

Supporting Information for
Effects of the Protein Environment on the Structure and Energetics of Active Sites of Metalloenzymes.
ONIOM Study of Methane Monooxygenase and Ribonucleotide Reductase.

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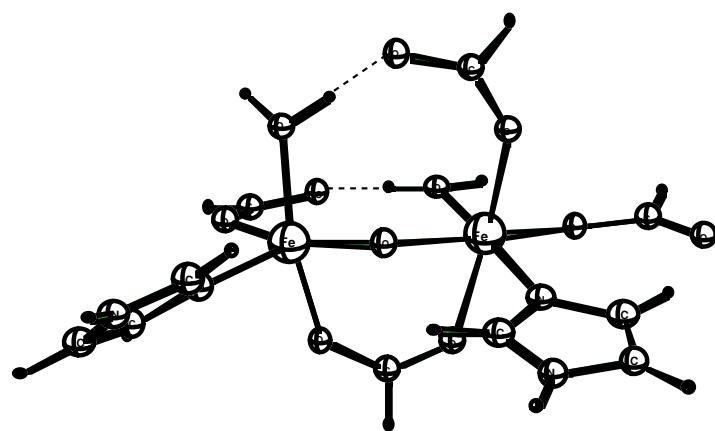
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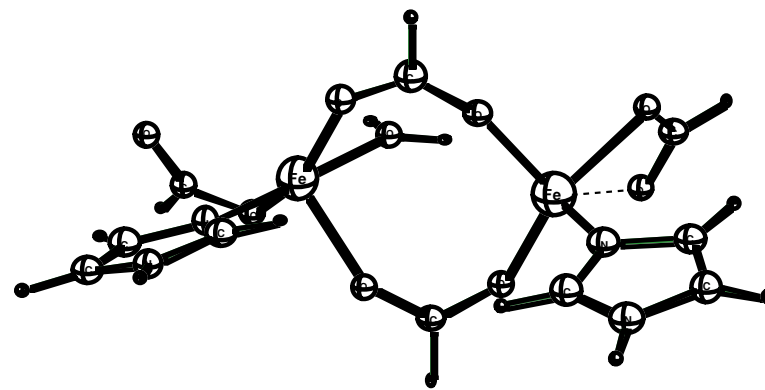
List of added Amber parameters for link atoms (“A” type = link atoms in carboxylate-like moieties; “B” type = link atoms in imidazole moieties):

$K_r(H_A-C) = 367.0$, $r_{eq}(H_A) = 1.080$, $K_\theta(H_A) = 70.0$, $\theta_{eq}(H_A-C-O2) = 117.0$, $V_n/2(H_A) = 10.5$, $\gamma(H_A) = 180.0$, $R(H_A) = 1.2870$, $\epsilon(H_A) = 0.0157$

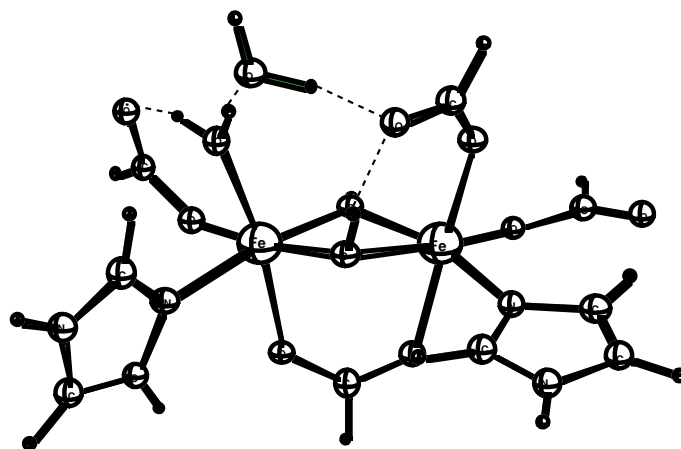
$K_r(H_B-C) = 367.0$, $r_{eq}(H_B) = 1.080$, $K_\theta(H_B) = 70.0$, $\theta_{eq}(H_B-CC-NB) = 120.0$, $\theta_{eq}(H_B-CC-CW) = 120.0$, $V_n/2(H_B) = 1.1$, $\gamma(H_B) = 180.0$, $R(H_B) = 1.4090$, $\epsilon(H_B) = 0.0150$.



