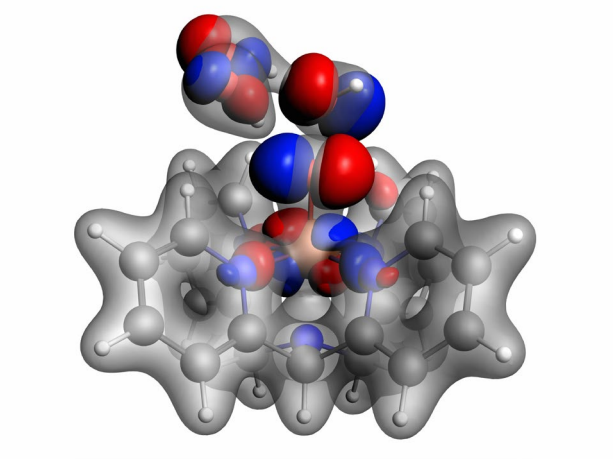
Reactive high-valent transition-metal complexes

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Oxidation processes of hydrocarbons in a selective, efficient and environment-friendly manner remains one of the major challenges at present today.[1] The majority of these studies is based on experiment, and computational chemistry plays sometimes an important role,[2-3] in giving a description of e.g. spectroscopy or transition states to lead to a deeper understanding of what is going on. This is in particular true for the influence of the spin state on reactivity.[3] Here I will give an overview of the spin-state consistent tools needed[2] and how these can be used for finding the pathways for the oxidation reactions of high-valent metal-oxo (Fe^{IV}=O, Ni^{IV}=O) species,[4-6] based on a consistent and accurate computational description of IR, Raman, UV-Vis, and Mössbauer spectroscopy. Furthermore, I will show how the barriers[5] can be decomposed in terms of ligand structure, orbital patterns and steric vs. electronic interactions.



Transition-metal oxygen complex

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