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Copying Nature: Chemical Synthesis of a Possible Catalytic Compound for H₂ Generation

The catalytic active iron-sulfur cluster of FeFe-hydrogenase can product hydrogen gas close to 10,000 molecules of H₂ per second per enzyme molecule. None of the currently known synthetic iron-sulfur cluster can even come close to this reactivity. A recent computer modeling study indicated that there is a new compound that may be able to meet this record activity. I propose to make this compound. The innovative part of the work is the attachment of a unsaturated ligand (olefinic and/or allylic) to the Fe₂S₂(CO)₆ 'parent' compound. I will use infrared and visible/ultraviolet spectroscopic techniques to characterize the compounds I will make. Using analytical techniques I will determine the reduction potential and protonation constant of the new compounds and will compare to other iron-sulfur compounds. The proposed work will be carried out with the help of a graduate student and with the guidance of faculty mentor, who has already secured funding for material and supplies related expenses.