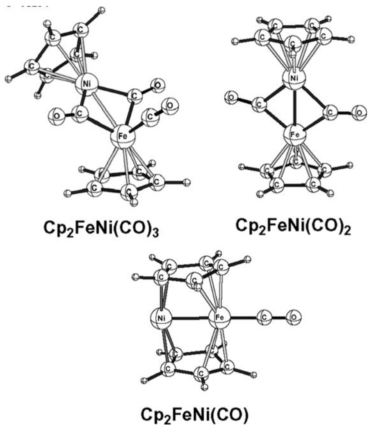
CONTENTS

Multiple Metal–Metal Bonds

J. D. Zhang, Z. Chen, R. B. King,*
H. F. Schaefer, III* 1219–1225

Comparison of Isoelectronic Heterometallic and Homometallic Binuclear Cyclopentadienylmetal Carbonyls: The Iron–Nickel vs. the Dicobalt Systems

Keywords: Iron / Nickel / Cyclopentadienyl complexes / Carbonyl ligands / Density functional theory



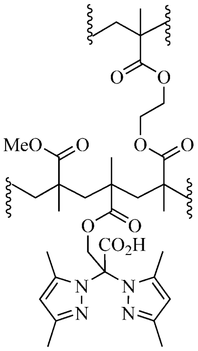
Using density functional theory (BP86) the global minima of both $Cp_2FeNi(CO)_3$ and $Cp_2FeNi(CO)_2$ are found to have two bridging CO groups. The coaxial structure of $Cp_2FeNi(CO)$ prefers an open-shell high spin state whereas the isoelectronic $Cp_2Co_2(CO)$ prefers a closed shell state with a Co≡Co triple bond. However, the global minimum for the monocarbonyl is a singlet perpendicular $Cp_2FeNi(CO)$ structure with an iron-bonded terminal CO group.

Solid Phase *N,N,O* Ligands

E. Hübner, G. Türkoglu, M. Wolf,
U. Zenneck, N. Burzlaff* 1226–1235

Novel *N,N,O* Scorpionate Ligands and Transition Metal Complexes Thereof Suitable for Polymerisation

Keywords: Solid phase / Immobilisation / Polymerisation / Tripodal ligands / *N,N,O* ligands / Tricarbonyl complexes



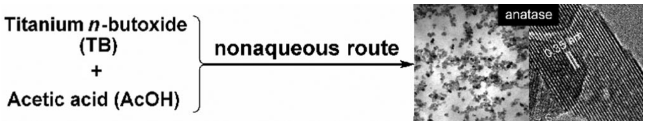
Addition of a methacryl linker to bis(3,5-dimethylpyrazol-1-yl)acetic acid leads to a new, polymerisation-active κ^3-*N,N,O* ligand. Copolymers with MMA and EGDMA as well as polymer-bound manganese, rhenium and copper complexes thereof are reported.

Nanocrystalline TiO_2

D. Jiang, Y. Xu,* B. Hou, D. Wu,
Y. Sun* 1236–1240

A Simple Non-Aqueous Route to Anatase TiO_2

Keywords: Titanium dioxide / Nonaqueous synthesis



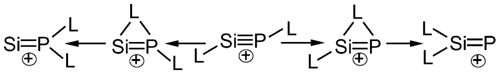
High-crystallized anatase TiO_2 was synthesized only using titanium *n*-butoxide (TB) and acetic acid (AcOH) as starting materials, by solvothermal treatment at 100 °C, without any cosolvent and additive.

Si–P Triple Bonds

C.-H. Chen, M.-D. Su* 1241–1247

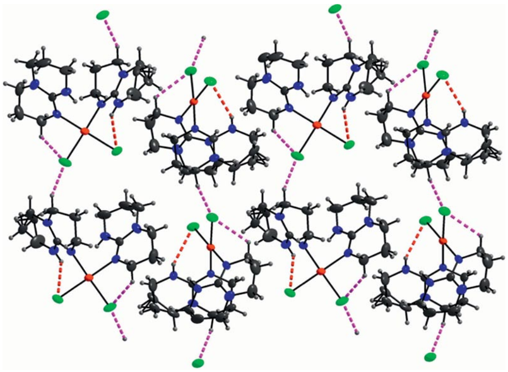
Theoretical Design of Silicon–Phosphorus Triple Bonds: A Density Functional Study

Keywords: Triple bonds / Phosphorus / Silicon / Density functional calculations



The B3LYP computational results suggest that the triply bonded molecule (L–Si≡P–L)$^{+1}$ lies at a minimum on the potential energy surface and can be stabilized and synthesized in both a kinetic and a thermodynamic sense, given a proper choice of bulky aryl ligands.

