Vinyl Polymerization of Norbornene on Nickel Complexes with Bis(imino)pyridine Ligands Containing Electron-Withdrawing Groups

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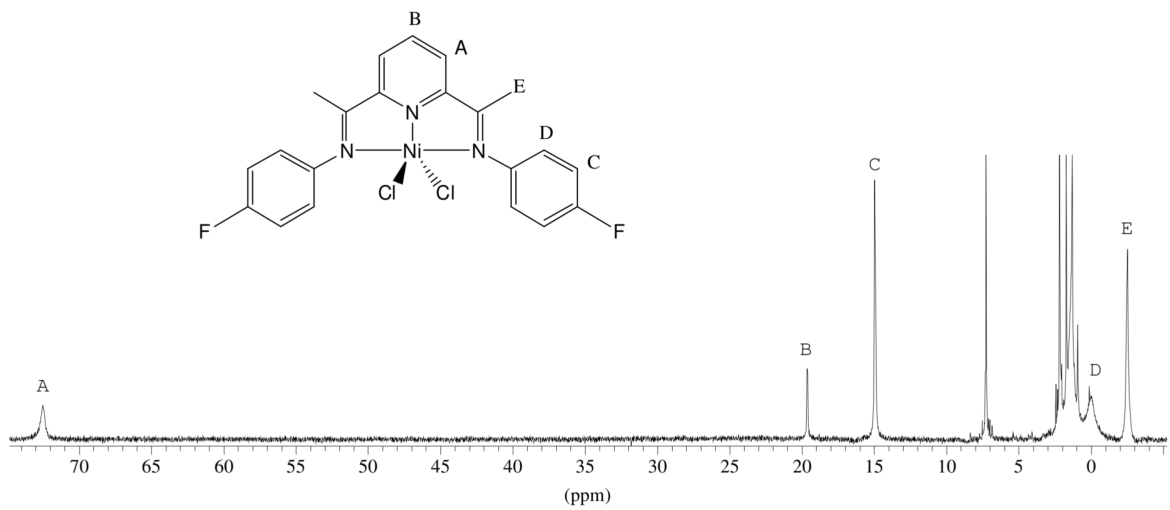
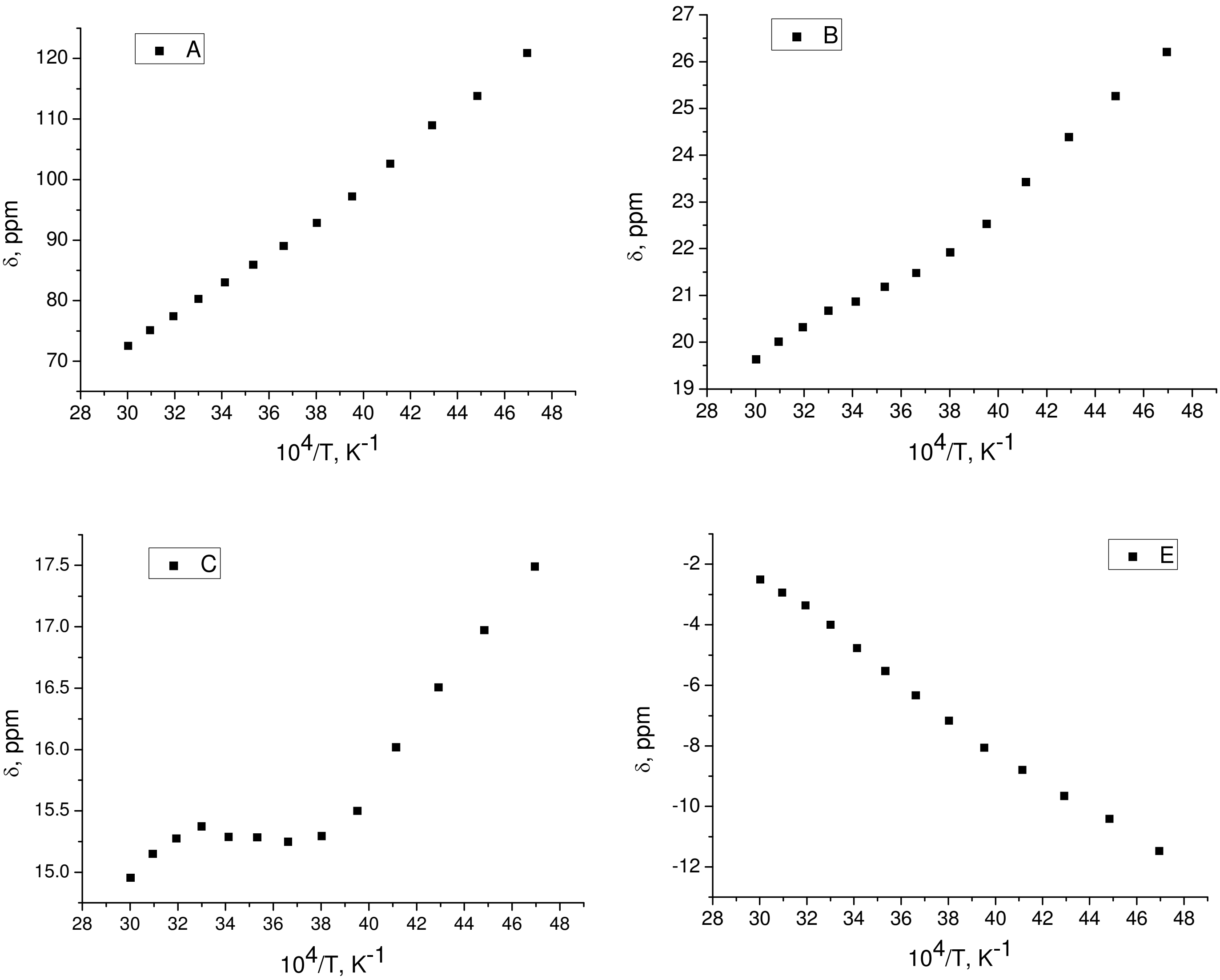
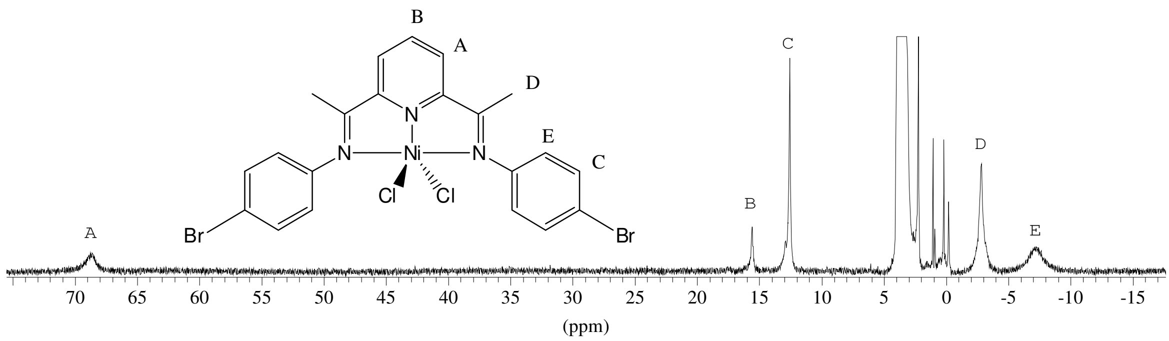
Electronic Supporting Information



