Exploring New Tripodal *N*-Heterocyclic Carbene Ligands Towards High- and Low-Valent Iron Complexes

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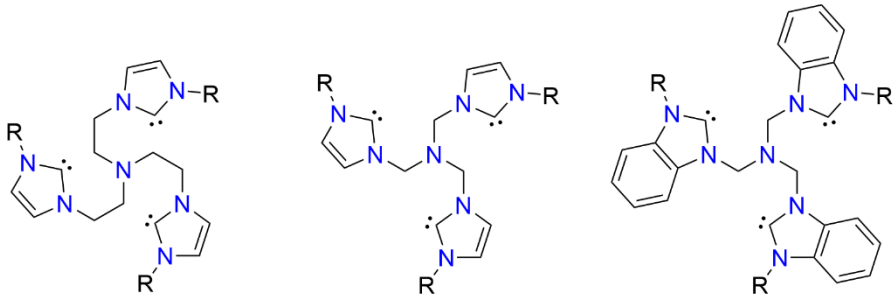
High-valent complexes of iron with terminal imido, nitrido and oxo ligands have been identified as active intermediates in both enzymatic and industrial catalytic processes of great interest, including the synthesis of ammonia.[1] The understanding of their molecular and electronic structures and reactivity, by means of isolating and studying well-defined model compounds, remains a challenging research topic. Towards that end, the utilization of tailored multidentate ligands (Scheme 1) with *N*-heterocyclic carbene (NHC) donors has been a milestone, allowing the structural characterization of once though to be elusive high-valent iron complexes, and the recent spectroscopic observation of an iron(VII) nitride.[2,3] In this work, we have employed different carbene donors to replace the classic imidazol-2-ylidenes and construct the new *tris*-carbene ligand scaffolds TBIMN^{R} (R = Mes, CH_2Cy). Their coordination to iron centers in different oxidation states has been probed following various synthetic strategies, and preliminary spectroscopic results on the characterization of the resulting complexes are reported.



Scheme 1: Nitrogen-anchored tripodal chelates established in metal coordination chemistry.

References: 1. J. Hohenberger, K. Ray, K. Meyer, *Nat. Commun.* 3 (**2012**) 720.
2. M. Keilwerth, L. Grunwald, W. Mao, F. W. Heinemann, J. Sutter, E. Bill, K. Meyer, *J. Am. Chem. Soc.* 143 (**2021**) 1458-1465.
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