

Electronic Supplementary Information for

Ni(II) Complexes Bearing Pyrrolide-Imine Ligands with Pendant O- and S-donor Groups: Synthesis, Structural Characterization and use in Ethylene Oligomerization

A. C. Pinheiro,^a A. H. Virgili,^a Thierry Roisnel,^b Evgueny Kirillov,^c Jean-François Carpentier^{c,*} and Osvaldo de L. Casagrande Jr.^{a,*}

^a *Laboratório de Catálise Molecular, Instituto de Química, Universidade Federal do Rio Grande do Sul, Av. Bento Gonçalves, 9500, Porto Alegre, RS 90501-970, Brazil*

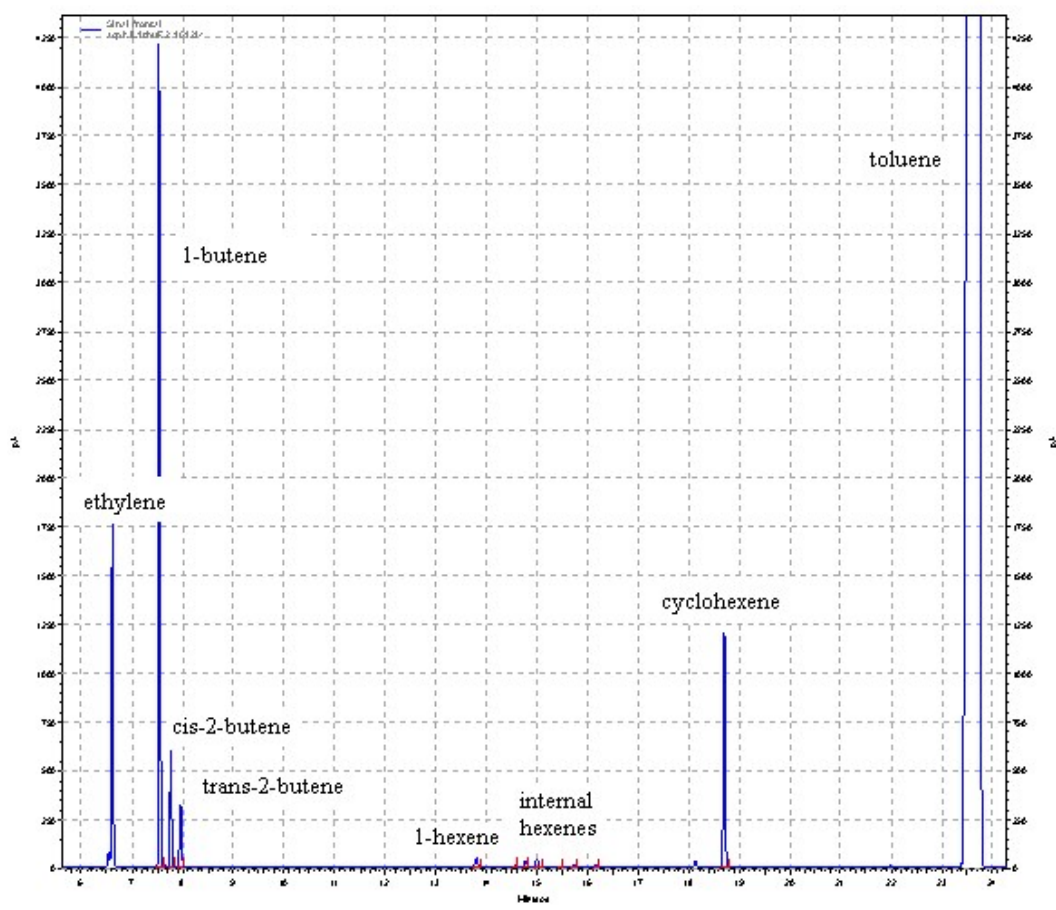
^b *Institut des Sciences Chimiques de Rennes, Centre de diffraction X, UMR 6226 CNRS-Université de Rennes 1, F-35042 Rennes Cedex, France*

^c *Institut des Sciences Chimiques de Rennes, Organometallics: Materials and Catalysis Dept., UMR 6226 CNRS-Université de Rennes 1, F-35042 Rennes Cedex, France*

* Corresponding authors: E-mail: jean-francois.carpentier@univ-rennes1.fr,
osvaldo.casagrande@ufrgs.br

S1. Table of crystallographic data for **Ni1**.