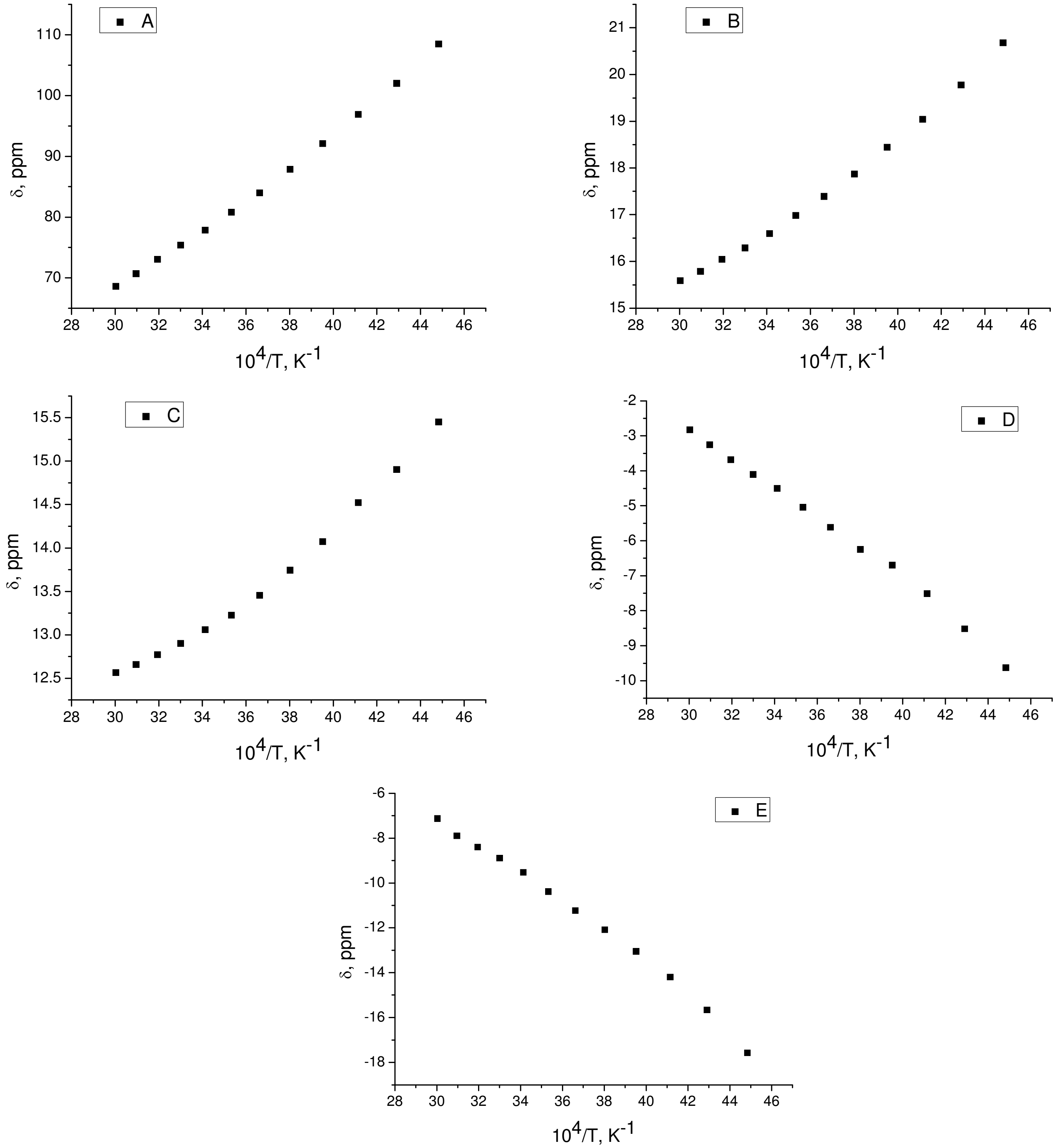
^{1}H NMR of complex **1** (T=333 K, $CDCl_3$)



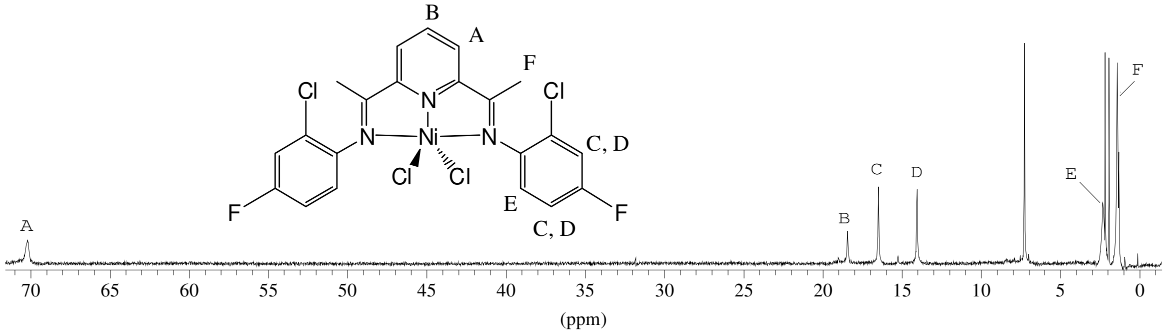
Temperature dependence of δ in ^{1}H NMR for complex **1**



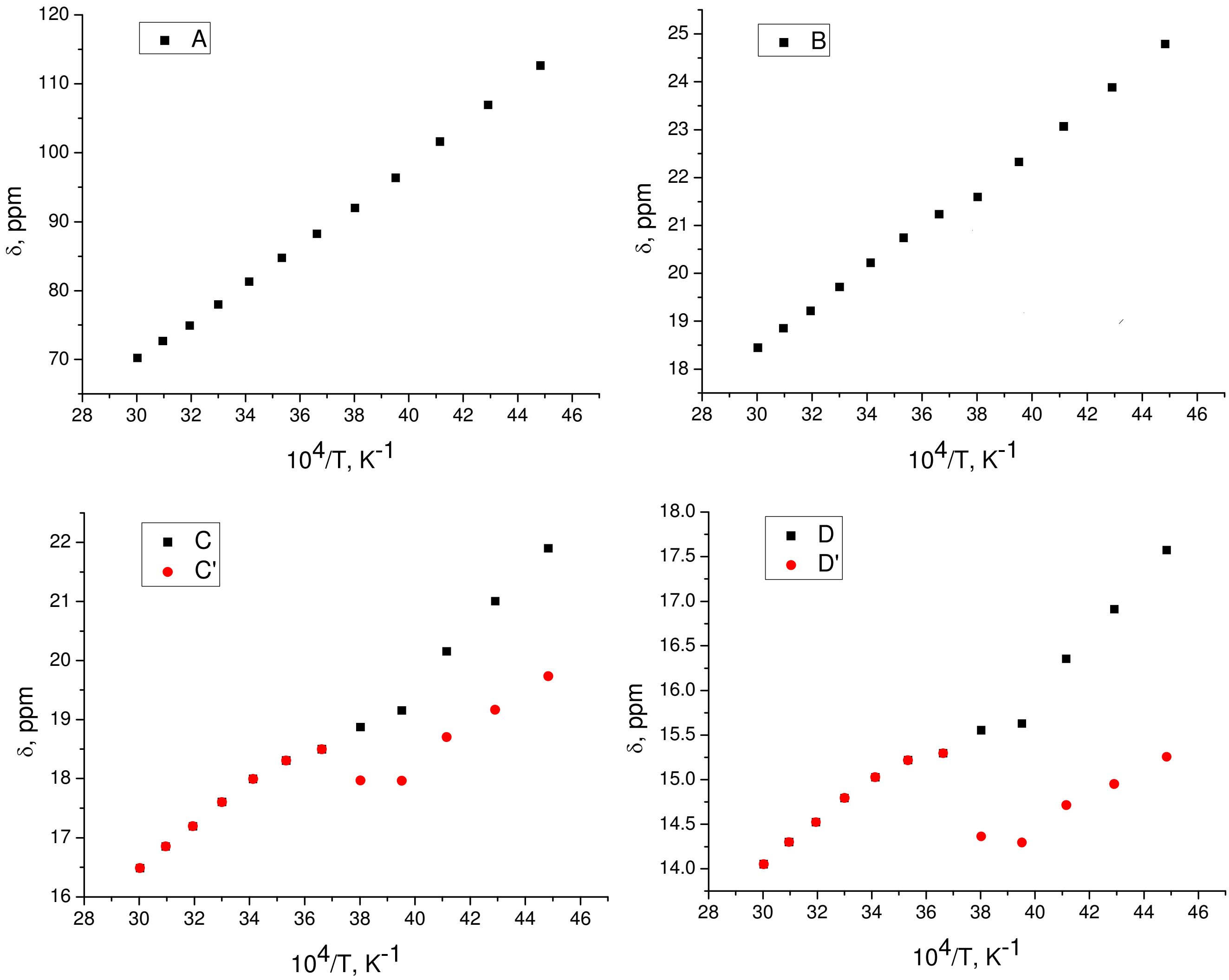
^{1}H NMR of complex **2** (T=333 K, CD_3OD)



