

Supporting information for

Olefin polymerization by zirconium enolatoimine complexes

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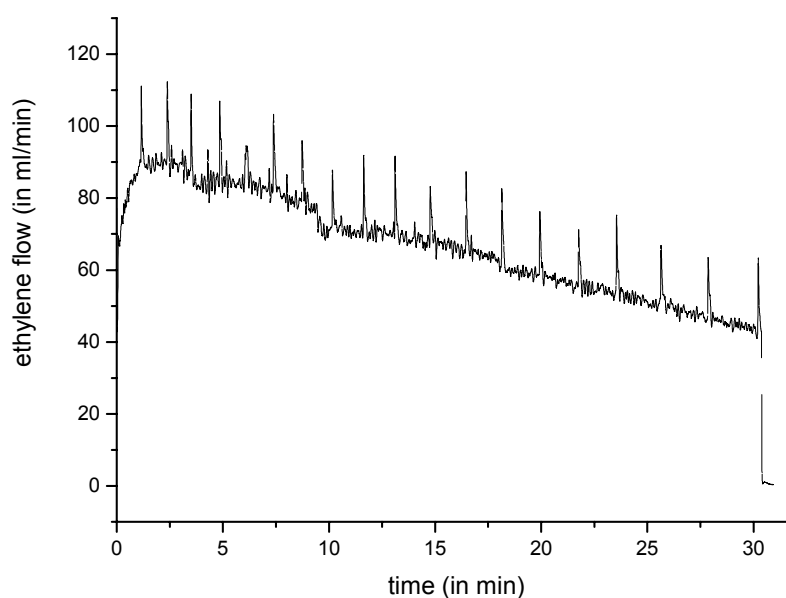


Figure S1. Ethylene mass flow of polymerization with **2b** at 25 °C (Table 2, entry 8).

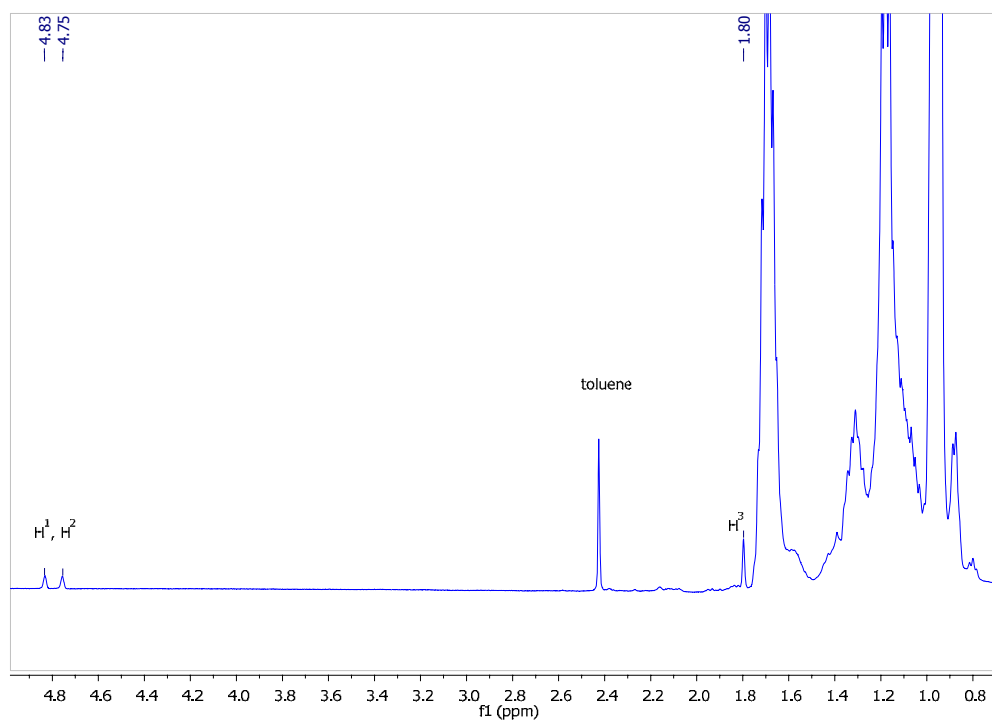


Figure S2. ^1H NMR spectrum of polypropylene obtained with complex **2b** at 25 °C; (measured at 100 MHz, solvent 1,1,2,2-tetrachloroethane- d_2 , T= 130 °C).

