Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supplementary Information

Synthesis of hyperbranched low molecular weight polyethylene oils by an iminopyridine nickel(II) catalyst

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Table S1: Selected bond lengths and angles for the crystal structure of **1**.

Bond lengths (Å)	**Bond angles (°)**	**Dihedral angles (°)**
Ni1- N1 2.012(3)	N1 - Ni1 - N2 81.7(1)	[PhMe2] - [Ni1] 78.4(1)
Ni1 - N2 2.012(3)	N1 - Ni1- Br1 124.77(9)	[Ph(i-Pr)2] - [Ni1] 71.3(1)
Ni1 - Br1 2.3360(6)	N2 - Ni1- Br1 119.14(8)	[Br1Ni1Br2] - [N1Ni1N2] 89.49(7)
Ni1 - Br2 2.3690(6)	N1 - Ni1- Br2 101.79(9)	
	N2 - Ni1 - Br2 100.72(8)	
	Br1 - Ni1 - Br2 120.47(2)	
	N1 Ni1 N2 81.7(1)	

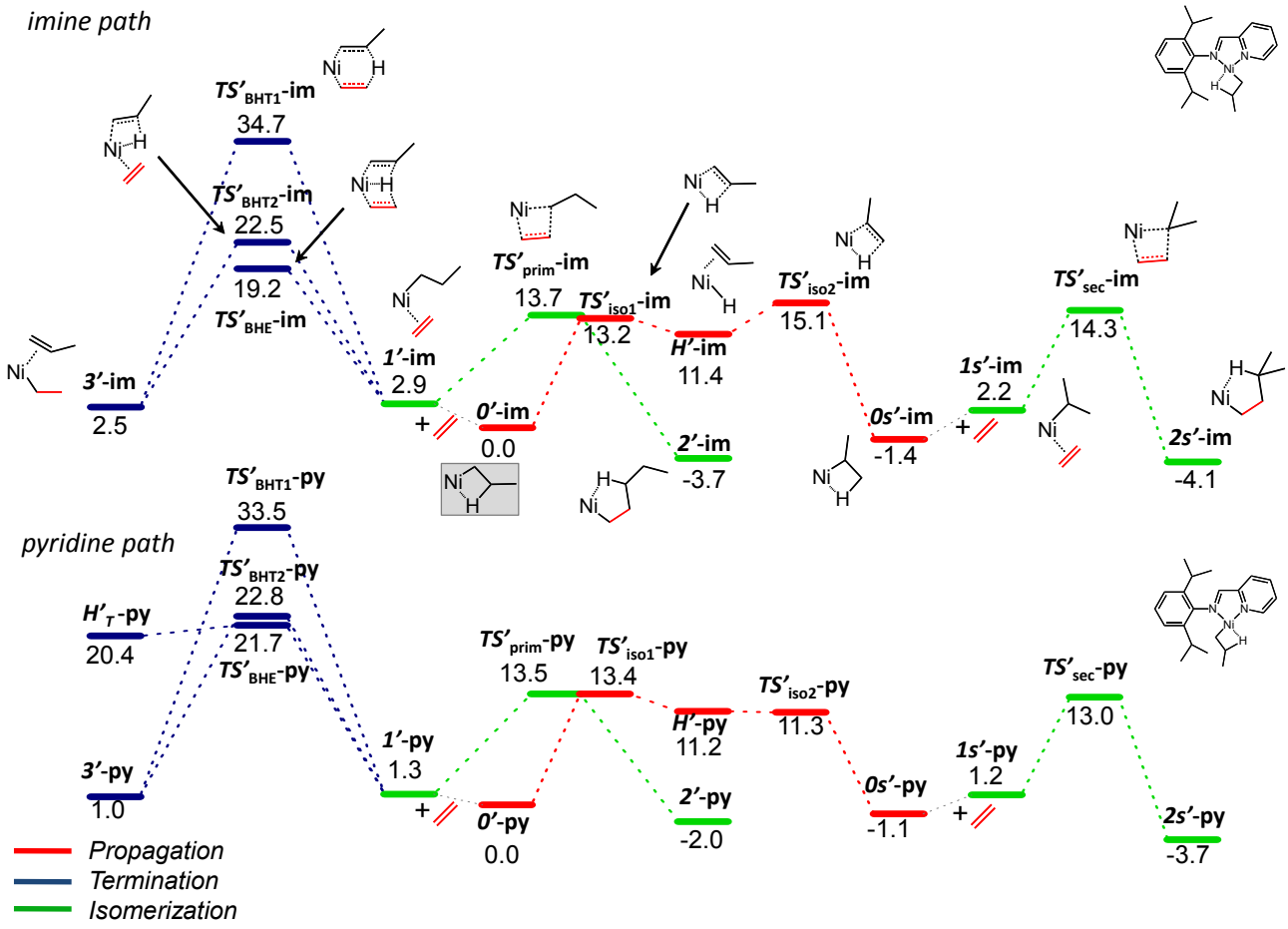
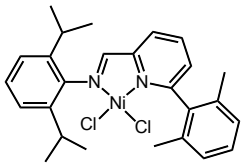
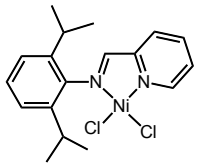


