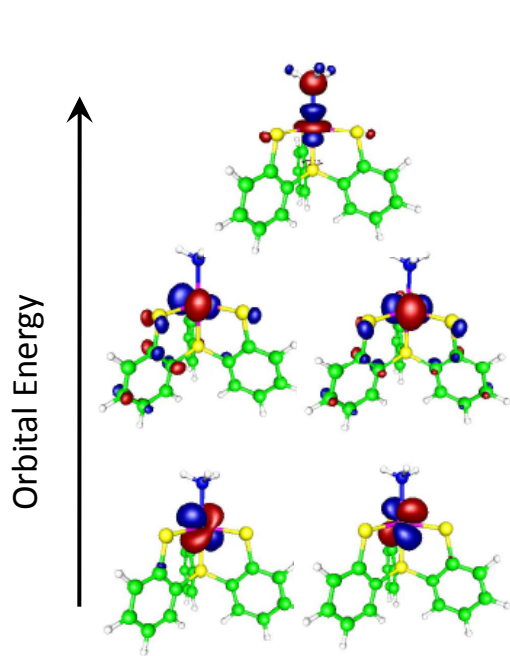




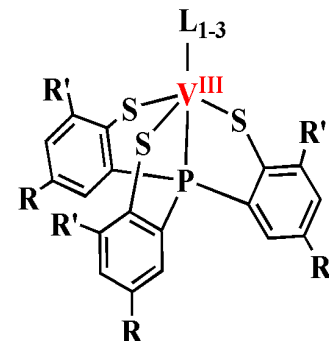
Vanadium(III)-Trithiolato Complexes Relevant to Functional Models of Vanadium Nitrogenase: Synthesis and Electronic Structure Investigations by HFEPR Coupled to Quantum Chemical Computations



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This project, which involved scientists in Europe, Asia, and North America, was directed towards the synthesis and characterization of a series of complexes of vanadium(III). The V(III) ion was coordinated by a quadridentate ligand with one phosphorus and three sulfur atoms, with variation in (an) additional ligand(s) providing the members of the series (see structure at right). Vanadium with sulfur coordination is thought to be present in the active site of the V-nitrogenase enzyme, which converts atmospheric nitrogen to ammonia. The combination of structural characterization by x-ray crystallography and spectroscopic characterization by high-frequency and -field electron paramagnetic resonance (HFEPR) allowed the application of the latest computational methods to provide a complete picture of the electronic structure of these complexes (see molecular orbital (MO) diagram at left).



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