Reactions of cationic palladium alpha-diimine complexes with nitrogen-containing olefins

Li, Weidong; Zhang, Xiaochun; Meetsma, Auke; Hessen, Bart

Published in:
Organometallics

DOI:
10.1021/om701059t

Publication date:
2008

Supporting Information to:

"Reactions of Cationic Palladium α-Diimine Complexes with Nitrogen-containing Olefins: Branched Polyethylene with Carbazole Functionalities"

by W. Li, X. Zhang, A. Meetsma and B.Hessen

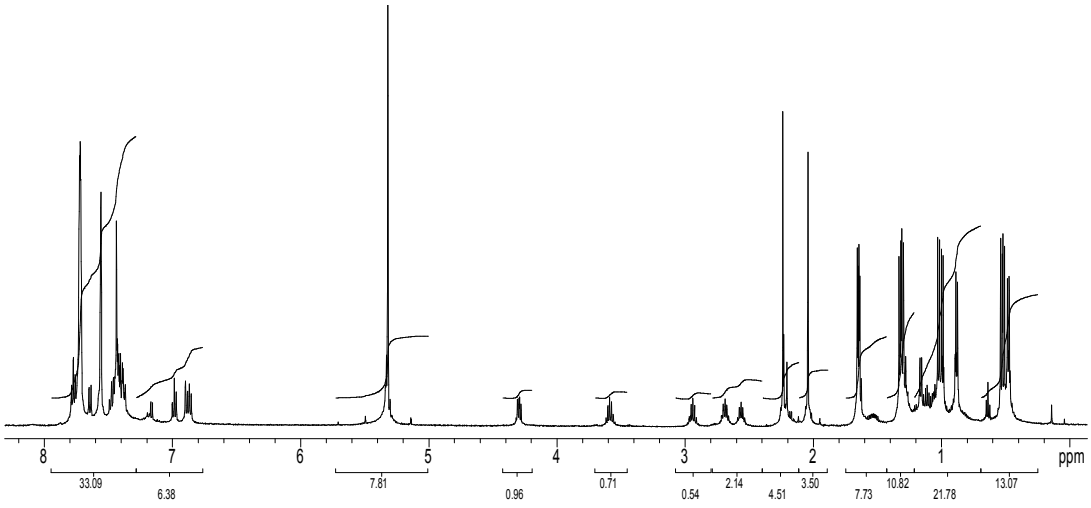

Figure S-1a. ^{1}H NMR spectrum of **2**. [500 MHz, CD_2Cl_2 solvent, 23°C]

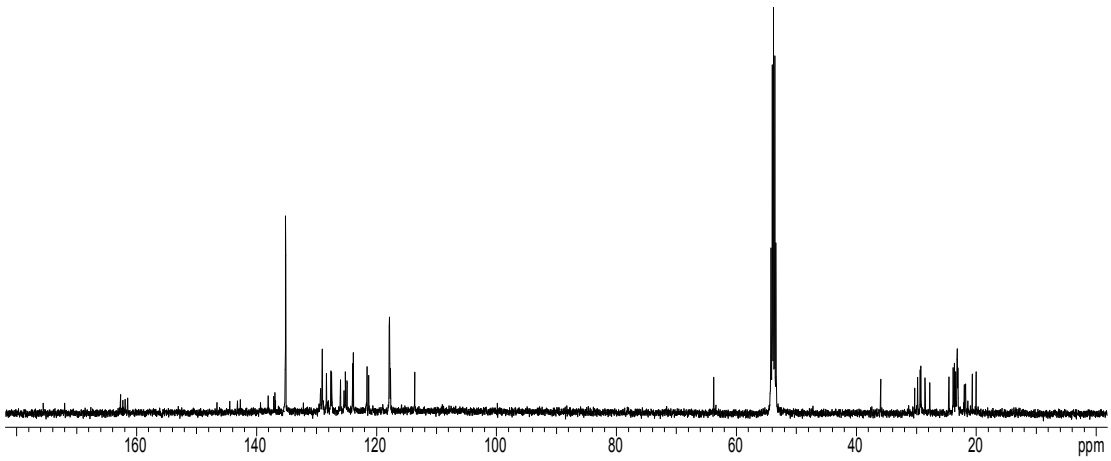

Figure S-1b. $^{13}C\{^{1}H\}$ NMR spectrum of **2**. [126 MHz, CD_2Cl_2 solvent, 23°C]

