Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary information for the paper:

Electrocatalytic dihydrogen evolution mechanism of $[Fe_2(CO)_4(\kappa^2\text{-}Ph_2PCH_2CH_2PPh_2)(\mu\text{-}S(CH_2)_3S)]$ and related models of the [FeFe]-hydrogenases active site: a DFT investigation

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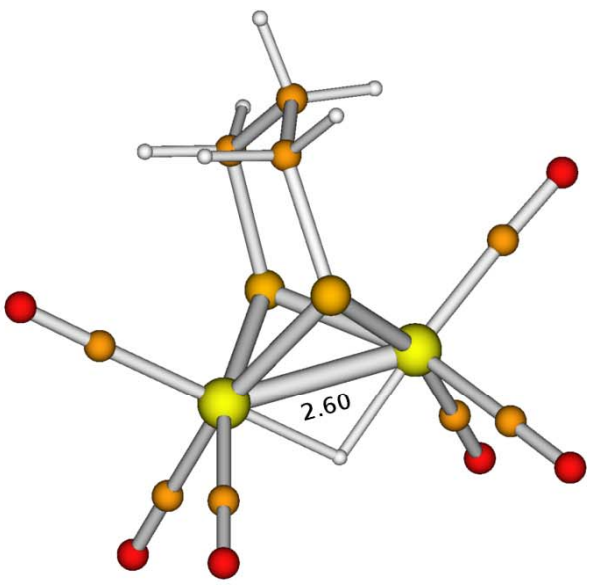
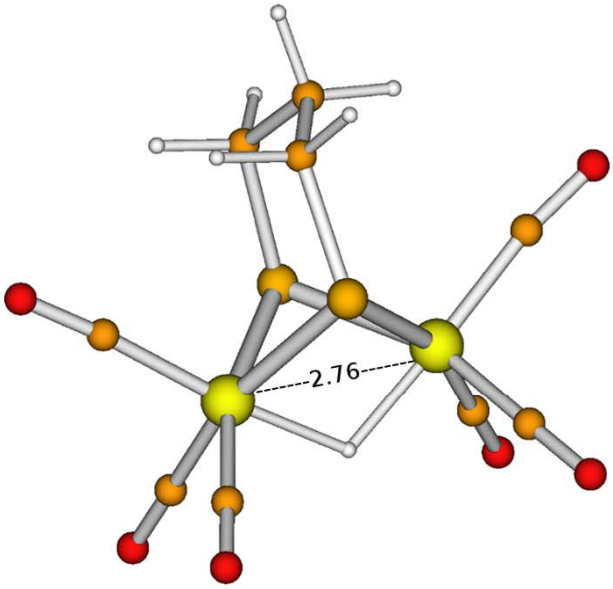
Figure S1. Optimized geometries of monoprotonated hexacarbonyl complexes. All distances in Å

