

# Synthesis and properties investigation of hydroxyl functionalized polyisoprene prepared by cobalt catalyzed co-polymerization of isoprene and hydroxylmyrcene

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**Figure 7S** The  $^1\text{H}$  NMR spectra of (a) polyisoprene, (b) poly(isoprene<sub>95.6</sub>-co-My-OH<sub>4.4</sub>), (c) poly(isoprene<sub>91.4</sub>-co-My-OH<sub>8.6</sub>), (d) poly(isoprene<sub>83.7</sub>-co-My-OH<sub>16.3</sub>), (e) poly(isoprene<sub>73.0</sub>-co-My-OH<sub>27.0</sub>) and (f) poly(isoprene<sub>68.5</sub>-co-My-OH<sub>31.5</sub>)

**Figure 8S** The  $^{13}\text{C}$  NMR spectra of (a) polyisoprene, (b) poly(isoprene<sub>95.6</sub>-co-My-OH<sub>4.4</sub>), (c) poly(isoprene<sub>91.4</sub>-co-My-OH<sub>8.6</sub>), (d) poly(isoprene<sub>83.7</sub>-co-My-OH<sub>16.3</sub>), (e) poly(isoprene<sub>73.0</sub>-co-My-OH<sub>27.0</sub>) and (f) poly(isoprene<sub>68.5</sub>-co-My-OH<sub>31.5</sub>) **Figure 9S** AFM topology of poly(IP-co-My-OH)s:

(a) polyisoprene, (b) poly(isoprene<sub>95.6</sub>-co-My-OH<sub>4.4</sub>),

(c) poly(isoprene<sub>91.4</sub>-co-My-OH<sub>8.6</sub>), (d) poly(isoprene<sub>83.7</sub>-co-My-OH<sub>16.3</sub>),

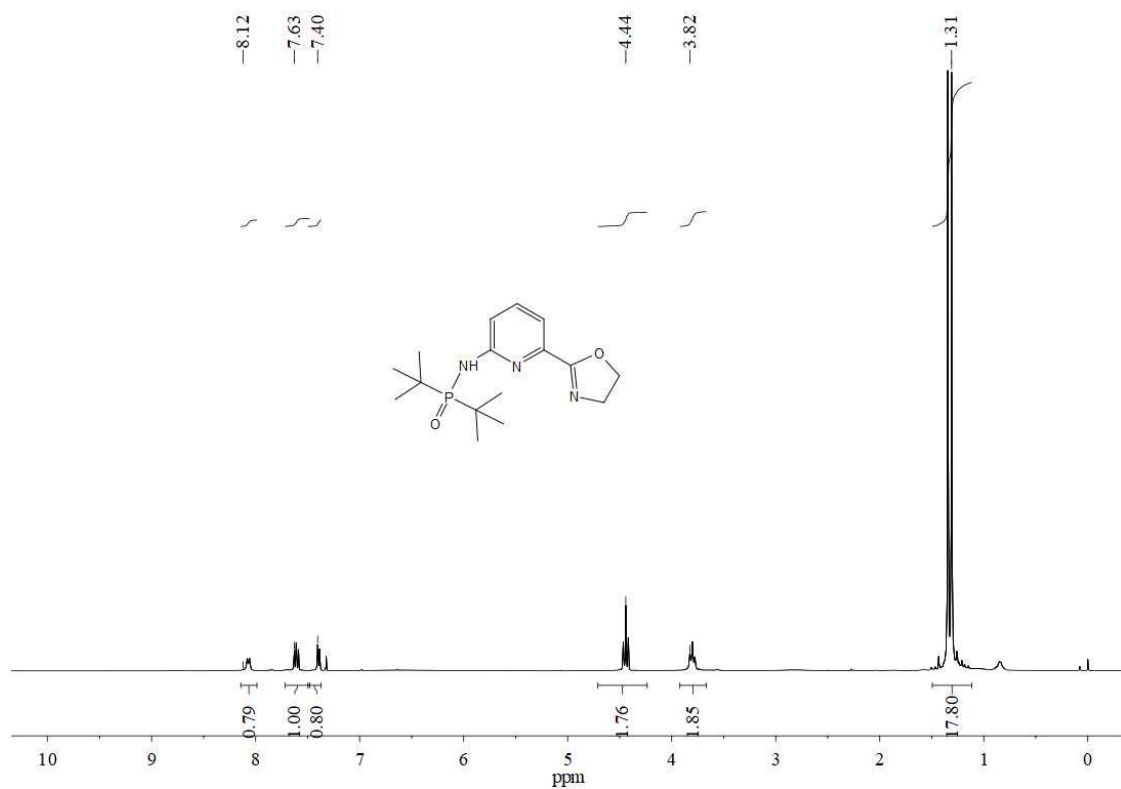
(e) poly(isoprene<sub>73.0</sub>-co-My-OH<sub>27.0</sub>) and (f) poly(isoprene<sub>68.5</sub>-co-My-OH<sub>31.5</sub>)

