

Supporting Information

Metal- and ligand-substitution-induced changes in the kinetics and thermodynamics of hydrogen activation and hydricity in a dinuclear metal complex

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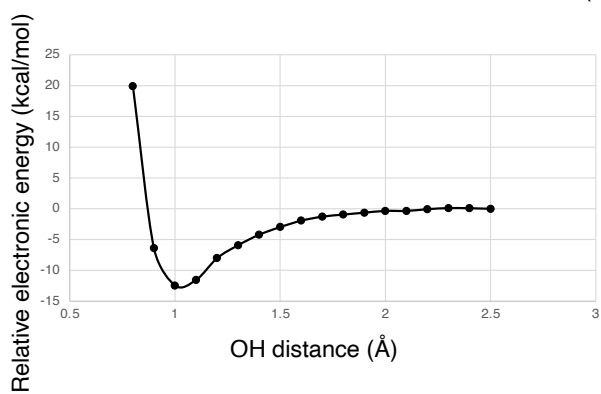
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Table S1. Reaction energies of $[M1M2(L2)] + H_2O \rightarrow [M1M2(H_2O)(L2)]$

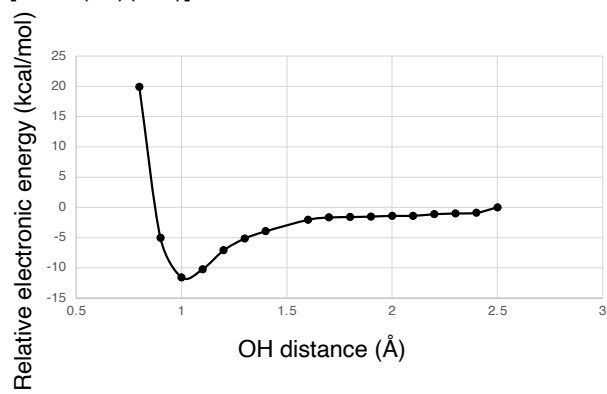
	Spin state		Spin state	ΔG
$[NiFe(CO)]^{2+}$	S = 0	$[NiFe(H_2O)(CO)]^{2+}$	S = 0	7.3
$[NiRu(CO)]^{2+}$	S = 0	$[NiRu(H_2O)(CO)]^{2+}$	S = 0	16.2
$[PdFe(CO)]^{2+}$	S = 0	$[PdFe(H_2O)(CO)]^{2+}$	S = 0	12.9
$[PdRu(CO)]^{2+}$	S = 0	$[PdRu(H_2O)(CO)]^{2+}$	S = 0	8.8
$[NiFe(CNMe)]^{2+}$	S = 0	$[NiFe(H_2O)(CNMe)]^{2+}$	S = 0	11.3
$[NiFe(NCS)]^+$	S = 0	$[NiFe(H_2O)(NCS)]^+$	S = 1	– ^a

^a H₂O is unbound.

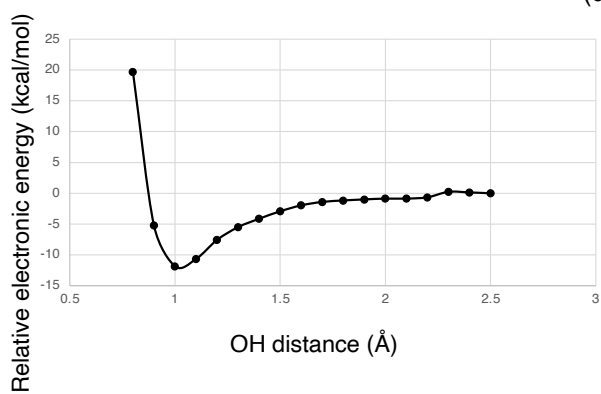
(a) $[\text{NiRu}(\text{H}_2)(\text{CO})]^{2+}$