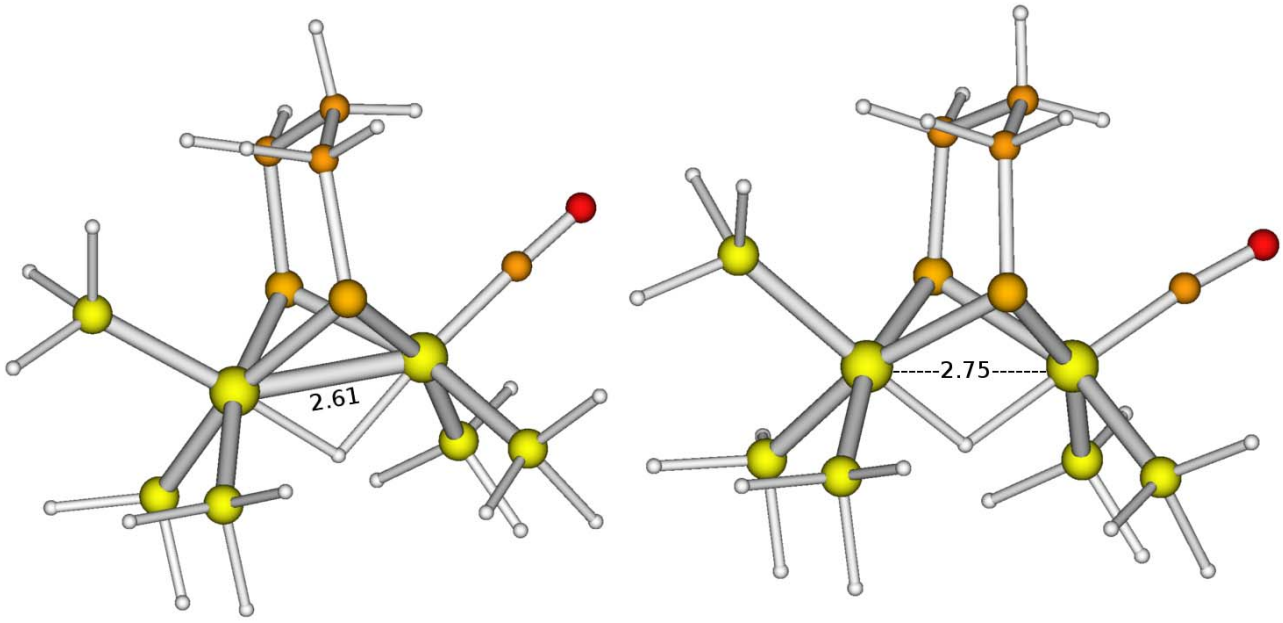


$[1\text{-}H]^{+}_{\{Fe(H)Fe\}}$



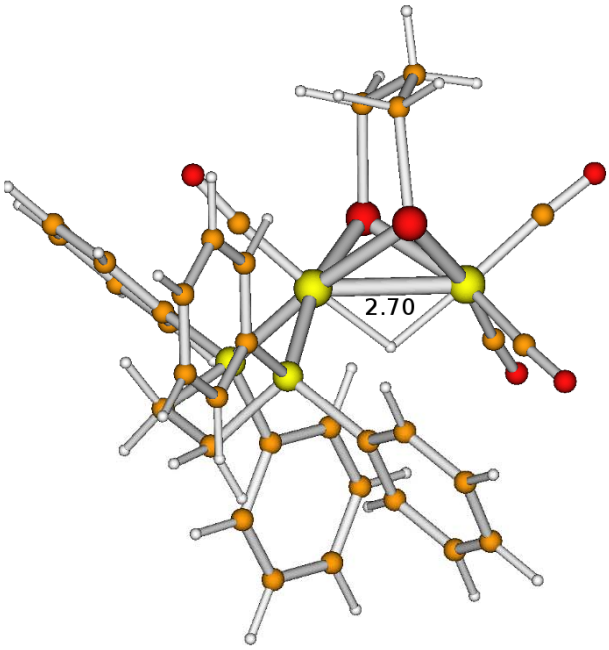
$[1\text{-}H(a)]_{\{Fe(H)Fe\}}$

Figure S2. Optimized geometries of monoprotonated pentaphosphine complexes. All distances in Å

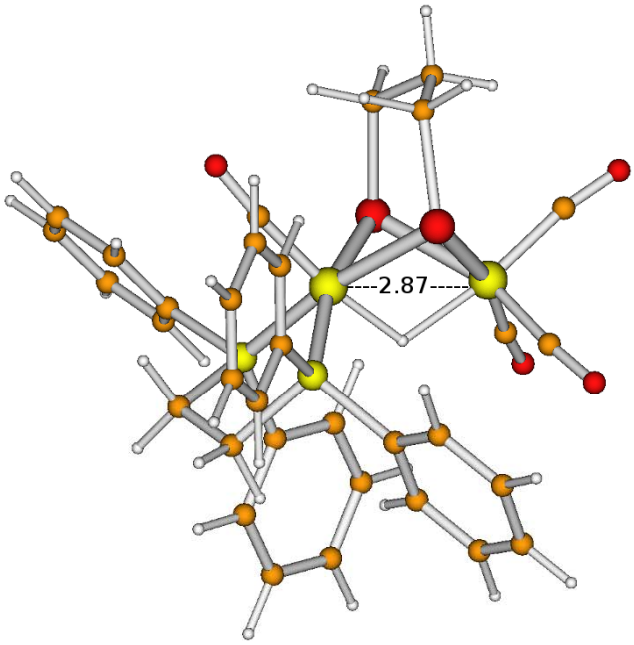


$[3\text{-}H]^{+}_{\{Fe(H)Fe\}}$ $[3\text{-}H(a)]_{\{Fe(H)Fe\}}$

Figure S3. Optimized geometries of monoprotonated complexes including dppe and propanediselenolate (pds). All distances in Å



