Supporting Information

DFT Calculations of Comparative Energetics and Mössbauer Properties for Two Protonation States of the Iron Dimer Cluster of Ribonucleotide Reductase Intermediate X

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pK\textsubscript{a} Calculations for Fe\textsuperscript{2+} and Fe\textsuperscript{3+} in Water

**Figure S1.** Structure of Fe\textsuperscript{2+} with 3 shells (6 + 12 + 24 = 42) of water molecules optimized with DFT/OPBE method using all-electron TZP Slater-type basis sets in COSMO solvation model with \(\varepsilon = 80\).

**Figure S2.** Structure of Fe\textsuperscript{2+}-OH\textsuperscript{-} with 3 shells (5 + 12 + 24 = 41) of water molecules.
Table S1. COSMO and DFT/PB-SCRF calculated energies ($E$, eV) for Fe(H$_2$O)$_{42}^{2+}$, Fe(OH)(H$_2$O)$_{41}^{+}$, Fe(H$_2$O)$_{42}^{3+}$, and Fe(OH)(H$_2$O)$_{41}^{2+}$ systems, and the calculated (cal) and experimental (exp) pK$_a$’s for the processes of Fe(H$_2$O)$_{42}^{2+}$ → Fe(OH)(H$_2$O)$_{41}^{+}$ + H$^+$, and Fe(H$_2$O)$_{42}^{3+}$ → Fe(OH)(H$_2$O)$_{41}^{2+}$ + H$^+$.

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$^a$ See section 3.5. The ∆ZPE terms are −7.1 kcal mol$^{-1}$ for Fe(H$_2$O)$_{42}^{2+}$ → Fe(OH)(H$_2$O)$_{41}^{+}$ + H$^+$, and −7.7 kcal mol$^{-1}$ for Fe(H$_2$O)$_{42}^{3+}$ → Fe(OH)(H$_2$O)$_{41}^{2+}$ + H$^+$, taken from “Li, J.; Fisher, C. L.; Chen, J. L.; Bashford, D.; Noodleman, L. Inorg. Chem. 1996, 35, 4694.”.

$^b$ In alkaline solution. Taken from “Baes, C. J.; Mesmer, R. E. The hydrolysis of Cations; Krieger: Malabar, India, 1986”.

$^c$ Ionic strength = 0. Taken from “Flynn, C. M., Jr. Chem. Rev. 1984, 84, 31”.

Cartesian coordinates of Fe(H$_2$O)$_{42}^{2+}$

(Using OPBE potential, optimized in COSMO solvation model with ε = 80)

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(Using OPBE potential, optimized in COSMO solvation model with $\varepsilon = 4$)

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(Using OPBE potential, optimized in COSMO solvation model with $\varepsilon = 4$)
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