	Ni1
Formula	C ₁₃ H ₁₄ ClN ₃ Ni
CCDC	1407832
Mol. wt.	306.43
Crystal System	Monoclinic
Space group	P2 ₁ /C
<i>a</i> (Å)	7.8815(2)
<i>b</i> (Å)	18.8766(5)
<i>c</i> (Å)	8.5933(2)
α (°)	90
β (°)	95.4990(10)
γ (°)	90
<i>V</i> (Å ³)	1272.59(6)
<i>Z</i>	4
Density (g/cm ³)	1.599
Abs. Coeff., (mm ⁻¹)	1.718
<i>F</i> (000)	632
Crystal size, (mm)	0.19 x 0.16 x 0.06
θ range, deg	3.21 to 27.48
Limiting indices	-10 ≤ <i>h</i> ≤ 10 -24 ≤ <i>k</i> ≤ 17 -11 ≤ <i>l</i> ≤ 11
Reflections collected/independent [<i>R</i> _(int)]	19895 / 2907 [<i>R</i> (int) = 0.0359]
Reflections [<i>I</i> > 2 σ]	2526
Completeness to θ (%)	99.7
Absorption correction type	Multi-scan
Max. and min. transmission	0.902 , 0.807
Data/ restraints/para.	2907 / 0 / 166
Goodness-of-fit	1.031
<i>R</i> ₁ [<i>I</i> > 2 σ (<i>I</i>)] (all data)	0.024
<i>wR</i> ₂ [<i>I</i> > 2 σ (<i>I</i>)] (all data)	0.0565
Largest diff. (e·Å ⁻³)	0.323 and -0.24



Fi

Figure S1. Typical GC trace for the toluene soluble fraction using Ni₂/MAO (Table 1, entry 2, [Al]/[Ni] = 250, oligomerization time = 20 min, P(ethylene) = 20 bar, T = 30°C).

