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Cover Artwork: One nitronyl nitroxide radical and its three lanthanide-based compounds have been prepared. Tb complex displays frequency-dependent signals at low temperature suggesting that it behaves as SMM.

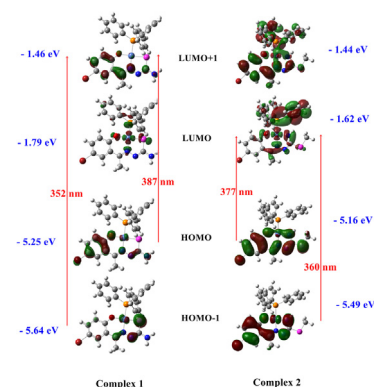
Corresponding Author: Feng-Ping Xiao. Page number: 40–45.

Işın Kılıç-Cıkla, Şükriye Güveli, Tülay Bal-Demirci, Muhittin Aygün, Bahri Ülküseven and Metin Yavuz

Polyhedron 130 (2017) 1

X-ray diffraction, spectroscopic and DFT studies on nickel(II)-triphenylphosphine complexes of 2-hydroxyacetophenone thiosemicarbazones

The results of IR and ^1H NMR spectra of 2-hydroxyacetophenone ligands show the ONS and ONN coordination modes of **L**¹ and **L**², respectively. Molecular geometries and intra- and inter-molecular interactions of **L**¹, **1** and **2** were defined by single crystal X-ray analysis. The electronic absorption spectra and electronic excitations were also calculated using the TD-DFT formalism.

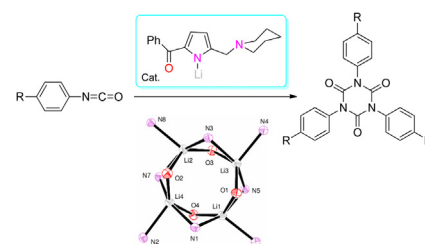


Zhiqiang Guo, Yakong Wang, Jihong Yang and Xuehong Wei

Polyhedron 130 (2017) 13

Lithium complex of 2-amino-functionalized benzoylpyrrole: Synthesis, structure, and catalytic activity for the cyclotrimerization of isocyanates

Lithium complex stabilised by 2-amino-functionalized benzoylpyrrole was synthesized, and its structural features were provided. The molecular structure shows a novel tetrameric cage structure, which includes a eight-membered (LiN)₄ ring and a eight-membered (LiO)₄ ring with the coordinating pyrrolyl ligands. It was proved to an efficient catalyst for the cyclotrimerisation of isocyanates in good to excellent yields under mild conditions.

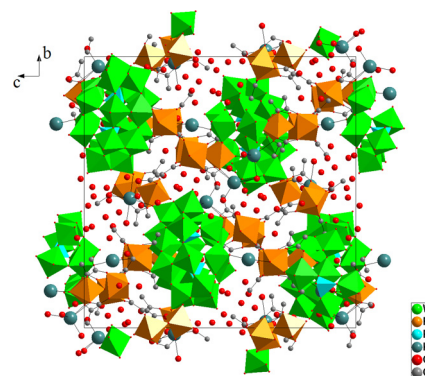


Fatma Dhifallah, Mohamed Salah Belkhiria, Nathalie Leclerc, Loic Parent, Israel-Martyr Mbomekalle and Emmanuel Cadot

Polyhedron 130 (2017) 18

A channeled 3D structure of a new polyoxometalate-based triiron(III) cluster: Synthesis, crystal structure and electrochemical properties

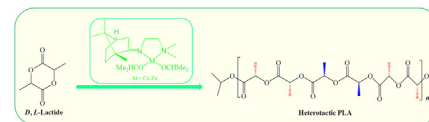
A novel and interesting hybrid compound based on Wells-Dawson polyanion and triiron macrocation was synthesized and characterized. This compound has a tridimensional structure with nanoscale channels running parallel to the c-axis and filled with crystallization water molecules.