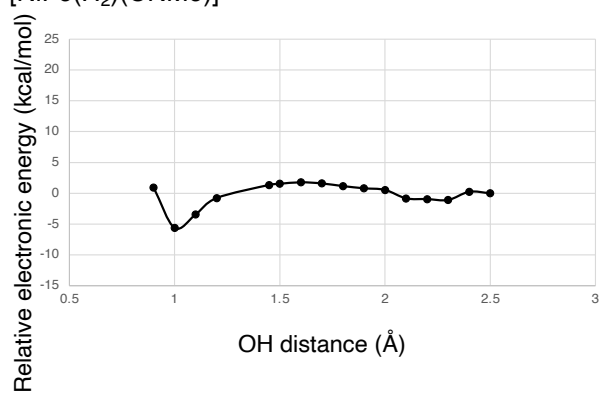
(b) $[\text{PdFe}(\text{H}_2)(\text{CO})]^{2+}$



(c) $[\text{PdRu}(\text{H}_2)(\text{CO})]^{2+}$



(d) $[\text{NiFe}(\text{H}_2)(\text{CNMe})]^{2+}$



(e) $[\text{NiFe}(\text{H}_2)\text{NCS}]^+$

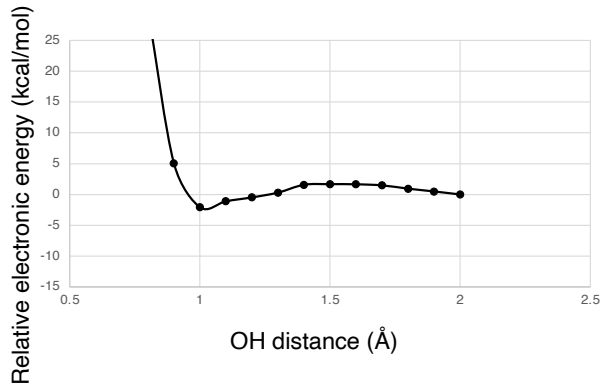
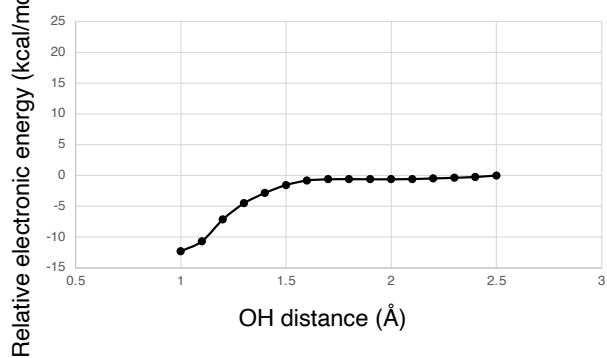
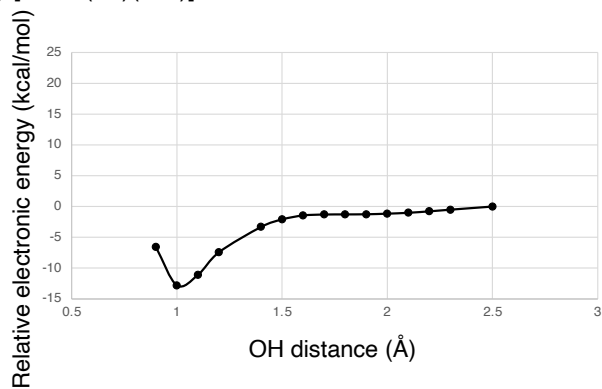


Figure S1. Relaxed potential energy surface scan for proton abstraction step by CH_3COO^- in H_2 activation.

