Supporting Information

Highly active half-sandwich chromium(III) catalysts bearing bis(imino)pyrrole ligands for ethylene (co)polymerization

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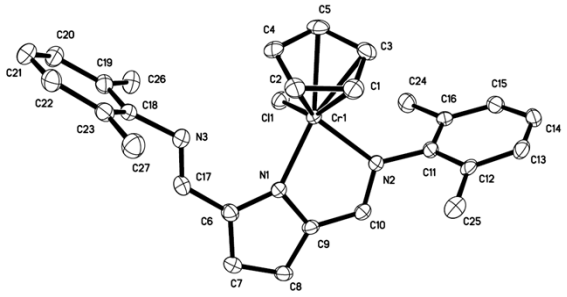

Fig. S1 Molecular structure of complex **2b** with thermal ellipsoids at 30% probability level. Hydrogen atoms are omitted for clarity.

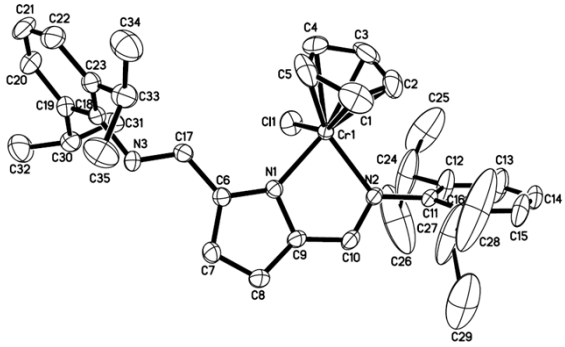

Fig. S2 Molecular structure of complex **2c** with thermal ellipsoids at 30% probability level. Hydrogen atoms are omitted for clarity.

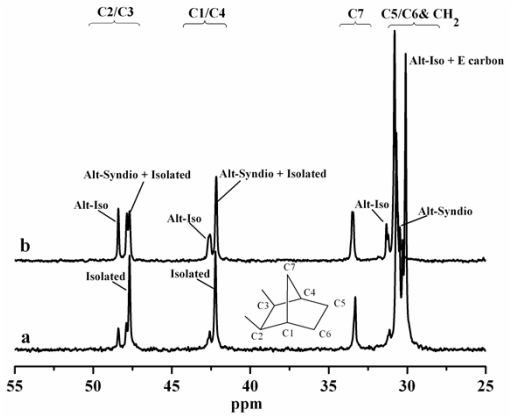

Fig. S3 ^{13}C NMR spectra of E/NBE copolymer with different NBE incorporations produced by **2c** (a: 18.1%, entry 3; b: 38.8%, entry 7 in Table 3, respectively).

Table S1. Crystal data and structure refinements of complexes **2a-c.**

	2a	**2b**	**2c**
Empirical formula	$C_{23}H_{19}ClCrN_3$	$C_{27}H_{27}ClCrN_3$	$C_{35}H_{43}ClCrN_3$
Formula weight	424.86	480.97	593.17
Crystal system	monoclinic	monoclinic	orthorhombic
Space group	P2(1)/c	P2(1)/c	Pbca
a (Å)	17.7884(12)	11.4826(9)	18.7272(13)
b (Å)	7.5640(5)	9.7676(8)	11.8149(8)
c (Å)	14.5599(10)	24.3114(19)	29.400(2)
α (°)	90.00	90.00	90.00
β (°)	92.5180(10)	98.2830(10)	90.00
γ (°)	90.00	90.00	90.00
V (Å^3), Z	1957.2(2), 4	2698.3(4), 4	6505.0(8), 8
$Density_{calcd}$ (Mg/m^3)	1.442	1.184	1.211
Absorption coefficient (mm^{-1})	0.734	0.540	0.461
F(000)	876	1004	2520
Crystal size/mm	0.34×0.21×0.14	0.28× 0.21×0.13	0.32× 0.23×0.15
θ range for data collection (°)	2.29 to 26.01	1.69 to 26.03	1.76 to 25.04
Reflections collected	12033	16758	36643
Independent reflections	3846 (R_{int} = 0.0218)	5297 (R_{int} = 0.0509)	5747 (R_{int} = 0.1032)
Data/restraints/ parameters	3846/0/253	5297/0/289	5747/0/369
Goodness-of-fit on F^2	1.036	1.043	1.018
Final R indices [I>2σ (I)]: R1, wR2	0.0363, 0.0940	0.0599, 0.1534	0.0742, 0.1683
Largest diff. Peak and hole (e Å^{-3})	0.342 and -0.266	0.474 and -0.434	0.660 and -0.594