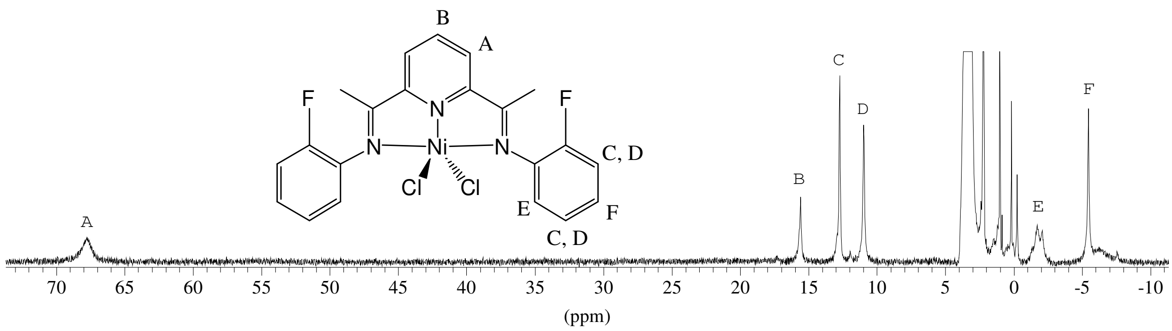
Temperature dependence of δ in ^{1}H NMR for complex **2**



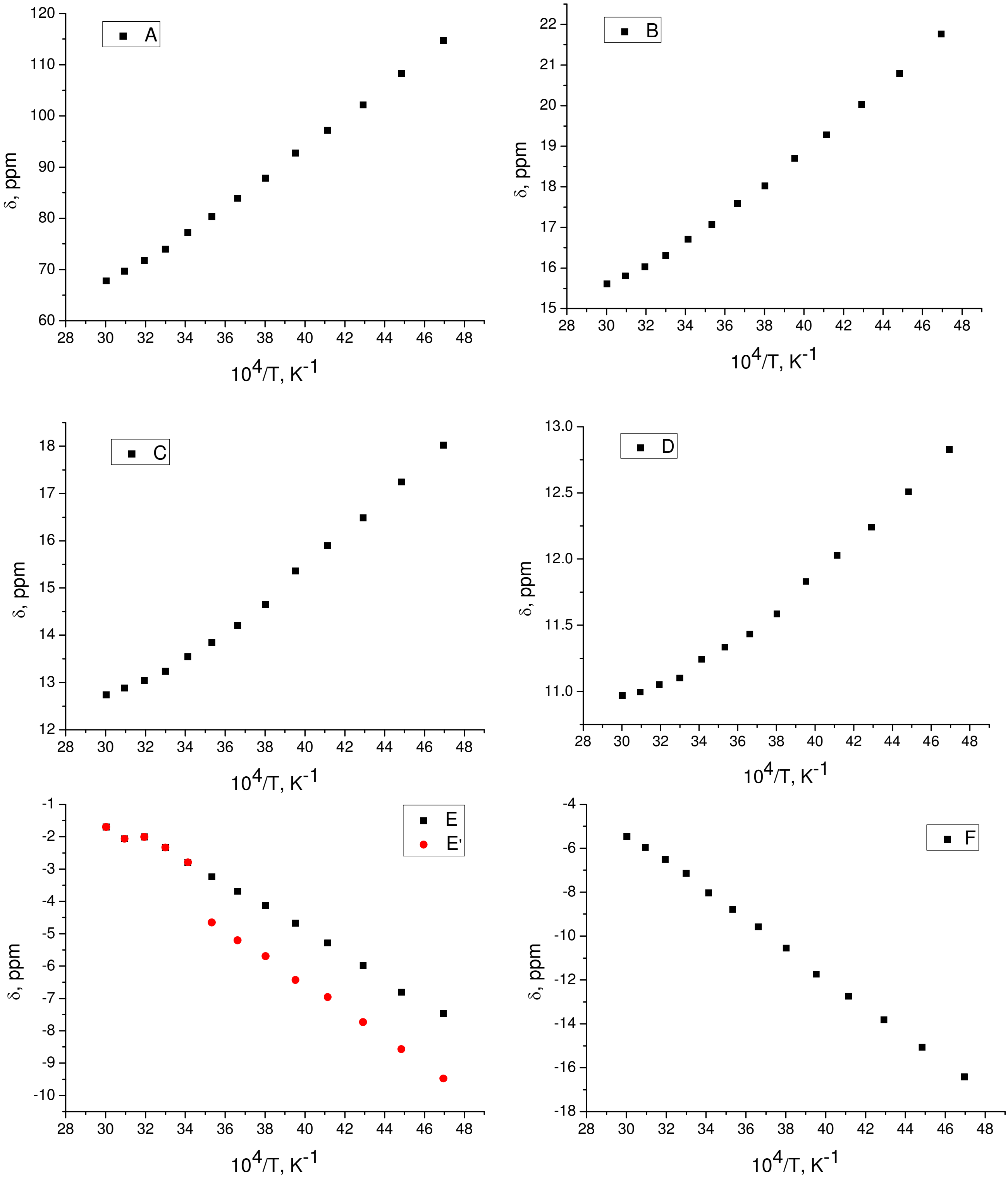
^{1}H NMR of complex **3** (T=333 K, $CDCl_3$)