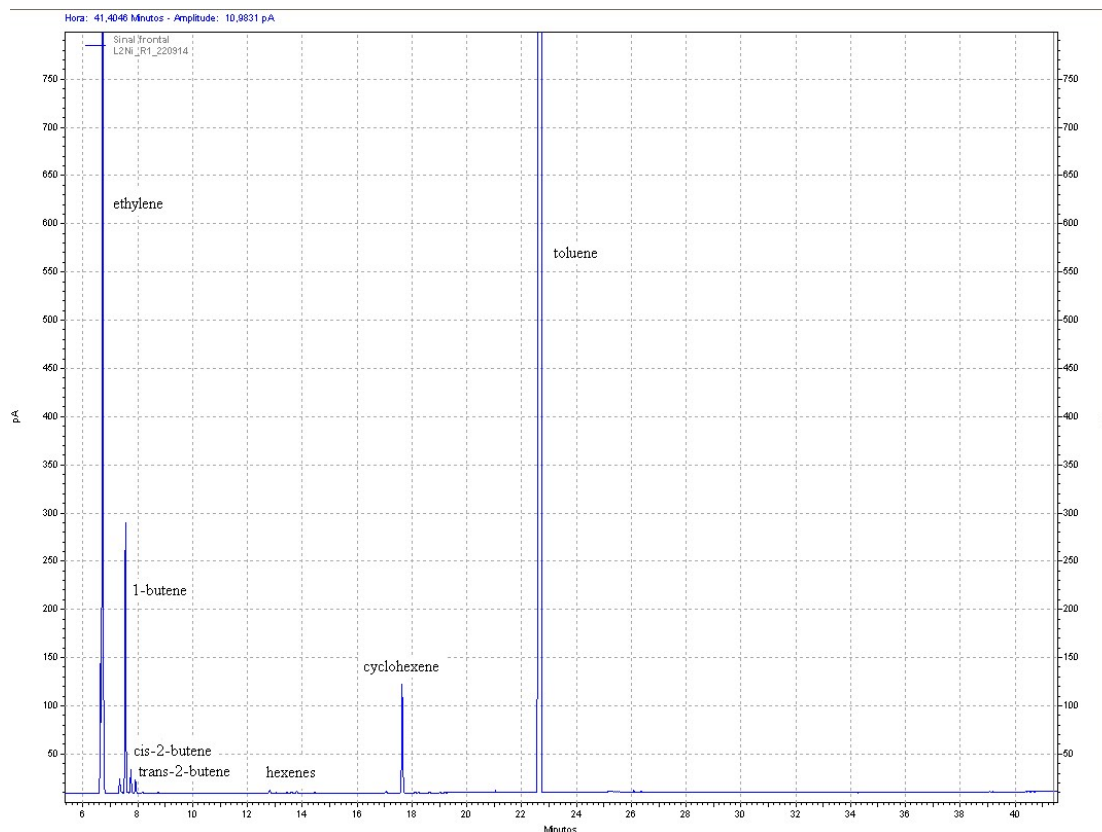


Figure S2. Typical GC trace for the toluene soluble fraction using Ni3/MAO (Table 1, entry 3, [Al]/[Ni] = 250, oligomerization time = 20 min, P(ethylene) = 20 bar, T = 30°C).

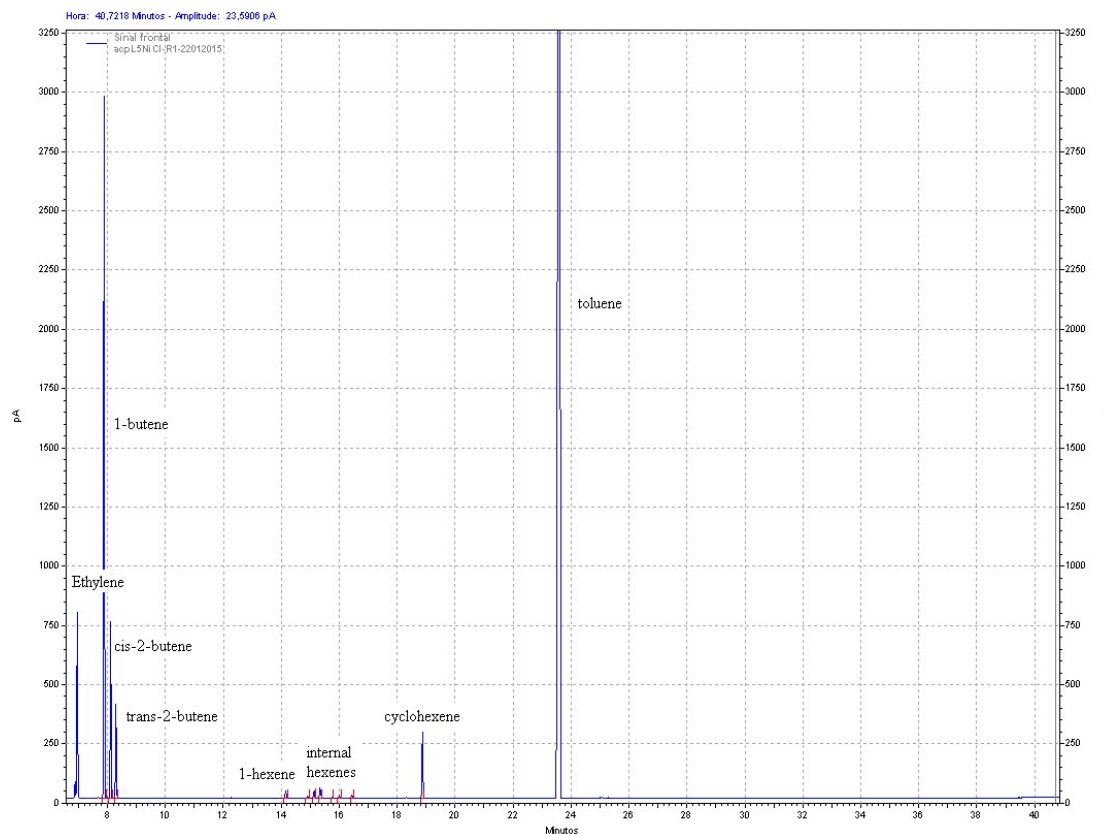


Figure S3. Typical GC trace for the toluene soluble fraction using Ni5/MAO (Table 1, entry 5, $[Al]/[Ni] = 250$, oligomerization time = 20 min, $P(\text{ethylene}) = 20$ bar, $T = 30^\circ\text{C}$).