

Supporting Information for:

Mechanistic Aspects of the Protonation [FeFe]- Hydrogenase Subsite Analogues

Aušra Jablonskytė, Joseph A. Wright and Christopher J. Pickett*

*Energy Materials Laboratory, School of Chemistry, University of East
Anglia, Norwich NR4 7TJ, United Kingdom*

c.pickett@uea.ac.uk

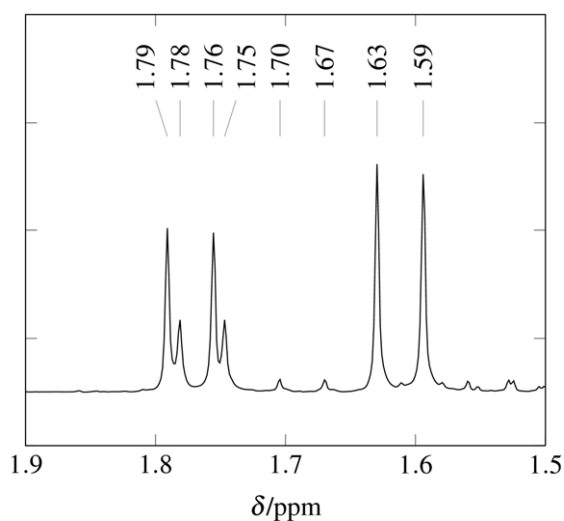


Figure S1. ^1H spectrum of reaction of **3** with $\text{HBF}_4\cdot\text{Et}_2\text{O}$ in $d_3\text{-MeCN}$ after approximately six minutes. $[\mathbf{3}]_0$ 40 mM, $[\text{HBF}_4\cdot\text{Et}_2\text{O}]_0$ 300 mM. Region for phosphorous-bound methyl groups.

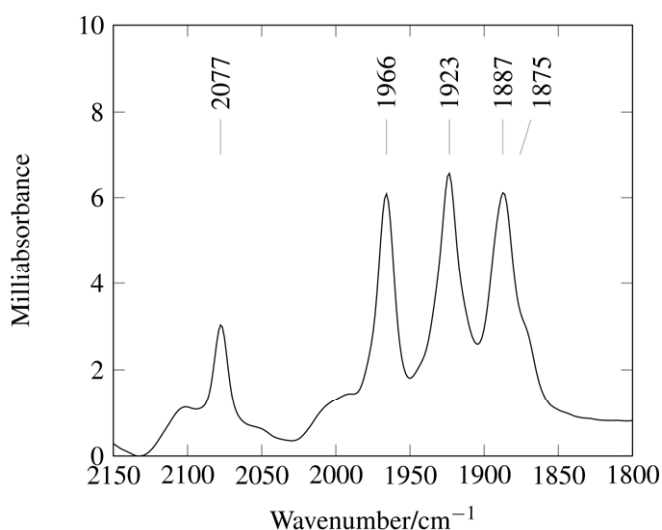


Figure S2. IR spectrum of $(\text{NEt}_4)[\text{Fe}_2(\text{edt})(\text{CO})_4(\text{CN})_2]$ in MeCN.

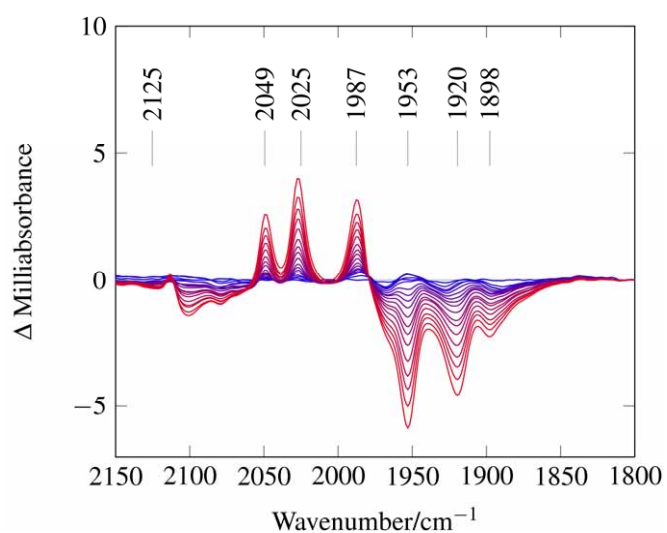


Figure S3. Difference spectrum for protonation of $(\text{NEt}_4)[\text{Fe}_2(\text{edt})(\text{CO})_4(\text{CN})_2]$ as observed by stop-flow IR, in the time range 3.2 s (blue) to 157 s (red) *versus* a scan at 2.9 s.