

Supporting information for:

## **Investigation of the reactions of small neutral iron oxide clusters with methanol**

Yan Xie,<sup>1</sup> Feng Dong,<sup>1</sup> Scott Heinbuch,<sup>2</sup> Jorge J. Rocca,<sup>2</sup> and Elliot R. Bernstein<sup>1\*</sup>

<sup>1</sup>Department of Chemistry

<sup>2</sup>Department of Electrical and Computer Engineering

<sup>1,2</sup>NSF ERC for Extreme Ultraviolet Science and Technology

Colorado State University, Fort Collins, CO 80523, USA

\*Corresponding email: [erb@lamar.colostate.edu](mailto:erb@lamar.colostate.edu)

## Figure Captions

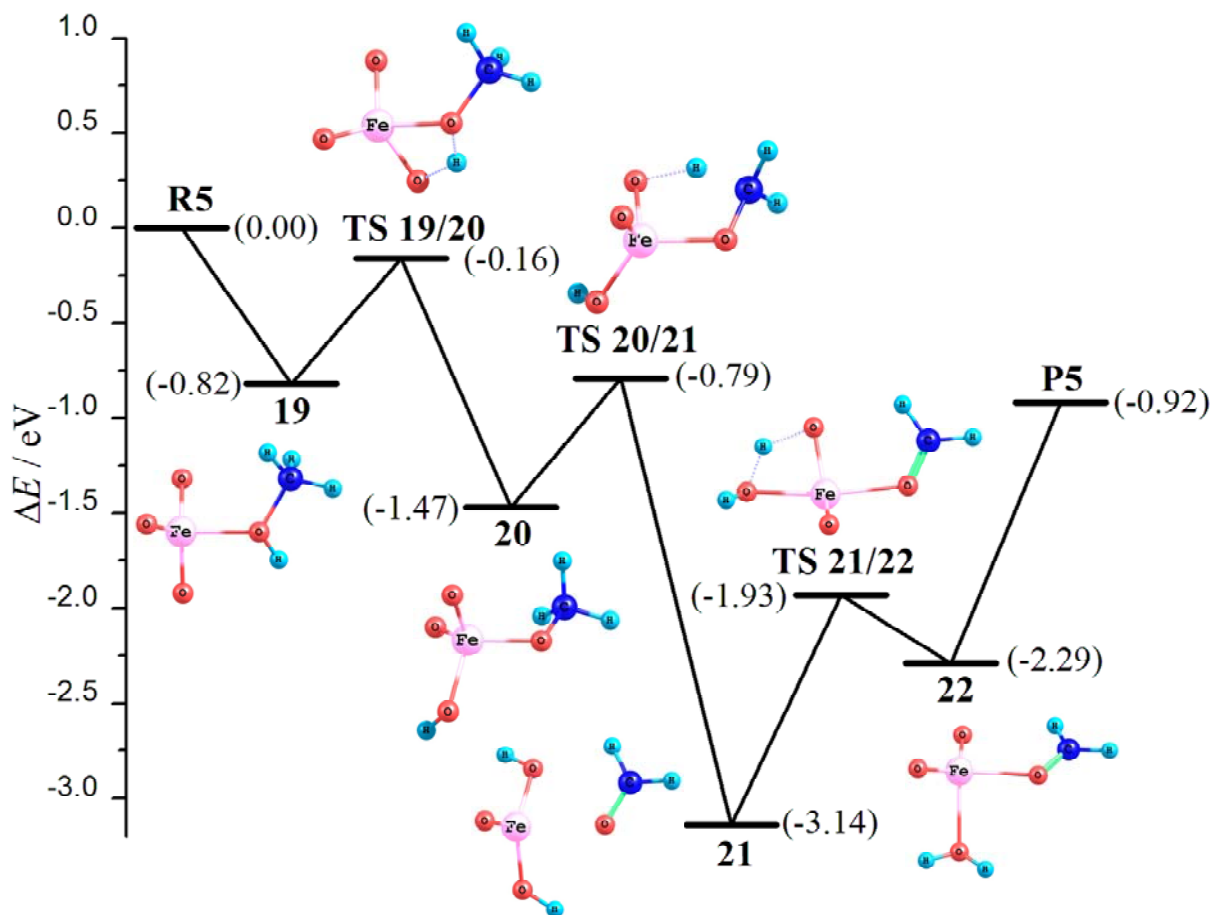
**Figure S1.** Reaction pathways for  ${}^3\text{FeO}_3 + \text{CH}_3\text{OH} \rightarrow {}^3\text{FeO}_2 + \text{H}_2\text{O} + \text{CH}_2\text{O}$  calculated at the B3LYP/6-311+G(d) level. Energies, including ZPE corrections, are given in eV and are relative to the initial energy of the  ${}^3\text{FeO}_3 + \text{CH}_3\text{OH}$  reactants. Note only Pathway A, hydrogen transfer from the O-H group followed by that from the C-H group, is presented in this figure. R5:  ${}^3\text{FeO}_3 + \text{CH}_3\text{OH}$ ; P5:  ${}^3\text{FeO}_2 + \text{CH}_2\text{O} + \text{H}_2\text{O}$ . Iron, oxygen, carbon, hydrogen are in pink, red, dark blue, and light blue, respectively.