Kyuong Seop Kwon, Saira Nayab and Jong Hwa Jeong
Polyhedron 130 (2017) 23

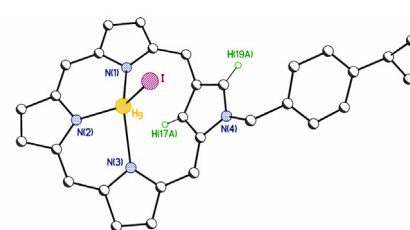
Synthesis, characterisation and X-ray structure of Cu(II) and Zn(II) complexes bearing *N,N*-dimethylethylenamine-camphorylimine ligands: Application in the polymerisation of *rac*-lactide

Novel Cu(II) and Zn(II) complexes based on the *N,N*-dimethylethylenamine-camphorylimine ligand have been synthesized and characterised by X-ray diffraction. Alkoxy derivatives, generated *in situ*, catalysed the ROP of *rac*-LA in controlled fashion yielding hetero-enriched PLA ($P_r = 0.85$).


Hsiang-Yin Lin, Chun-Yeh Lin, Chun-Chia Chiu, Hsueh-Ju Li, Jyh-Horung Chen, Shin-Shin Wang and Jo-Yu Tung
Polyhedron 130 (2017) 30

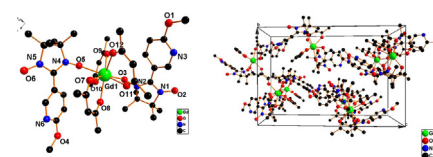
Weak $\eta^2\text{-C-H}\cdots\text{Hg}$ interactions. Crystal structures of Hg(II) 2-N substituted N-confused porphyrin: Hg(2-NCH₂-*p*-C₆H₄-CH₃-21-H-NCTPP)I and Hg(2-NCH₂-*p*-C₆H₄-isoC₃H₇-21-H-NCTPP)I·C₆H₅CH₃

The rare examples of weak $\eta^2\text{-C-H}\cdots\text{Hg}$ agostic interactions with coupling constants J ($\text{Hg-H}'_{\text{ago}}$) of 34.5 ± 0.3 Hz have been found from the X-ray structures of Hg(2-NCH₂-*p*-C₆H₄-CH₃-21-H-NCTPP)I and Hg(2-NCH₂-*p*-C₆H₄-isoC₃H₇-21-H-NCTPP)I·C₆H₅CH₃.


Peng Hu, Yuan-Yuan Gao, Feng-Ping Xiao, Li-Li Zhu, Li-Na Wang, Fen Su and Miao Zhang
Polyhedron 130 (2017) 40

Three lanthanide–nitronyl nitroxide complexes: Syntheses, crystal structures and magnetic properties

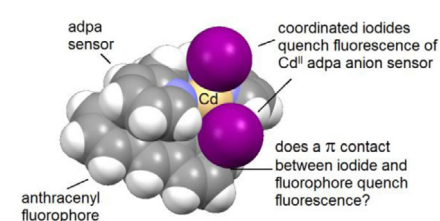
One nitronyl nitroxide radical and its three mononuclear tri-spin compounds have been successfully prepared. The magnetic studies reveal that Tb complex displays frequency-dependent signals at low temperature suggesting that it behaves as SMM.


Joseph W. Nugent, Hyunjung Lee, Joseph H. Reibenspies, Hee-Seung Lee and Robert D. Hancock
Polyhedron 130 (2017) 47

Effects of anion coordination on the fluorescence of a photo-induced electron transfer (PET) sensor complexed with metal ions

The Cd^{II} adpa complex shows increased fluorescence intensity when coordinated to Cl[−], Br[−], SCN[−] and S₂O₃^{2−}, allowing it to act as an anion sensor. Coordination of I[−] causes a strong decrease in fluorescence intensity, which might

be due to formation of an I \cdots C π contact with the fluorophore, in line with studies that show that M \cdots C π contacts can quench fluorescence. Crystal structures of the M^{II}(adpa)₂ complexes (M = Zn, Cd, Hg) show that such I \cdots C and M \cdots C π contacts are not present. Density functional theory (DFT) studies show a structural change in the excited state of the Cd^{II}(adpa)₂ complex, reordering the frontier molecular orbitals. This introduces charge transfer from the fluorophore to the iodine into the S₁ \rightarrow S₀ transition, which becomes forbidden, thus quenching the fluorescence.



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