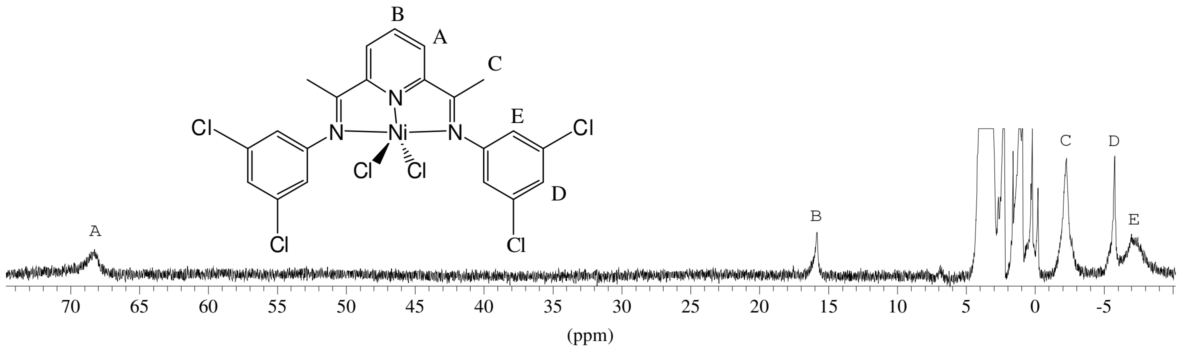
Temperature dependence of δ in ^{1}H NMR for complex **3**. Signals assigned to H_C and H_D decoalesce into doublets below 263 K. This fact may be explained by hindered rotation of phenyl rings at low temperature.



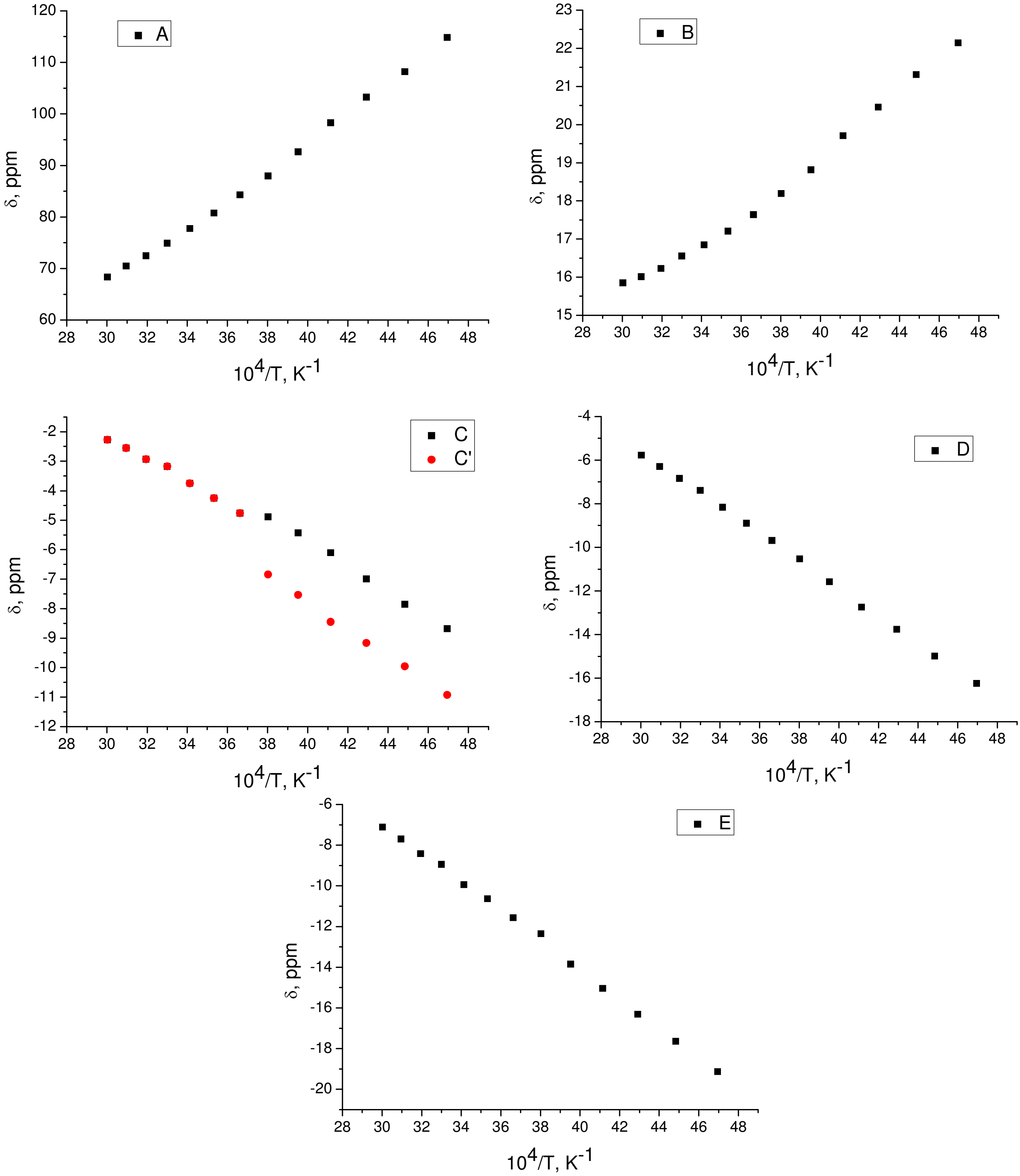
^{1}H NMR of complex **4** (T=333 K, CD_3OD)



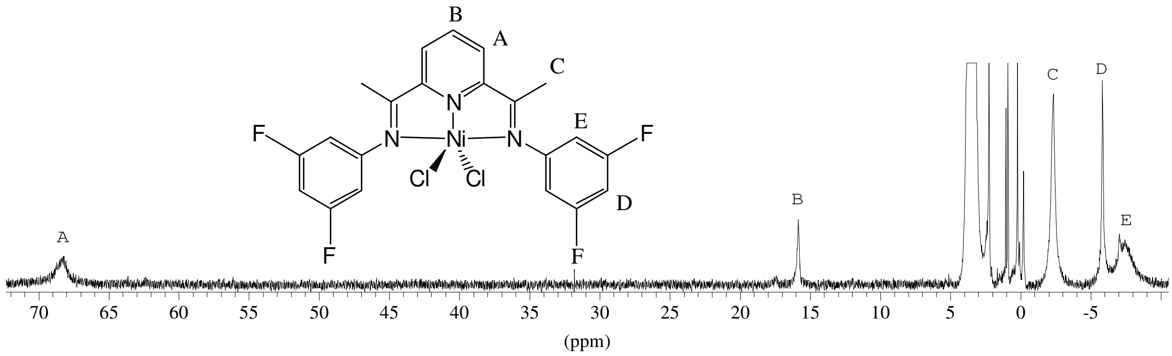
Temperature dependence of δ in ^{1}H NMR for complex **4**



