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Novel High and Ultrahigh Molecular Weight Poly(propylene) Plastomers by Asymmetric Hafnocene Catalysts

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Crystal structure of catalyst 7b

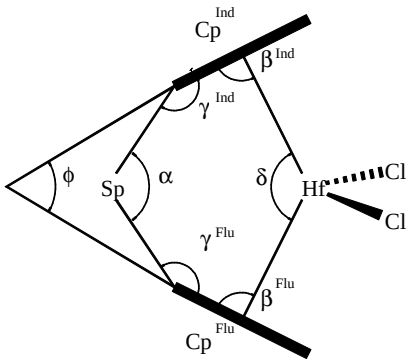

Figure 10 Schematic illustration of relevant bond angles

The Cp^{Flu}-Hf-Cp^{Ind} angle (δ:128.51°, Table 6 Supp. Inf.) is in between those of the complexes **6b** [11] (δ: 128.04°) and **6a** [5] (δ: 128.6°). The γ-angles, slightly smaller than 180° (γ^{Flu} = 171.51°, γ^{Ind} =178.6°), are in good agreement with the results previously reported for other bridged indenyl and fluorenyl complexes.[11] The Hf-fluorenyl centroid bond of **7b** (2.59 Å) is distinctly longer than the distance between Hf(V) and the indenyl centroid (2.50 Å) leading to a non-symmetric positioning of the Hf(IV)-center between the two Cp planes. A β^{Ind} value of 87.14° points toward a nearly ideal η^5-coordination of the indenyl ring to Hf(IV). This is different for the fluorenyl fragment. The value of β^{Flu} close to 80° (80.42°) and the corresponding Hf-C distances (ranging from 2.405 to 2.707 Å) clearly indicate a reduced hapticity of the fluorenyl fragment toward η^3 coordination. Therein, complex **7b** exhibits a structural characteristic that was also observed for unbridged and bridged bisfluorenyl zirconium complexes.

Table 5 Summary of Crystal Data and Structure Refinement Parameters for **7b**

chemical formula	$C_{27}H_{24}Cl_2Hf$
Fw	597.85
cryst color and form	yellow plate
cryst syst	monoclinic
space group	$P2_1/n$
a(Å)	12.1940(12)
b(Å)	15. 2188(11)
c(Å)	12.2284(13)
α (deg)	90.0
β(deg)	102.066
γ(deg)	90.0
V(Å^3)	2219.2(4)
Z	4
D_C (Mg/m^3)	1.789
Abs coeff μ (mm^{-1})	4.953
F(000)	1168
cryst size (mm)	0.34×0.28×0.24
scan mode	2θ/ω
θ_{max} (deg)	25.92
index ranges	$0 \le h \le 11$
	$-17 \le k \le 17$
	$-10 \le l \le 10$
no. of unique/all reflns	4284/4284
no. of params	272
goodness-of-fit on S(F^2)[a]	1.038
final R indices [I>2σ(I)][b]	R_1 = 0.0340, wR_2 = 0.0807
R indices (all data)[b]	R_1 = 0.0429, wR_2 = 0.0841
Largest differential peak and hole (e/Å^3)	2.299 and –2.915

[a] $S = [\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters. [b] $R(F) = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR(F^2) = [\Sigma(w(F_o^2 - F_c^2)^2/\Sigma wF_o^4]^{1/2}$.

Table 6 Relevant Geometrical Parameters for **7b**

β^{Flu}	80.42(5)
β^{Ind}	87.14(5)
γ^{Flu}	171.51(5)
γ^{Ind}	178.6(5)
ϕ	62.93(5)
δ	128.51(5)
Cl-Hf-Cl	97.14(4)
Hf-Cl(1)	2.3909(12)
Hf-Cl(2)	2.4027(12)
av. Hf-centroid(Cp^{Flu})[a]	2.582(6)
av. Hf-centroid(Cp^{Ind})[a]	2.508(4)
Hf1-C4 (Cp^{Flu})	2.707(5)
Hf1-C5 (Cp^{Flu})	2.533(5)
Hf1-C7 (Cp^{Flu})	2.688(5)
Hf1-C8 (Cp^{Flu})	2.560(5)
Hf1-C9 (Cp^{Flu})	2.405(5)
Hf1-C14 (Cp^{Ind})	2.537(4)
Hf1-C19 (Cp^{Ind})	2.584(5)
Hf1-C20 (Cp^{Ind})	2.484(5)
Hf1-C21 (Cp^{Ind})	2.477(4)
Hf1-C22 (Cp^{Ind})	2.458(4)