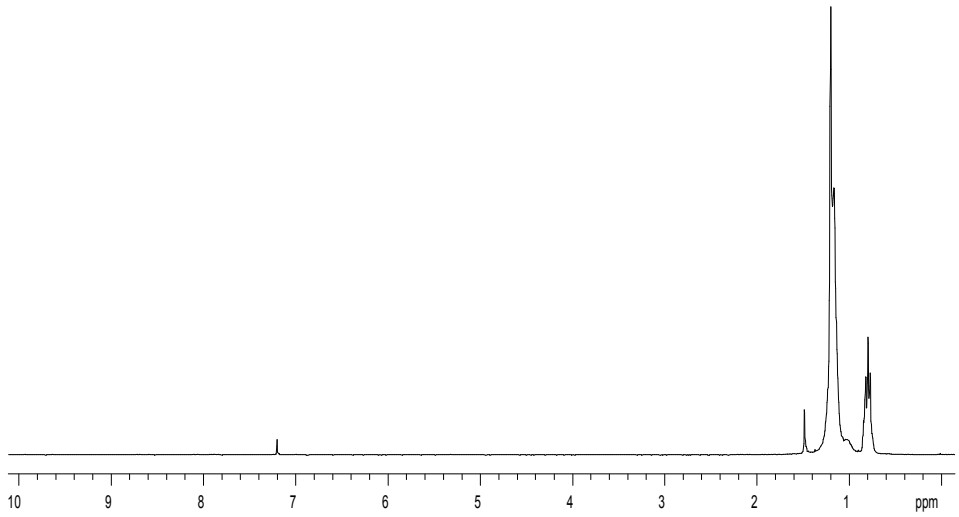

Figure S-2. ^{1}H NMR spectrum of the polymer produced in the attempted copolymerization of ethylene and *N*-allyl carbazole (NAC), using **5** as catalyst at 5 bar ethene, CH_2Cl_2 solvent, 1.1 M NAC, 50^{o}C. No NAC incorporation is visible. [500 MHz, $CDCl_3$ solvent, 23^{o}C]

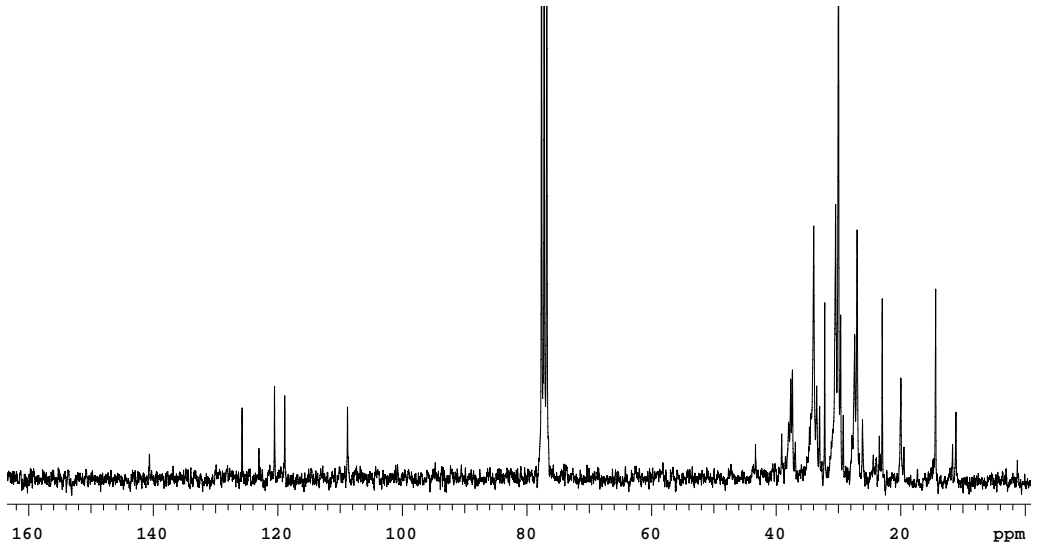

Figure S-3. ^{13}C{^{1}H} NMR spectrum of the ethylene/*N*-pentenylcarbazole (NPC) copolymer with 18.8 wt% incorporated comonomer. [75 MHz, $CDCl_3$ solvent, 23^{o}C].

Table S-1. Crystallographic data for complex **1** and **2**.

Compound	**1**	**2**
Formula	$C_{66}H_{66}N_3BF_{24}Pd$	$C_{78}H_{71}N_3BF_{24}Pd$
FW	1474.46	1623.61
Crystal system	monoclinic	monoclinic
Space group	*C*2/c	$P2_1/n$
a (Å)	41.414(2)	12.8846(6)
b (Å)	12.7965(5)	15.7270(7)
c (Å)	26.010(1)	36.571(2)
β (deg)	103.000(1)	91.951(1)
V (Å^3)	13430.8(10)	7406.3(6)
θ-range (deg)	2.20-20.53	2.26-24.27
Z	8	4
ρ_{calc} (g.cm^{-3})	1.458	1.456
F(000)	6000	3308
μ(Mo $K\bar{\alpha}$), cm^{-1}	3.85	3.57
Temp (K)	100(1)	100(1)
Reflections	11866	15141
Parameters	907	1003
wR(F^2)	0.1664	0.2061
Weighting (*a, b*)	0.0644, 65.10	0.0926, 20.0630
R(*F*)	0.0618	0.0762
GooF	1.028	1.057