

Title: Data to support Study of Ligand-Directed Metallation of a Gold Pyrazolate Cluster

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Rights-holder(s): Malcolm A. Halcrow

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Description: Metallation of $[\text{Au}_n(\mu\text{-L})_n]$ ($\text{HL} = 3\text{-[pyrid-2-yl]-5-tertbutyl-1H-pyrazole}$; $n = 3$ or 4) with AgBF_4 yields $[\text{Ag}_2\text{Au}_4(\mu\text{-L})_4][\text{BF}_4]_2$, where two edges of the Au_4 square are spanned by Ag^+ ions coordinated to its pendant pyridyl groups. Treatment of $[\text{Au}_n(\mu\text{-L})_n]$ with $[\text{Cu}(\text{NCMe})_4]\text{PF}_6$ affords a metalloligand helicate $[\text{Au}_2\text{Cu}_2(\mu\text{-L})_4][\text{PF}_6]_2$, *via* oxidation of the copper and partial fragmentation of the cluster.

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Related publication: Smith, Ryan A., Kulmaczewski, Rafal, and Halcrow, Malcolm A. (2023). Ligand-Directed Metallation of a Gold Pyrazolate Cluster. *Inorganic Chemistry*, doi: 10.1021/acs.inorgchem.3c01667.

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2. TERMS OF USE

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3. PROJECT AND FUNDING INFORMATION

Title: Understanding and Engineering Function in Switchable Molecular Crystals

Dates: 2013-2018

Funding organisation: EPSRC

Grant no.: EP/K012576/1

4. CONTENTS

The dataset contains data for this study:

NMR spectra (raw and processed data – *NMR.zip*).

Elemental microanalyses (*microanalysis.zip*).

Electrospray mass spectra (*ESMS.zip*).

X-ray powder diffraction data (measured and simulated – *XRPD.zip*).

X-ray crystallographic data (*crystal.zip*):

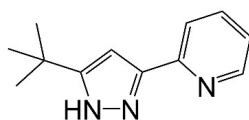
- Structure of **1a** at 120 K (CCDC 2238818)
- Structure of **1b**·xEt₂O at 120 K (CCDC 2238819)
- Structure of **2**·yC₂H₄Cl₂ at 120 K (CCDC 2238820)
- Structure of **3**·zEt₂O at 120 K (CCDC 2238821)

Solution UV/visible absorption and emission spectra (*UVvis.zip*).

5. METHODS

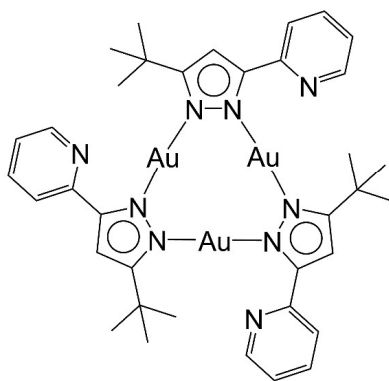
Full details are provided in the related publication, listed above.

Compounds referred to in this dataset



HL

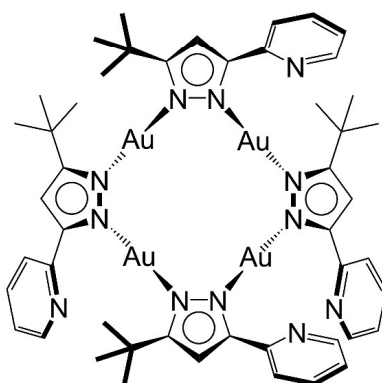
3{5}-(Pyrid-2-yl)-5{3}-(*tert*butyl)pyrazole
 $C_{12}H_{14}N_3$



1a

$[Au_3(\mu-L)_3]$

Tris[3{5}-(pyrid-2-yl)-5{3}-(*tert*butyl)pyrazolato]trigold(I)
 $C_{36}H_{42}Au_3N_9$

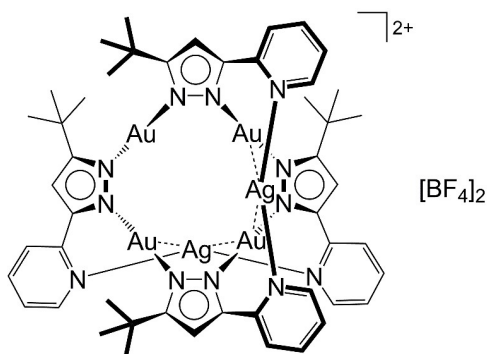


1b

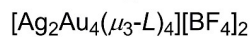
$[Au_4(\mu-L)_4]$

Tetrakis[3{5}-(pyrid-2-yl)-5{3}-(*tert*butyl)pyrazolato]tetragold(I)
 $C_{48}H_{56}Au_4N_{12}$

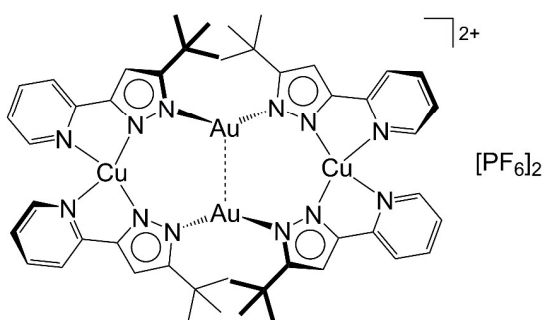
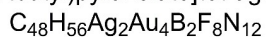
Compounds referred to in this dataset (continued)



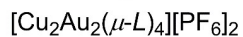
2



Tetrakis[3{5}-(pyrid-2-yl)-5{3}-(*tert*butyl)pyrazolato]tetragold(I)disilver(I) ditetrafluoroborate



3



Tetrakis[3{5}-(pyrid-2-yl)-5{3}-(*tert*butyl)pyrazolato]digold(I)dicopper(II) bis[hexafluorophosphate]