**Figure 10S** The vulcanization profiles of  $\text{SiO}_2$  reinforced  $\text{SiO}_2$ /PIP composites and  $\text{SiO}_2$ /poly(IP-co-My-OH)s composites

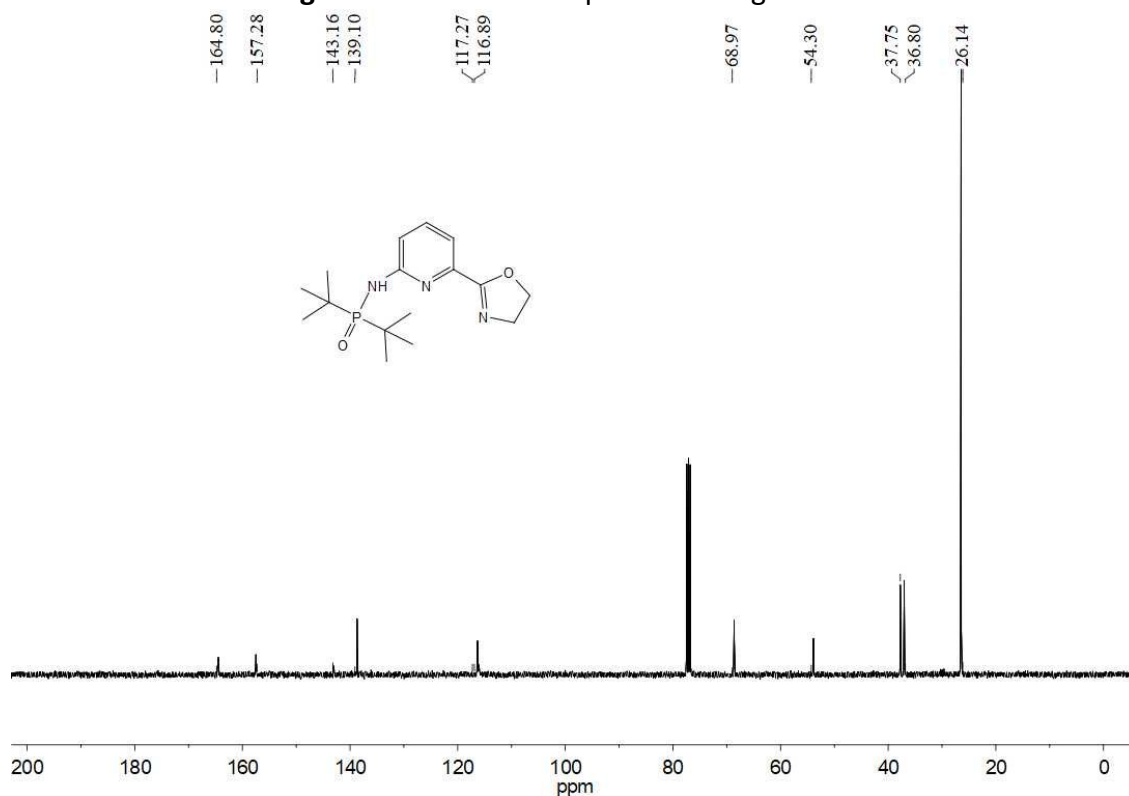
**Figure 11S** The loss storage of  $\text{SiO}_2$  reinforced  $\text{SiO}_2$ /PIP composites and  $\text{SiO}_2$ /poly(IP-co-My-OH)s composites

