Reduced-dimensionality quantum dynamics study of the $^3Fe(CO)_4 + H_2 \rightarrow {}^1FeH_2(CO)_4$ spin-inversion reaction

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Supplementary Material

Table S1. Comparison of the singlet-triplet energy gap (ΔE in kcal/mol) in the $Fe(CO)_4$ reactant obtained from various DFT functionals (without zero-point energy correction).

DFT functional	ΔE (kcal/mol)
TPSSh / def2-TZVPP	7.18
M06-2X / def2-TZVPP	24.24
M06L / def2-TZVPP	8.30
M06 / def2-TZVPP	5.14
OPBE / def2-TZVPP	–0.095
OLYP / def2-TZVPP	0.74
B97D / def2-TZVPP	0.83
ωB97XD / def2-TZVPP	8.53
CCSD(T)	4.02–5.03[a]

[a] Taken from the paper by Carreón-Macedo and Harvey (*Phys. Chem. Chem. Phys*. **2006**, *8*, 93–100).