Figure S1. Relative Gibbs free energy profiles corresponding to the competitive reactions for the 2-(2,6-diisopropylphenyl)iminopyridine Ni(II) complex **2.** Energies are given in kcal/mol.

Table S2. Heights of the propagation, insertion and isomerization barriers for the nickel (II) complexes featuring the N-(2,6-diisopropyl-phenyl)-6-(2,6-dimethyl-phenyl)-pyridine-2-carboxaldiimine or the N-(2,6-diisopropyl-phenyl)-pyridine-2-carboxaldiimine as examined in this study. Energies are given in kcal mol^{-1}.

				
	imine path	*pyridine path*	*imine path*	*pyridine path*
Propagation				
$\boldsymbol{TS}_{\mathbf{prim}}$	6.7	9.8	10.8	12.2
$\boldsymbol{TS}_{\mathbf{sec}}$	11.7	11.1	12.1	11.8
Termination				
$\boldsymbol{TS}_{\mathbf{BHE}}$	15.6	16.9	16.3	20.4
$\boldsymbol{TS}_{\mathbf{BHT1}}$	30.5	31.2	31.8	32.2
$\boldsymbol{TS}_{\mathbf{BHT2}}$	18.6	19.5	19.6	21.5
Isomerization				
$\boldsymbol{TS}_{\mathbf{iso1}}$	15.6	15.3	13.2	13.4
$\boldsymbol{TS}_{\mathbf{iso2}}$	1.6	0.2	3.7	0.1