**Table 1S** The crystal data and structure refinements of complex **Co1·CH<sub>3</sub>OH**

**Table 2S** The summarized properties of  $\text{SiO}_2$  reinforced  $\text{SiO}_2$ /PIP composites and  $\text{SiO}_2$ /poly(IP-co-My-OH)s composites



**Figure 1S** The  $^1\text{H}$  NMR spectrum of ligand L1



**Figure 2S** The  $^{13}\text{C}$  NMR spectrum of ligand L1

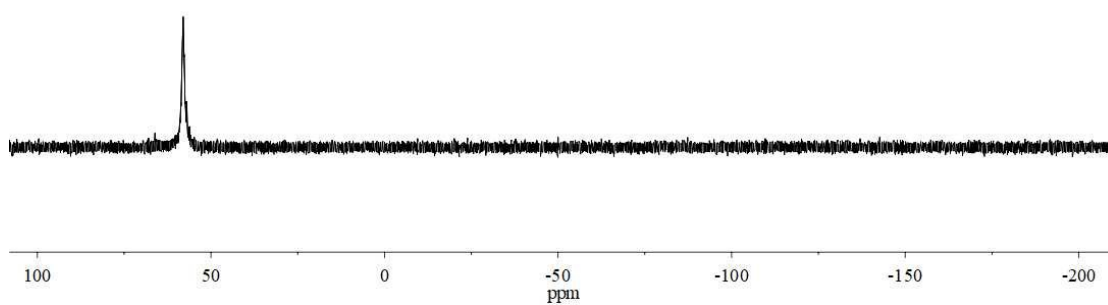
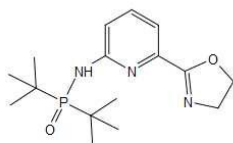


