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Contents

Special Issue In Honor of Professor Jerry L. Atwood

Note

Jamie N. Jones, Charles L.B. Macdonald, John D. Gorden, Alan H. Cowley

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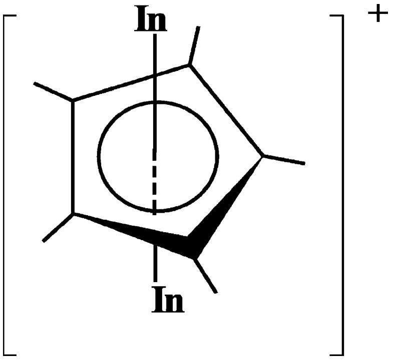
Use of a smaller counterion results in an 'inverse sandwich' diindium cation

Reducing the size of the counterion from $[(C_6F_5)_3BO(H)B(C_6F_5)_3]^-$ to $[B(C_6F_5)_4]^-$ 'squeezes' the toluene molecules from the triple decker cation $[\eta^6\text{-}C_7H_8)In(\mu\text{-}\eta^5\text{-}C_5Me_5)In(\eta^6\text{-}C_7H_8)]^+$ and results in the 'inverse sandwich' diindium cation, $[In(\mu\text{-}\eta^5\text{-}C_5Me_5)In]^+$. The latter exhibits short In···F and In···(η^6-C_6F_5) contacts with $[B(C_6F_5)_4]^-$ anions.



Regular Papers

Jason K. Vohs, L. Ellen Downs, Michael E. Barfield, Kirk Latibeaudiere, Gregory H. Robinson

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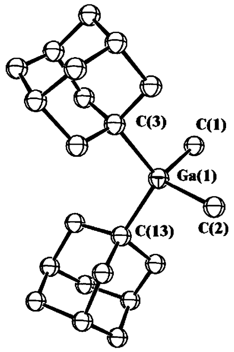
Unusual trimetallic magnesium cations and adamantyl anions of aluminum and gallium

Reaction of adamantylmagnesium bromide, AdaMgBr, with $AlCl_3$, $GaCl_3$, Me_2AlCl, and Me_2GaCl gives $[Mg_3BrCl_3(OEt)(OEt_2)_6][Ada_3AlBr]$ (**I**), $[Mg_3Br_2Cl_3(OEt_2)_6][Ada_2GaBr_2]$ (**II**), $[Mg_3Br_4(OEt)(OEt_2)_6][Ada_2GaMe_2]$ (**III**), and $[Mg_3Br_4(OEt)(OEt_2)_6][Ada_2AlMe_2]$ (**IV**), respectively. These compounds contain trimetallic magnesium cations with each metal residing in distorted octahedral environments while the aluminum and gallium atoms in the adamantyl-based anions reside in distorted tetrahedral environments.



Jonathan R. Nitschke, T. Don Tilley

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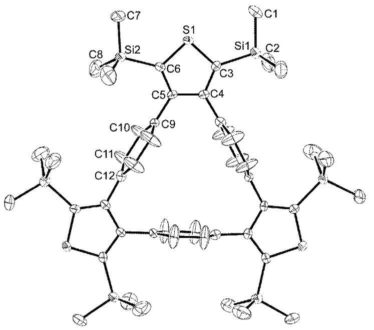
Convenient, zirconocene-coupling routes to germole- and thiophene-containing macrocycles with triangular geometries

Reactions of zirconacyclopentadiene-coupled macrocycles with S_2Cl_2 or $GeCl_4$ gave new macrocycles containing thiophene and dichlorogermole groups, respectively The germoles, synthesized in high yields, possess labile chloride substitutents that are readily displaced via nucleophilic substitution reactions. These germole-containing macrocycles are potentially useful as supramolecular building blocks..



