

Supporting Information: Mononuclear Nickel(II) Complexes with Schiff Base Ligands: Synthesis, Characterization, and Catalytic Activity in Norbornene Polymerization

Xu Yi-Mei, Kuan Li, Yuhong Wang and Wei Deng and Zi-Jian Yao

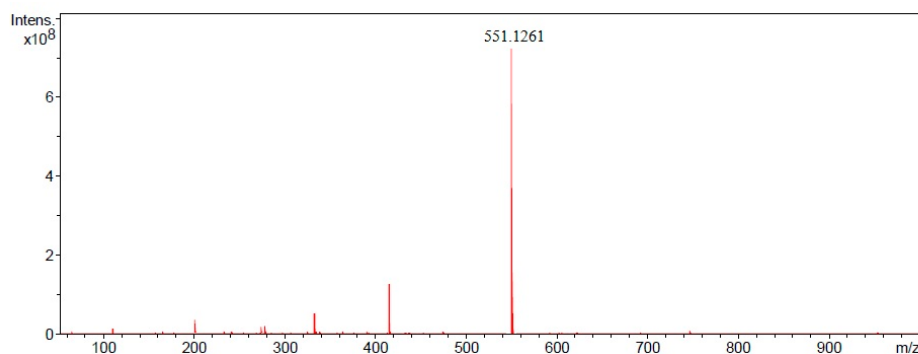


Figure S1. HRMS of complex 1.

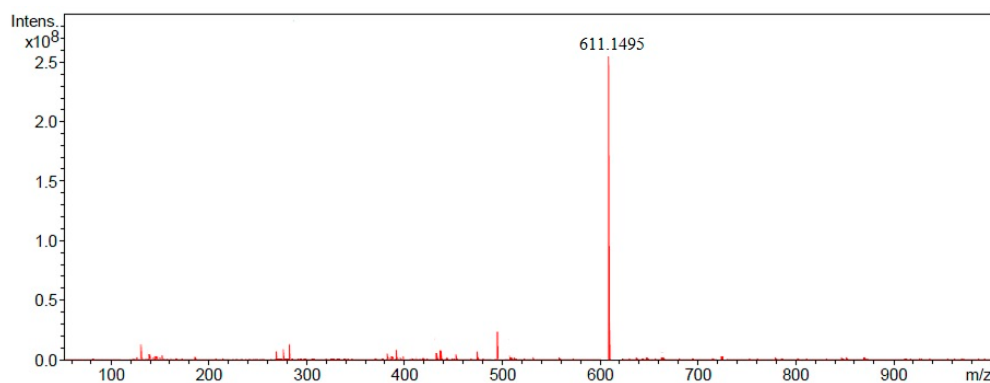


Figure S2. HRMS of complex 2.

