

Supporting information

Synthesis of Bis(N-arylcarboximidoylchloride)pyridine Cobalt(II) Complexes and Their Catalytic Behavior for 1,3-Butadiene Polymerization

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Table S1. Crystallographic data of complexes **4a-e** and **5a**.

	4a · 2CH ₂ Cl ₂	5a · 2CH ₂ Cl ₂	4b · CH ₂ Cl ₂	4c · CH ₂ Cl ₂	4d	4e · CH ₂ Cl ₂
formula	C ₂₆ H ₂₈ Cl ₁₇ CoN ₃	C ₂₉ H ₃₅ Cl ₆ CoN ₃	C ₃₁ H ₃₇ Cl ₄ CoN ₃	C ₂₄ H ₂₃ Cl ₆ CoN ₃	C ₁₉ H ₁₃ Cl ₄ CoN ₃	C ₂₄ H ₂₁ Cl ₈ CoN ₃
fw	681.44	697.23	652.37	625.08	484.05	693.97
color	green	green	brown	green	green	green
cryst. Syst.	trigonal	Monoclinic	Triclinic	Monoclinic	Orthorhombic	Monoclinic
space	R3c	P2(1)/c	P-1	P2(1)/n	P2(1)2(1)2(1)	P2(1)/n
<i>a</i> , (Å)	24.8916(7)	8.8565(12)	8.8292(5)	12.9379 (7)	8.998(4)	8.1076 (7)
<i>b</i> , (Å)	24.8916(7)	14.5920(18)	9.7126(5)	15.0989 (8)	13.785(6)	22.7160 (18)
<i>c</i> , (Å)	25.6814(11)	26.249(3)	21.0607(12)	14.3818 (7)	16.476(7)	16.3196 (13)
<i>α</i> , (deg)	90.00	90.00	82.7520(10)	90.00	90.00	90.00
<i>β</i> , (deg)	90.00	92.697(3)	87.6250(10)	108.177 (1)	90.00	101.821 (1)
<i>γ</i> , (deg)	120	90.00	65.7340(10)	90.00	90.00	90.00
<i>V</i> , Å ³	13780.2(8)	3388.5(8)	1633.22(16)	2669.3 (2)	2043.7(14)	2941.9 (4)
<i>Z</i>	18	4	2	4	4	4
<i>T</i> , K	185(2)	293(2)	293(2)	188	293(2)	188
<i>D</i> _{calcd} , (g	1.478	1.367	1.327	1.555	1.573	1.567
<i>μ</i> (Mo Kα),	1.16	1.00	0.88	1.26	1.37	1.33
<i>F</i> (000)	6246	1436	678	1268	972	1396
<i>θ</i> range,	1.64-26.05	2.30-17.74	2.4–25.9	2.3–26.0	2.6–22.0	2.2–22.5
no. of rflns	23065	19836	8969	16725	12128	17177
no. of	4852(R _{int} =0.045	6026(R _{int} =0.073	6291(R _{int} =0.014	5238(R _{int} =0.023	3617(R _{int} =0.041	5205(R _{int} =0.068
No. of	4852/0/343	6026/0/360	6291/0/360	5238/0/311	3617/0/244	5205/0/329
Goodness	1.094	0.988	1.027	1.024	0.999	0.974
R ₁ (I>2σ(I)	0.056	0.062	0.038	0.032	0.037	0.051
wR ₂	0.157	0.158	0.103	0.080	0.084	0.109

Figure S1. GPC curves for runs 8 to 12 in Table 4.

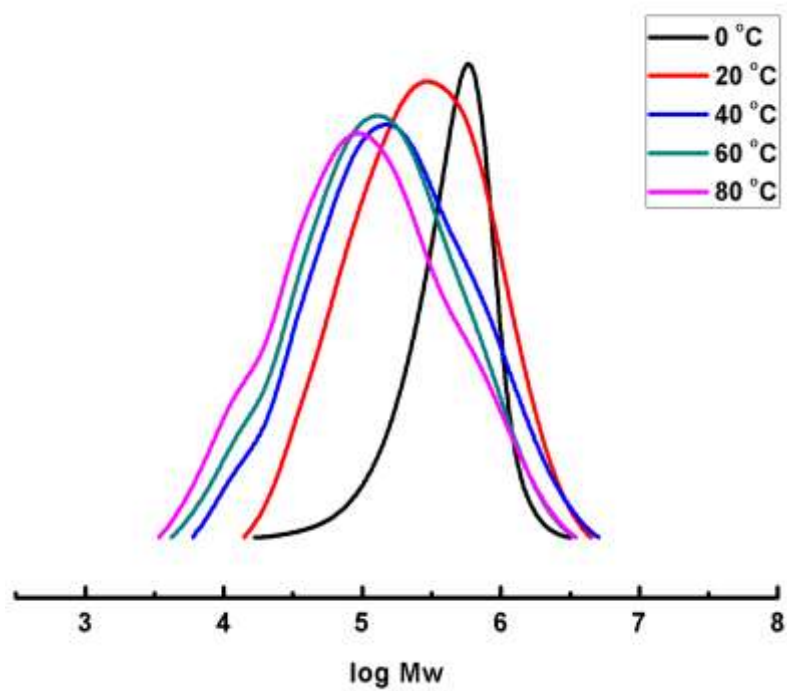


Figure S2. GPC curves for runs 13 to 16 in Table 4.

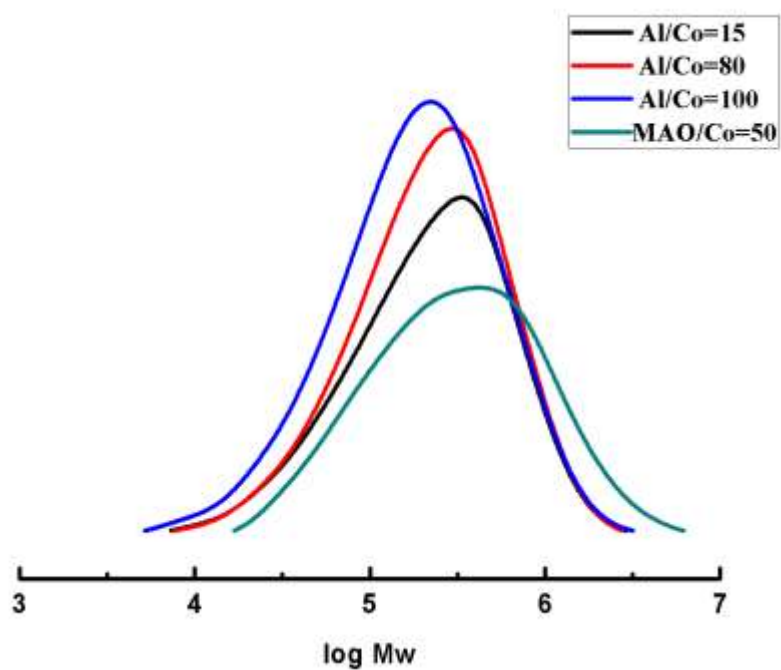


Figure S3. DSC curves of the polybutadienes obtained at various temperatures.