$[^{pds}2\text{-}H]^{+}_{\{Fe(H)Fe\}}$



$[^{pds}2\text{-}H(a)]_{\{Fe(H)Fe\}}$

Figure S4. Optimized geometries of selected diprotonated cationic complexes. All distances in Å.

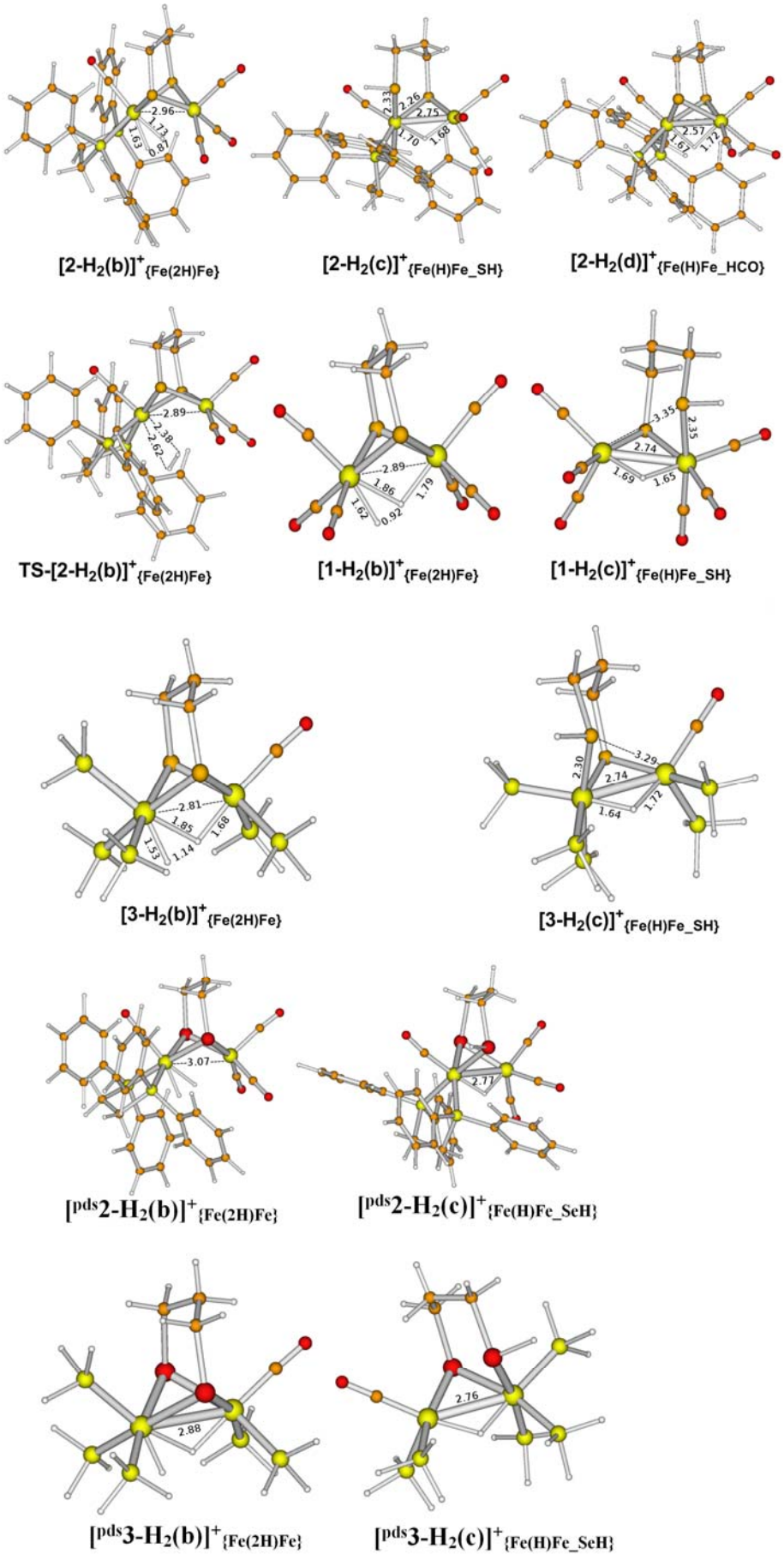


Figure S5. Optimized geometries of selected diprotonated neutral complexes. All distances in Å.

