Supporting Information for

Chromium (III)-bis(iminophoshoranyl) methanido Complexes – Synthesis, X-ray Crystal Structures and Catalytic Ethylene Oligomerization

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Table T1: Crystal structure data for **3a**-**c**.

Compound	**3a**	**3b**	**3c**
Crystal size [mm]	0.22 × 0.22 × 0.10	0.26 × 0.16 × 0.12	0.22 × 0.10 × 0.06
Empirical formula	$C_{62}H_{70}Cl_4Cr_2N_4P_4$. $6(CH_2Cl_2)$	$C_{66}H_{78}Cl_4Cr_2N_4P_4$. (C_4H_8O)	$C_{39}H_{35}Cl_2O_4CrN_2O_2P_2.2(C_4H_8O)$
Molecular mass	1750.46	1441.26	893.78
Crystal system	triclinic	monoclinic	triclinic
space group	*P-1*	$P2_1/c$	*P-1*
a [Å]	12.779(1)	11.078(1)	9.412(1)
b [Å]	12.956(1)	22.191(1)	13.128(1)
c [Å]	13.700(1)	14.487(1)	18.731(1)
α [°]	77.252(1)	90.000	72.651(1)
β [°]	69.776(1)	97.136(1)	83.444(1)
γ[°]	69.642(1)	90.000	80.124(1)
V [Å]^3	1982.4(3)	3533.8(3)	2171.5(3)
Z	1	2	2
Calcd. Dens. [g.cm^{-3}]	1.466	1.354	1.367
Abs. Coeff. [cm^{-1}]	0.936	0.598	0.506
θ_{max} [deg.]	30.03	27.46	25.35
F(000)	898	1516	936
Index ranges	-17 17; -18 17; -16 19	-14 14; -26 28; -13 18	-10 11; -15 15; -22 21
Refl. coll./indep.	29661/11583	25183/8075	16829/7856
Refl. used	9507	6023	5263
(R_{int})	0.0219	0.0331	0.0422
Abs. corr.	multi-scan, 0.8205 min, 0.9122 max	multi-scan, 0.8600 min, 0.9317 max	multi-scan, 0.8967 min, 0.9703 max
Parameters refined	429	412	525
Reflection/parameter	22	14	10
Final R1[a]/	0.0354/0.1001	0.0449/0.1360	0.0732/0.2266
*w*R2 [I>2σ(*I*)] [b]			
Goodness-of-fit on F^2	1.051	1.048	1.022
Diff. peak/hole	0.895(0.064)/	0.955(0.074)/	1.037(0.100)/
[e.Å^{-3}]	-0.783(0.064)	-0.618(0.074)	-0.729(0.100)

[a] $R1 = \Sigma \left| |F_o| - |F_c| \right| / \Sigma |F_o|$, [b] $wR2 = (\Sigma w \left| |F_o| - |Fc| \right|^2 / \Sigma w |F_o|^2)^{1/2}$

