ADDITIONS AND CORRECTIONS

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Andreas Heyden,* Baron Peters, Alexis T. Bell,* and Frerich J. Keil: Comprehensive DFT Study of Nitrous Oxide Decomposition over Fe-ZSM-5

Pages 1866, 1867, 1869, and 1870. Figures 2−5 should have been printed in color when this manuscript was published on the Web on January 19, 2005 (ASAP) and in the print version (Vol. 109, No. 5, February 3, p 1857). The corrected figures appear below, and the electronic version was corrected on February 25, 2005.

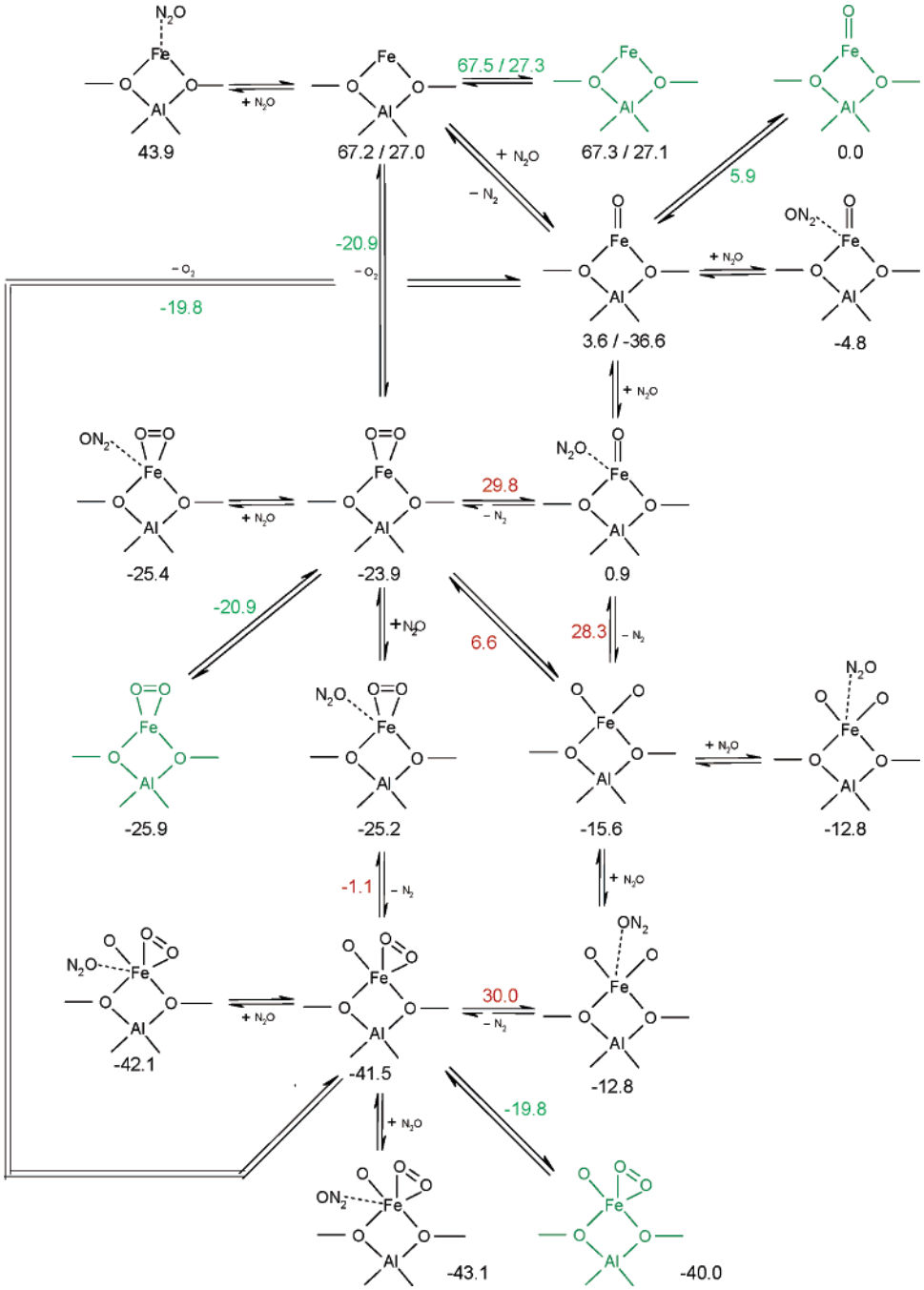

Figure 2. Reaction network of the N_2O dissociation on mononuclear iron oxo species. All energies are zero-point corrected, in kcal/mol and with reference to $Z^-[FeO]^+$ $\{M_S = 6\}$ with the appropriate amounts of N_2O, O_2, N_2, H_2O. Energies of potential energy minima are in black. Energies of transition states are in red. Energies of minima on the seam of two PES ($M_S = 4$ and $M_S = 6$) are in green. Structures in black are on the PES with $M_S = 4$. Structures in green are on the PES with $M_S = 6$.