**Figure S2.** Reaction pathways for  ${}^9\text{Fe}_2\text{O}_4 + \text{CH}_3\text{OH} \rightarrow {}^9\text{Fe}_2\text{O}_4 + \text{H}_2\text{O} + \text{CH}_2\text{O}$  calculated at the B3LYP/6-311+G(d) level. Energies, including ZPE corrections, are given in eV and are relative to the initial energy of the  ${}^9\text{Fe}_2\text{O}_4 + \text{CH}_3\text{OH}$  reactants. Note only Pathway A, hydrogen transfer from the O-H group followed by that from the C-H group, is presented in this figure. R6:  ${}^9\text{Fe}_2\text{O}_4 + \text{CH}_3\text{OH}$ ; P6:  ${}^9\text{Fe}_2\text{O}_3 + \text{CH}_2\text{O} + \text{H}_2\text{O}$ . Iron, oxygen, carbon, hydrogen are in pink, red, dark blue, and light blue, respectively.

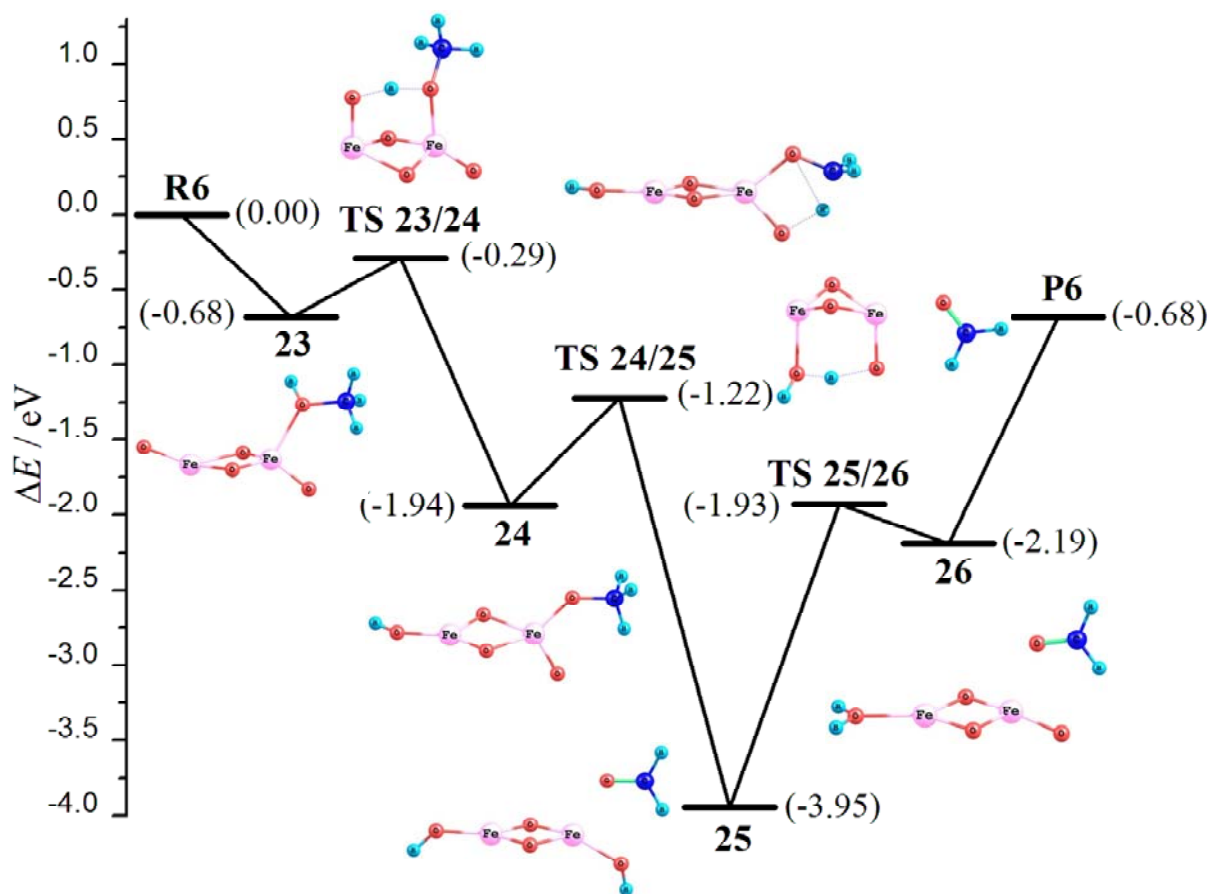
**Figure S3.** Reaction pathways for  ${}^9\text{Fe}_2\text{O}_5 + \text{CH}_3\text{OH} \rightarrow {}^9\text{Fe}_2\text{O}_4 + \text{H}_2\text{O} + \text{CH}_2\text{O}$  calculated at the B3LYP/6-311+G(d) level. Energies, including ZPE corrections, are given in eV and are relative to the initial energy of the  ${}^9\text{Fe}_2\text{O}_5 + \text{CH}_3\text{OH}$  reactants. Note only Pathway A, hydrogen transfer from the O-H group followed by that from the C-H group, is presented in this figure. R7:  ${}^9\text{Fe}_2\text{O}_5$  (Conformer B) +  $\text{CH}_3\text{OH}$ ; P7:  ${}^9\text{Fe}_2\text{O}_4 + \text{CH}_2\text{O} + \text{H}_2\text{O}$ . Iron, oxygen, carbon, hydrogen are in pink, red, dark blue, and light blue, respectively.

