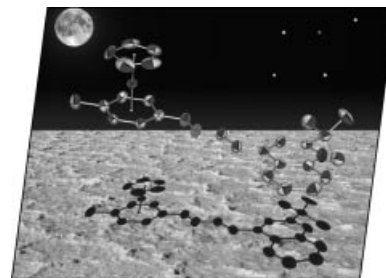


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## COVER PICTURE

**The cover picture shows** the crystal structure of the cationic organometallic  $\pi$ -conjugated push–pull chromophore combining the mixed sandwich acceptor group  $[\text{CpFe}(\eta^6\text{-}p\text{-MeC}_6\text{H}_4)]^+$ , associated with the 2-*tert*-butyl-4*H*-chromen-4-ylidene donor through the asymmetric hydrazone spacer  $-\text{NH}-\text{N}=\text{CH}-$ . This dipolar chromophore exhibits solvatochromic properties, low-lying intramolecular charge-transfer transition and enhanced second-order NLO properties ( $\mu\beta$ ), as measured with the EFISH technique at  $1.907\ \mu\text{m}$ . The scientific cooperation between researchers from the Southern Hemisphere (Chile) and the Northern Hemisphere (France) is symbolised not only by the Southern Cross but also by the NaCl crystals of the salt desert El Salar de Atacama. Details are discussed in the article by C. Manzur, D. Carrillo, B. Caro, J.-R. Hamon et al. on p. 1131 ff.



## MICROREVIEW

Contents

### 1111 B. Smarsly, M. Antonietti\*

Block Copolymer Assemblies as Templates for  
 the Generation of Mesoporous Inorganic Materials  
 and Crystalline Films

**Keywords:** Block copolymers / Mesoporous materials /  
 Self-assembly / Sol–gel processes

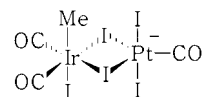


## SHORT COMMUNICATIONS

- 1121** S. Gautron, N. Lassauque, C. Le Berre,  
P. Serp, L. Azam, R. Giordano,  
G. Laurenczy, D. Thiébaud, P. Kalck\*



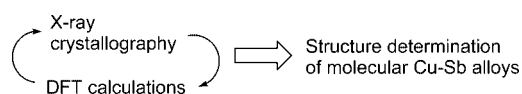
Analysis of the Synergistic Effect of Carbonyl-platinum Complexes on the Iridium-Catalysed Carbonylation of Methanol to Acetic Acid



**Keywords:** Homogeneous catalysis / Carbonylation / Iridium / Platinum / Reaction mechanism

- 1127** R. Ahlrichs, D. Fenske,\* A. Rothenberger,\*  
C. Schrod, S. Wieber

Atom Assignment in Solid-State Structures on the Basis of X-ray Crystallography and DFT Calculations – A Case Study on a Molecular Cu–Sb Alloy



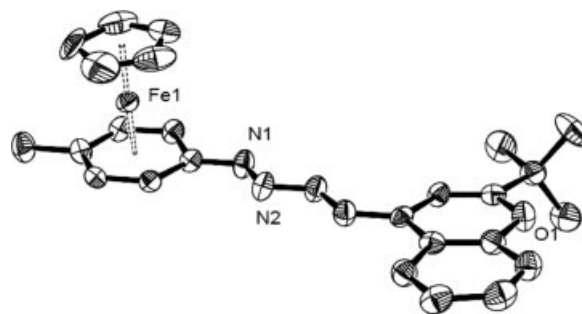
**Keywords:** DFT calculations / Molecular alloys / Sb ligands

## FULL PAPERS

- 1131** L. Millán, M. Fuentealba, C. Manzur,\*  
D. Carrillo,\* N. Faux, B. Caro,\*  
F. Robin-Le Guen, S. Sinbandhit,  
I. Ledoux-Rak, J.-R. Hamon\*



Dipolar Organoiron Pyranilideneacetaldehyde Hydrazone Complexes: Synthesis, Characterization, Crystal Structure, Linear and Nonlinear Optical Properties

