Supporting Information to "Encapsulating [FeFe]-hydrogenase model compounds in peptide hydrogels dramatically modifies stability and photochemistry"

Pim W. J. M. Frederix,[1,2] Rafal Kania,[1] Joseph A. Wright,[3] Dimitrios A. Lamprou,[4] Rein V. Ulijn,[2]* Christopher J. Pickett[3]* and Neil T. Hunt[1]*

Full reference 48:

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, *Gaussian 03 Revision C.02*.

Figure S1. Comparison between a fresh (2 hours) and 13 day-old gel sample containing (μ-$S(CH_2)_3S)Fe_2(CO)_4(PMe_3)_2$

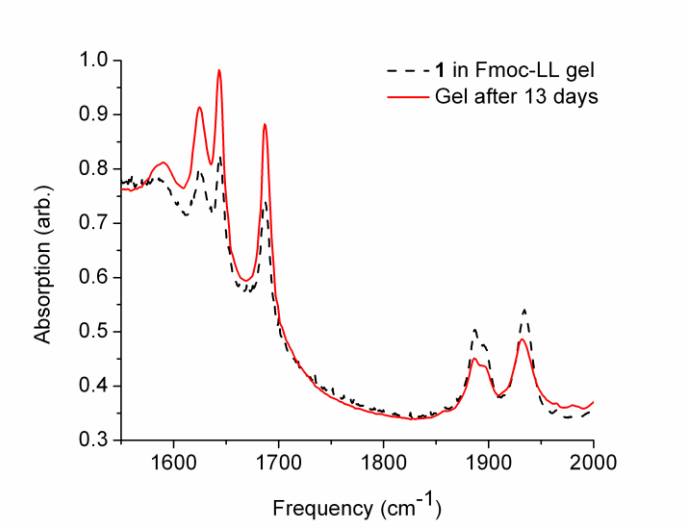

Figure S2. Comparison of FTIR spectra for (μ-S(CH$_2$)$_3$S)Fe$_2$(CO)$_4$(PMe$_3$)$_2$ in the gel phase, in the pre-gel solution (without Fmoc-LL gelator) and the gel without the metal carbonyl. Dramatic line broadening is observed for the carbonyl stretch region in the pre-gel solution. However, this solution is unstable and precipitates out completely within 20 minutes of preparation by sonication.

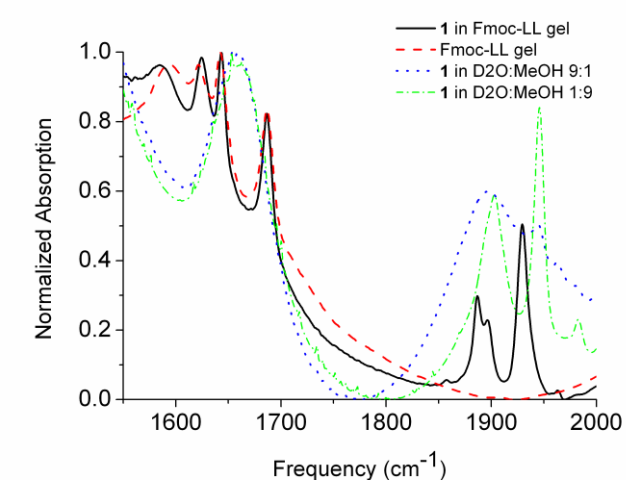

Figure S3. Peak heights in the amide I (~1600-1700 cm^{-1}) and CO stretch region (~1850-2050 cm^{-1}) of the IR spectrum for (μ-$S(CH_2)_3S)Fe_2(CO)_4(PMe_3)_2$ in the gel phase. The decrease in the CO region occurs at a different temperature from the decrease in the amide I region. The peak at 1590 cm^{-1} is attributed to COO^- absorption from the deprotonated C-termini of Fmoc-LL.

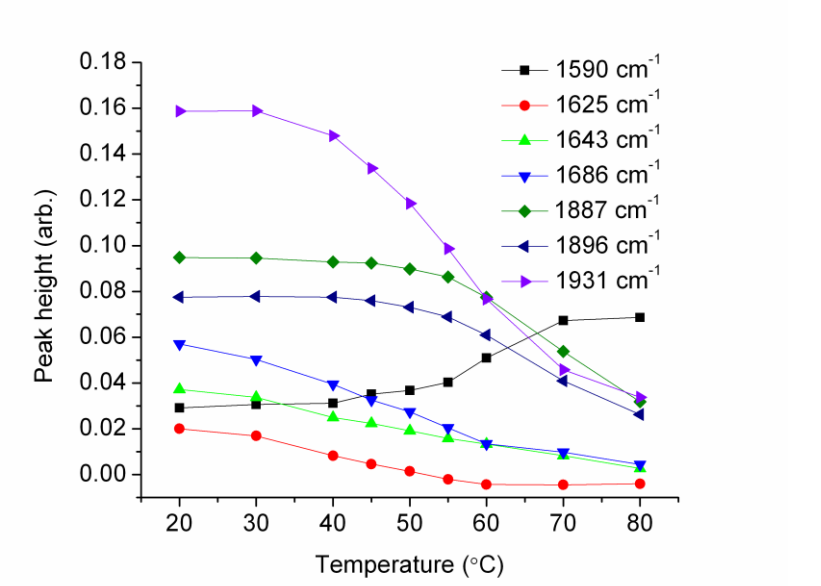

Figure S4. Fluorescence emission spectra of an Fmoc-LL hydrogel at various temperatures. The dashed line represents the emission in methanol at 20 °C. The inset shows the intensity at 386 nm as function of temperature.