Figure 3S The  $^{31}\text{P}$  NMR spectrum of ligand L1

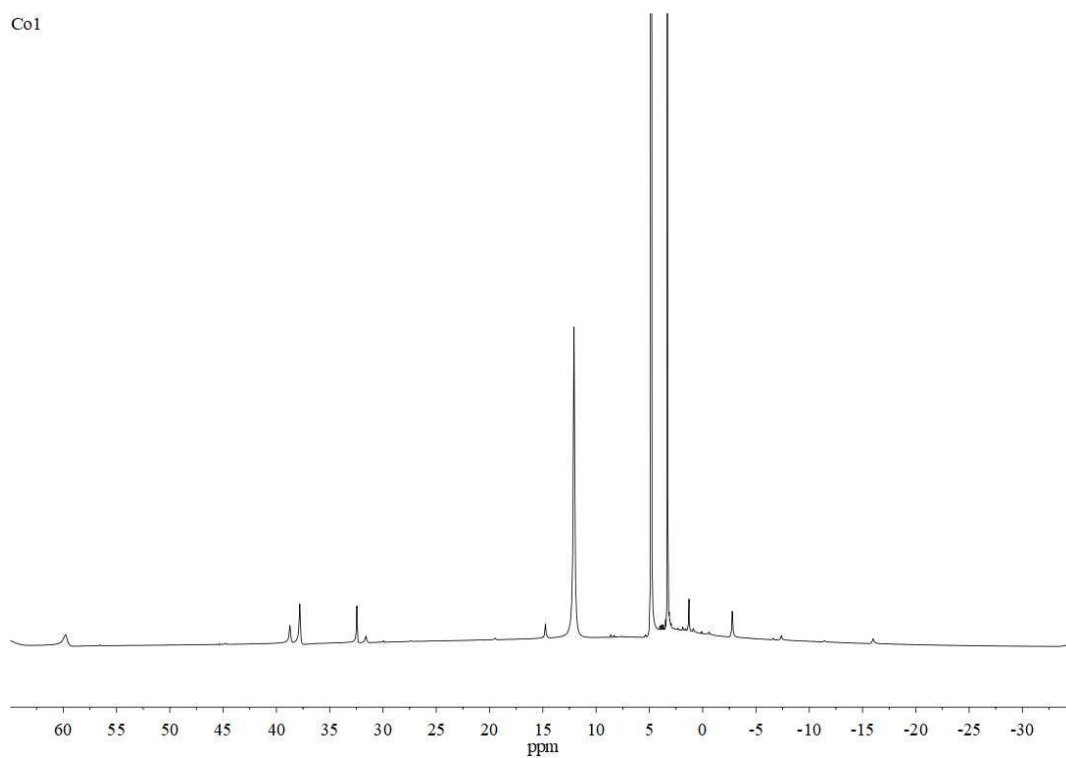


Figure 4S The  $^1\text{H}$  NMR spectrum of the Co1 complex