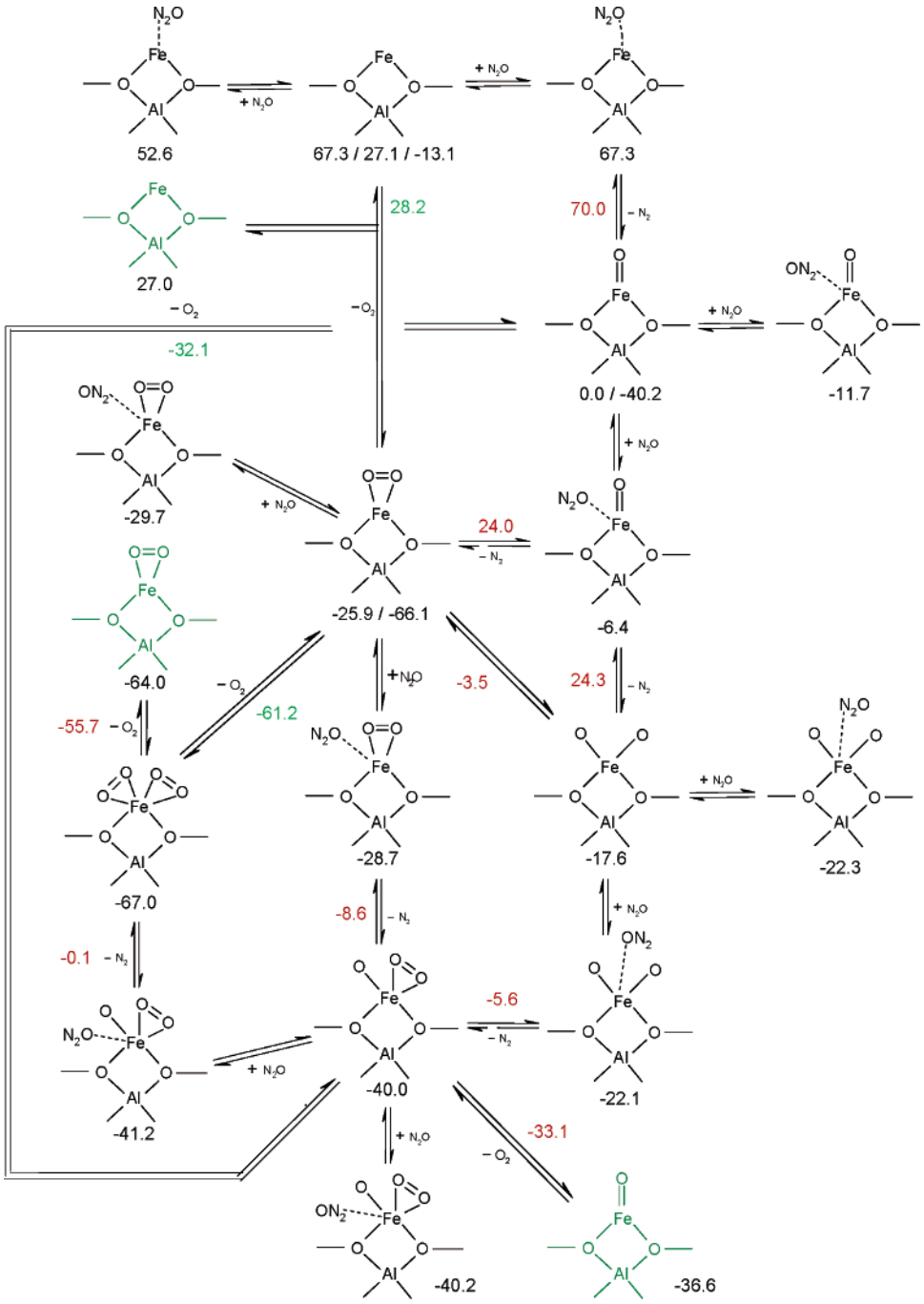

Figure 3. Reaction network of the N_2O dissociation on mononuclear iron oxo species. All energies are zero-point corrected, in kcal/mol and with reference to $Z^-[FeO]^+$ $\{M_S = 6\}$ with the appropriate amounts of N_2O, O_2, N_2, and H_2O. Energies of potential energy minima are in black. Energies of transition states are in red. Energies of minima on the seam of two PES ($M_S = 6$ and 8) are in green. Structures in black are on the PES with $M_S = 6$. Structures in green are on the PES with $M_S = 4$.

