

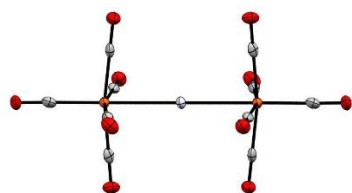
Seminar

Ligand-Stabilised Complexes from the Computational Perspective

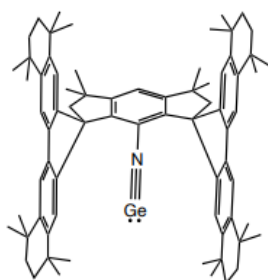
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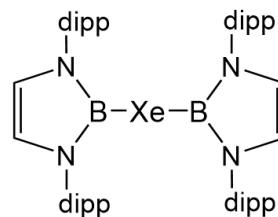
Both bonding and oxidation state are fuzzy concepts in Chemistry. The IUPAC definition of oxidation state using the ionic approximation is not very helpful in many cases. In this lecture, I will present a few case studies to show how computational tools play an important, complementary role to experiments in understanding the bonding and oxidation state of an element in ligand-stabilised complexes. I will also talk about bulky ligand-stabilised noble gas complexes.



$\text{Hg}[\text{Fe}(\text{CO})_5]_2^{2+}$



germa-isonitrile



Bis(diazaborolyl) xenon

Keywords: Ligand stabilisation; Dative bonding; Oxidation state; Zero-valent element.

Friday, Sep 18th 2026

14:30 Hrs (Tea / Coffee 14:15 Hrs)

Auditorium, TIFRH