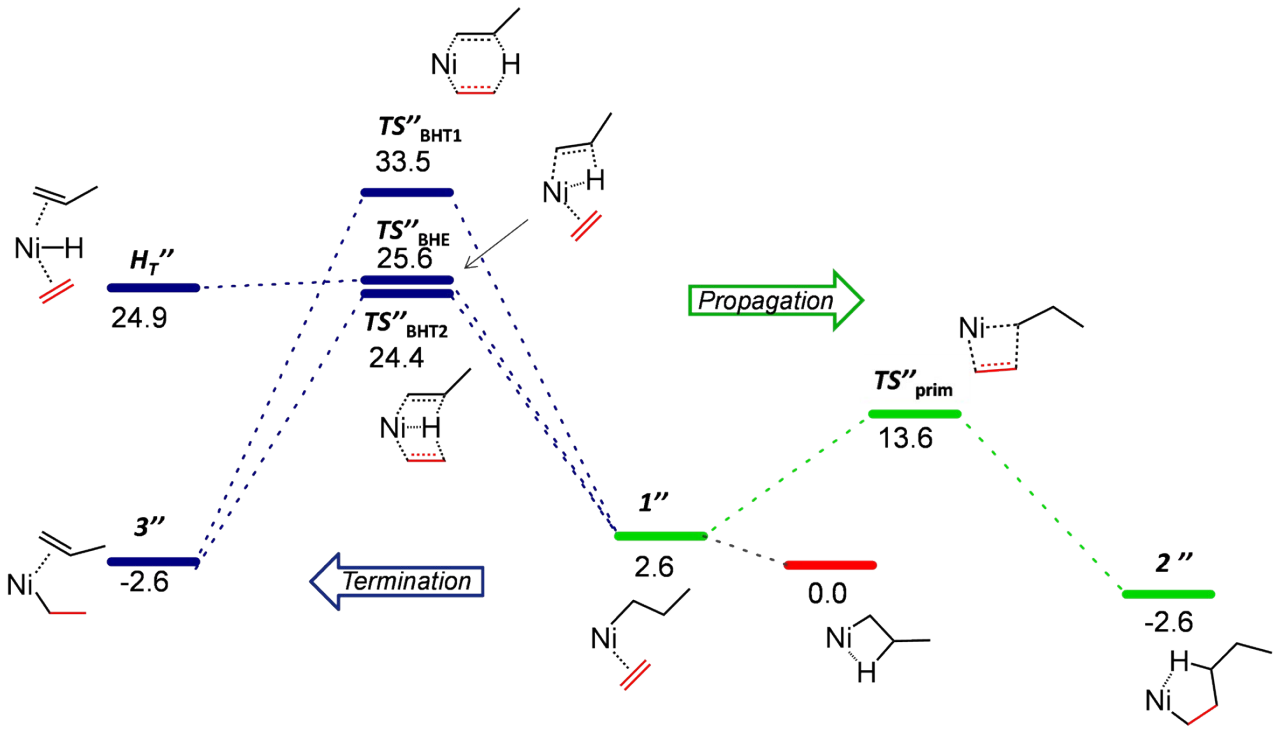


Figure S2. Relative Gibbs free profiles corresponding to the competitive reactions for the N,N'-(2,6-diisopropylphenyl)ethylenediimine Ni(II) Brookhart catalyst. Energies are given in kcal/mol.

