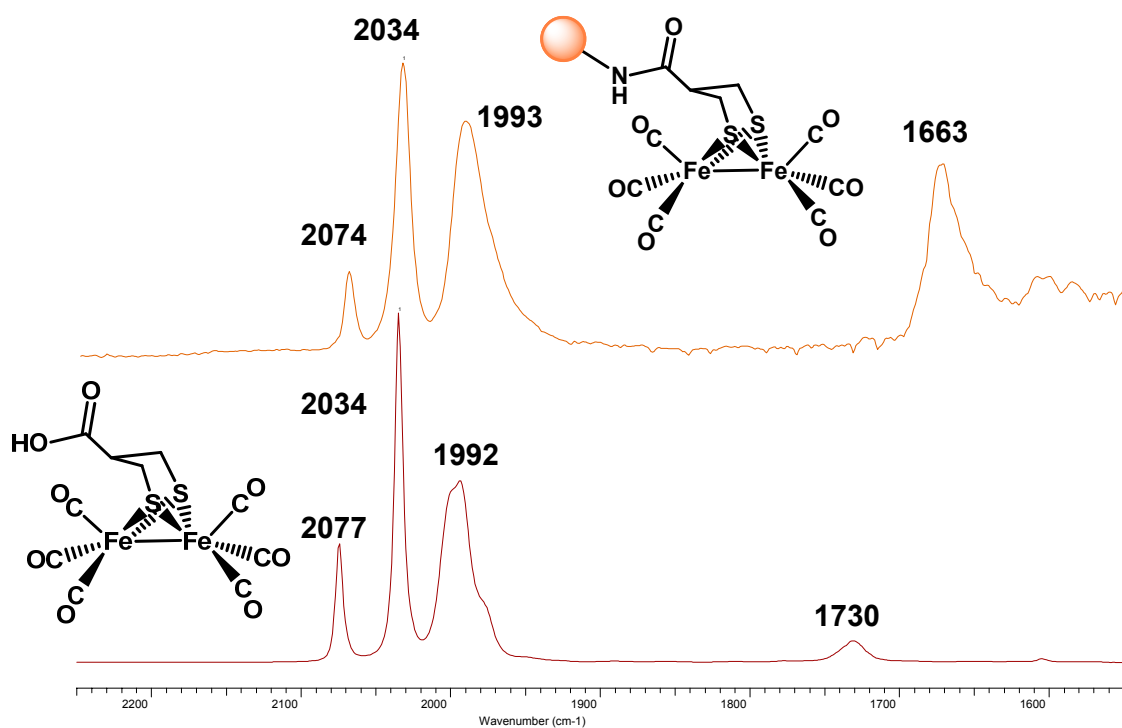


Supplementary Information

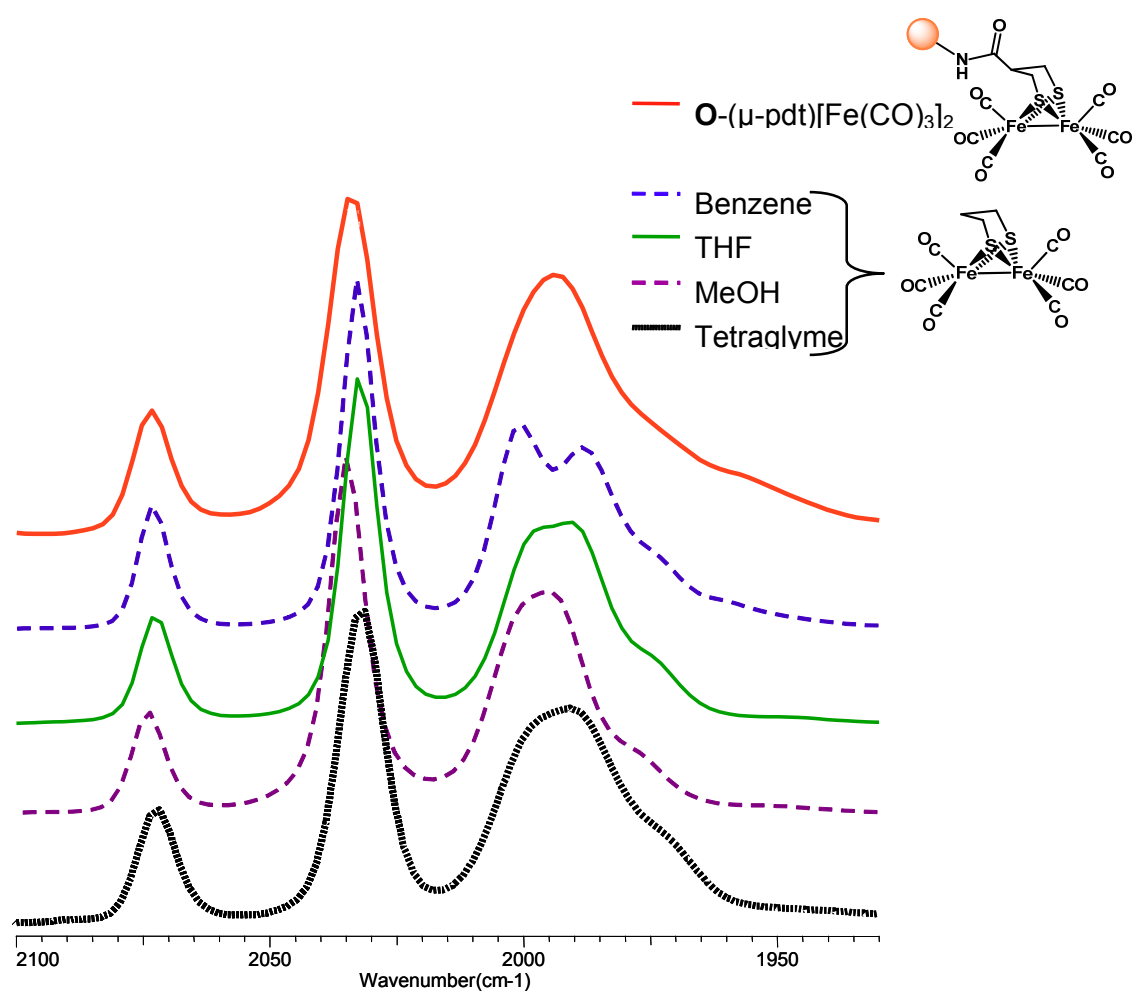
Resin-bound models of the [FeFe]-hydrogenase enzyme active site and studies of their reactivity