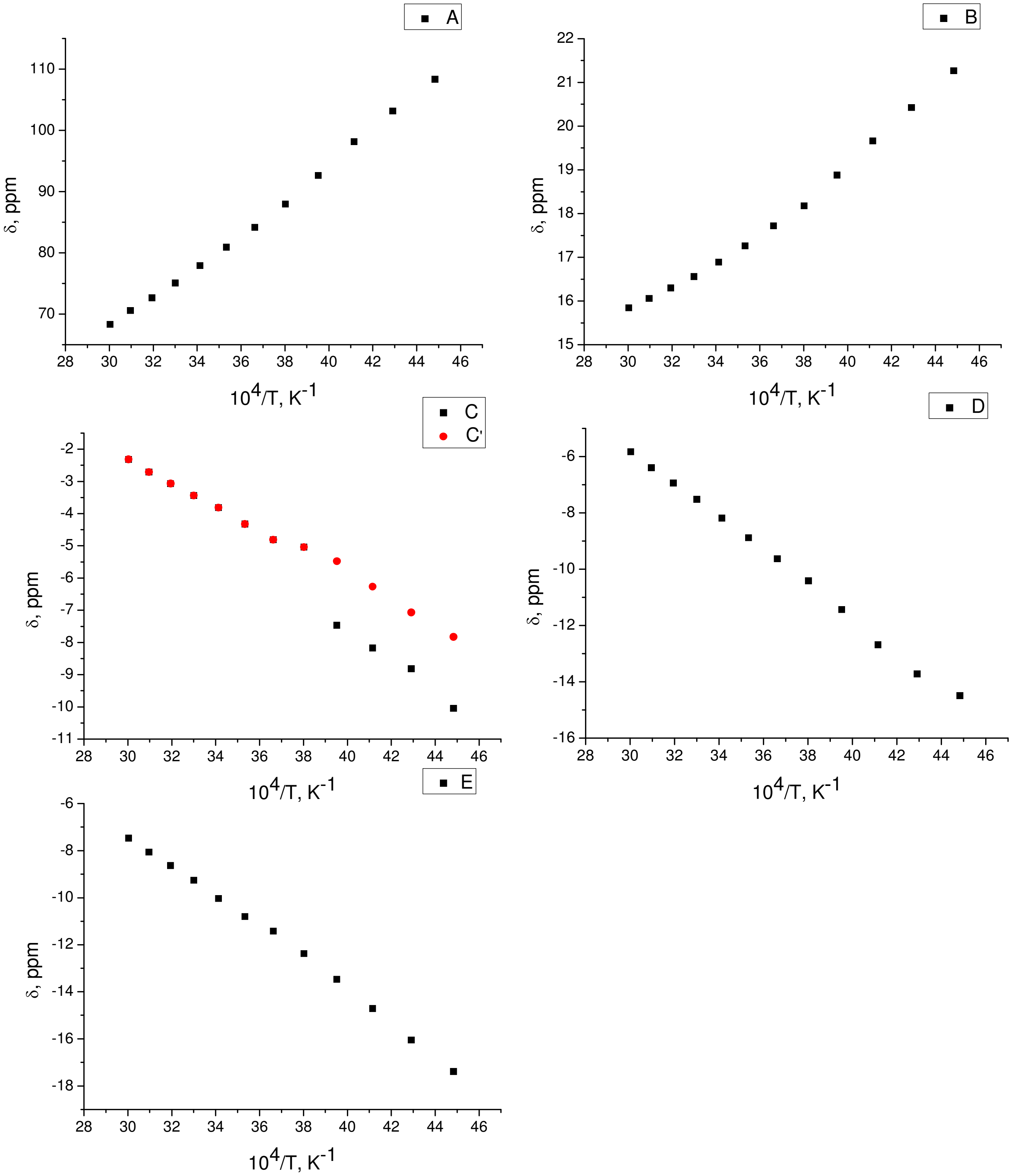
^{1}H NMR of complex **5** (T=333 K, CD_3OD)



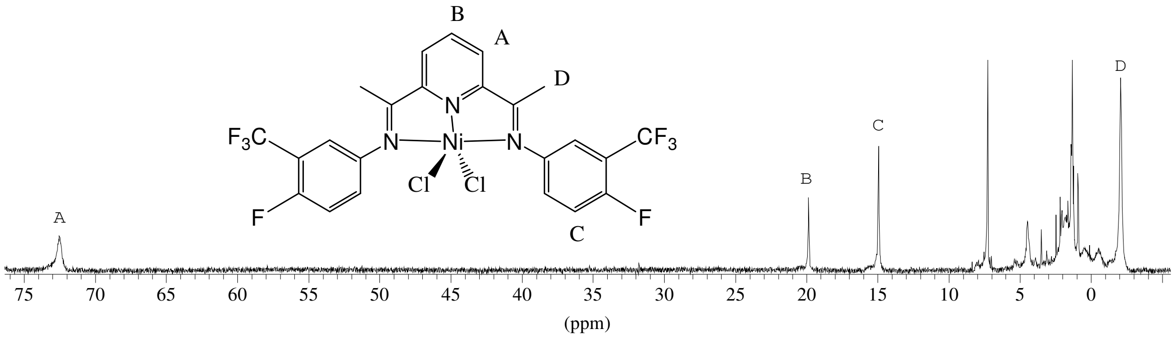
Temperature dependence of δ in ^{1}H NMR for complex **5**



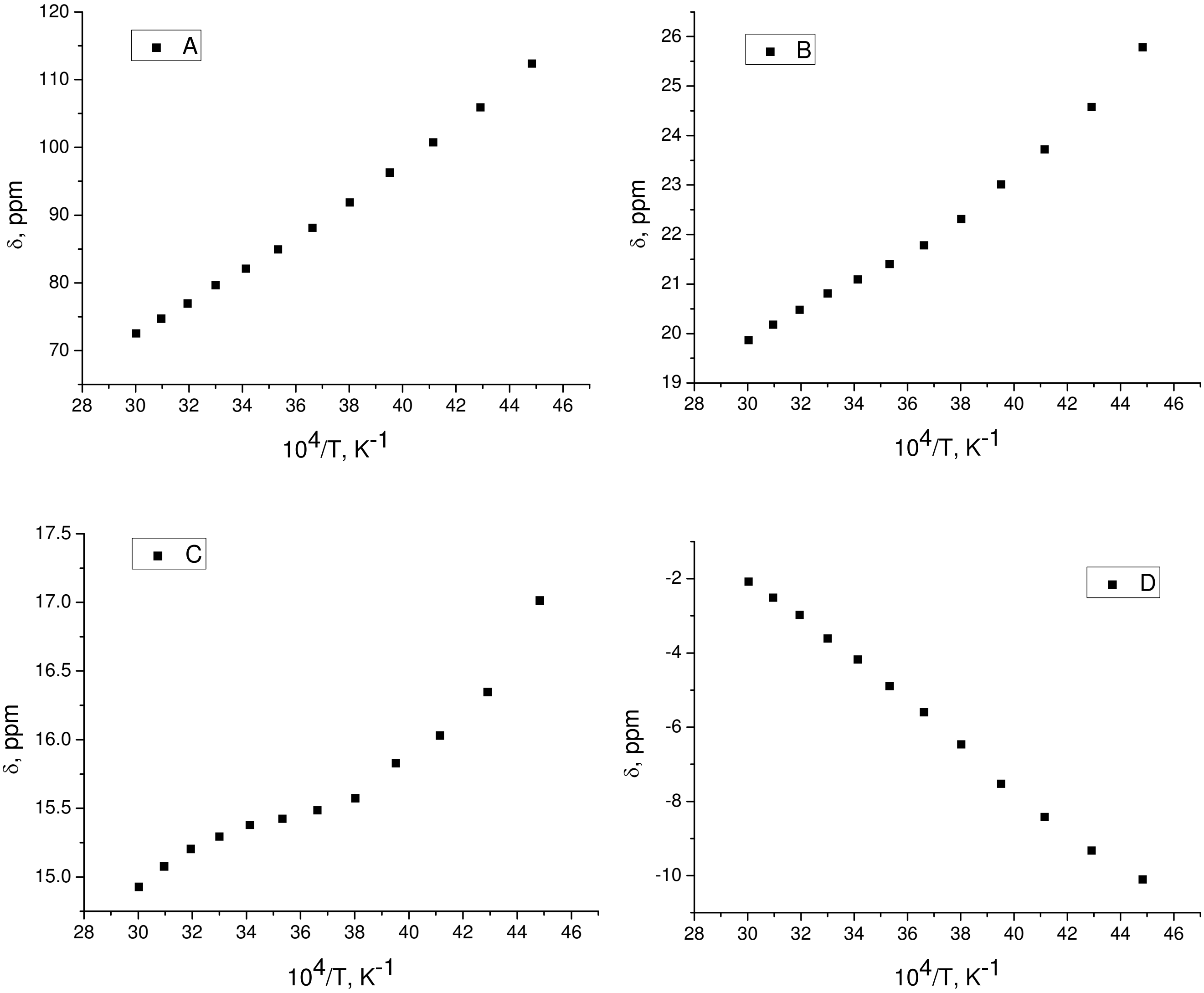
^{1}H NMR of complex **7** (T=333 K, CD_3OD)