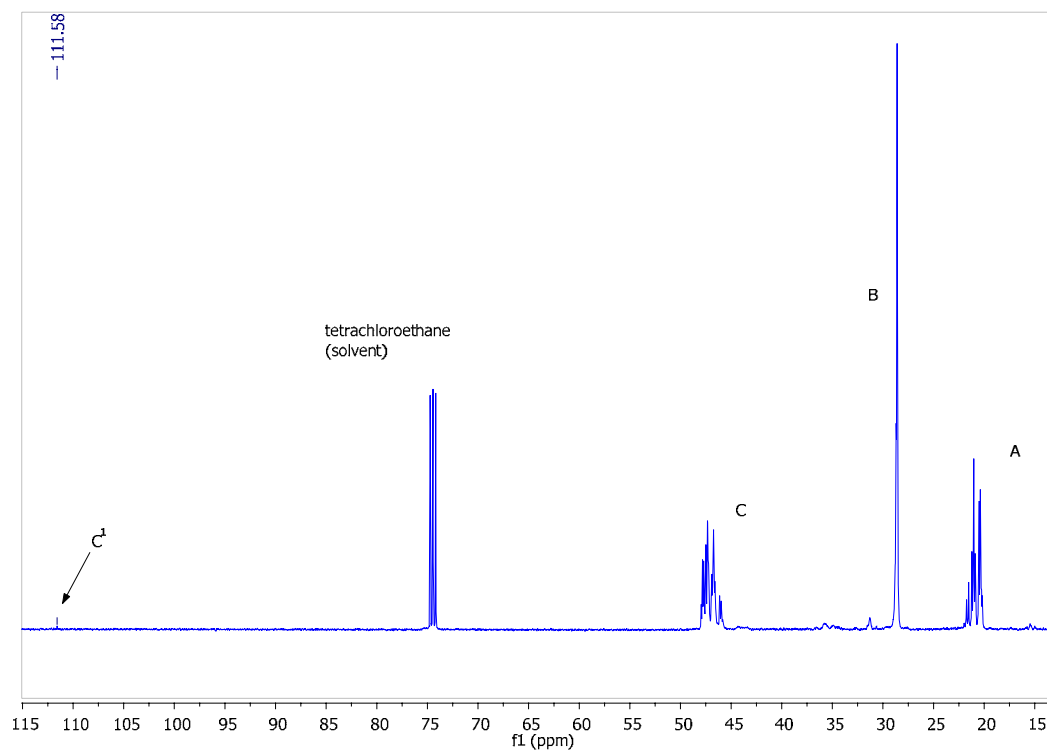


Figure S3. ^{13}C NMR spectrum of polypropylene obtained with complex **2b** at 25 °C; (measured at 100 MHz, solvent 1,1,2,2-tetrachloroethane - d_2 , T= 130 °C; A= CH_3 , B= CH , C= CH_2).