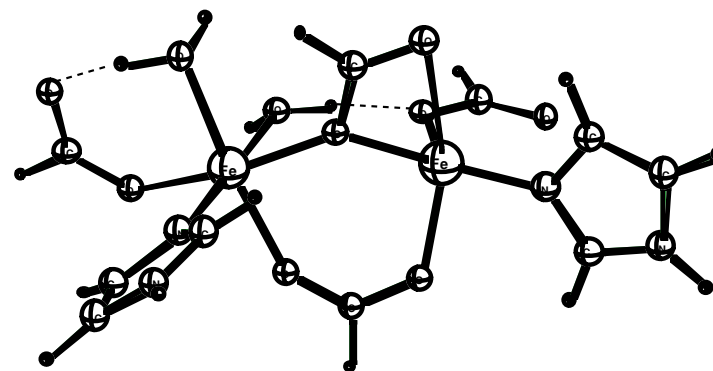
R2_{met}



R2_{red}



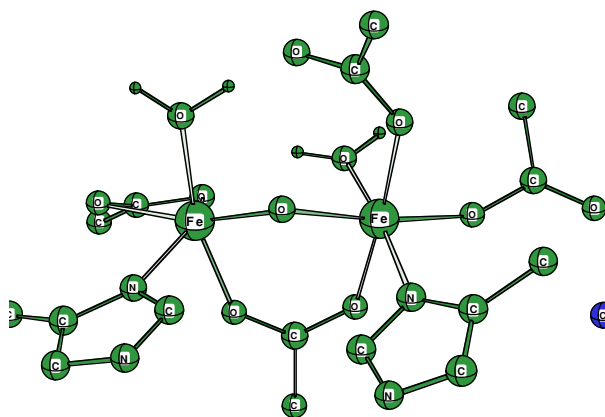
MMOH_{ox}



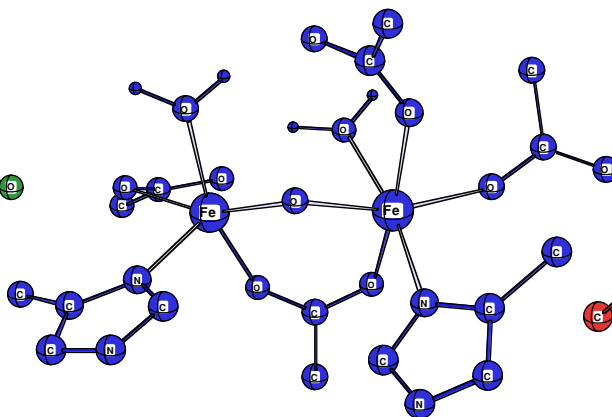
MMOH_{red}

Figure S1. Biomolecular models for the active sites of R2 (top) and MMOH (bottom) including only the first-shell ligands.

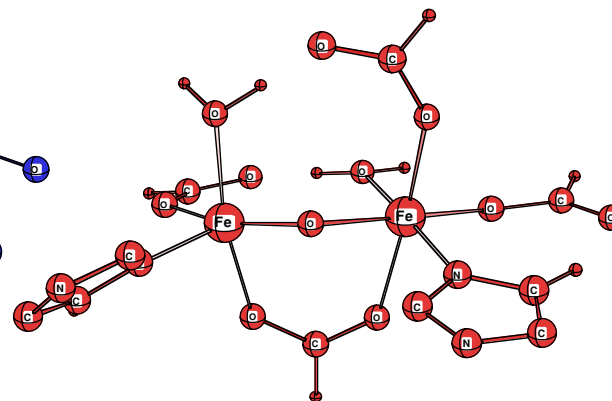
R2_{met} - Comparison of optimized active sites with X-ray



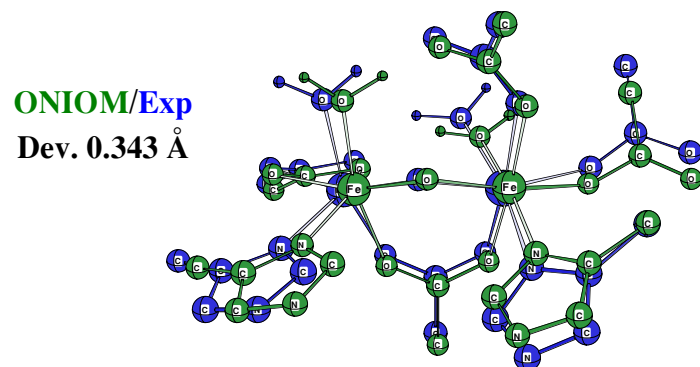
ONIOM(QM:MM)
with selected MM atoms frozen



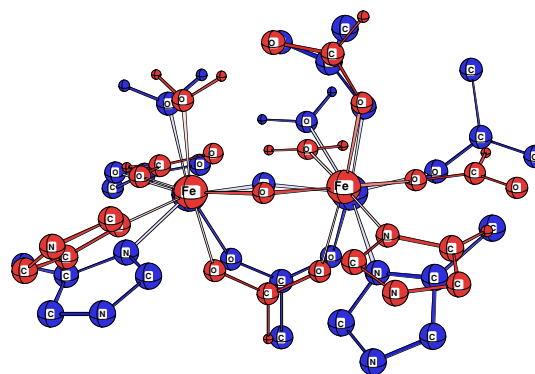
Experimental
(X-ray)



Pure QM
(small model)



ONIOM/Exp
Dev. 0.343 Å



QM/Exp
Dev. 0.796 Å