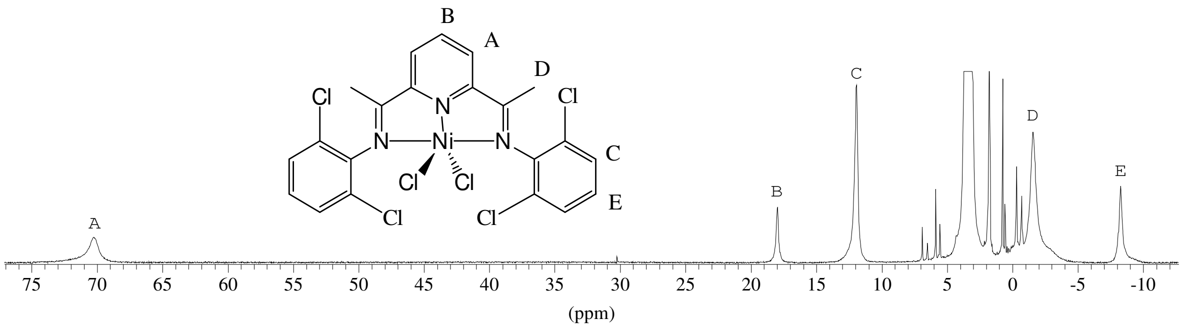
Temperature dependence of δ in ^{1}H NMR for complex **7**



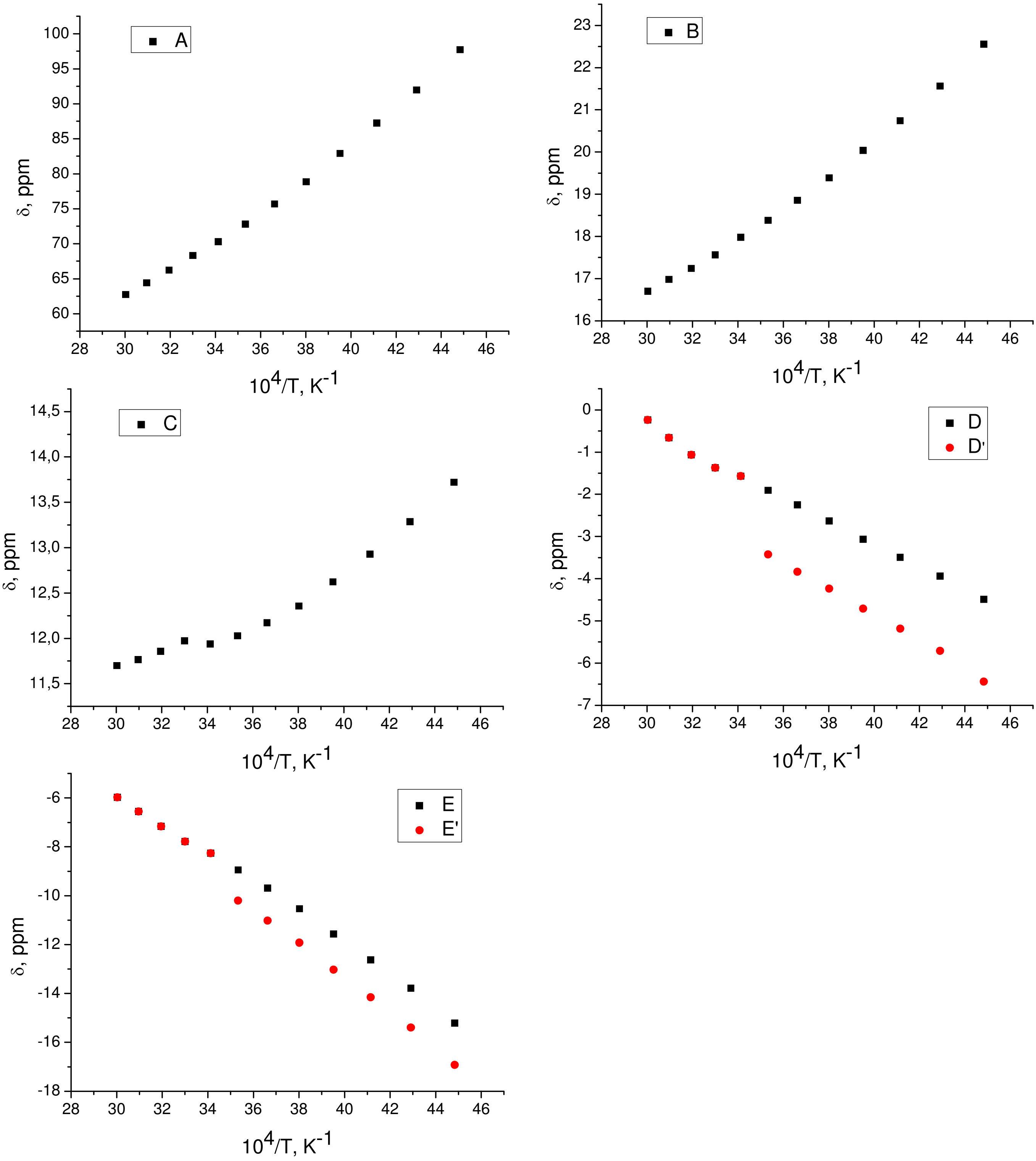
^{1}H NMR of complex **9** (T=333 K, $CDCl_3$)



