Supporting Information

Is $[FeO]^{2+}$ the Active Center also in Iron Containing Zeolites? A Density Functional Theory Study of Methane Hydroxylation Catalysis by Fe–ZSM-5 Zeolite

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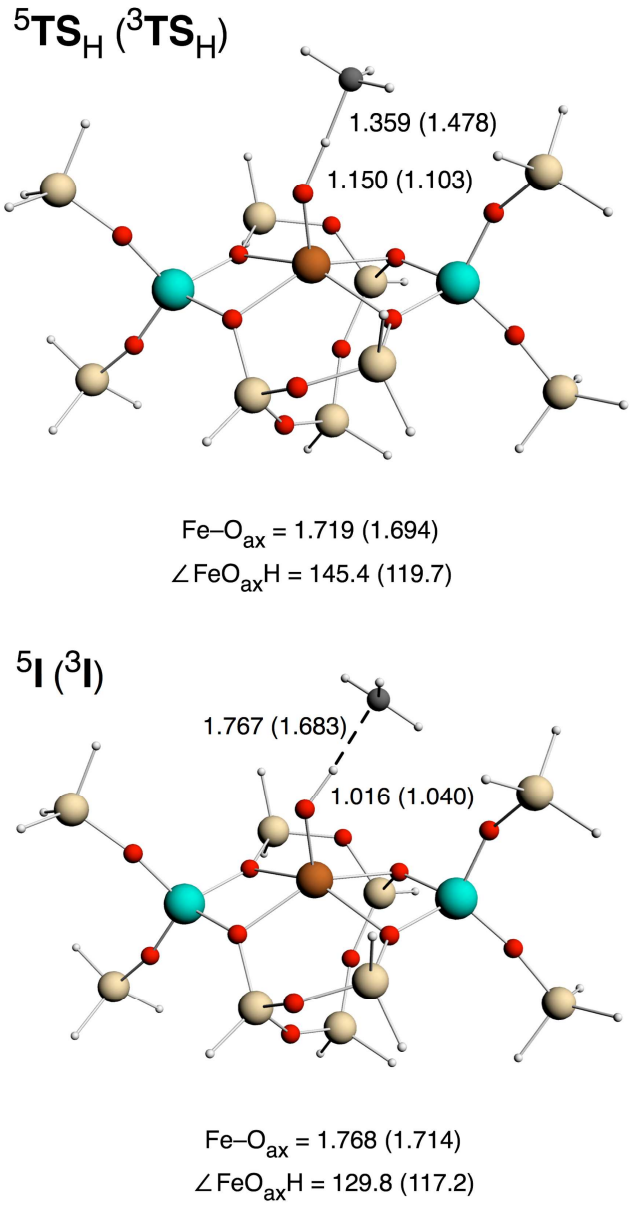

Figure S1. DFT/BP86/def2-TZVP optimized geometries (Å and degrees) of the species involved in the H-abstraction from methane by ^{3,5}**1**.