**Figure S4.** Reaction pathways for  ${}^9\text{Fe}_2\text{O}_5 + \text{CH}_3\text{OH} \rightarrow {}^9\text{Fe}_2\text{O}_4 + \text{H}_2\text{O} + \text{CH}_2\text{O}$  calculated at the B3LYP/6-311+G(d) level. Energies, including ZPE corrections, are given in eV and are relative

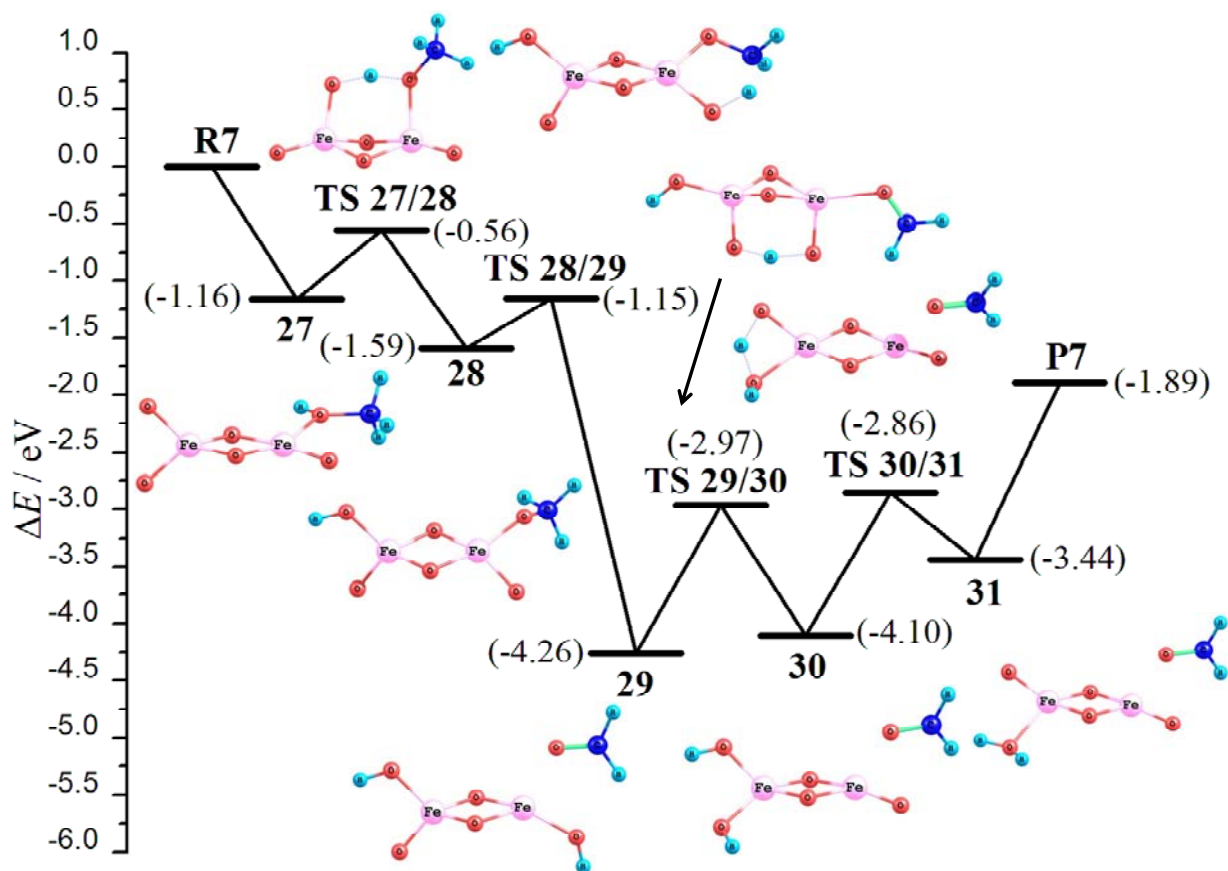
to the initial energy of the  ${}^9\text{Fe}_2\text{O}_5 + \text{CH}_3\text{OH}$  reactants. Note only Pathway A, hydrogen transfer from the O-H group followed by that from the C-H group, is presented in this figure. R8:  ${}^9\text{Fe}_2\text{O}_5$  (Conformer A) +  $\text{CH}_3\text{OH}$ ; P8:  ${}^9\text{Fe}_2\text{O}_4 + \text{CH}_2\text{O} + \text{H}_2\text{O}$ . Iron, oxygen, carbon, hydrogen are in pink, red, dark blue, and light blue, respectively.



