Supporting Information (Entry B)
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 conver gence 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 DLPNO-CCSD(T0) and the def2-TZVP basis set and def2-TZVPP/C auxiliary basis set. The RI JCOSX approximation is used with the def2/J auxiliary basis set. 3s3p electrons of iron were correlated. Furthermore, *TightSCF* and *SlowConv* convergence criteria were used. All the DLPNO-CCSD(T0) calculations (*NormalPNO*) were performed with ORCA5.0.3.