Platinum Complexes



The guanidine derivative 1,3,4,6,7,8-hexahydro-2*H*-pyrimido[1,2-*a*]pyrimidine (hppH) forms both *cis*- and *trans*-$[(\text{hppH})_2\text{PtCl}_2]$ complexes, although from different platinum-containing starting materials. hppH also readily forms salts that have different degrees of hydrogen bonding.

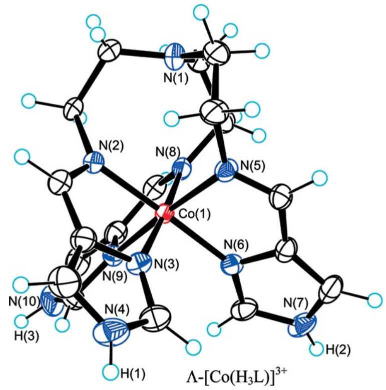
U. Wild, P. Roquette, E. Kaifer, J. Mautz, O. Hübner, H. Wadepohl, H.-J. Himmel* 1248–1257

Synthesis and Structural Characterisation of *cis*- and *trans*-$[(\text{hppH})_2\text{PtCl}_2]$, $[(\text{hppH})_3\text{-PtCl}]^+\text{Cl}^-$ and Some New Salts of the $[\text{hppH}_2]^+$ Cation (hppH = 1,3,4,6,7,8-Hexahydro-2*H*-pyrimido[1,2-*a*]pyrimidine): The Importance of Hydrogen Bonding

Keywords: Platinum / Hydrogen bonding / Quantum chemical calculations / N ligands

Chiral Resolution

Optical resolution of $[\text{Co}(\text{H}_3\text{L})]^{3+}$ was carried out by fractional crystallization of the diastereomeric salt with $[\text{Sb}_2\{(R,R)\text{-tart}\}_2]^{2-}$. Λ-$[\text{Co}(\text{H}_2\text{L})][\text{Sb}_2\{(R,R)\text{-tart}\}_2]\cdot 4\text{H}_2\text{O}$, which was isolated from the less soluble part, gave Λ-$[\text{Co}(\text{H}_3\text{L})](\text{ClO}_4)_3\cdot 1.5\text{H}_2\text{O}$ and Λ-[Co(L)] upon further treatment. The crystal structures of these latter complexes are compared with those of the racemic structures.



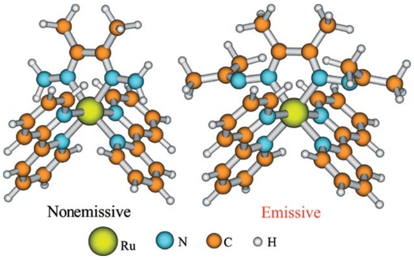
H. Nakamura, M. Fujii, Y. Sunatsuki, M. Kojima,* N. Matsumoto 1258–1267

Cobalt(III) Complexes of a Tripodal Ligand Containing Three Imidazole Groups: Properties and Structures of Racemic and Optically Active Species

Keywords: Cobalt / Crystal structure / Chiral resolution / Schiff bases / N ligands / Tripodal ligands

Phosphorescence in Ru$^{\text{II}}$ Complexes

Theoretical studies on the ground- and excited-state geometries, electronic structures, absorptions, and phosphorescence mechanisms of $\text{Ru(bpy)}_2(\text{N}^\wedge\text{N})$ [$\text{N}^\wedge\text{N}$ = hydrazone (**1**) and azine (**2**)] were performed. Compound **2** displays phosphorescence, whereas **1** does not; this can be rationalized on the basis of the compositions of the ^{3}MLCT excited states of the two compounds.

