

Supporting Information

Naked Five-coordinate Fe^{III}(NO) Porphyrin Complexes: Vibrational and Reactivity Features

Francesco Lanucara,^{†,‡} Barbara Chiavarino,[†] Maria Elisa Crestoni,[†] Debora Scuderi,[§] Rajeev K. Sinha,^{§,#} Philippe Maître,^{*,§} and Simonetta Fornarini,^{*,†}

Dipartimento di Chimica e Tecnologie del Farmaco, Università di Roma “La Sapienza”, P.le A. Moro 5, I-00185, Roma (Italy) and Université Paris Sud - Laboratoire de Chimie Physique - UMR8000 CNRS Faculté des Sciences - Bâtiment 350 - 91405 Orsay Cedex (France)
E-mail: simonetta.fornarini@uniroma1.it; philippe.maitre@u-psud.fr

[†] Università di Roma “La Sapienza”

[§] Université Paris Sud

[‡] Present address: School of Chemistry, University of Manchester, Manchester Interdisciplinary Biocentre, 131 Princess Street, Manchester M1 7ND (UK)

[#] Present address: Department of Chemistry and Biochemistry University of Bern, Freistrasse 3, CH-3012 Bern (Switzerland)

Complete reference 29

Figures S1-S5

Full citation for Reference 29:

Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, **2004**.

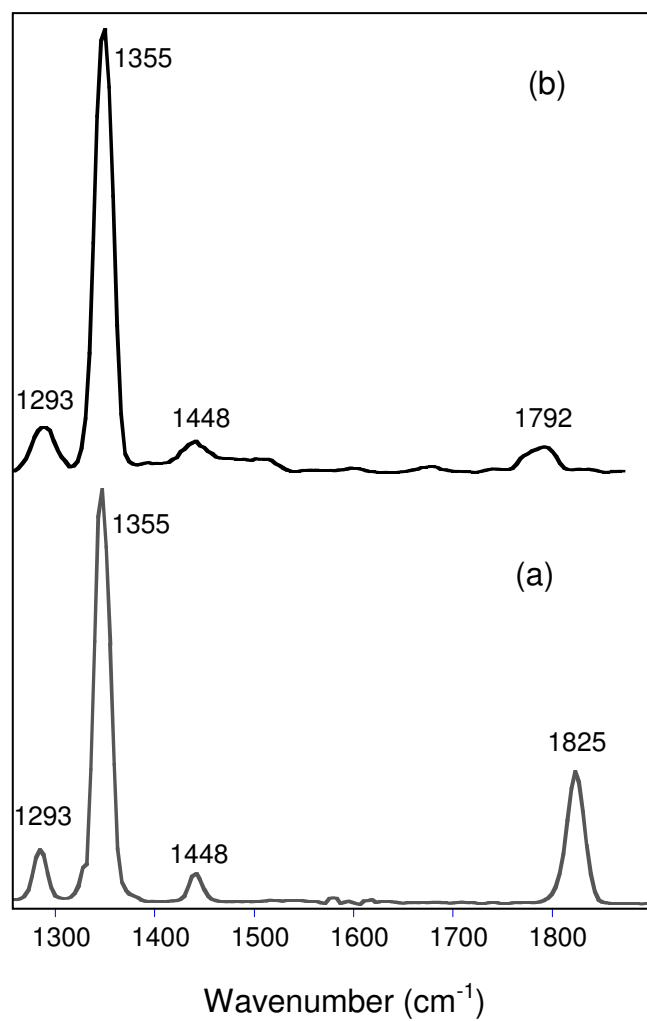


Figure S1. IRMPD spectrum of unlabelled $[\text{Fe}(\text{TPP})(\text{NO})]^+$ (a) and of the $[\text{Fe}(\text{TPP})(^{15}\text{NO})]^+$ complex (b).

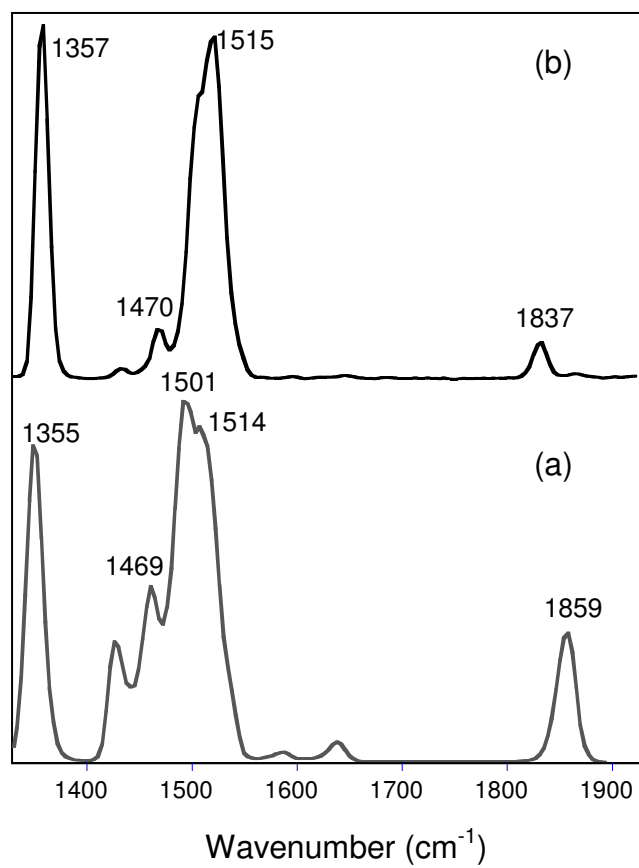


Figure S2. IRMPD spectrum of unlabelled $[\text{Fe}(\text{TPFPP})(\text{NO})]^+$ (a) and of the $[\text{Fe}(\text{TPFPP})(^{15}\text{NO})]^+$ complex (b).