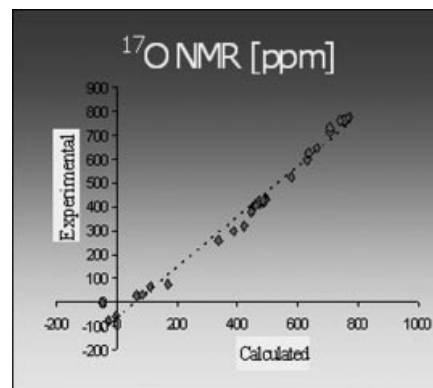


**Keywords:** Donor–acceptor systems / Iron / Pyranilideneacetaldehyde / Nonlinear optics / Sandwich complexes

- 1139** J. Gracia, J. M. Poblet,\* J. Autschbach,  
L. P. Kazansky\*



Density-Functional Calculation of the  $^{183}\text{W}$  and  $^{17}\text{O}$  NMR Chemical Shifts for Large Polyoxotungstates



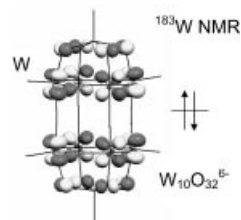
**Keywords:** Density-functional calculations / NMR spectroscopy / Oxygen / Polyoxometalates / Tungsten

**1149** J. Gracia, J. M. Poblet,\* J. Autschbach,  
L. P. Kazansky\*



DFT Calculations of the  $^{183}\text{W}$  NMR Chemical Shifts in Reduced Polyoxotungstates

**Keywords:** Density functional calculations / NMR spectroscopy / Oxygen / Polyoxometalates / Tungsten

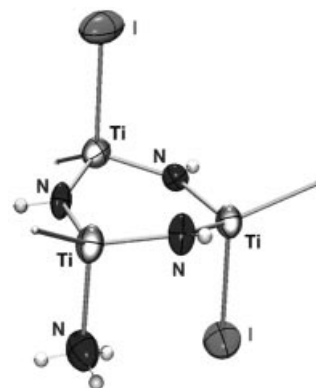


**1155** M. García-Castro, A. Martín, M. Mena,\*  
J.-M. Poblet, C. Yélamos



Iodine Attack on the Metalloligand  $[\{\text{Ti}(\eta^5\text{-C}_5\text{Me}_5)(\mu\text{-NH})\}_3(\mu_3\text{-N})]$ : Surprising Formation of the  $[\text{Ti}_3(\eta^5\text{-C}_5\text{Me}_5)_3\text{I}_2(\mu\text{-NH})_3(\text{NH}_3)]^+$  Cation

**Keywords:** Iridium / Iodine / N ligands / Nitrido complexes / Titanium

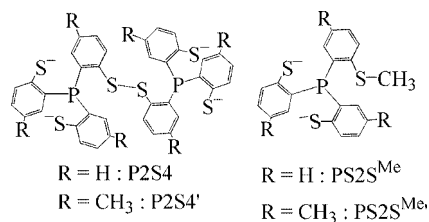


**1161** H.-F. Hsu,\* C.-L. Su, N. O. Gopal,  
C.-C. Wu, W.-C. Chu, Y.-F. Tsai,  
Y.-H. Chang, Y.-H. Liu, T.-S. Kuo,  
S.-C. Ke\*



Redox Chemistry in the Reaction of Oxovanadium(v) with Thiolate-Containing Ligands: the Isolation and Characterization of Non-Oxo Vanadium(IV) Complexes Containing Disulfide and Thioether Groups

**Keywords:** Vanadium / S ligands / Bioinorganic chemistry / EPR spectroscopy

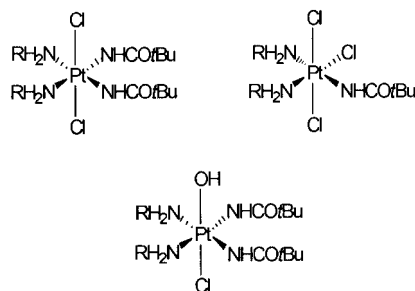


**1168** F. Liu, W. Chen\*



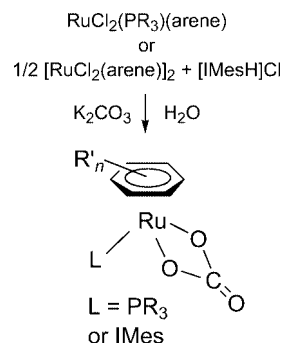
Oxidative Addition of  $\text{Cl}_2$ ,  $\text{HClO}$  to Square-Planar  $\text{Pt}^{\text{II}}$  Complexes: Synthesis and Structural Characterization of Platinum(II) and Platinum-(IV) Bis(amidate) Complexes

