Supporting Information

One-pot Synthesis of Cobalt Complexes with 2,6-Bis(arylimino)phenoxyl/phenthioxyl Ligands and Catalysis on Isoprene Polymerization

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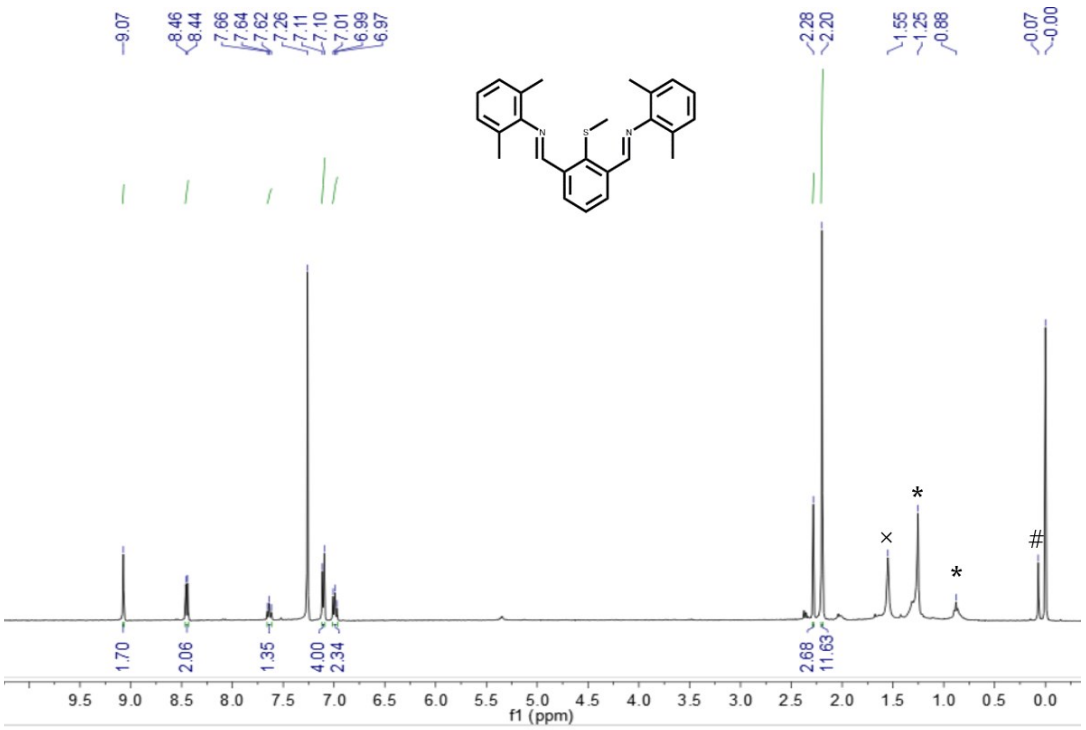
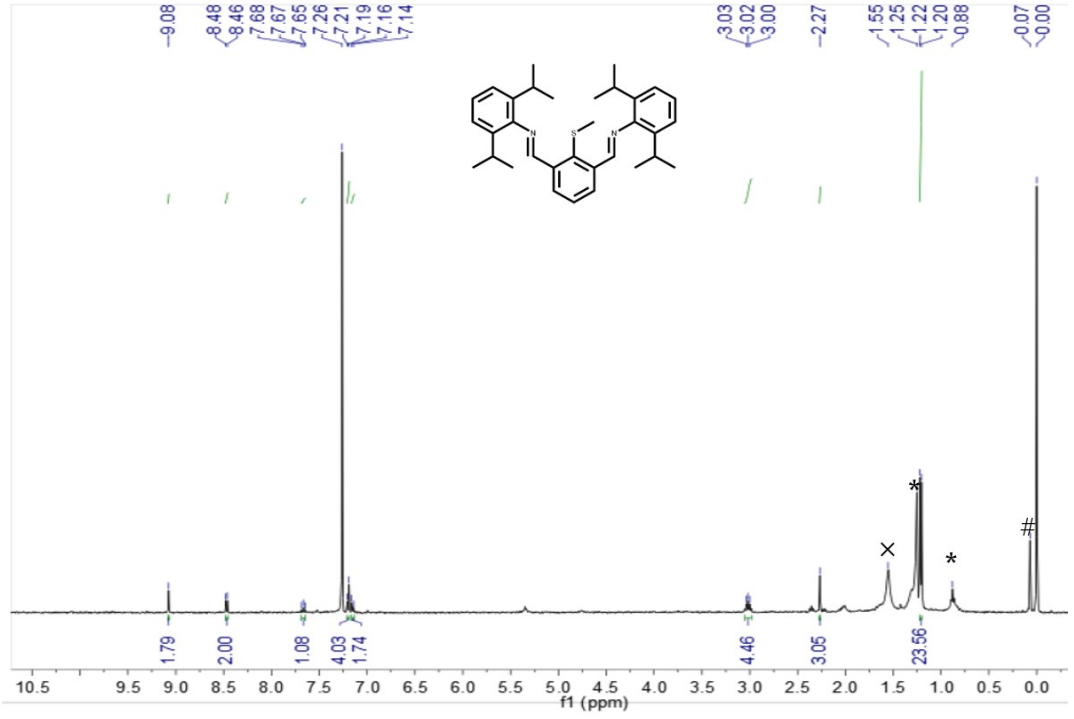
S**Table 1.** Summary of crystallographic data for complexes **1b′**, **3b′**, **4a**, and **4b**.