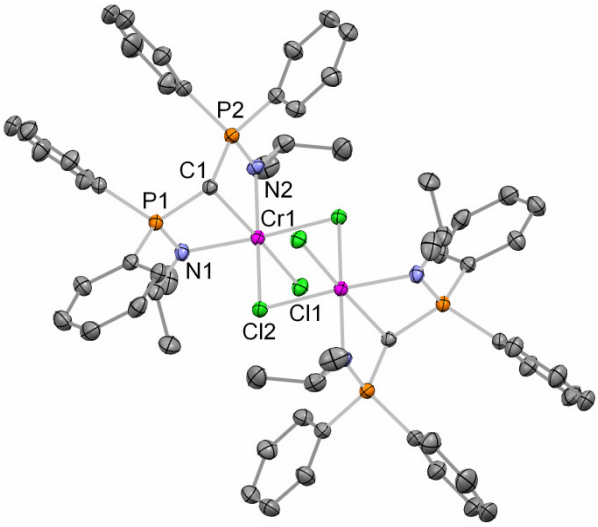
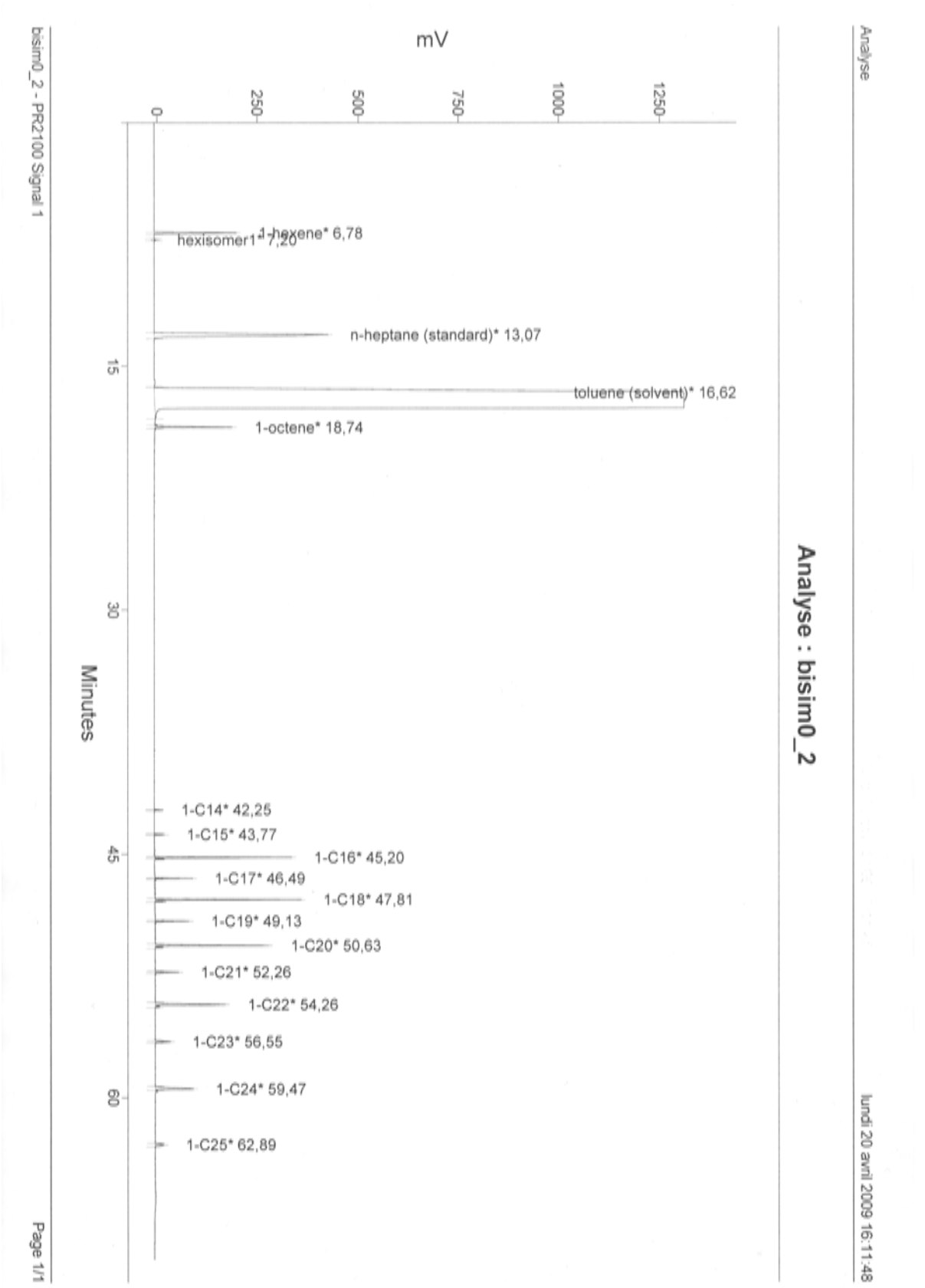
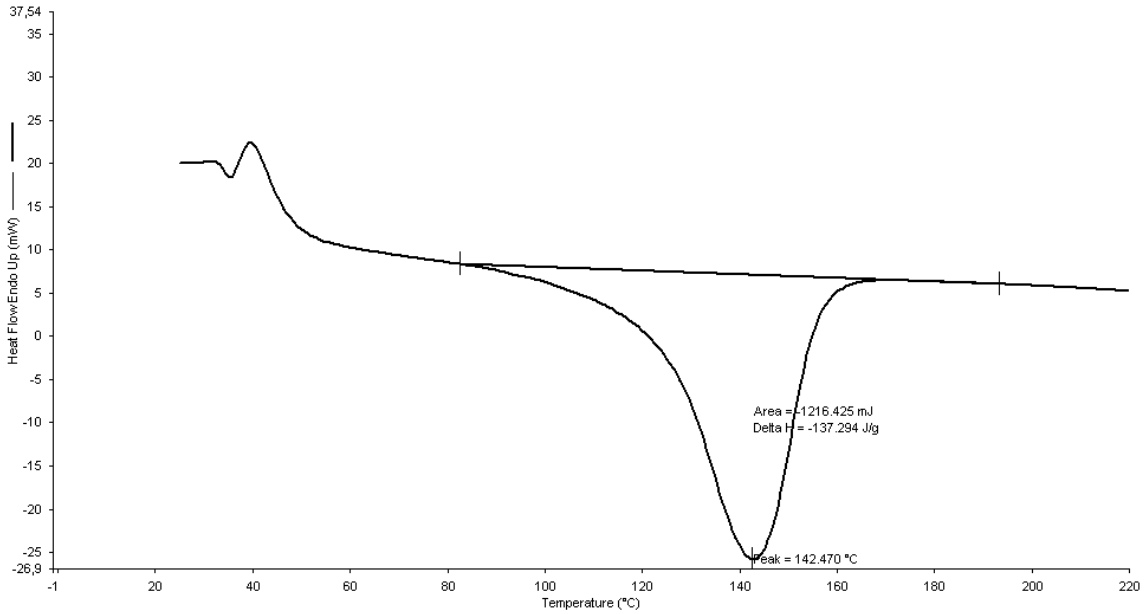


Figure S1: Ortep plot of **3a** which lies about an inversion centre. Hydrogen atoms and six dichloromethane solvent molecules have been omitted for clarity. Ellipsoids are drawn at the 50% probability level.



Scheme S2: GC plot of run 2. This analysis is made from an effluent recovered by vacuum flash distillation of the product mixture at the end of the catalytic run. The distillation resulted in the complete loss of the C4 fraction, and partial loss of the C6 fraction, which thus cannot be quantified from the present GC trace.



Scheme S3: DSC graph of polymer obtained from run 2.

The DSC were recorded using a Perkin-Elmer DSC-7 calorimeter. The samples were heated twice from ambient temperature (a.t.) to 220°C at a rate of 20°C per minute, then cooled down to a.t. at 20°C per minute. The third run (equally from a.t. to 220°C) was used to determine the polymer melting point. Sample quantities of 7.4 to 8.9 mg were employed in stamped Al pans (50 µL) with pierced holes.

Table T2: Recorded melting points of polymer obtained from catalytic runs 1-7.

Catalytic run	T_m/°C
1	138.3
2	142.5
3	149.8
4	127.1
5	133.8
6	136.5
7	138.5