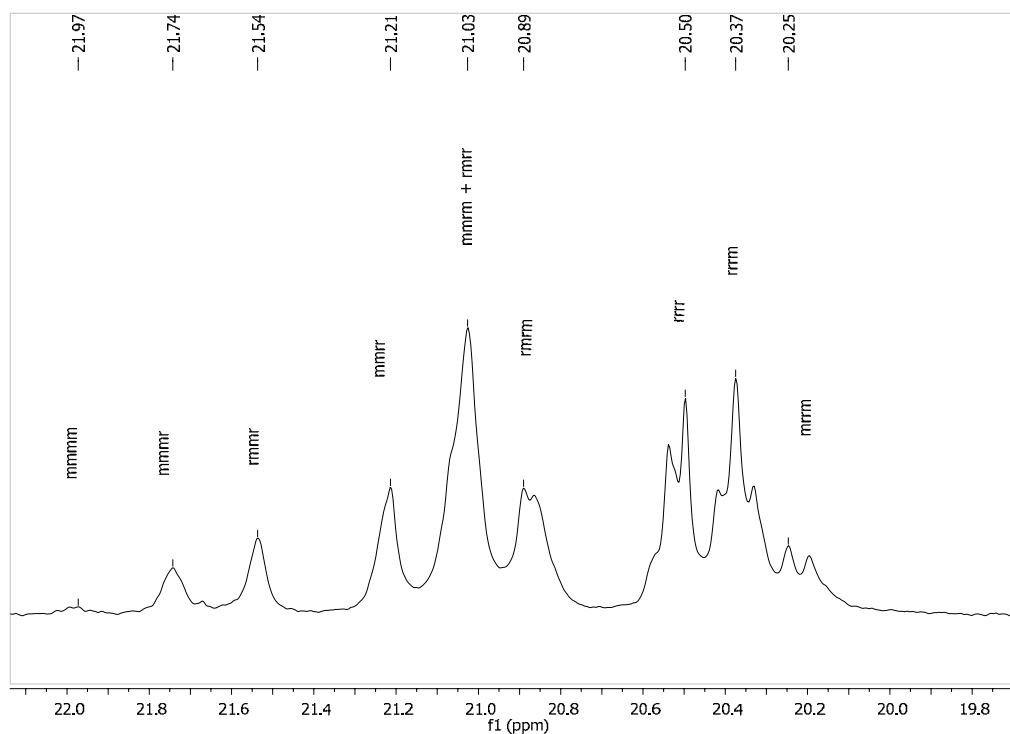


Figure S4. Assignment of the methyl resonances of regioregular sequences of polypropylene prepared with **2b**/MAO, cf. ref [1].

