

Supporting Information for

A Structure and Reactivity Analysis of Monomeric Ni(II)—Hydroxo Complexes

Prepared from Water

Darla Powell-Jia, Joseph W. Ziller, and A. S. Borovik*

Department of Chemistry, University of California-Irvine, 1102 Natural Science II,

Irvine, CA 92697

Table S1. Crystallographic Data for $\text{K}[\text{Ni}^{\text{II}}\text{H}_2\mathbf{1}^{\text{Bu}'}(\text{OH})]$ and $[\text{NMe}_4][\text{Ni}^{\text{II}}\text{H}_2\mathbf{1}^{\text{iPr}}(\text{OH})]$

Salt	$\text{K}[\text{Ni}^{\text{II}}\text{H}_2\mathbf{1}^{\text{Bu}'}(\text{OH})]\cdot\text{DMA}$	$[\text{NMe}_4][\text{Ni}^{\text{II}}\text{H}_2\mathbf{1}^{\text{iPr}}(\text{OH})]$	$[\text{NMe}_4][\text{Ni}^{\text{II}}\text{H}_2\mathbf{1}^{\text{iPr}}(\text{OBu}^t)]$
Molecular formula	$\text{C}_{13}\text{H}_{28}\text{KN}_5\text{NiO}_3$		$\text{C}_{21}\text{H}_{48}\text{N}_6\text{NiO}_3$
Formula weight (g/mol)	400.12		491.36
<i>T</i> (K)	163(2)		148(2)
Space group	<i>P</i> -1		<i>P</i> 4 ₃ 2 ₁ 2
<i>a</i> (Å)	9.6492(9)		17.6716(10)
<i>b</i> (Å)	9.8057(9)		17.6716(10)
<i>c</i> (Å)	10.2370(9)		21.525(3)
α (deg)	86.824(2)		90
β (deg)	88.467(2)		90
γ (deg)	74.471(2)		90
<i>Z</i>	2		8
<i>V</i> (Å ³)	931.73(15)		6722.1(9)
δ_{calcd} (Mg/m ³)	1.427		0.971
<i>R</i> 1 ^a	0.0286		0.0996
w <i>R</i> 2 ^b	0.716		0.3029
GOF ^c	1.050		1.471

^a $R1 = \sum ||F_o| - |F_c|| / \sum |F_o|$. ^b $wR2 = [\sum [\omega(F_o^2 - F_c^2)^2] / \sum [\omega(F_o^2)^2]]^{1/2}$. ^c $GOF = [\sum [\omega(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$ where *n* is the number of reflections and *p* is the total number of parameters refined.

Table S2. Selected Metrical Parameters for the $\text{K}[\text{Ni}^{\text{II}}\text{H}_2\mathbf{1}^{\text{Bu}'}(\text{OH})]$, $[\text{NMe}_4][\text{Ni}^{\text{II}}\text{H}_2\mathbf{1}^{\text{iPr}}(\text{OH})]$, and $[\text{NMe}_4][\text{Ni}^{\text{II}}\text{H}_2\mathbf{1}^{\text{iPr}}(\text{OBu}')]$.

Complex	$[\text{Ni}^{\text{II}}\text{H}_2\mathbf{1}^{\text{Bu}'}(\text{OH})]^-$	$[\text{Ni}^{\text{II}}\text{H}_2\mathbf{1}^{\text{iPr}}(\text{OH})]^-$	$[\text{Ni}^{\text{II}}\text{H}_2\mathbf{1}^{\text{iPr}}(\text{OBu}')]^-$
<u>Distances (Å)</u>			
Ni—O1	1.857(1)		1.874(4)
Ni—N1	1.928(1)		1.907(6)
Ni—N2	1.917(1)		1.914(5)
Ni—N3	1.914(2)		1.925(5)
O1⋯N4	2.649(2)		2.746(8)
O1⋯N5	2.757(2)		2.714(7)
O1⋯K1	3.251(2)		—
<u>Angles (°)</u>			
N1—Ni—O1	172.49(6)		172.8(3)
N1—Ni—N2	86.21(6)		84.1(2)
N1—Ni—N3	84.71(6)		85.0(2)
N2—Ni—N3	168.91(6)		166.9(2)
N2—Ni—O1	94.59(6)		95.8(2)
N3—Ni—O1	95.24(6)		95.9(2)