Catherine S. Branch, Simon G. Bott, Andrew R. Barron

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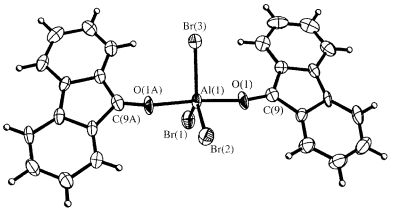
Group 13 trihalide complexes of 9-fluorenone: a comparison of methods for assigning relative Lewis acidity

A correlation of the results for the five structurally characterized compounds MX$_3$(9-fluorenone) (M = B, X = Cl; M = Al, X = Cl, Br; M = Ga, X = Cl, Br) was used to examine the suitability of the following parameters to measuring Lewis acidity: IR $\nu_{C=O}$, UV λ_{max}, and ^{13}C-NMR $\delta_{C=O}$, K_{eq} at 298 K, ΔH, ΔG, and a variety of structural parameters. It appears important to differentiate, the ability of a Lewis acidic compound to bind a Lewis base from the effect the metal compound has upon that Lewis base once coordinated.



Ziyun Wang, Colin D. Abernethy, Alan H. Cowley, Jamie N. Jones, Richard A. Jones, Charles L.B. Macdonald, Lilu Zhang

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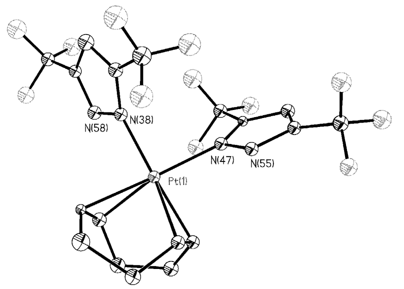
Synthesis and structures of 3,5-bis(trifluoromethyl)pyrazol derivatives of Rh(I), Ir(I), Pd(II) and Pt(II)

The reaction of Li 3,5-(CF$_3$)$_2$Pz with [Rh(COD)Cl]$_2$, IrCl(CO)$_3$, [PdCl(η^3-C$_3$H$_5$)]$_2$ and PtCl$_2$(COD) in diethylether solution at 0 °C results in the formation of [Rh(COD)-(μ-3,5-(CF$_3$)$_2$Pz)]$_2$ (**1**), [Ir(CO)$_2$(μ-3,5-(CF$_3$)$_2$Pz)]$_2$ (**2**), [Pd(η^3-C$_3$H$_5$)(μ-3,5-(CF$_3$)$_2$-Pz)]$_2$ (**3**), and Pt(COD)(η^1-3,5-(CF$_3$)$_2$Pz)$_2$ (**4**), respectively (3,5-(CF$_3$)$_2$Pz = 3,5-(CF$_3$)$_2$ pyrazolate; COD = 1,5-cyclooctadiene).



Tomislav Friščić, Leonard R. MacGillivray

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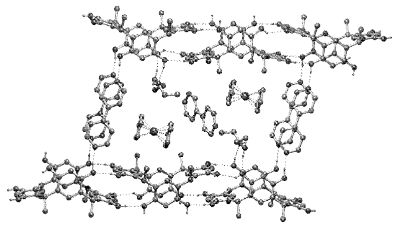
Double inclusion of ferrocene within a doubly interpenetrated three-dimensional framework based on a resorcin[4]arene

A doubly interpenetrated 3D hydrogen-bonded framework based on resorcin[4]arene is revealed to accommodate two molecules of ferrocene within box-shaped cavities of nanometer-scale dimensions.



Donald J. Darensbourg, Andrea L. Phelps, M. Jason Adams, Jason C. Yarbrough

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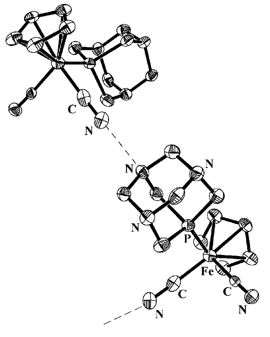
Intermolecular hydrogen-bonding in the solid-state structure of CpFe(CN)$_2$(PTAH) Structural and spectral comparisons with its [K][CpFe(CN)$_2$PTA] salt

K[CpFe(CN)$_2$PTA] has been synthesized from K[CpFe(CN)$_2$CO] and PTA and its structure determined by X-ray crystallography. Protonation of K[CpFe(CN)$_2$PTA] yielded CpFe(CN)$_2$PTAH which was also structurally characterized by X-ray crystallography. The latter complex exhibits hydrogen bonding between the cyanide nitrogen of one and a PTA nitrogen of another with a N···N distance of 2.686 Å.



