

Mössbauer , XANES and DFT characterization of an aqueous $\text{Fe}^{\text{IV}}=\text{O}$ species

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Mössbauer spectra and the X-ray absorption near edge structure of a short-lived intermediate, **Z**, generated from $\text{Fe}(\text{H}_2\text{O})_6^{2+}$ and ozone at pH 1 are reported. The Mössbauer parameters indicate that **Z** is a high-spin $\text{Fe}^{\text{IV}}=\text{O}$ complex, an interpretation supported by density functional theory calculations. The question as to whether aqueous $\text{Fe}^{\text{IV}}=\text{O}$ participates in the Fenton reaction is addressed.