Electronic Supplementary Information (ESI) for

Zwitterionic Ni(II) Complexes Bearing Pyrazolyl-Ether-Imidazolium Ligands: Synthesis, Structural Characterization and use in Ethylene Oligomerization

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Table S1. Crystallographic data for **L1^{PF6}**·and **L3^{PF6}**.

	L1^{PF6}	**L3^{PF6}**
Formula	C_{13} H_{21} N_4 O, F_6 P	C_{14} H_{23} N_4 O, F_6 P
CCDC	1055620	1055623
Mol. wt.	394.31	408.33
Temperature (K)	120 (2)	100(2)
Crystal System	Triclinic	Monoclinic
Space group	P-1	P 2_1/n
a (Å)	7.3802	9.8869 (4)
b (Å)	8.3070	8.5977 (3)
c (Å)	14.538	21.7613 (9)
α (°)	93.277	90 °
β (°)	99.516	94.160 (2) °
γ (°)	96.900	90 °
V (A^3)	870.0 (2)	1844.94 (12)
Z	2	4
Density (g/cm^3)	1.505	1.47
Abs. Coeff., (mm^{-1})	0.228	0.218
F (000)	408	848
Crystal size, (mm)	0.15 x 0.14 x 0.13	0.33 x 0.26 x 0.15
θ range, deg	3.5 – 27.48 °	3,02 – 27.48 °
Limiting indices	$-9 \leq h \geq 9$	$-9 \leq h \geq 12$
	$-10 \leq k \geq 10$	$-10 \leq k \geq 6$
	$-18 \leq l \geq 18$	$-28 \leq l \geq 26$
Reflections collected/indepent [$R_{(int)}$]	15450/3980 [$R_{(int)}$=0.0477]	9900/4181 [$R_{(int)}$= 0.0343]
Reflections [I>2σ]		
Completeness to θ (%)	99.5	99.2
Absorption correction type	Multi-scan	Multi-scan
Max. and min. transmission	0.971; 0.957	0.968; 0.866
Data/ restraints/para.	3980 / 0 / 232	4181 / 0 / 238
Goodness-of-fit	1.046	1.021
R_1[I>2σ(*I*)] (all data)	0.0348	0.0409
wR_2[I>2σ(*I*)] (all data)	0.0978	0.097
Largest diff. (e·$Å^{-3}$)	0.296 and -0.42	0.269 and -0.358

Table S2. Crystallographic data for **Ni1, Ni2** and **Ni3**.

	Ni1	**Ni2**	**Ni3**
Formula	$2(C_{13}\ H_{21}\ Cl_3\ N_4\ Ni\ O)$	$C_{14}\ H_{19}\ Cl_3\ N_4\ Ni\ O$	$C_{14}\ H_{23}\ Cl_3\ N_4\ Ni\ O$
CCDC	1055629	1055632	1406895
Mol. wt.	828.8	400.37	428.42
Temperature (K)	150 (2)	150(2)	100(2)
Crystal System	Orthorhombic	Monoclinic	Monoclinic
Space group	$Pc2_1b$	$P\ 2_1/c$	$P\ 2_1/n$
a (Å)	8.1781(2)	13.3573 (4)	8.08500(10)
b (Å)	15.6069(3)	7.7215 (2)	17.5163(3)
c (Å)	28.0616(6)	17.1025 (4)	13.4475(2)
α (°)	90	90	90
β (°)	90	104.3550 (10)	99.5100(10)
γ (°)	90	90	90
V (A^3)	3581.64(14)	1708.85 (8)	1878.25(5)
Z	4	4	4
Density (g/cm^3)	1.537	1.556	1.515
Abs. Coeff., (mm^{-1})	1.536	1.607	1.467
F (000)	1712	824	888
Crystal size, (mm)	0.28 x 0.18 x 0.07	0.38 x 0.29 x 0.13	0.26 x 0.19 x 0.09
θ range, deg	3.56 – 27.44°	1.57 – 27.49	2.99 – 27.48
Limiting indices	$-10 \le h \ge 10$	$-17 \le h \ge 17$	$-10 \le h \ge 10$
	$-20 \le k \ge 20$	$-9 \le k \ge 10$	$-22 \le k \ge 22$
	$-36 \le l \ge 36$	$-22 \le l \ge 22$	$-17 \le l \ge 13$
Reflections collected/indepent	54557 / 8156	14787 / 3902	15723 / 4278
$[R_{(int)}]$	[R(int) = 0.0338]	[R(int) = 0.0417]	[R(int) = 0.0251]
Completeness to θ (%)	99.7	99.7	99.1
Absorption correction type	Multi-scan	Multi-scan	Multi-scan
Max. and min. transmission	0.898; 0.767	0.811; 0.685	0.876 ; 0.695
Data/ restraints/para.	8156 / 1 / 403	3092/ 0 / 194	4278 / 0 / 212
Goodness-of-fit	1.034	1.019	1.021
R_1[I>2σ(*I*)] (all data)	0.0192	0.0279	0.0258
wR_2[I>2σ(*I*)] (all data)	0.0467	0.0678	0.0638
Largest diff. ($e \cdot Å^{-3}$)	0.293 and -0.191	0.286 and -0.267	0.777 e -0.285