Marcus L. Cole, Peter C. Junk

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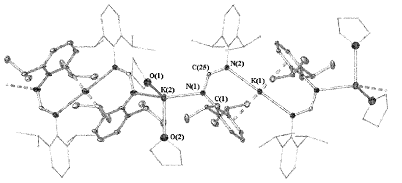
Potassium complexes of the 'super' formamidine $(2,6-\mathrm{Pr}^i_2\mathrm{C}_6\mathrm{H}_3)\mathrm{NC(H)NH}(2,6-\mathrm{Pr}^i_2\mathrm{C}_6\mathrm{H}_3)$, HDippForm.
Synthesis and molecular structure of $[\{\mathrm{K(DippForm)_2K(THF)_2}\}_n]\cdot n\mathrm{THF}$ and $[\mathrm{K(DippForm)(THF)_3}]\cdot\mathrm{HDippForm}$

Ambient temperature treatment of the new 'super' formamidine $(2,6-\mathrm{Pr}^i_2\mathrm{C}_6\mathrm{H}_3)-\mathrm{NC(H)NH}(2,6-\mathrm{Pr}^i_2\mathrm{C}_6\mathrm{H}_3)$, HDippForm, with one equivalent of potassium bis(trimethylsilyl)amide yields the polymeric potassium formamidinate complex $[\{\mathrm{K}(\eta^6{:}\eta^1\text{-}\mathrm{DippForm})_2\mathrm{K(THF)_2}\}_n]\cdot n\mathrm{THF}$ (**1**). Addition of a further equivalent of HDippForm to **1** results in the formation of hydrogen bound species; $[\mathrm{K}(\eta^6{:}\eta^1\text{-}\mathrm{DippForm})\text{-}(\mathrm{THF})_3]\cdot\mathrm{HDippForm}$ (**2**). The supra-, macro- and solution-state molecular structures of both **1** and **2** are discussed.



Karl J. Wallace, Rachvinder Daari, Warwick J. Belcher, Lagili O. Abouderbala, Martyn G. Boutelle, Jonathan W. Steed

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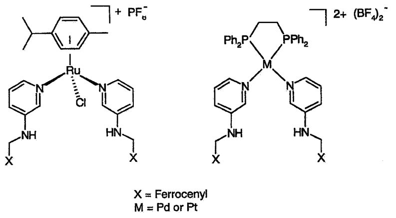
Oxo-anion binding by metal containing molecular 'clefts'

Metal-based molecular clefts have been synthesised and their ability to bind oxo-anions has been studied.



Dennis L. Lichtenberger, Hua-Jun Fan, Nadine E. Gruhn

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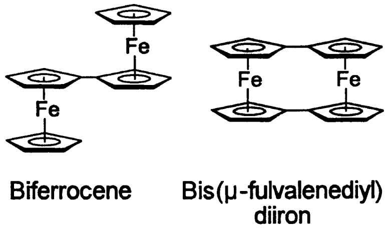
Ligand-mediated metal–metal interactions and localized versus delocalized mixed-valence cation states of biferrocene and bis(μ-fulvalenediyl)diiron characterized in the gas phase by valence photoelectron spectroscopy

Gas-phase photoelectron spectroscopy is used to investigate metal–metal interactions and the mixed-valence positive ion states of the title molecules. The initial ionization bands of both bimetallic molecules are spread over a wide energy range, indicating delocalization across the two metal halves of the molecule and formal oxidation states of $+2^1/_2$ for each metal atom in these cation states.