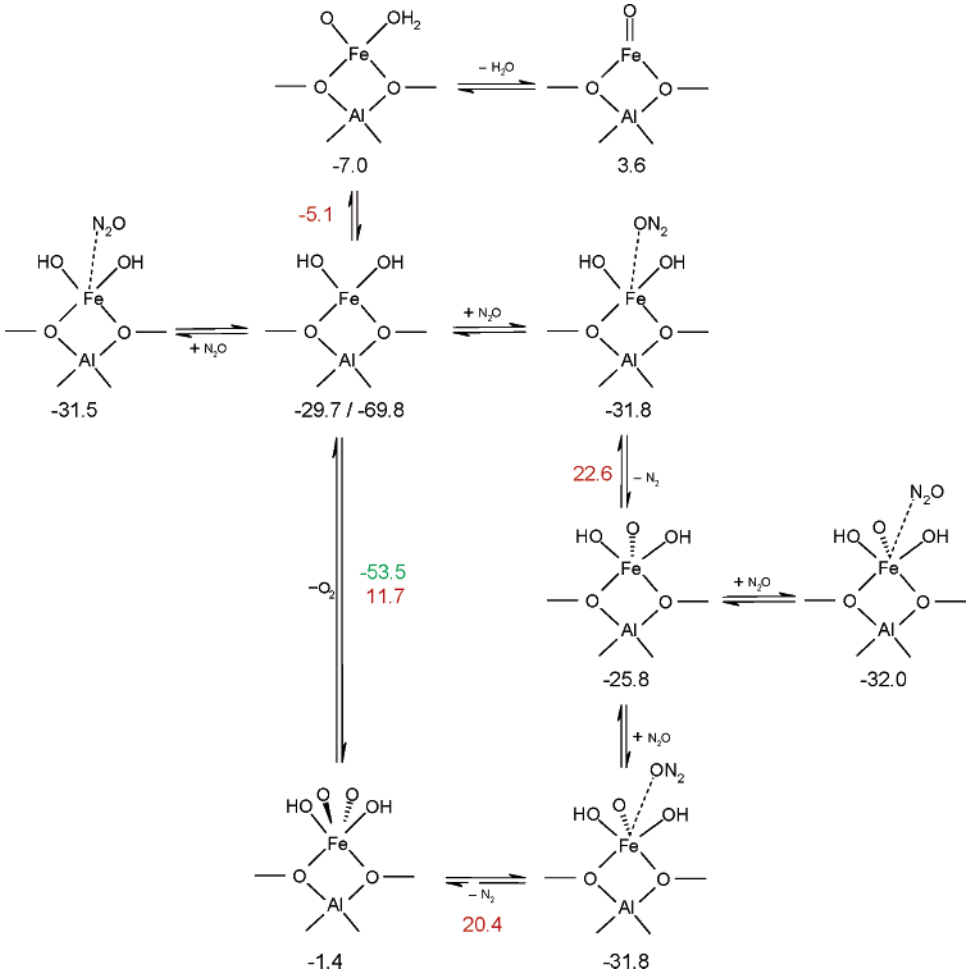

Figure 4. Reaction network of the N2O dissociation on mononuclear iron hydroxo species. All energies are zero-point corrected, in kcal/mol and with reference to $Z^{-}[FeO]^{+}$ $\{M_S = 6\}$ with the appropriate amounts of N_2O, O_2, N_2, H_2O. Energies of potential energy minima are in black. Energies of transition states are in red. Energies of minima on the seam of two PES ($M_S = 4$ and $M_S = 6$) are in green. Structures in black are on the PES with $M_S = 4$.