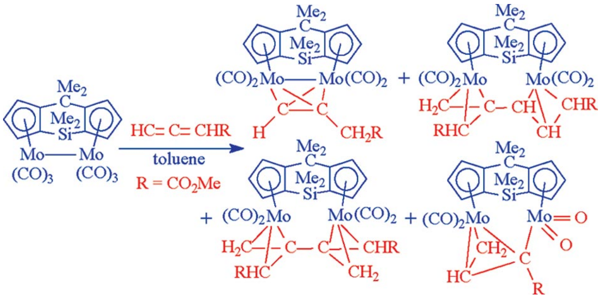


T. Liu, H.-X. Zhang,* X. Zhou, B.-H. Xia 1268–1276

Theoretical Studies on $[\text{Ru(bpy)}_2(\text{N}^\wedge\text{N})]^{2+}$ [$\text{N}^\wedge\text{N}$ = Hydrazone and Azine]: Ground- and Excited-State Geometries, Electronic Structures, Absorptions, and Phosphorescence Mechanisms

Keywords: Ruthenium / Electronic structure / Spectroscopic properties / Density functional calculations

Mo Complex Reactivity



Reaction of $(\text{Me}_2\text{C})(\text{Me}_2\text{Si})[(\eta^5\text{-C}_5\text{H}_3)\text{Mo}(\text{CO})_3]_2$ with $\text{H}_2\text{C=C=CHCO}_2\text{Me}$ gave four unexpected products, including two allene C–C coupled complexes. Diversity in the products revealed the different reactivities of this complex.

B. Li, C. Zhang, S. Xu, H. Song, B. Wang* 1277–1286

Reactions of the Doubly Bridged Bis(cyclopentadienyl) Dinuclear Molybdenum Complex $(\text{Me}_2\text{C})(\text{Me}_2\text{Si})[(\eta^5\text{-C}_5\text{H}_3)\text{Mo}(\text{CO})_3]_2$ with a Carboxylate-Substituted Allene

Keywords: Molybdenum / Allenes / C–C coupling / Bridging ligands / X-ray diffraction

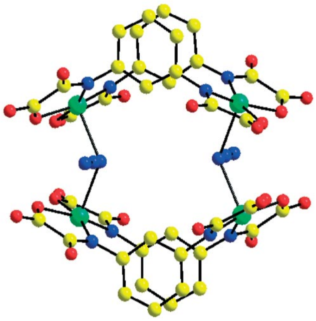
CONTENTS

Cu^{II} Metallacyclophane Complexes

X. Qu, X. Song, W. Li, Y. Xu, L. Li,*
D. Liao, Z. Jiang 1287–1292

Structural and Magnetic Properties of Two Copper(II) Complexes Based on Dinuclear Copper(II) Metallacyclophane

Keywords: Oxamates / Crystal structures / Metallacyclophanes / Azides / Magnetic properties



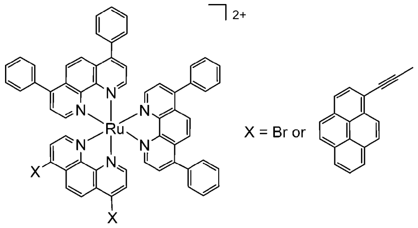
Two new (oxamato)copper(II) complexes have been synthesized in the presence of the azido ligand. The first complex has a metallamacrocycle structure in which two dinuclear copper(II) metallacyclophane anions are linked by two azido ligands, and the second is a 2D brick-wall-like layer structure. The magnetic properties of the metallamacrocycle complex are analyzed in connection with its structure.

Luminescent Ru^{II} Complexes

C. Goze, C. Sabatini, A. Barbieri,
F. Barigelletti,* R. Ziessel* 1293–1299

Synthesis, Electrochemical and Optical Properties of Ru^{II}–Diphenylphenanthroline–Ethynylpyrenephenanthroline Systems

Keywords: Ruthenium / Pyrenes / Energy conversion / Electrochemistry / Photophysics



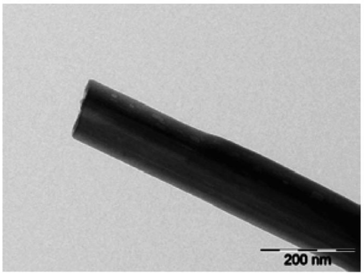
Ru^{II} complexes bearing bromo or ethynylpyrene substituents were synthesised. The complexes are stable, redox active and highly coloured. With a pyrene unit, the luminescence is strongly quenched at room temperature, whereas with a bromo substituent, intense ^{3}MLCT luminescence is found.