**Keywords:** Platinum / Amidates / Amines



**1174 B. Demerseman,\* M. D. Mbaye, D. Sémeril,  
L. Toupet, C. Bruneau, P. H. Dixneuf**

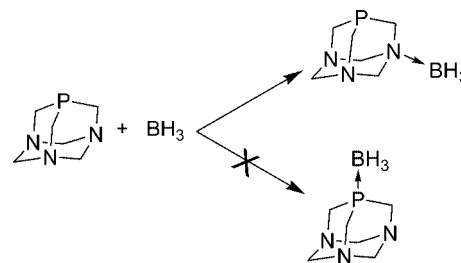
Direct Preparation of  $[\text{Ru}(\eta^2\text{-O}_2\text{CO})(\eta^6\text{-arene})\text{-}(\text{L})]$  Carbonate Complexes ( $\text{L}$  = Phosphane, Carbene) and Their Use as Precursors of  $[\text{RuH}_2(p\text{-cymene})(\text{PCy}_3)]$  and  $[\text{Ru}(\eta^6\text{-arene})(\text{L})\text{-(MeCN)}_2][\text{BF}_4]_2$ : X-ray Crystal Structure Determination of  $[\text{Ru}(\eta^2\text{-O}_2\text{CO})(p\text{-cymene})(\text{PCy}_3)] \cdot 1/2\text{CH}_2\text{Cl}_2$  and  $[\text{Ru}(\eta^2\text{-O}_2\text{CO})(\eta^6\text{-C}_6\text{Me}_6)\text{-(PMe}_3)] \cdot \text{H}_2\text{O}$



**Keywords:** Arene ligands / Hydrides / O ligands / Reactive intermediates / Ruthenium

**1182 B. J. Frost,\* C. A. Mebi, P. W. Gingrich**

Boron–Nitrogen Adducts of 1,3,5-Triaza-7-phosphaadamantane (PTA): Synthesis, Reactivity, and Molecular Structure

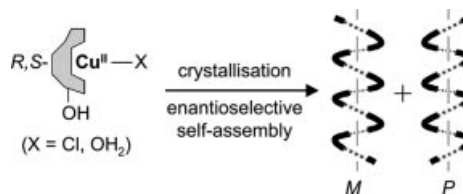


**Keywords:** Borane adducts / Boroxine / N,P ligands / Coordination modes / Structure elucidation

**1190 D. G. Lonnon, S. B. Colbran,\* D. C. Craig**



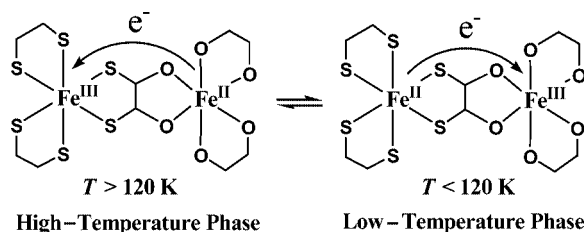
Programmed Helicity in Self-Assembled Hydrogen-Bonded Chains of Chiral Copper(II) Complexes



**Keywords:** Hydrogen bonds / Supramolecular / Self-assembly / Copper / Helical structures

**1198 M. Itoi,\* Y. Ono, N. Kojima,\* K. Kato,  
K. Osaka, M. Takata**

Charge-Transfer Phase Transition and Ferromagnetism of Iron Mixed-Valence Complexes  $(n\text{-C}_n\text{H}_{2n+1})_4\text{N}[\text{Fe}^{\text{II}}\text{Fe}^{\text{III}}(\text{dto})_3]$  ( $n = 3\text{--}6$ ;  $\text{dto} = \text{C}_2\text{O}_2\text{S}_2$ )



**Keywords:** Mixed-valence compounds / Iron / Magnetic properties / Charge transfer

**1208** J. Yang, J.-F. Ma,\* Y.-Y. Liu, J.-C. Ma,  
H.-Q. Jia, N.-H. Hu



Two New Cu<sup>II</sup> Coordination Polymers: Studies of Topological Networks and Water Clusters