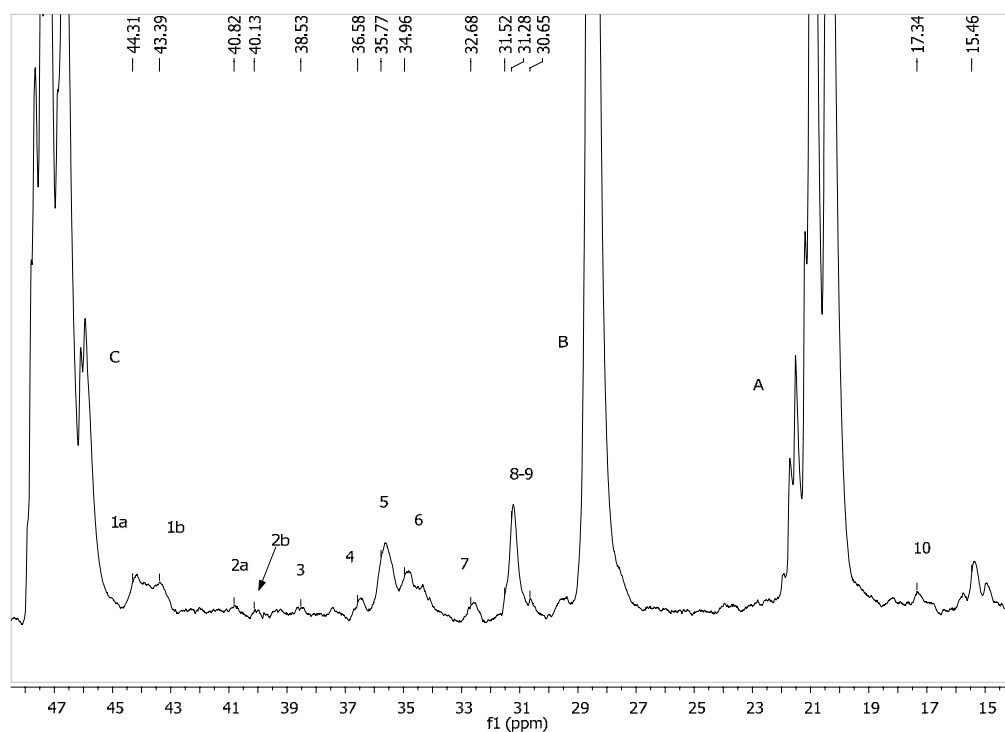


Figure S5. Resonances of regioirregular sequences (1 to 10) of polypropylene prepared with **2b**/MAO (A= CH_3 , B= CH , C= CH_2), cf. ref [2].

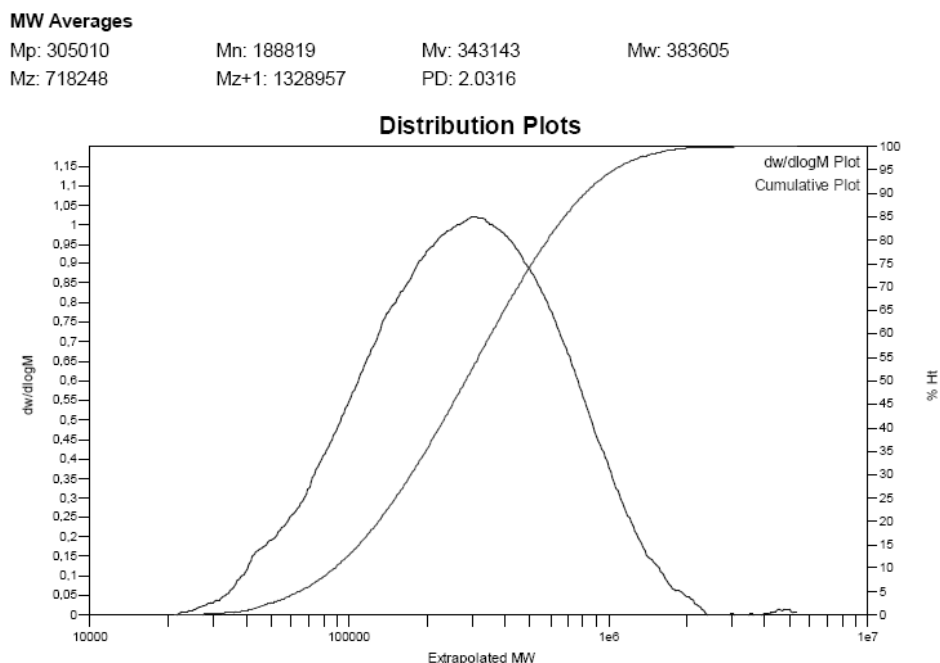


Figure S6. GPC profile of PE obtained with complex **2b** at 25 °C (Table 2, entry 6).

