

Supporting Information

Rational Tuning of the Thiolate Donor in Model Complexes of Superoxide Reductase: Direct Evidence for a Trans Influence in Fe^{III}-OOR Complexes

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CIF files for **2**, **3**, **4** and **5**

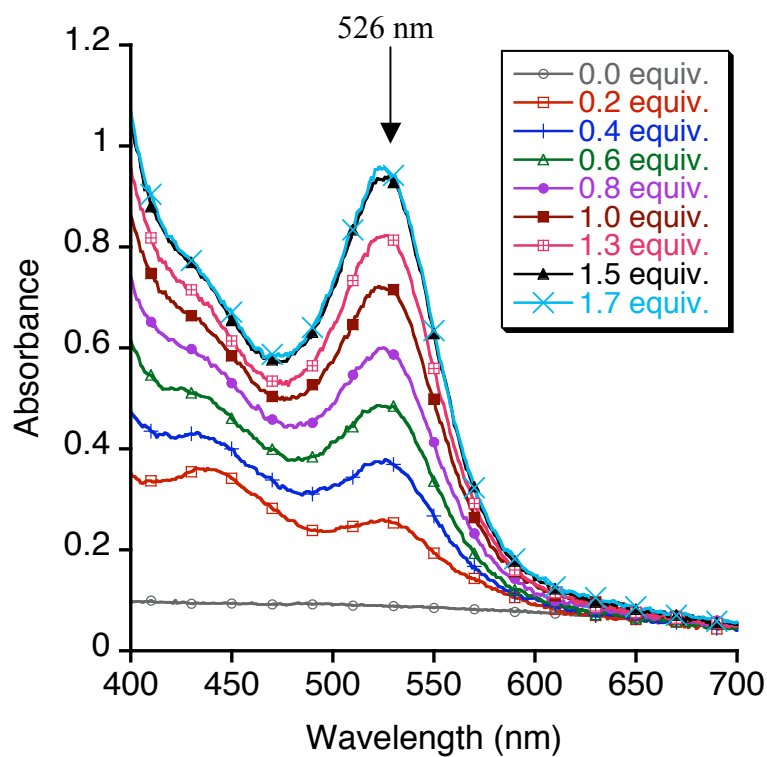


Figure S1: UV-vis spectra of the reaction of $[\text{Fe}^{\text{II}}([\text{15}] \text{aneN}_4)(\text{SPh})](\text{BF}_4)$ with ${}^t\text{BuOOH}$ (stock solution in *n*-decane) (0 – 1.7 equiv) in CH_2Cl_2 at $-78\text{ }^\circ\text{C}$. The reaction was allowed to stir after each addition of ${}^t\text{BuOOH}$ until no further change in the absorption at 526 nm was observed.

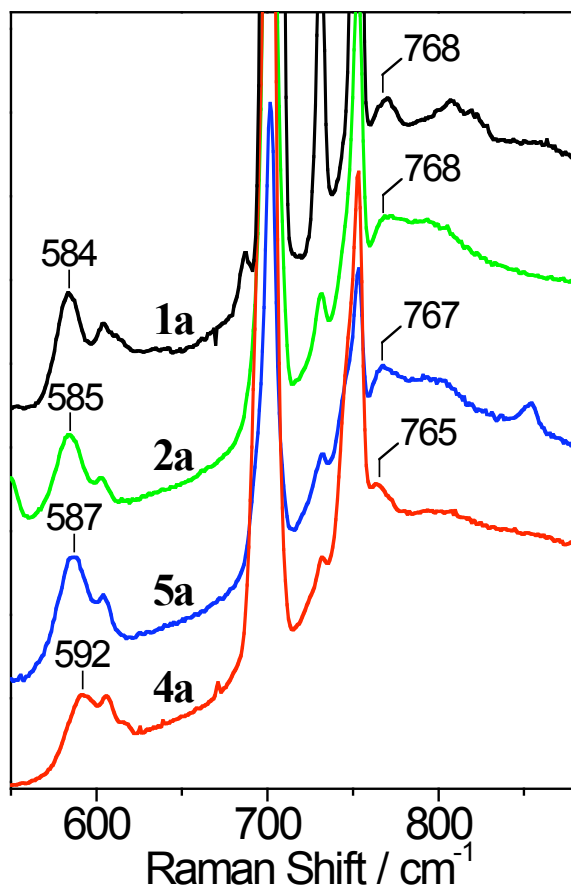


Figure S2. RR spectra of $[\text{Fe}^{\text{III}}([\text{15}]\text{aneN}_4)(\text{SAr})(^{18}\text{O}^{18}\text{O}^t\text{Bu})]^+$ complexes **1a** (black), **2a** (green), **5a** (blue), and **4a** (red) (same experimental conditions as in Figure 6).

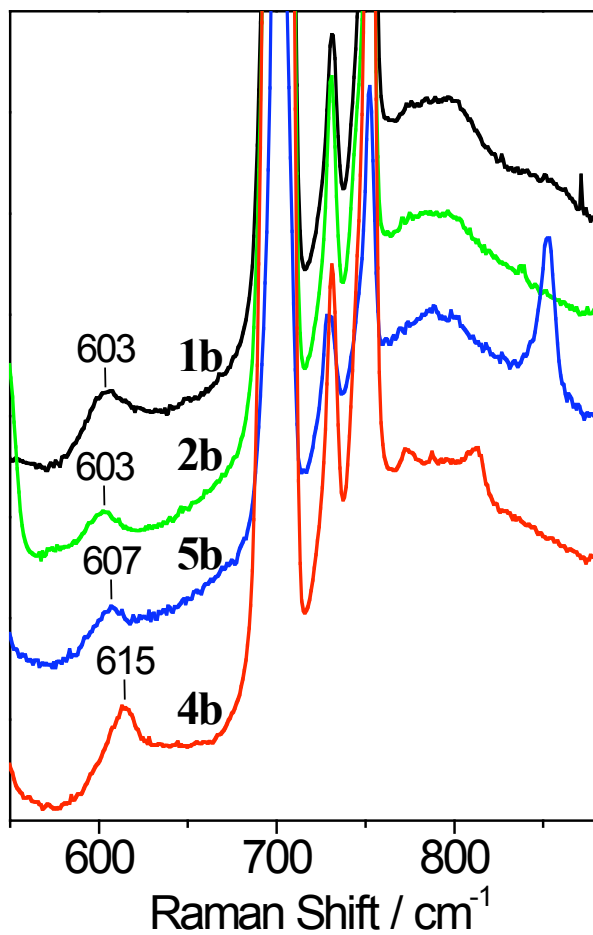


Figure S3. RR spectra of $[\text{Fe}^{\text{III}}([\text{15}]\text{aneN}_4)(\text{SAr})(^{18}\text{O}^{18}\text{OCm})]^+$ complexes **1b** (black), **2b** (green), **5b** (blue), and **4b** (red) (same experimental conditions as in Figure 7).

Complete ref 56: http://www.gaussian.com/citation_g03.htm

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.