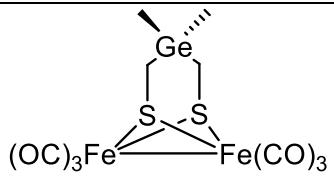
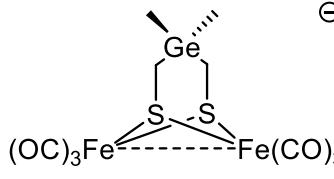
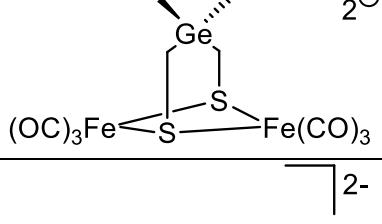
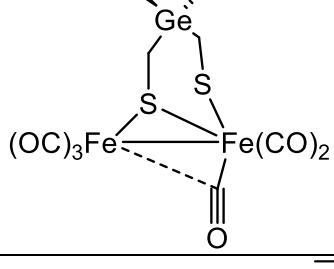
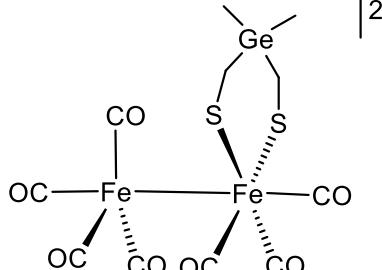


Supplementary Materials: Electrochemical and Computational Insights into the Reduction of $[\text{Fe}_2(\text{CO})_6\{\mu\text{-}(\text{SCH}_2)_2\text{GeMe}_2\}]$ Hydrogenase H-Cluster Mimic

Hassan Abul-Futouh, Wolfgang Imhof, Wolfgang Weigand and Laith R. Almazahreh

Table S1. Calculated energies and numbers of imaginary frequencies.

| Compound | Structure | HF [a.u.] | NImag |
|--------------------------------|---|--------------|-------|
| 1 |  | -1886.826914 | 0 |
| 1⁻ |  | -1886.952107 | 0 |
| 1²⁻ |  | -1887.039823 | 0 |
| 1²⁻ (isomer) |  | -1887.041611 | 0 |
| P1 |  | -2000.404315 | 0 |
| CO | CO | -113.363848 | 0 |