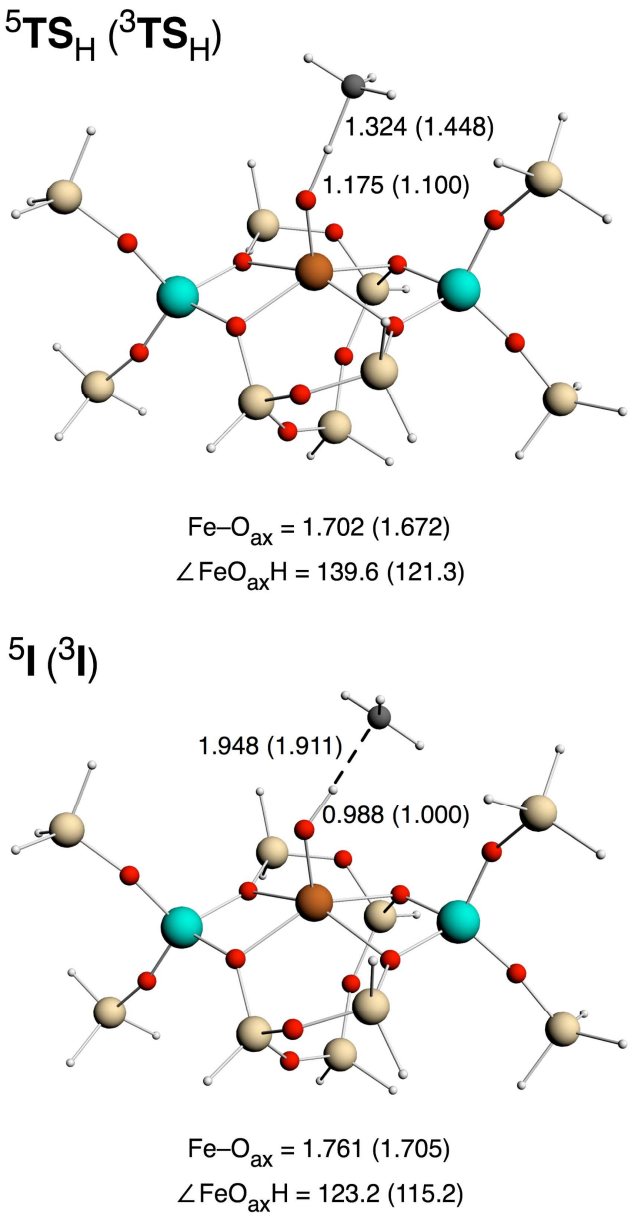

Figure S2. DFT/ZORA/OPBE/TZ2P optimized geometries (Å and degrees) of the species involved in the H-abstraction from methane by ^{3,5}**1**.

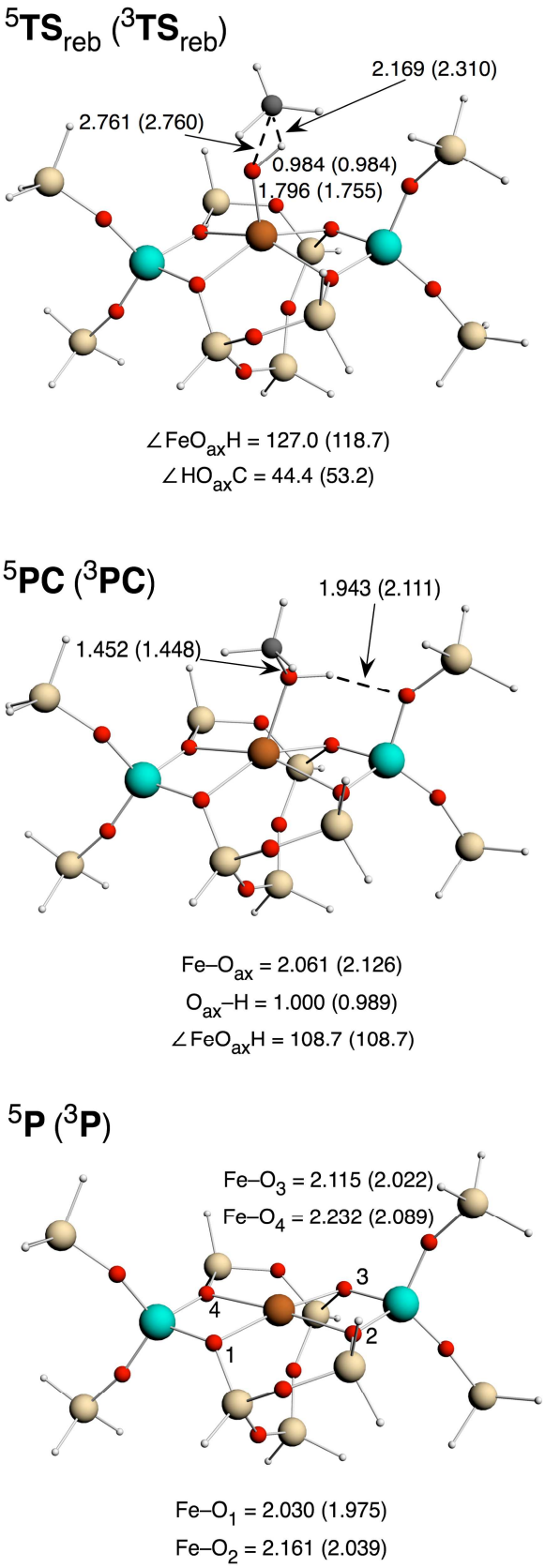

Figure S3. DFT/BP86/def2-TZVP optimized geometries (Å and degrees) of the species involved in the rebound phase of methane hydroxylation by ^{3,5}**1**.

