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Organometallic Chemistry of Methanogenesis: Modeling the Fe(CO)₂ GP Cofactor in the Hmd

With this grant we have made breakthroughs in modeling the active site of the “third hydrogenase,” Hmd, which consists of a Fe(CO)₂ center bound to a thiolate and the nitrogen of the guanylylpyridinol (GP) cofactor. The advances provide new insights that are revealing new catalytic sites. Acyl ligands are rarely encountered in bioinorganic chemistry, and their coexistence with thiolato ligands defines a novel platform from the perspective of homogeneous catalysis. The new structural information – i.e. Fe(SR)(N-donor)(CO)₂(acyl) – provided sufficient information to enable the design of a first generation model for this active site.