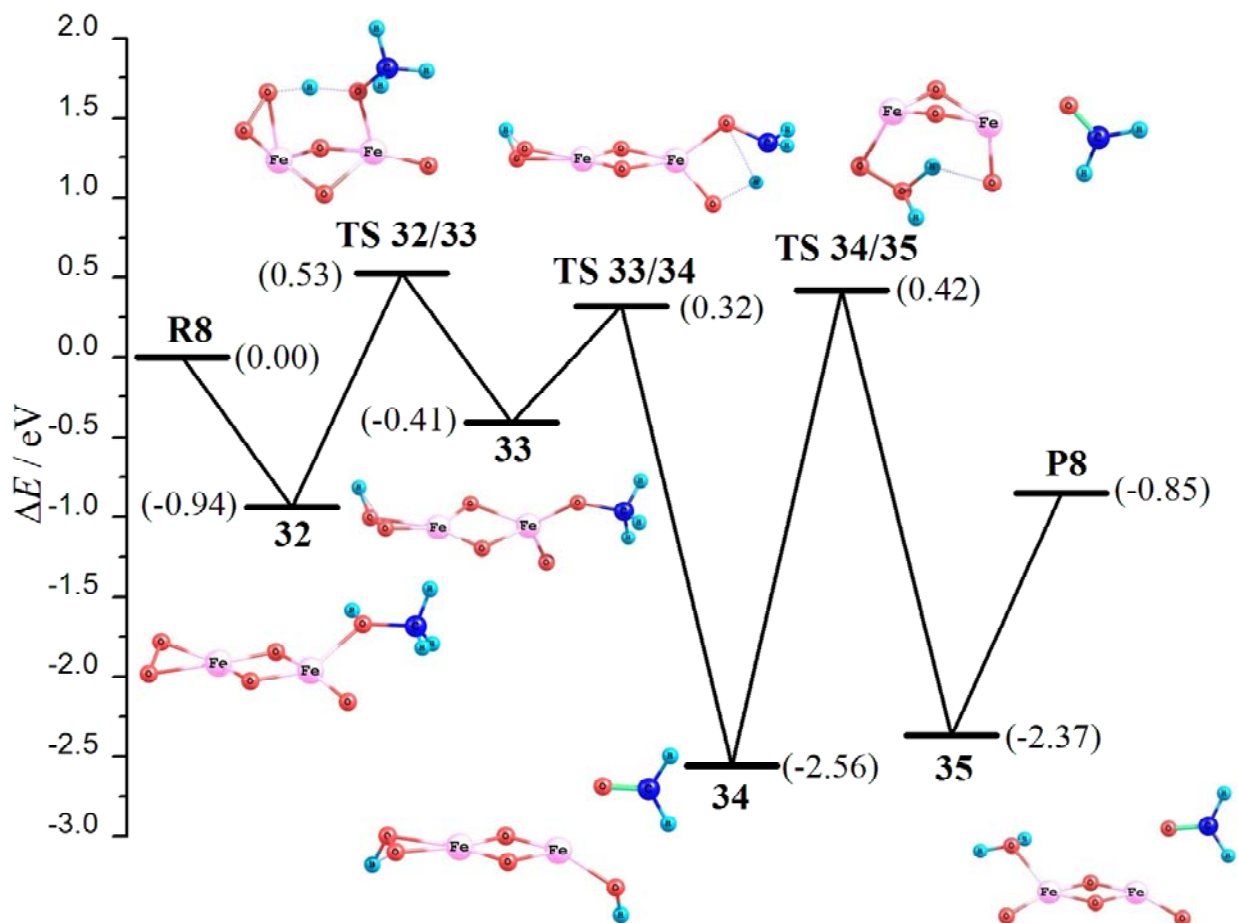
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