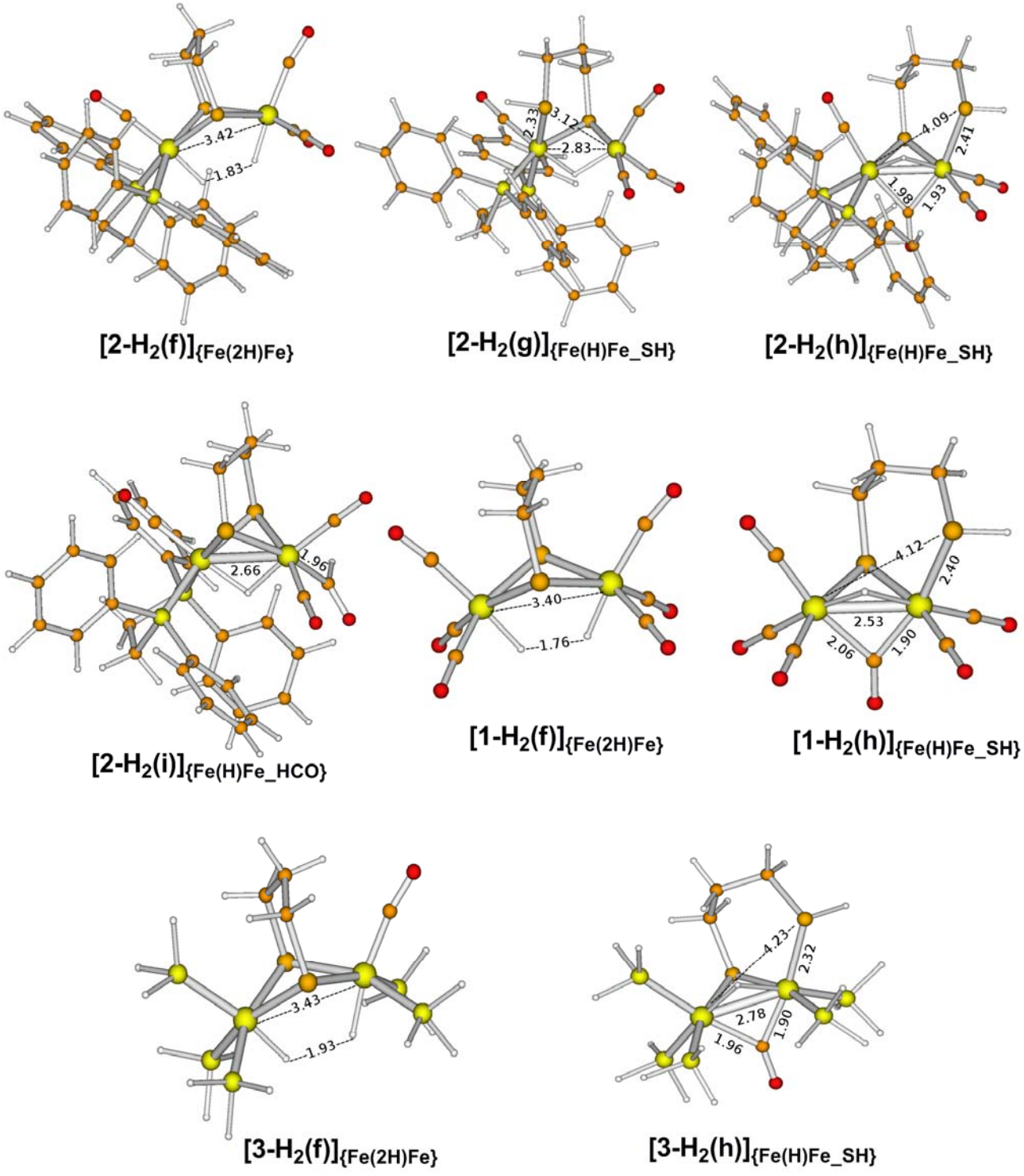


Figure S6. Optimized geometries of selected diprotonated anionic complexes. All distances in Å.