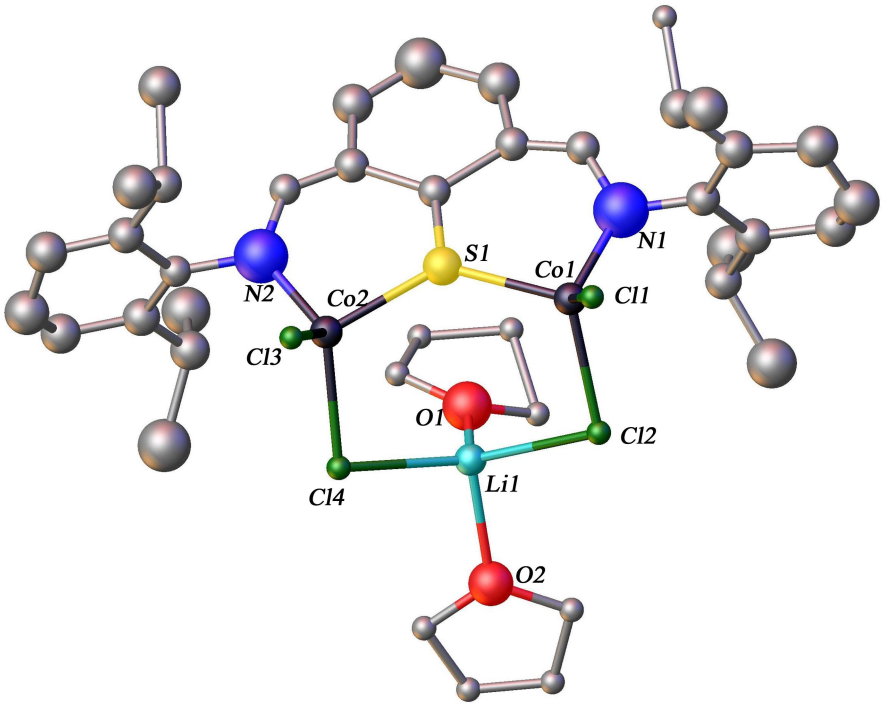
	1b′	**3b′**	**4a**	**4b**
Formula	$C_{39}H_{48}Cl_2CoN_2O$	$C_{64}H_{80}Cl_4Co_2Li_2N_4O_2$	$C_{34}H_{43}Cl_4Co_2LiN_2O_{3.5}$	$C_{48}H_{70}Cl_4Co_2LiN_2O_5$
F_w	690.62	1210.86	802.30	1021.66
cryst syst	Monoclinic	Triclinic	Monoclinic	Monoclinic
space group	P2(1)/c	P-1	P2(1)/n	P2(1)/c
a (Å)	14.2116(7)	10.7411(7)	18.5708(10)	16.092(5)
b (Å)	15.6053(8)	11.4789(7)	23.5866(12)	17.586(2)
c (Å)	18.0770(10)	13.3274(8)	20.4402(11)	19.569(6)
α (deg)	90	80.2670(10)	90	90
β (deg)	111.560(2)	77.5960(10)	108.7030(10)	108.843(4)
γ (deg)	90	88.4920(10)	90	90
v (Å^3)	3728.5(3)	1581.67(17)	8480.5(8)	5241(3)
Z	4	1	8	4
D_{calcd}(gcm^{-3})	1.230	1.271	1.257	1.295
μ (mm^{-1})	0.635	0.738	1.066	0.880
F(000)	1460.0	636.0	3312	2148
$2\theta_{max}$(deg)	50.068	52.044	46.098	52.4
collected reflns	35937	8499	41708	32019
Uniq reflns	6578	6067	11840	10327
R_{int}	0.0909	0.0141	0.0776	0.0864
GOF	1.063	1.041	1.031	1.038
*R*1	0.0756	0.0401	0.0824	0.0758
w*R*2	0.2031	0.1125	0.2430	0.2089
Largest diff peak, hole (e A^-3)	1.32, –0.93	0.83, –0.26	1.92, –0.54	1.06, –0.90



SFigure 1. ^{1}H NMR spectrum of ^{Me}S-CH$_3$ (400 MHz, CDCl$_3$, 25 ºC). #, *, and × stand for residual signals of silicone grease, n-hexane, and H_2O respectively.



SFigure 2. ^{1}H NMR spectrum of ^{iPr}S-CH$_3$ (400 MHz, CDCl$_3$, 25 ºC). #, *, and × stand for residual signals of silicone grease, n-hexane, and H_2O respectively.



SFigure 3. Molecular structure of **5b**