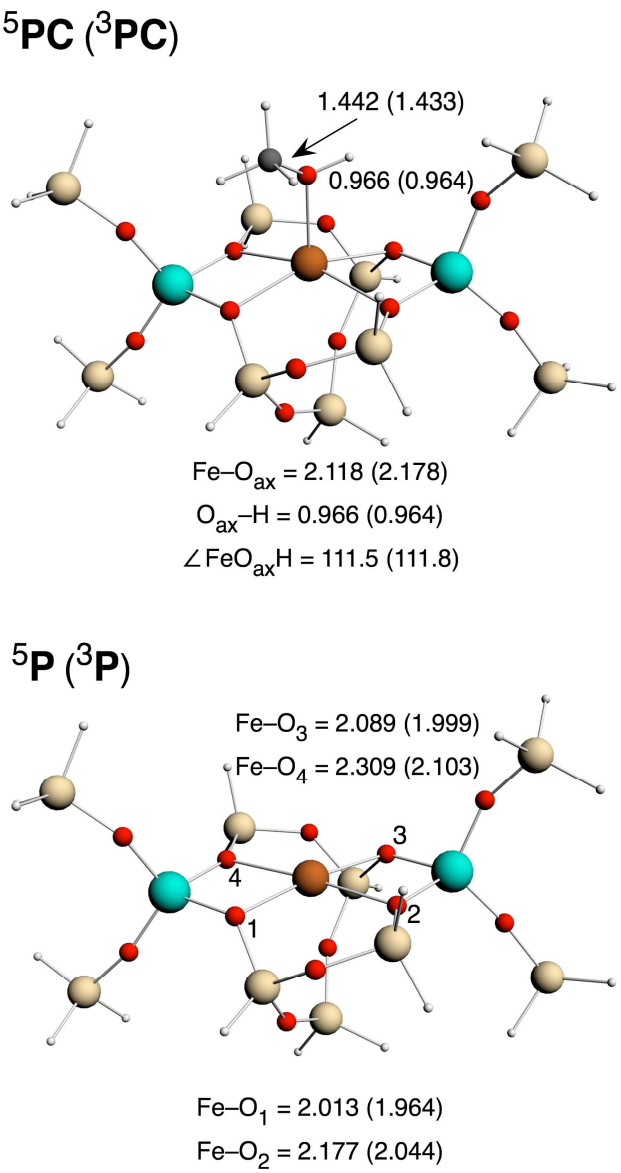

Figure S4. DFT/ZORA/OPBE/TZ2P optimized geometries (Å and degrees) of the species involved in the H-abstraction from methane by ^{3,5}**1**