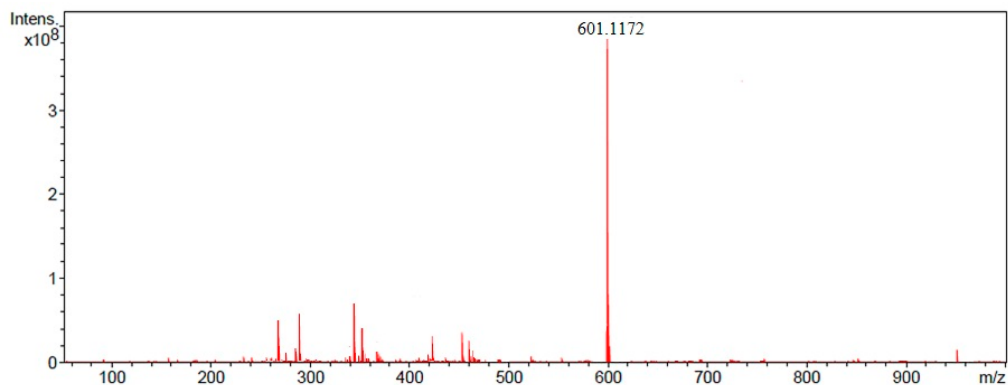
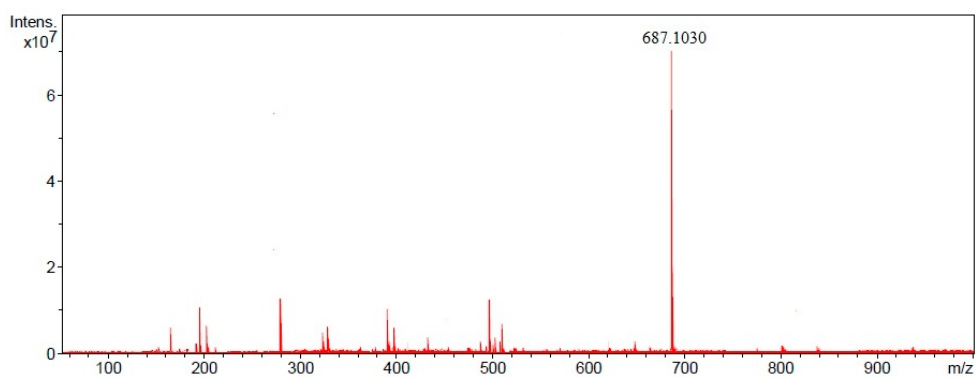
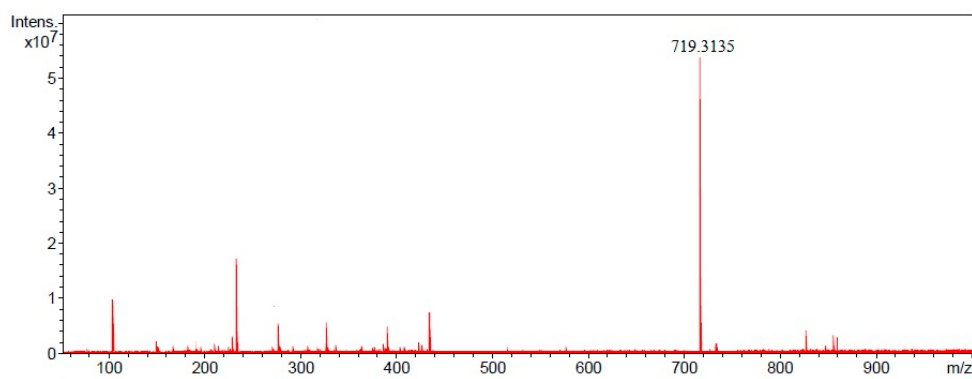
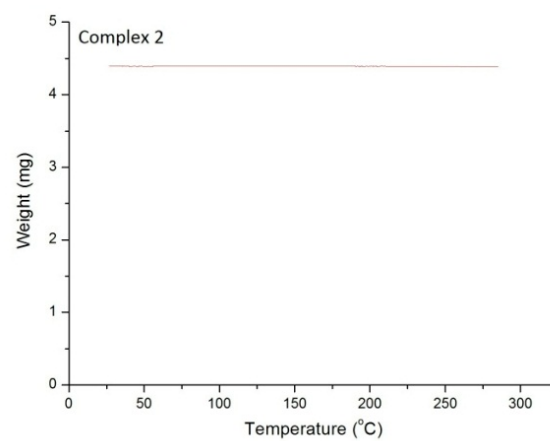
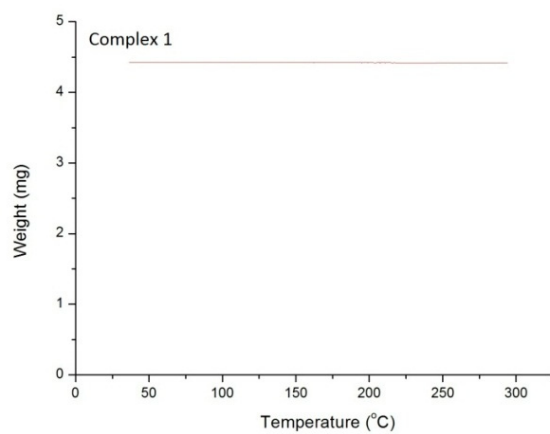


Figure S3. HRMS of complex 3.