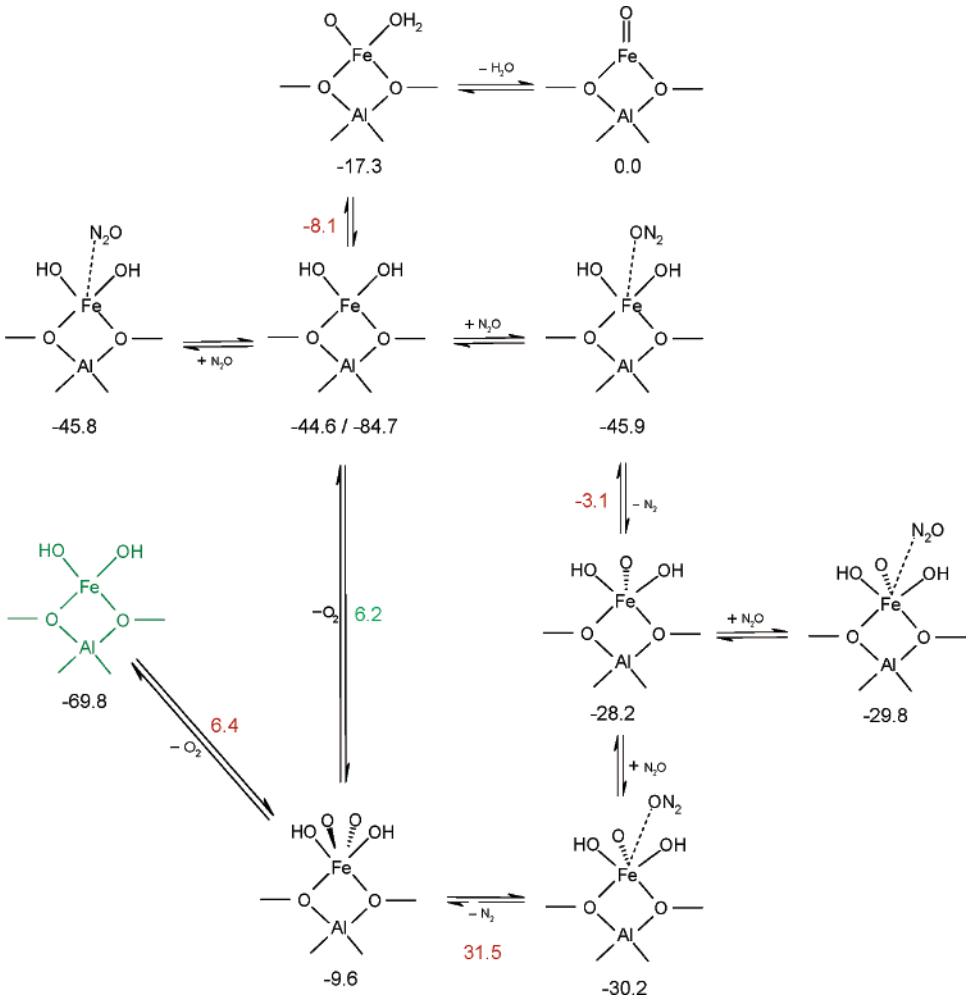

Figure 5. Reaction network of the N_2O dissociation on mononuclear iron hydroxo species. All energies are zero-point corrected, in kcal/mol and with reference to $Z^-[FeO]^+$ $\{M_S = 6\}$ with the appropriate amounts of N_2O, O_2, N_2, H_2O. Energies of potential energy minima are in black. Energies of transition states are in red. Energies of minima on the seam of two PES ($M_S = 6$ and 8) are in green. Structures in black are on the PES with $M_S = 6$. Structures in green are on the PES with $M_S = 4$.

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