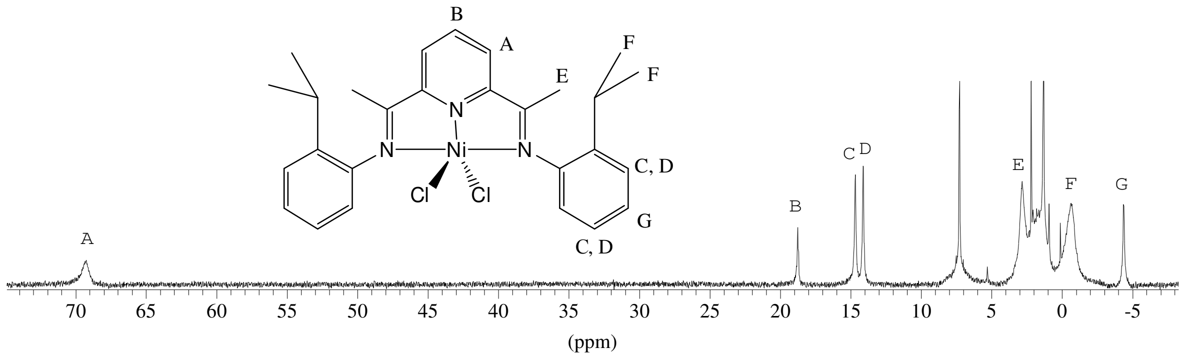
Temperature dependence of δ in ^{1}H NMR for complex **9**



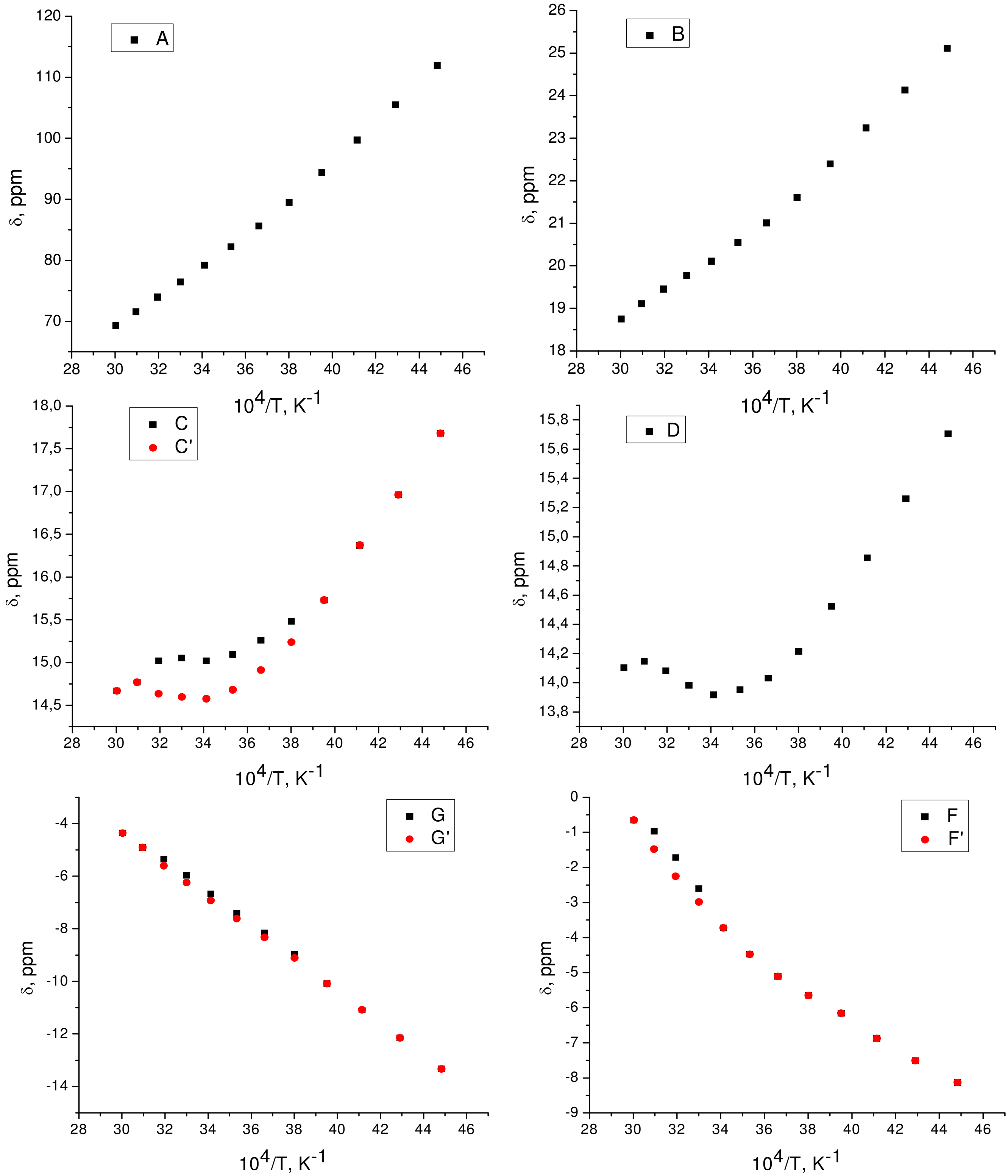
^{1}H NMR of complex **11** (T=293 K, CD_3OD)



Temperature dependence of δ in ^{1}H NMR for complex **11**



^{1}H NMR of complex **12** (T=333 K, $CDCl_3$)



Temperature dependence of δ in ^{1}H NMR for complex **12**

Table S1: MWD data of polynorbornenes from entries 14, 17 of Table 2.

Sample	$M_n \times 10^{-3}$	$M_w \times 10^{-3}$	$M_z \times 10^{-3}$	M_w/M_n	M_z/M_w
Entry 17	1700	3750	6100	2.2	1.6
Entry 14	2100	4500	7150	2.1	1.6