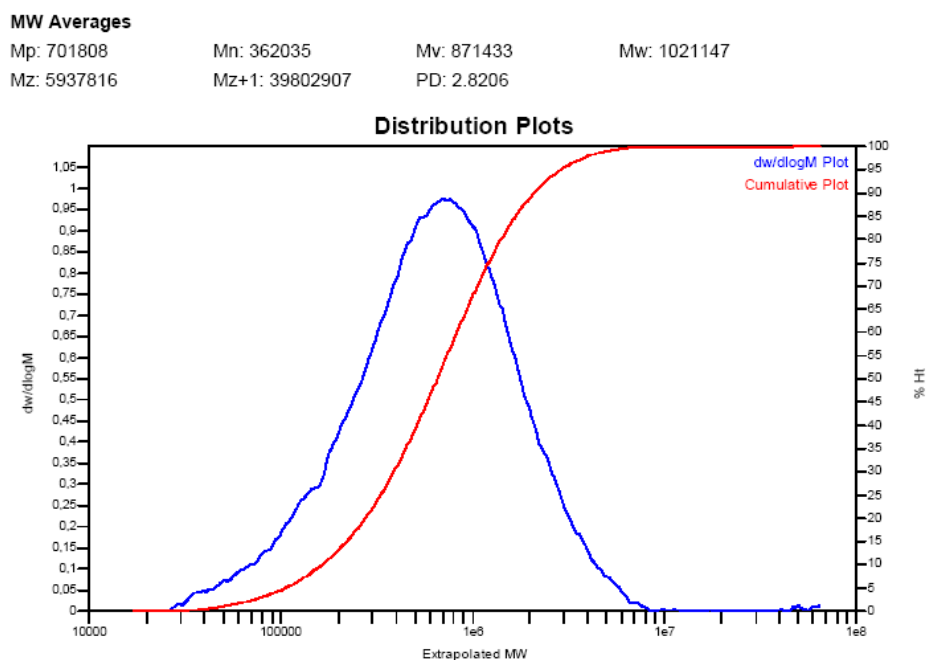


Figure S7. GPC profile of PE obtained with complex **2c** at 50 °C (Table 2, entry 11).

References

- 1) V. Busico, R. Cipullo, G. Monaco, M. Vacatello, A. L. Segre, *Macromolecules* 1997, **30**, 6251.
- 2) H. N. Cheng, *Polymer Bulletin*, 1985, **14**, 347.

Table S1 Details of the crystal structure determination of **1d**, **2a**, **2b** and **2d**.

	1d	2a	2b	2d
formula	C ₁₇ H ₂₂ F ₃ N O	C ₂₂ H ₁₈ Cl ₂ F ₆ N ₂ O ₂ Zr	C ₂₂ H ₁₄ Cl ₂ F ₁₀ N ₂ O ₂ Zr	C ₃₄ H ₄₂ Cl ₂ F ₆ N ₂ O ₂ Zr
fw	313.36	618.50	690.47	786.82
cryst. size, mm	0.4 x 0.367 x 0.3	0.4 x 0.383 x 0.35	0.38 x 0.36 x 0.35	0.3 x 0.23 x 0.15
space group	C2/c	C2/c	C2/c	<i>P</i> -1
a, Å	19.4589(11)	9.7961(6)	10.313(9)	11.652(3)
b, Å	16.3091(10)	14.0461(8)	13.317(1)	11.781(2)
c, Å	11.5997(6)	18.3236(12)	19.161(2)	13.684(2)
α, deg.	90.00	90.00	90.00	74.216(12)
β, deg.	112.240(4)	95.011(5)	95.468(9)	82.723(17)
γ, deg.	90.00	90.00	90.00	86.135(17)
V, Å ³	3407.4(3)	2511.6(3)	2619.8(5)	1791.9(6)
Z	8	4	4	2
δ _{calc} , g cm ⁻³	1.222	1.636	1.751	1.458
T, K	100	100	100	100
μ, mm ⁻¹	0.98	0.717	0.719	0.52
F(000)	1328	1232	1360	808
Θ _{max} , deg.	27.45	28.06	26.84	27.72
no. of rflns measd.	26306	18366	17115	28369
no. of unique rflns	3859	3015	2789	8067
no. of rflns I > 2σ(I)	2937	2643	2428	6610
R ₁ , I > 2σ(I) ^a	0.0455	0.0394	0.0301	0.0364
R ₁ , all data	0.0681	0.0473	0.0386	0.0516
wR ₂ ^a	0.1216	0.0736	0.072	0.0949
diff. Fourier peak min./ max., e Å ⁻³	-0.27/ 0.26	-0.50/ 0.45	-0.81/ 0.36	-0.69/ 0.74

$$^a R_1 = \sum |F_0 - F_c| / \sum |F_0|, wR_2 = [\sum (w(F_0^2 - F_c^2)^2) / \sum (w(F_0^2)^2)]^{1/2}$$