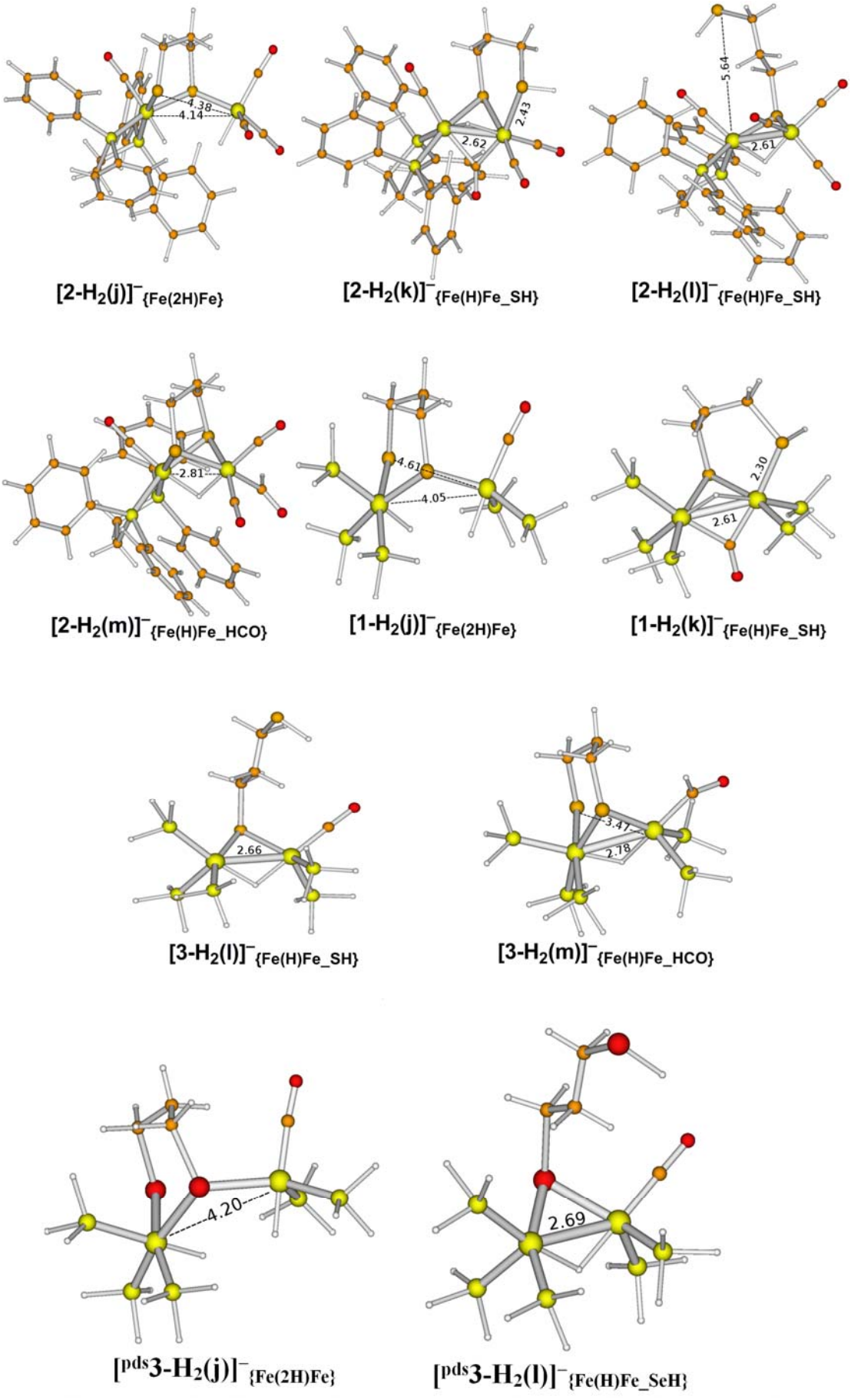


Figure S7. Optimized geometries of selected triprotonated cationic complexes. All distances in Å.