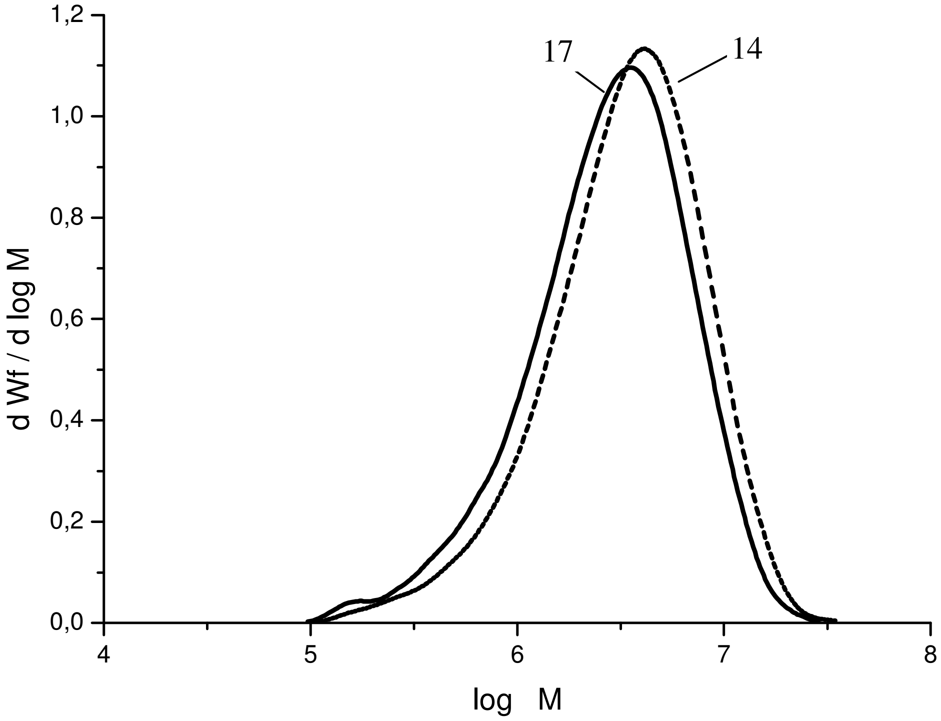
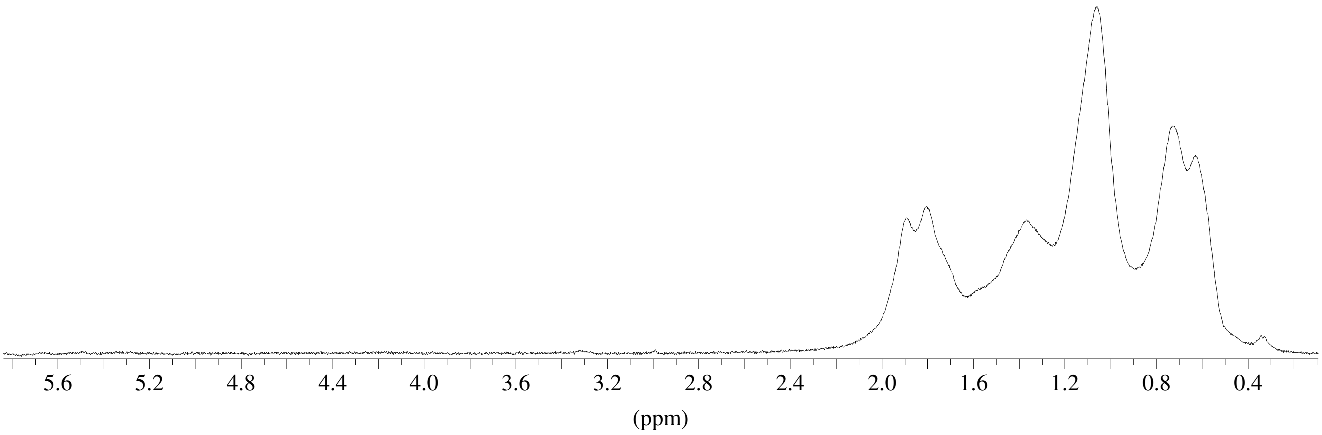
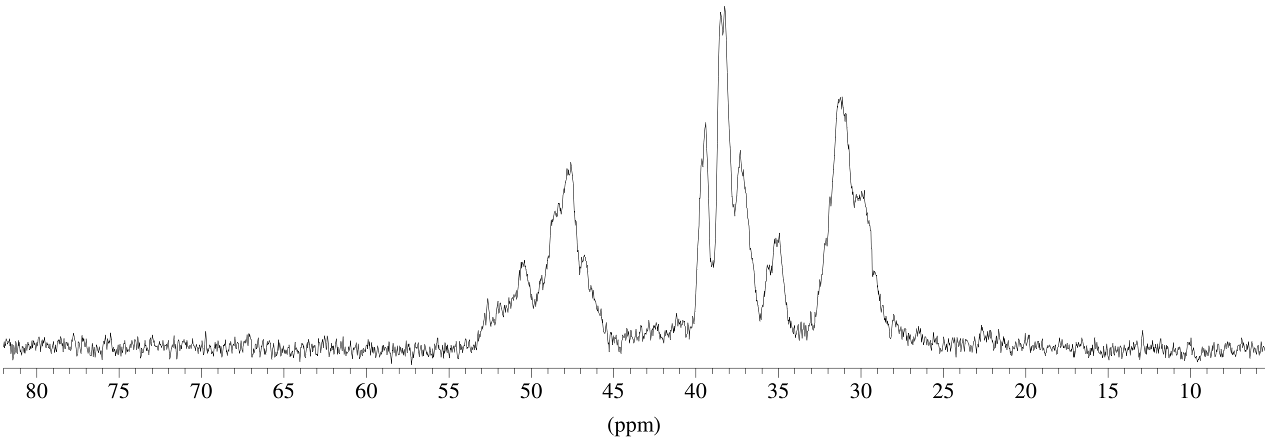


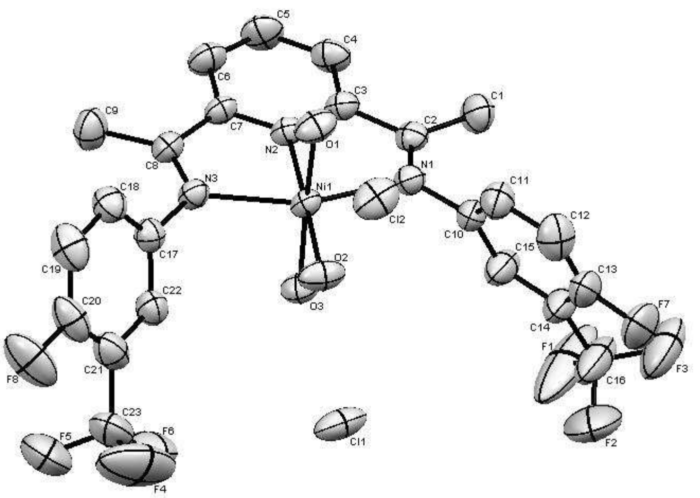
Figure S1. Molecular weight distribution of polynorbornenes.



^{1}H NMR of polynorbornene (obtained on Ni-2-iPr (**12**)) in *o*-dichlorobenzene at 99 ^{o}C



^{13}C NMR of polynorbornene (obtained on Ni-2-iPr (**12**)) in *o*-dichlorobenzene at 99 ^{o}C



Molecular structure of complexs **9**. Hydrogen atoms omitted for clarity.

Table S1. Crystal Data and Refinement Details for **5** and **6**

	5	**6**
Empirical formula	$C_{21}H_{19}Cl_6N_3NiO_2$	$C_{23}H_{17}Cl_2F_6N_3Ni$
Formula weight	616.80	579.01
Crystal color	yellow	red
Temperature (K)	173(2) K	293(2) K
Wavelength (Å)	0.71073	0.71073
Crystal system	Orthorhombic	Orthorhombic
space group	Pna2(1)	Pbca
a (Å)	18.740(4)	15.329(3)
b (Å)	10.387(2)	17.834(4)
c (Å)	26.300(5)	19.773(4)
α (°)	90	90
β (°)	90	90
γ (°)	90	90
Volume (Å^3)	5119.3(18)	5405.7(19)
Z	8	8
*D*calc(Mg m^{-3})	1.601	1.423
μ (mm^{-1})	1.409	0.972
F(000)	2496	2336
Crystal size (mm)	0.12 x 0.08 x 0.05	0.25× 0.20×0.12
θ range (°)	1.55 to 27.48	2.03-27.45
Limiting indices	-24<=h<=24, -13<=k<=12, -16<=l<=34	-9<=h<=19, -23<=k<=14, -25<=l<=14
No. of rflns collected	20265	13272
No. of unique rflns	8076	6129
Rint	0.0599	0.0439
Completeness to θ	99.7 %	99.3%
Goodness-of-fit on	1.081	1.135
Final R indices [I>2σ	R1 = 0.0641, wR2 = 0.1414	R1 = 0.0803, wR2 = 0.2035
R indices (all data)	R1 = 0.0691, wR2 = 0.1461	R1 = 0.0975, wR2 =0.2188
Largest diff peak, hole (e Å^{-3})	1.171, -0.499	0.923, -0.448