**Keywords:** Coordination polymers / Copper / Materials science / Topology / Water clusters

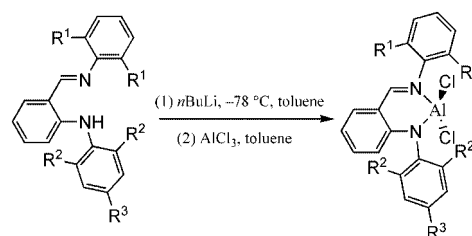


**1216** X. Liu, H. Xia, W. Gao, L. Ye, Y. Mu,\*  
Q. Su, Y. Ren



Synthesis, Structures, and Luminescent Properties of Aluminum Complexes with Chelating Anilido-Imine Ligands

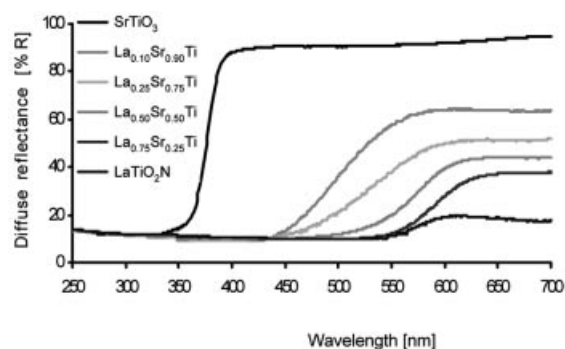
**Keywords:** Aluminum / N ligands / Luminescence



**1223** F. Cheviré, F. Tessier,\* R. Marchand

Optical Properties of the Perovskite Solid Solution LaTiO<sub>2</sub>N–ATiO<sub>3</sub> (A = Sr, Ba)

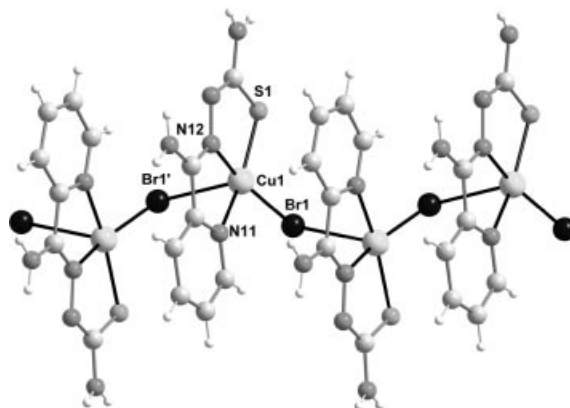
**Keywords:** Oxynitrides / Perovskites / Solid solution / Optical properties



**1231** M. del Carmen Aguirre, J. Borrás,  
A. Castiñeiras,\* J. M. García-Montegudo,  
I. García-Santos, J. Niclós, D. X. West

Synthesis, Characterization, and Properties of Some Copper(II) Complexes of 2-Pyridineformamide Thiosemicarbazone (HAm4DH)

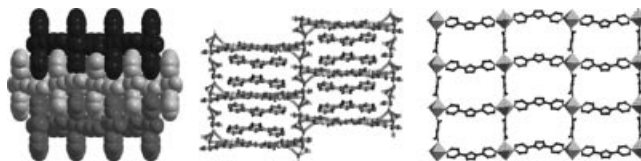
**Keywords:** Thiosemicarbazones / Copper complexes / One-dimensional chains / Cyclic voltammetry / DNA cleavage



**1245** M. Du,\* X.-J. Jiang, X.-J. Zhao, H. Cai, J. Ribas

Novel Metallosupramolecular Networks Constructed from Cu<sup>II</sup>, Ni<sup>II</sup>, and Cd<sup>II</sup> with Mixed Ligands: Crystal Structures, Fluorescence, and Magnetism

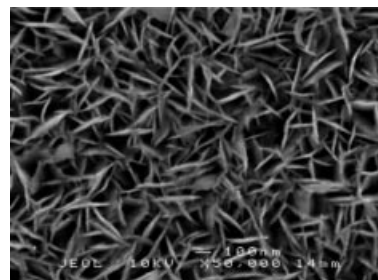
**Keywords:** Coordination polymers / Inclusion complexes / Supramolecular chemistry / Noncovalent interactions