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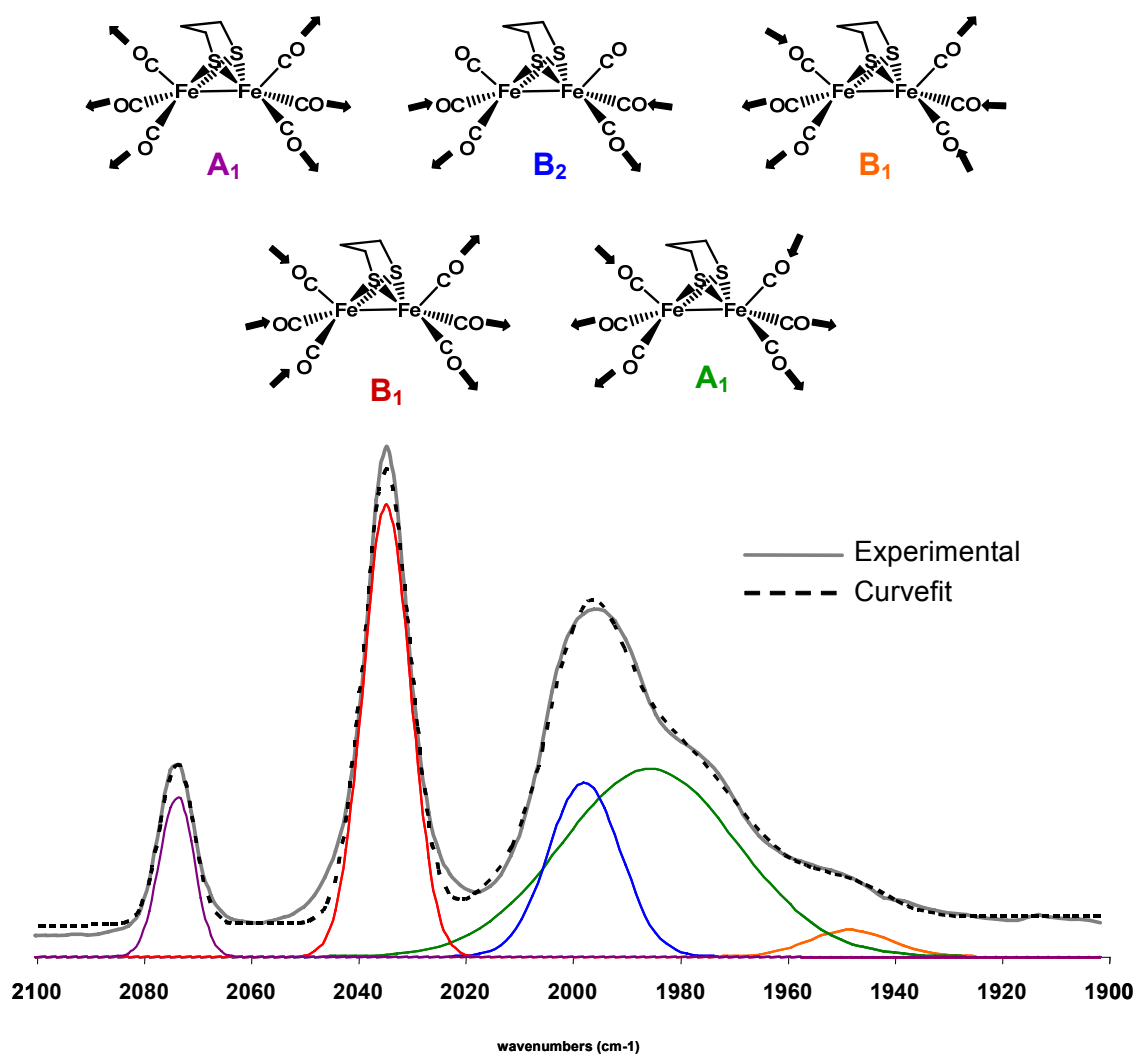
- S1.** Comparison of infrared spectra of **O-am-[A]** (ATR-FTIR, top) and **[A]** (THF solution FTIR, bottom).
- S2.** Overlay of infrared spectra of **O-am-[A]** and $(\mu\text{-pdt})[\text{Fe}(\text{CO})_3]_2$ dissolved in polar to non-polar solvents.
- S3.** Assignment of vibrational modes for the $(\mu\text{-pdt})[\text{Fe}(\text{CO})_3]_2$ molecule (top) and deconvoluted IR spectrum of **O-am-[A]** with the resulting fitted spectrum (---) and the experimental ATR-FTIR spectrum (—) overlaid (bottom).



S1. Comparison of infrared spectra of **O-am-[A]** (ATR-FTIR, top) and **[A]** (THF solution FTIR, bottom).



S2. Overlay of infrared spectra of **O-am-[A]** and $(\mu\text{-pdt})[\text{Fe}(\text{CO})_3]_2$ dissolved in polar to non-polar solvents.



S3. Assignment of vibrational modes for the $(\mu\text{-pdt})[\text{Fe}(\text{CO})_3]_2$ molecule (top) and deconvoluted IR spectrum of **O-am-[A]** with the resulting fitted spectrum (---) and the experimental ATR-FTIR spectrum (—) overlaid (bottom).