

# Soft X-ray Spectroscopy as a Neat Tool to Assign Electronic Structures of {FeNO} Complexes

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{FeNO} complexes are a family of compounds that contain both iron (Fe) and nitric oxide (NO) as active sites, and are largely used as models to study O<sub>2</sub> and NO metabolism. The detailed electronic structures of the {FeNO} complexes are always controversial, due to the lack of robust tools for characterization. In this work, N K-edge and Fe L-edge XAS are combined to unambiguously assign the charge and spin state of both Fe and NO in a pair of {FeNO}<sub>6</sub> and {FeNO}<sub>7</sub> compounds, and showed that the one electron redox occurred on the NO side. At beamline 8.0.1 at Advanced Light Source (ALS), the technique can also be applied to other systems under different conditions.

**Keywords [optional]:** Iron Nitrosyl compounds, X-ray absorption spectroscopy, electronic structures, charge and spin density, density functional theory.

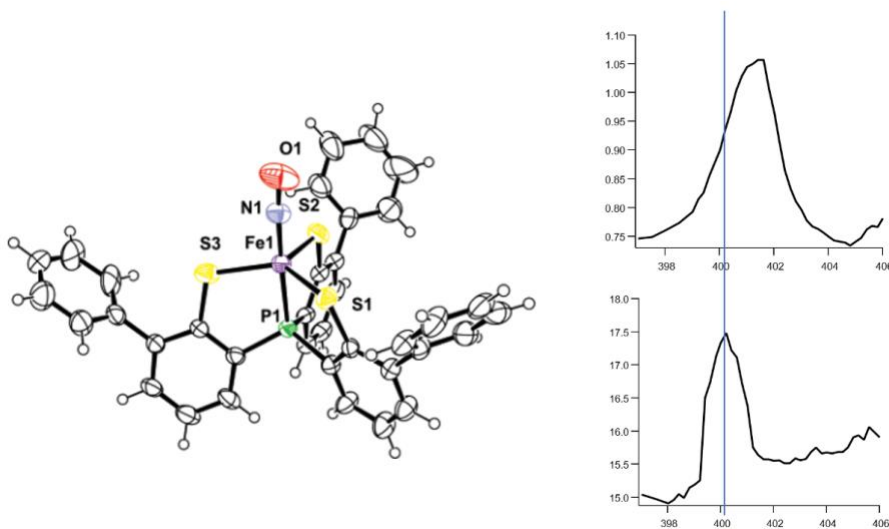


Figure 1. Structure of an {FeNO} complex and the corresponding XAS data.