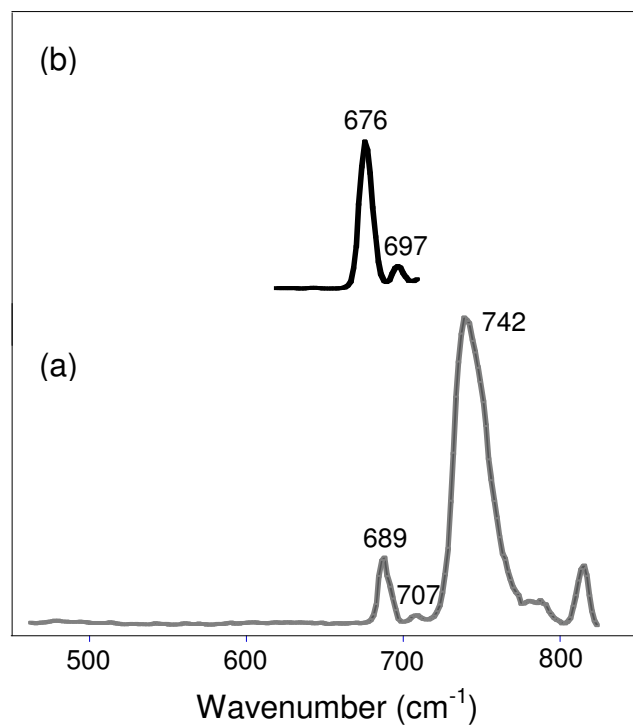


Figure S3. IRMPD spectrum of unlabelled $[\text{Fe}(\text{TPFPP})(\text{NO})]^+$ (a) in the 450-850 cm^{-1} region and of the $[\text{Fe}(\text{TPFPP})(^{15}\text{NO})]^+$ complex (b) in the 620-710 cm^{-1} range.

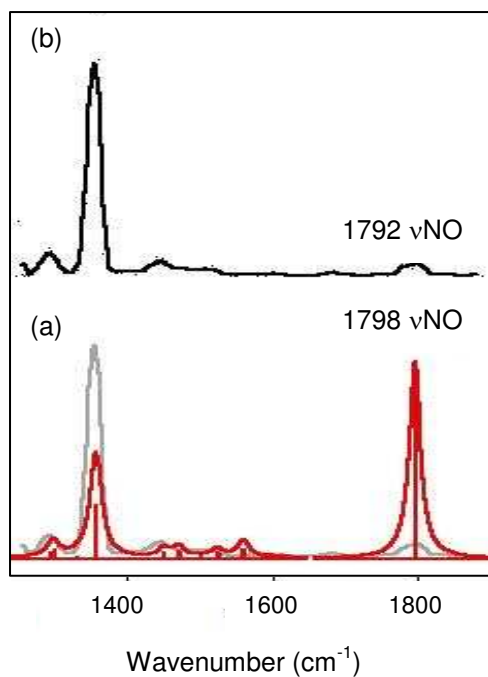


Figure S4. Calculated IR spectrum of the $[\text{Fe}(\text{TPP})(^{15}\text{NO})]^+$ complex (a) and experimental IRMPD spectrum (b).

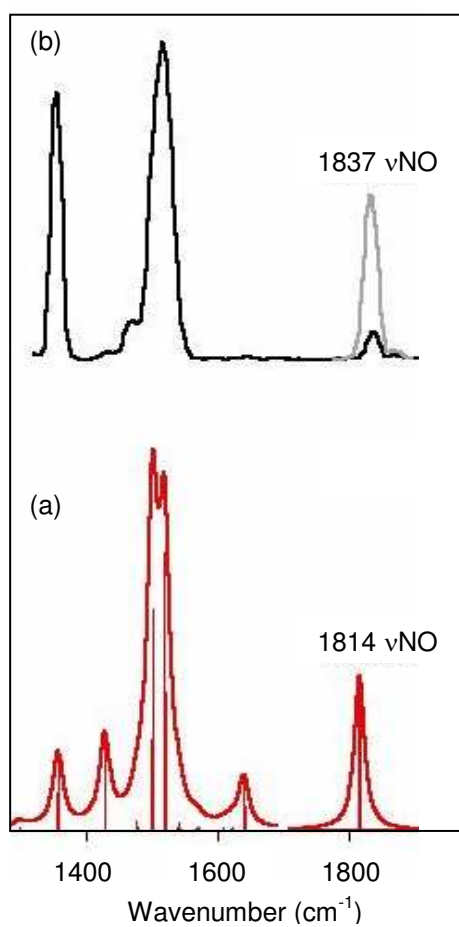


Figure S5. Calculated IR spectrum of the $[\text{Fe}(\text{TPFPP})(^{15}\text{NO})]^+$ complex (a) and experimental IRMPD spectrum (b).