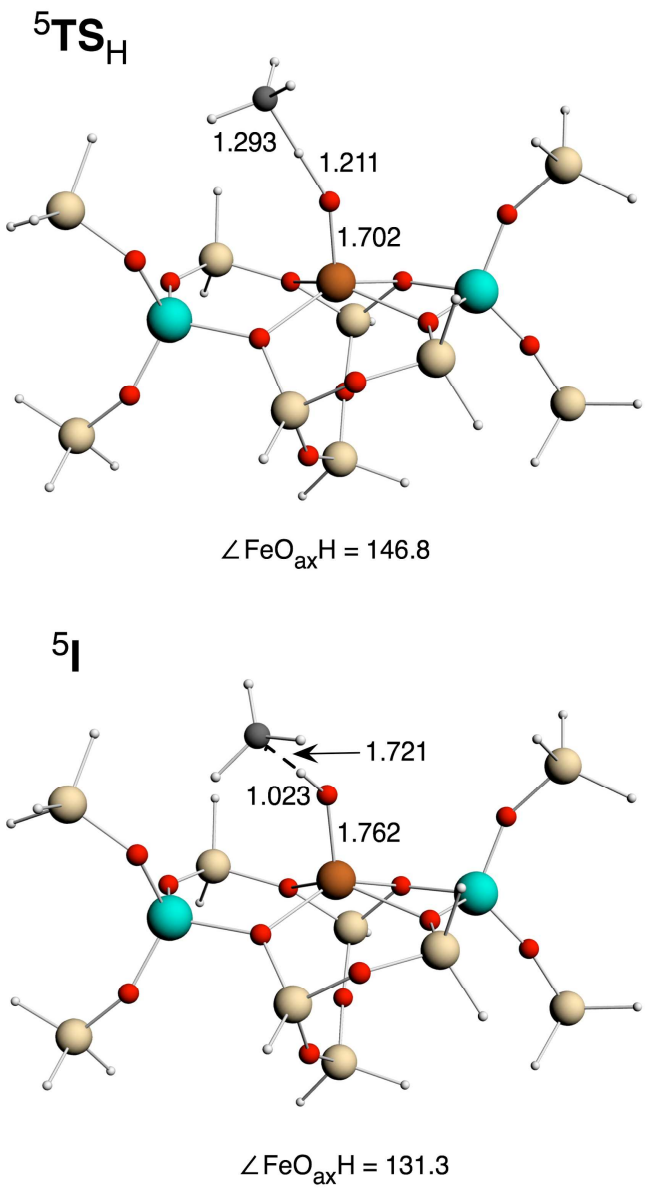

Figure S5. DFT/BP86/def2-TZVP optimized geometries (Å and degrees) of the species involved in the H-abstraction from methane by ^{5}**2**.

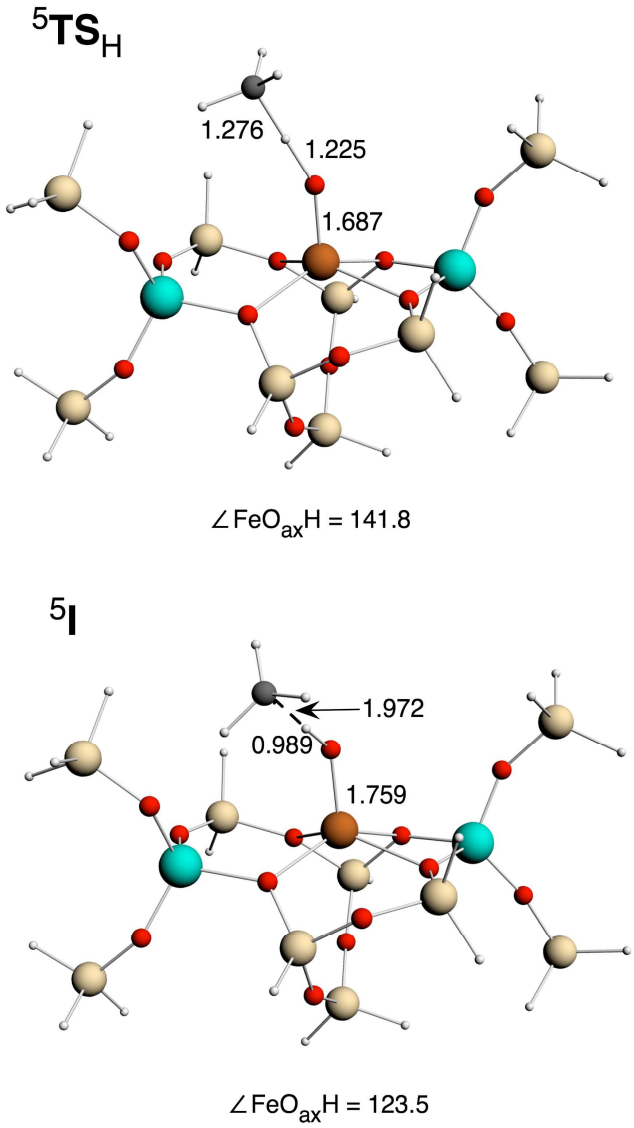

Figure S6. DFT/ZORA/OPBE/TZ2P optimized geometries (Å and degrees) of the species involved in the H-abstraction from methane by ^{5}**2**.

