Supporting Information (Entry C)
The Fe-MAN Challenge: Ferrates – Microkinetic Assessment of Numerical Quantum Chemistry

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1 Computational Details

All structures were optimized with the ωB97X-D3 functional and the def2-TZVP basis set. For the convergence the following criteria were used: *VeryTightSCF TightOpt SlowConv*. ZPE corrections were obtained from these calculations. Standard atomic weights were used for the atomic masses for vibrational calculations. All optimization calculations were performed with ORCA 5.0.3.

For all ωB97X-D3/def2-TZVP optimized structures, electronic single-point energy calculations were carried out with PNO-LCCSD(T)-F12 (pair natural orbitals) with the def2-TZVP basis set and default parameters. Preliminary DFT calculations (using B-LYP or BP86) were carried out to improve the convergence of the subsequent HF calculations. Density fitting was applied in DFT and HF calculations in combination with corresponding basis sets (def2-TZVP/JKFIT). The CABS singles correction was added to the reference energy. All the PNO-LCCSD(T)-F12 calculations were performed with Molpro 2022.1.