Daniel L. Reger, Radu F. Semeniuc, Mark D. Smith

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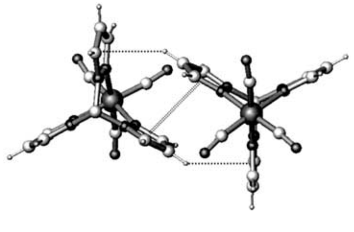
Structurally adaptive multitopic ligands containing tris(pyrazolyl)methane units as supramolecular synthons: manganese carbonyl complexes

The compounds $\{p\text{-}\mathrm{C_6H_4[CH_2OCH_2C(pz)_3]_2[Mn(CO)_3]_2}\}(\mathrm{BF_4})_2$ (**1**, pz = pyrazolyl ring), $\{p\text{-}\mathrm{C_6H_4[CH_2OCH_2C(pz)_3]_2[Mn(CO)_3]_2}\}(\mathrm{OTf})_2$ (**2**, $\mathrm{OTf^-} = \mathrm{CF_3SO_3^-}$), $\{m\text{-}\mathrm{C_6H_4[CH_2OCH_2C(pz)_3]_2[Mn(CO)_3]_2}\}(\mathrm{BF_4})_2$ (**3**) and $\{\mathit{1,2,4,5}\text{-}\mathrm{C_6H_2[CH_2OCH_2C(pz)_3]_4[Mn(CO)_3]_4}\}(\mathrm{BF_4})_2$ (**4**) have been prepared. The structurally adaptive ligands in all four complexes support extended 3D supramolecular structures. An important organizational feature for the three $\mathrm{BF_4^-}$ complexes is a double π–π and C–H···π interaction involving the pyrazolyl rings, see Figure.



Timothy S. Keizer, Lauren J. De Pue, Sean Parkin, David A. Atwood

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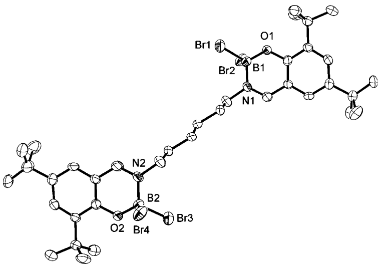
Dealkylation with boron bromide chelates

Potential two-point Lewis acids compounds can be formed by combining the salen(^{t}Bu)H_2 ligands (N,N'-alkylenene-bis(3,5-di-tertbutyl(2-hydroxy)benzylidenimine) and its derivatives with boron tribromide. In the present study compounds having the formula, salen(^{t}Bu)$(BBr_2)_2$ were prepared (the structure of one is shown). These compounds are active towards the dealkylation of alkyl phosphates and are catalytic when stoichiometric amounts of BBr_3 and trimethylphosphate are introduced to the chelate ligand.



Milja S. Hannu-Kuure, Jarno Komulainen, Raija Oilunkaniemi, Risto S. Laitinen, Reijo Suontamo, Markku Ahlgrén

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An experimental and theoretical study of the isomerization of mononuclear bis(arylselenolato)bis(triphenylphosphine)platinum complexes $[Pt(SeR)_2(PPh_3)_2]$

$[Pt(SeR)_2(PPh_3)_2]$ (R = furyl, thienyl, phenyl) can be prepared from *cis*-$[PtCl_2(PPh_3)_2]$ and NaSeR or LiSeR. Initially, *cis*-$[Pt(SeR)_2(PPh_3)_2]$ is formed. Upon prolonged standing in solution it isomerizes to *trans*-$[Pt(SeR)_2(PPh_3)_2]$. Solid *cis*,*anti*- and *trans*,*syn*-$[Pt(SeFu)_2(PPh_3)_2]$, *cis*,*syn*- and *trans*,*anti*-$[Pt(SeTh)_2(PPh_3)_2]$ have been isolated and structurally characterized. Ab initio MO calculations have been carried out to $[Pt(SeR)_2(PH_3)_2]$ isomers to model the structures and energetics of the mononuclear selenolato platinum complexes.