**1255** N. D. Boscher, C. J. Carmalt, I. P. Parkin\*

Atmospheric Pressure Chemical Vapour Deposition of NbSe<sub>2</sub> Thin Films on Glass

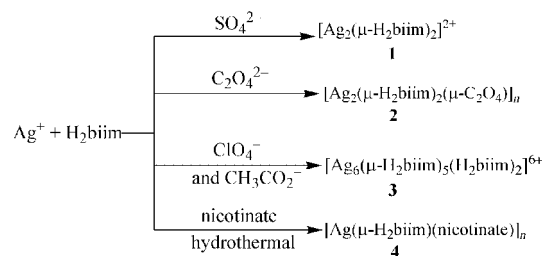
**Keywords:** Chemical vapour deposition / Metal selenide / Thin film



**1260** R.-L. Sang, L. Xu\*

Counteranion-Induced Formation of *cis* and *trans* Singly and Doubly H<sub>2</sub>biim-Bridged Di-, Hexa-, and Polymeric Ag–H<sub>2</sub>biim Complexes

**Keywords:** Crystal engineering / Luminescence / Metal–metal interactions / N ligands / Silver

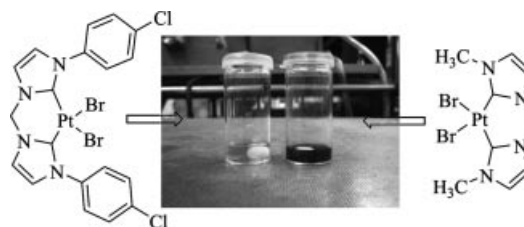


**1268** S. Ahrens, E. Herdtweck, S. Goutal, T. Strassner\*



Synthesis, Structure and Stability of New Pt<sup>II</sup>–Bis(N-Heterocyclic Carbene) Complexes

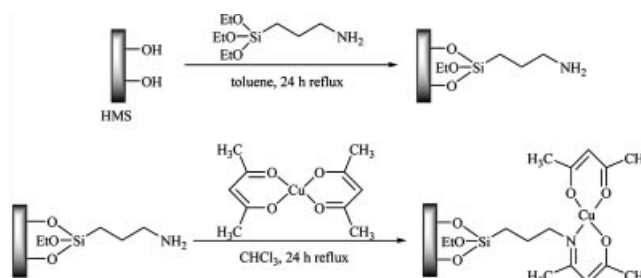
**Keywords:** Carbene ligands / NMR spectroscopy / Platinum / Synthesis design



**1275** A. R. Silva, K. Wilson, A. C. Whitwood, J. H. Clark, C. Freire\*

Amine-Functionalised Hexagonal Mesoporous Silica as Support for Copper(II) Acetylacetonate Catalyst

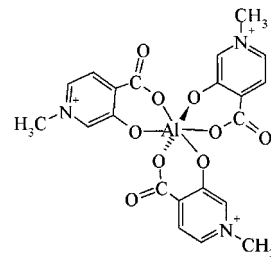
**Keywords:** Copper / Anchoring / Mesoporous silica / EPR spectroscopy / Aziridination



**1284** V. B. Di Marco,\* A. Dean, M. G. Ferlin,  
R. A. Yokel, H. Li, A. Venzo, G. G. Bombi

Methyl-Hydroxypyridinecarboxylic Acids as Possible Bidentate Chelating Agents for Aluminium(III): Synthesis and Metal–Ligand Solution Chemistry

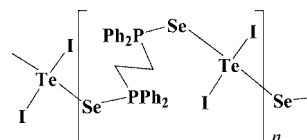
**Keywords:** Aluminium / Carboxylate ligands / Potentiometry / Chelation therapy



**1294** C. G. Hrib, P. G. Jones, W.-W. du Mont,\*  
V. Lippolis, F. A. Devillanova

Complexes of Bidentate Phosphane Selenide Ligands with Mesitylenetellurenyl Iodide and with Tellurium Diiodide

**Keywords:** Phosphane selenides / Tellurium iodides / Heteronuclear NMR / Raman spectroscopy / Soft–soft interactions



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