



Synthesis and reactivity of low-valent Zn^I - Zn^I complexes: a combined DFT and experimental study

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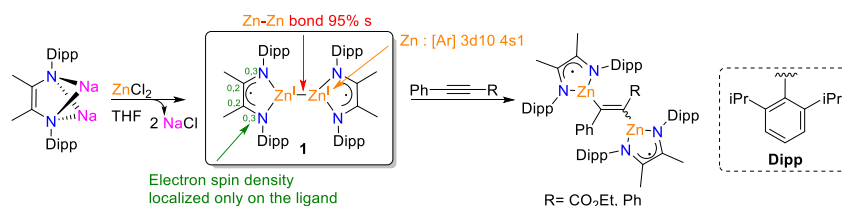
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Main-group organometallic compounds bearing a metal-metal M-M bonds are well known in the literature in the case of group 13 metals, such as boron or aluminum. More particularly di-boron compounds, which are easy to handle and relatively stable compounds, are used in a varied applications because of their ability to achieve 1,2-diboration reactions with unsaturated compounds.^[1]

Since the first discovery of $Cp^*_2Zn_2$,^[2] some low valent Zn^I - Zn^I complexes presenting an unusual formal oxidation state have been disclosed. A limited number of LZn - ZnL species have been synthesized and characterized by experimental and theoretical Zn-Zn bonding analysis.^[3] Indeed, as those species are highly sensitive to moisture and oxygen, their synthesis and the study of their reactivity are challenging.

In this communication, we will present a combined experimental and DFT theoretical investigations on the synthesis and reactivity of the low valent Zn^I - Zn^I species **1**, where each zinc center is bearing a radical α -diimine ligand.^[4] The formation of this Zn-Zn di-radical complex was studied by DFT calculations and the intermediates of the mechanism were characterized using Natural Bonding Orbitals.

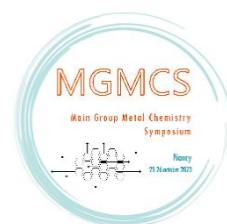
The reduction process is exergonic but as it implies radical species as open shell system, it is necessary to use a representative model, method and chemical environment, in particular the solvent, in adequation with the electronic structure of the species. The addition onto alkynes was theoretically explored using a concerted mechanism in only one step, suggesting the feasibility of such reactivity. In parallel, experimental work is ongoing to prove such an *in silico* discovery.



Scheme 1: Synthesis and proposed reactivity of LZn-ZnL complex **1**.

References :

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