**Figure S4.** HRMS of complex 4.**Figure S5.** HRMS of complex 5.

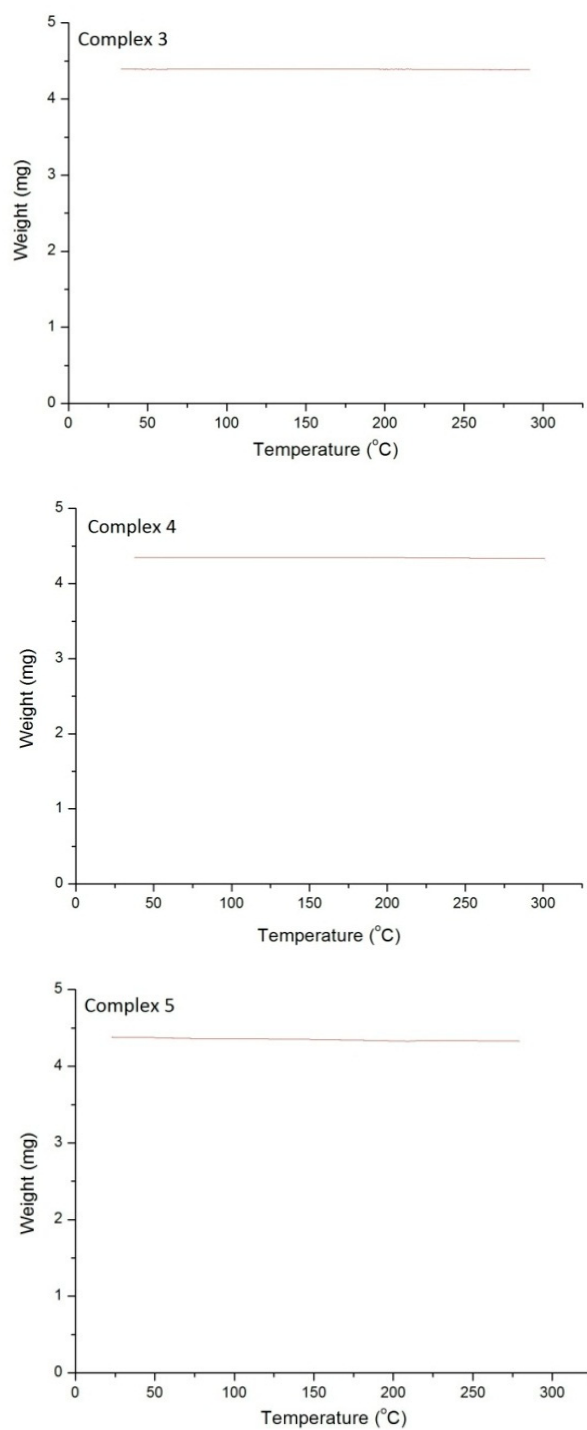


Figure S6. TGA curves of complexes 1–5.

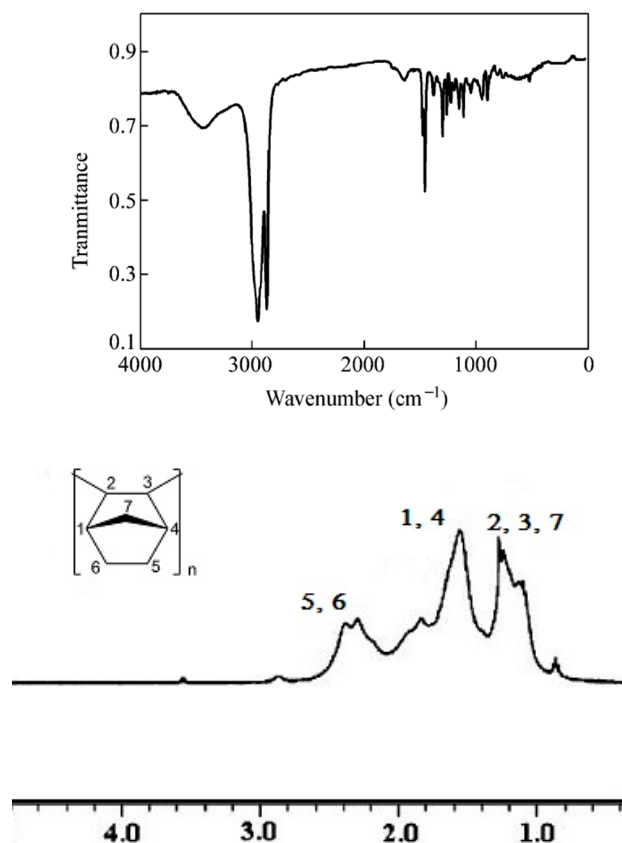
Figure S7. IR spectrum and ¹H NMR spectrum of PNB.