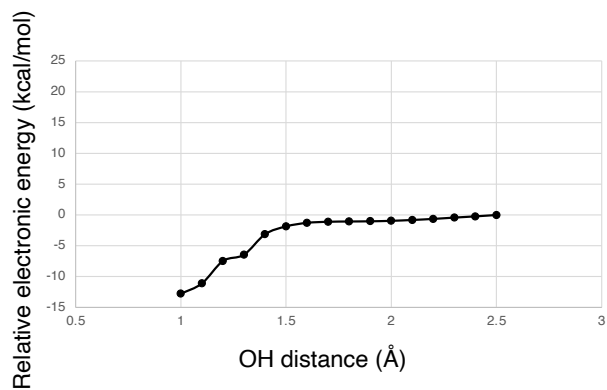
(a) $[\text{NiRu}(\text{H}_2)(\text{CO})]^{2+}$



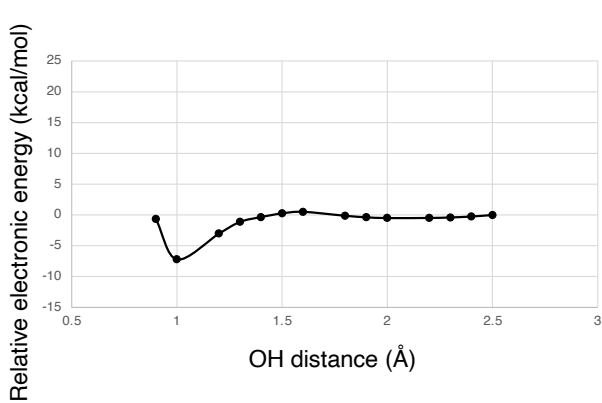
(b) $[\text{PdFe}(\text{H}_2)(\text{CO})]^{2+}$



(c) $[\text{PdRu}(\text{H}_2)(\text{CO})]^{2+}$



(d) $[\text{NiFe}(\text{H}_2)(\text{CNMe})]^{2+}$



(e) $[\text{NiFe}(\text{H}_2)\text{NCS}]^+$

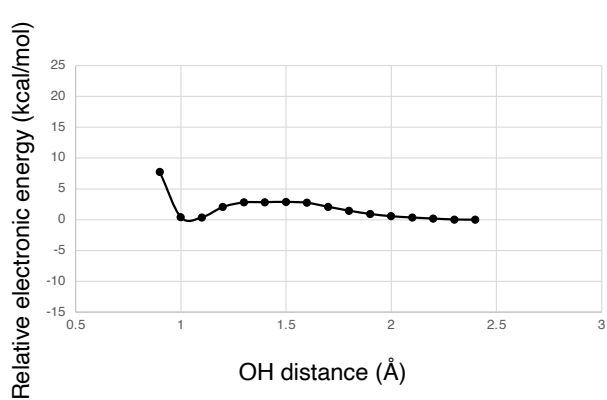
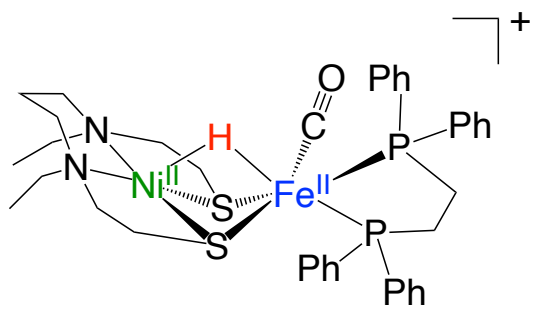
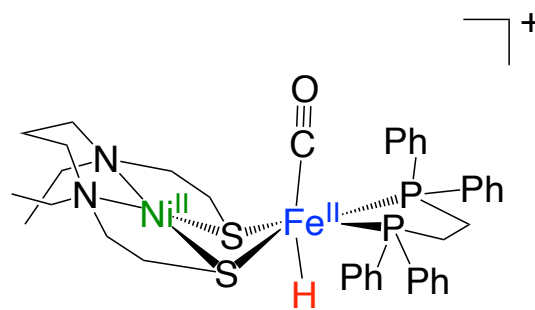


Figure S2. Relaxed potential energy surface scan for proton abstraction step by HPO_4^{2-} in H_2 activation.



Bridging hydride complex



Terminal hydride complex

Figure S3. Isomers of NiFe hydride complexes.