

W0158

A Nitrosyl Heme Thiolate Product from a Heterogeneous Reaction. Douglas R. Powell, Nan Xu, Lin Cheng, and George B. Richter-Addo, Dept. of Chemistry and Biochemistry, Univ. of Oklahoma, 620 Parrington Oval, Norman, OK 73019-3051.

Heme thiolate proteins display rich and diverse reactivities that include nitric oxide (NO) biosynthesis, NO reduction, hydroxylation, and detoxification of xenobiotics. Attempts to make model nitrosyl heme thiolate compounds by solution methods have, so far, been unsuccessful. However, such a model compound has been prepared from a heterogeneous reaction of crystals of $[\text{Fe}^{\text{III}}(\text{oep})(\text{thiolate})]$ and NO gas.¹ The resulting crystal diffracted to only 1.0 Å resolution. The volume of the crystal lattice increased from 2266.3(6)Å³ for the crystal without NO to 2360(2)Å³ after NO addition. The NO ligand is bent with an angle of 159.6(8)°. The nitrosyl N is tilted 9.1° from the normal to the porphyrin plane. The Fe atom is displaced 0.05 Å toward the NO ligand from the porphyrin plane. This work was supported by the U.S. National Institutes of Health (GM64476).

¹Nan Xu, Douglas R. Powell, Lin Cheng, and George B. Richter-Addo, *Chem. Comm.*, 2006, submitted.