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# Electronic structure and excited state properties of iron carbene photosensitizers - a combined X-ray absorption and quantum chemical investigation

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**Abstract**

The electronic structure and excited state properties of a series of iron carbene photosensitizers are elucidated through a combination of X-ray absorption measurements and density functional theory calculations. The X-ray absorption spectra are discussed with regard to the unusual bonding environment in these carbene complexes, highlighting the difference between ferrous and ferric carbene complexes. The valence electronic structure of the core excited $Fe^{III} - 3d^5$ complex is predicted by calculating the properties of a $Co^{III} - 3d^6$ carbene complex using the Z+1 approximation. Insight is gained into the potential of sigma-donating ligands as strategy to tune properties for light harvesting applications.

## Introduction

Favorable excited state properties of many transition metal complexes have made them popular choices as photosensitizers in several applications including solar energy conversion, light-emitters, and photodynamic therapy [1]. Strategies involving metal-to-ligand charge transfer (MLCT) excitations and associated long-lived MLCT-excited states in $Ru^{II}(bpy)_3$ and other octahedral $d^6$ complexes of several 2nd and 3rd row transition metals including $Os^{II}$, $Rh^{III}$, and $Ir^{III}$ have been particularly successful, and the photophysics and photochemistry of many complexes of these metals have been thoroughly investigated in the last several decades [2].

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