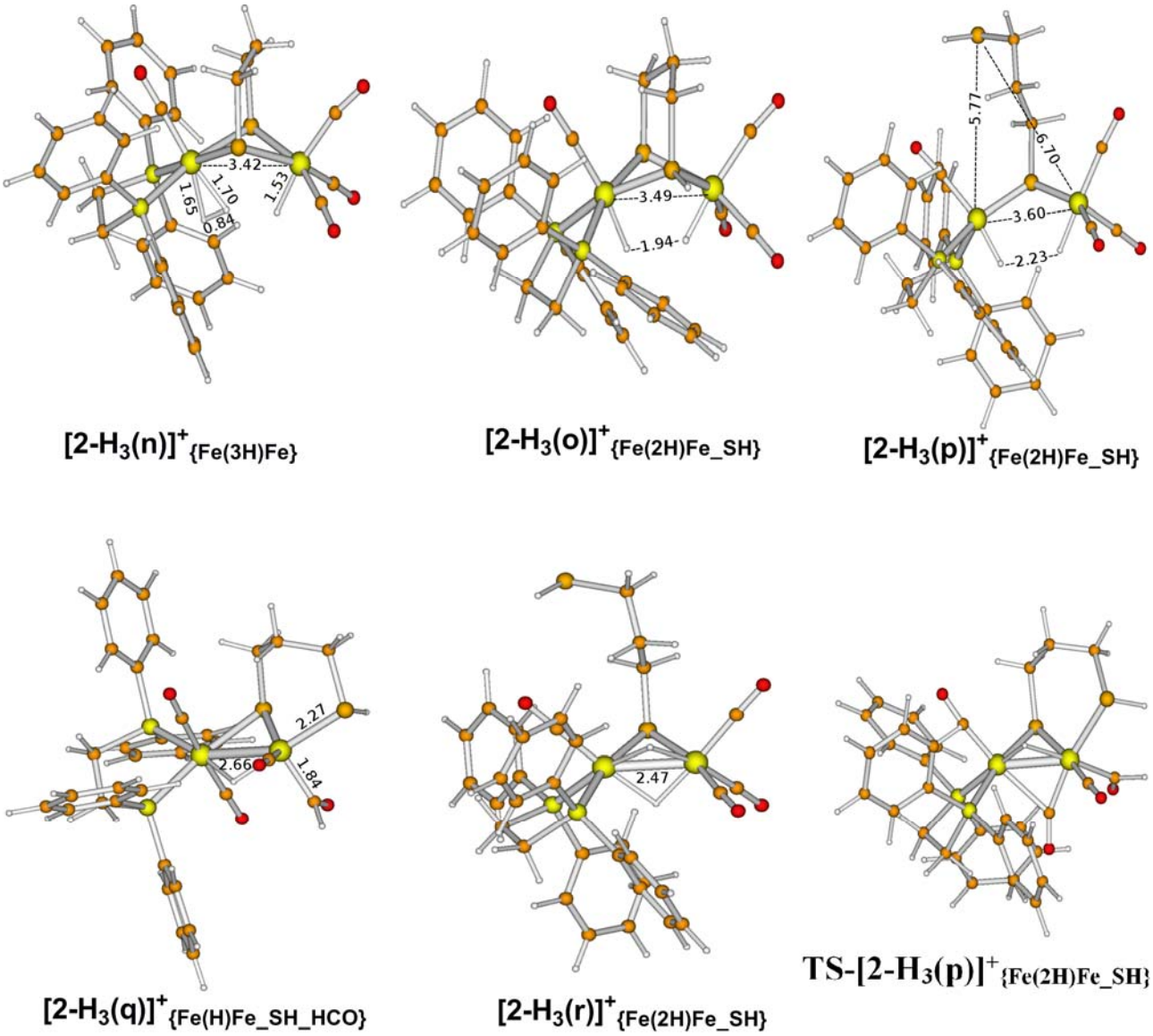


Figure S8. Optimized geometries of selected triprotonated neutral complexes. All distances in Å.