Table S1. Selected Bond Lengths (Å) and Angles (°) for Complexes 2, 4, and 5.

Bond lengths (Å) and angles	2	4	5
Ni(1)–N(1)	1.899(3)	1.901(3)	1.906(4)
Ni(1)–N(1A)	1.899(3)	1.901(3)	1.906(4)
Ni(1)–O(1)	1.833(2)	1.832(2)	1.819(4)
Ni(1)–O(1A)	1.833(2)	1.832(2)	1.819(4)
N(1)–C(11)	1.300(4)	1.310(5)	1.301(6)
O(1)–C(1)	1.308(4)	1.295(4)	1.298(6)
O(1)–Ni(1)–N(1)	88.25(11)	87.44(11)	87.76(16)
O(1)–Ni(1)–N(1A)	91.75(11)	92.56(11)	92.24(16)
O(1A)–Ni(1)–N(1)	89.69(6)	92.56(11)	92.24(16)
O(1A)–Ni(1)–N(1A)	90.31(6)	87.44(11)	87.76(16)
N(1)–Ni(1)–N(1A)	180.00(16)	180.00(2)	180.00(2)
O(1)–Ni(1)–O(1A)	180.00(9)	180.00(2)	180.00(1)

Table S2. Crystal data for Complexes **2**, **4**, and **5**^a.

	2	4	5
	2	4	5
Formula	C ₃₆ H ₂₈ N ₂ NiO ₄	C ₃₆ H ₂₂ F ₆ N ₂ NiO ₂	C ₄₆ H ₄₈ N ₂ NiO ₂
Fw	611.31	687.27	719.57
T/K	293(2)	293(2)	293(2)
Crystal system	monoclinic	monoclinic	triclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>C</i> 2/ <i>c</i>	<i>P</i> -1
<i>a</i> /Å	10.5790(4)	24.966(3)	9.3981(7)
<i>b</i> /Å	9.6679(3)	5.8753(6)	9.7509(13)
<i>c</i> /Å	14.3723(6)	21.035(3)	11.4639(15)
α /°	90.00	90.00	80.721(11)
β /°	95.790(4)	101.040(10)	72.344(9)
γ /°	90.00	90.00	83.028(8)
<i>V</i> /Å ³	1462.45(60)	3028.37(594)	985.03(319)
<i>Z</i>	2	4	1
ρ /g.cm ⁻³	1.38814	1.50731	1.21296
μ /mm ⁻¹	0.707	0.715	0.528
<i>F</i> (0 0 0)	636	1400	336
θ range/°	2.85–26.01	2.81–26.01	2.99–25.01
Reflections collected	5938	12106	6497
Completeness to θ	99.8%	99.8%	99.7%
Data/restraints/param.	2861/0/196	2976/0/214	3466/0/232
Goodness-of-fit on <i>F</i> ²	0.712	0.756	0.906
Final <i>R</i> indices	<i>R</i> ₁ = 0.0434	<i>R</i> ₁ = 0.0520	<i>R</i> ₁ = 0.0844
[<i>I</i> > 2 σ (<i>I</i>) ^a]	<i>wR</i> ₂ = 0.1066	<i>wR</i> ₂ = 0.1698	<i>wR</i> ₂ = 0.2145
	<i>wR</i> ₁ = 0.1066		
λ /Å	0.71073	0.71073	0.71073

^a $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$ (based on reflections with $F_o^2 > 2\sigma F^2$). $wR_2 = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$; $w = 1 / [\sigma^2(F_o^2) + (0.095P)^2]$; $P = [\max(F_o^2, 0) + 2F_c^2] / 3$ (also with $F_o^2 > 2\sigma F^2$).