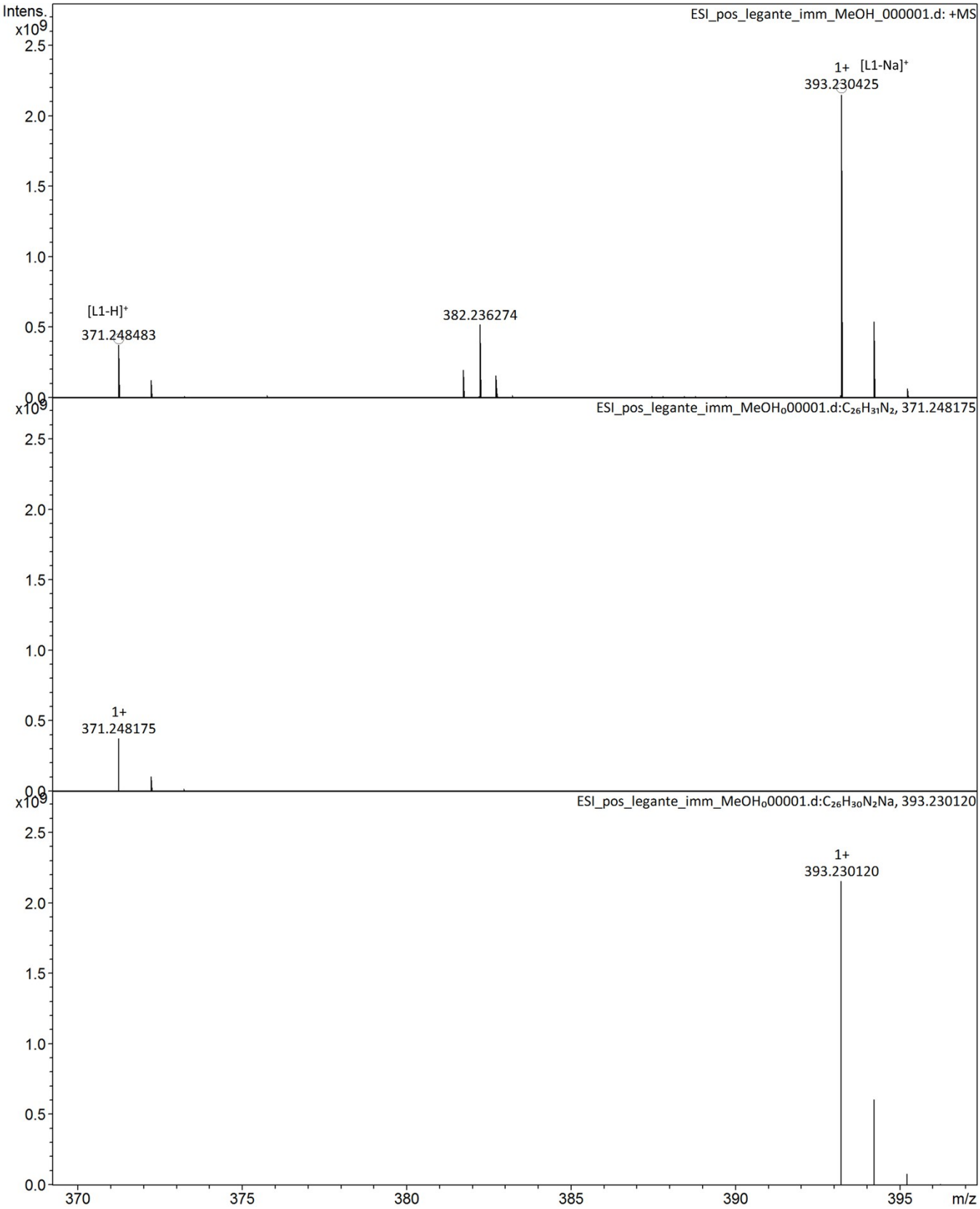


Figure S3. HR ESI FT-ICR mass spectrum of **L1**

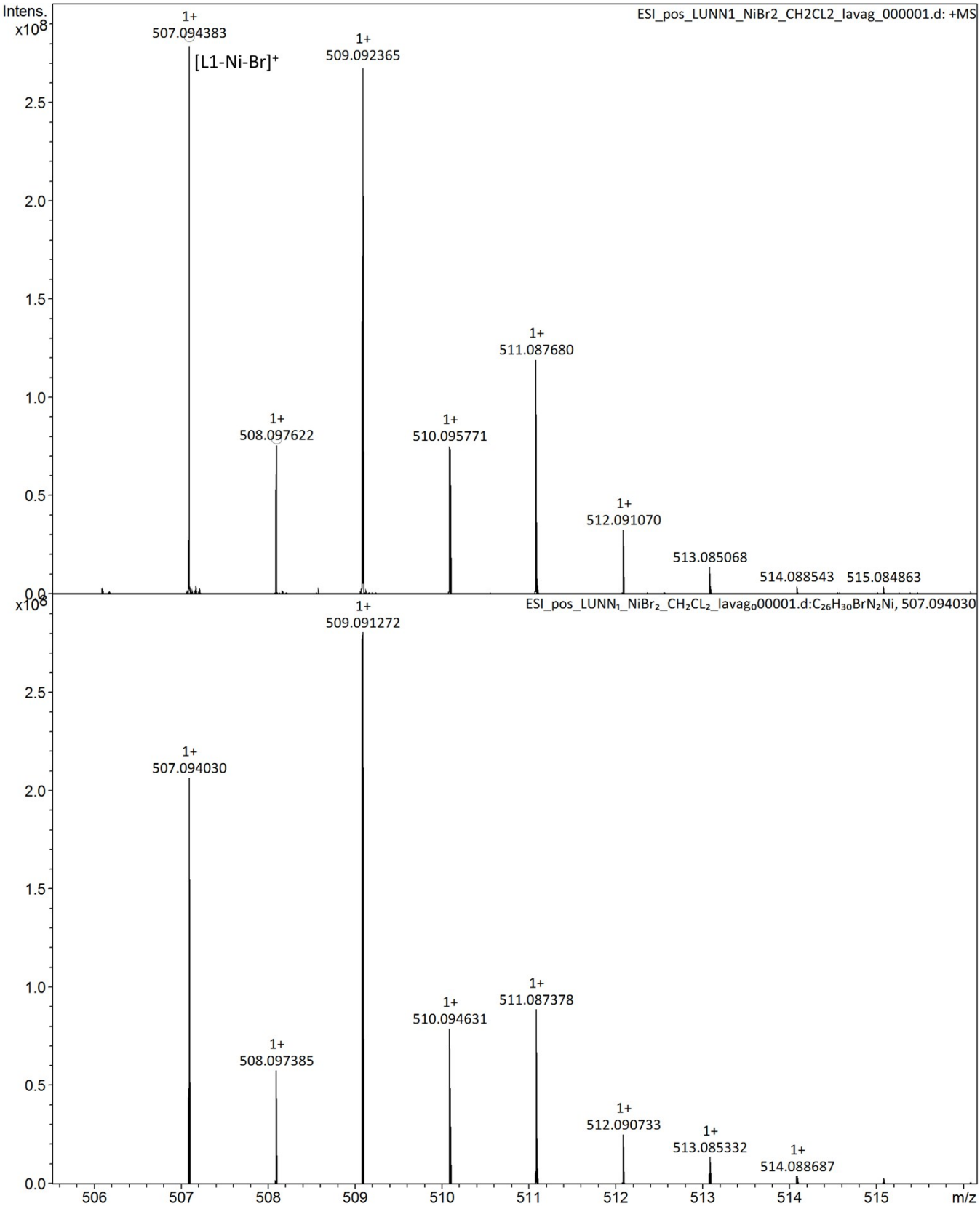


Figure S4. HR ESI FT-ICR mass spectrum of complex **1** [L1-Ni-Br]$^+$ showing the isotope distribution.