Sodium Niobates

A. J. Paula,* M. A. Zaghete, E. Longo,
J. A. Varela 1300–1308

Microwave-Assisted Hydrothermal Synthesis of Structurally and Morphologically Controlled Sodium Niobates by Using Niobic Acid as a Precursor

Keywords: Hydrothermal synthesis / Crystal growth / Niobates / Crystal morphology



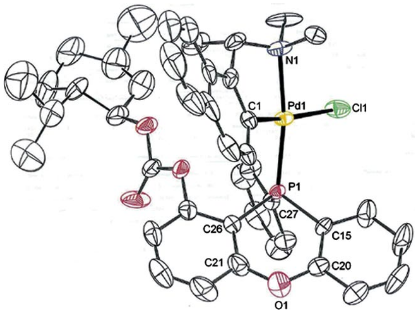
In a microwave-assisted hydrothermal system, the reaction between niobic acid ($Nb_2O_5 \cdot nH_2O$) and sodium hydroxide produced sodium niobium oxide powders with different structures and morphologies. These variations were a result of changes in the concentration of the reactant or the duration of the reaction.

Chiral Phosphacycles

F. Doro, M. Lutz, J. N. H. Reek,
A. L. Spek,
P. W. N. M. van Leeuwen* 1309–1317

P-Chirogenic Benzo-Fused Phenoxaphosphane: Synthesis, Resolution and Study of the Stereochemical Properties of the Corresponding Palladium Complexes

Keywords: Phosphacycles / P-Chirogenic ligands / Spectroscopic studies



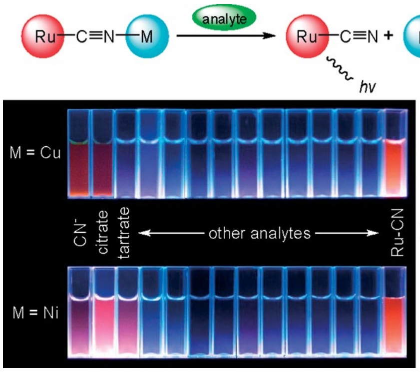
Phenoxaphosphane **3**, a chiral cyclic analogue of triphenylphosphane, has been synthesized and resolved in its two enantiomeric forms. The stereochemical properties of the corresponding palladium complexes have been extensively studied, both at the solid state and in solution.

Chemosensors

C.-K. Koo, C.-F. Chow, B. K.-W. Chiu, N.-Y. Lei, M. H.-W. Lam,* W.-Y. Wong 1318–1325

A Pair of Coordination Donor–Acceptor Ensembles for the Detection of Tartrate in Aqueous Media

Keywords: Chemosensing ensembles / Chemodosimetry / Donor–acceptor complexes / Tartrate / XOR logic



An "XOR" logic response from the two coordination donor–acceptor ensembles enables the specific detection of tartrate.

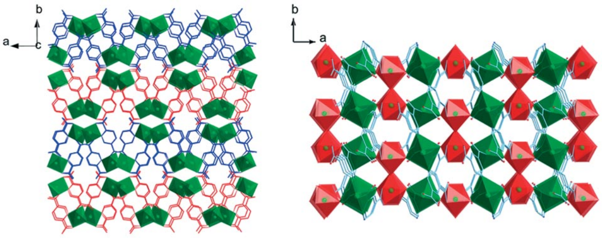
A pair of new trinuclear, heterodimetallic donor–acceptor complexes, {Ru(*t*Bubpy)(CN)$_4$[Cu(cyclen)]$_2$}(ClO$_4$)$_2$ ([Ru-Cu]) and {Ru(*t*Bubpy)(CN)$_4$[Ni(cyclen)]$_2$}(ClO$_4$)$_2$ ([Ru-Ni]), have been designed and synthesized for the specific chemodosimetric detection of tartrate through the use of XOR logic.

Hybrid Inorganic–Organic Compounds

Z. Guo, Y. Li, W. Yuan, X. Zhu, X. Li, R. Cao* 1326–1331

Syntheses, Structures, and Characterizations of Two New Indium(III) Compounds from 1D ···In–OH–In–OH··· Chains and Pyridinedicarboxylic Ligands

Keywords: Indium / Self-assembly / Luminescence



Two hybrid inorganic–organic compounds of indium(III) were hydrothermally prepared by the assembly of indium(III) with pyridinedicarboxylic acid, and were characterized by IR, XRPD, elemental analysis, and photoluminescent studies. Both of the compounds possess the similar 1D ···In–OH–In–OH··· SBU that has not yet been documented in nitrogen-donor aromatic carboxylates of indium.