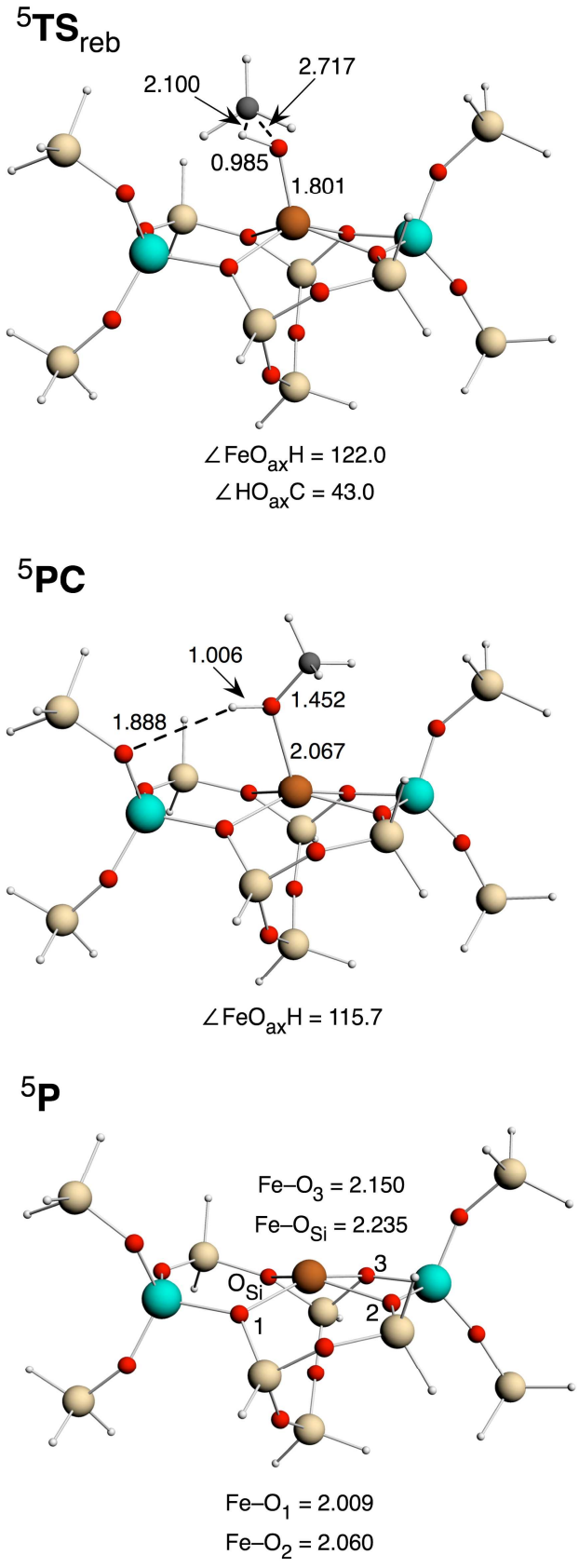

Figure S7. DFT/BP86/def2-TZVP optimized geometries (Å and degrees) of the species involved in the rebound phase of methane hydroxylation by ^{5}**2**.

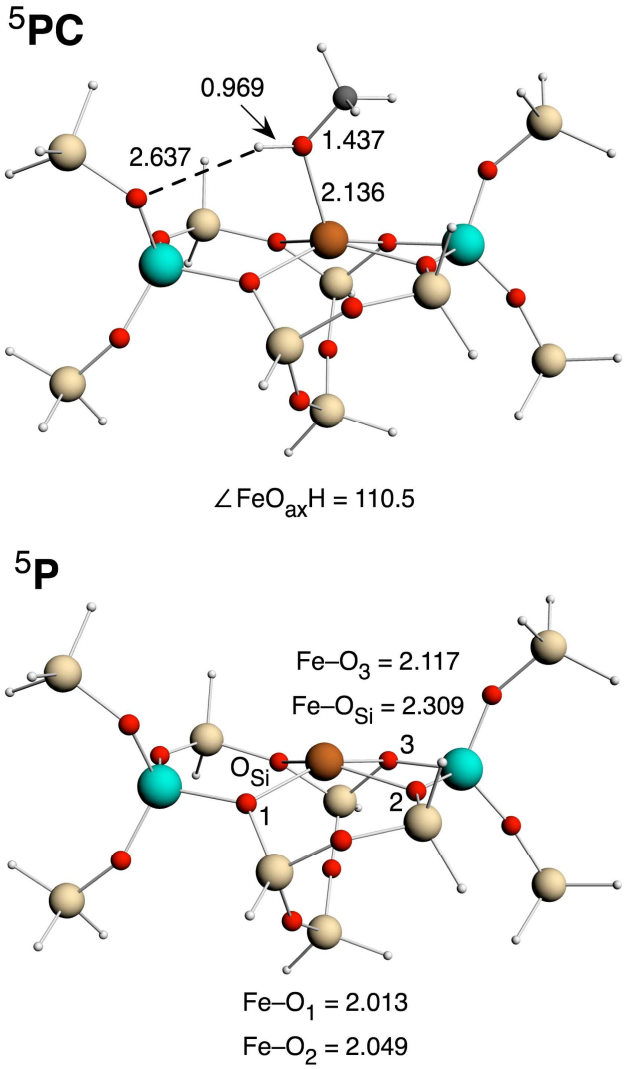

Figure S8. DFT/ZORA/OPBE/TZ2P optimized geometries (Å and degrees) of the species involved in the rebound phase of methane hydroxylation by ^{5}**2**.