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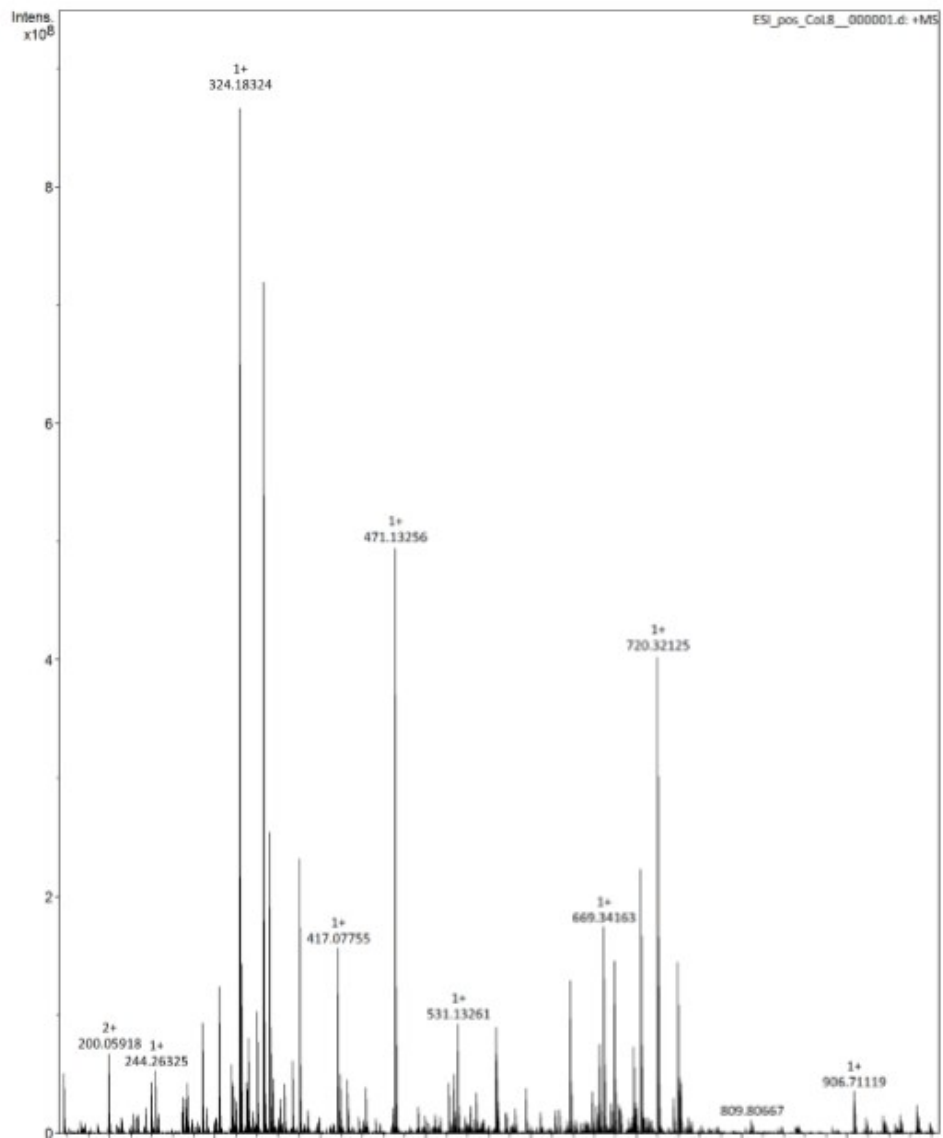
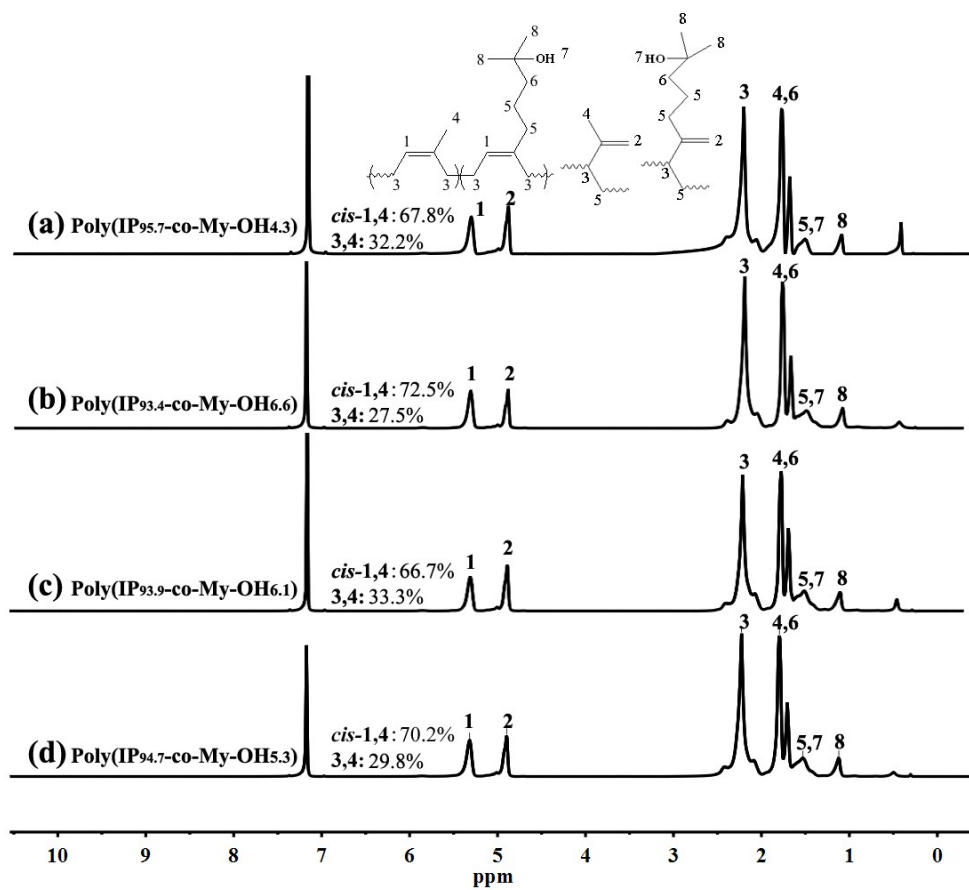
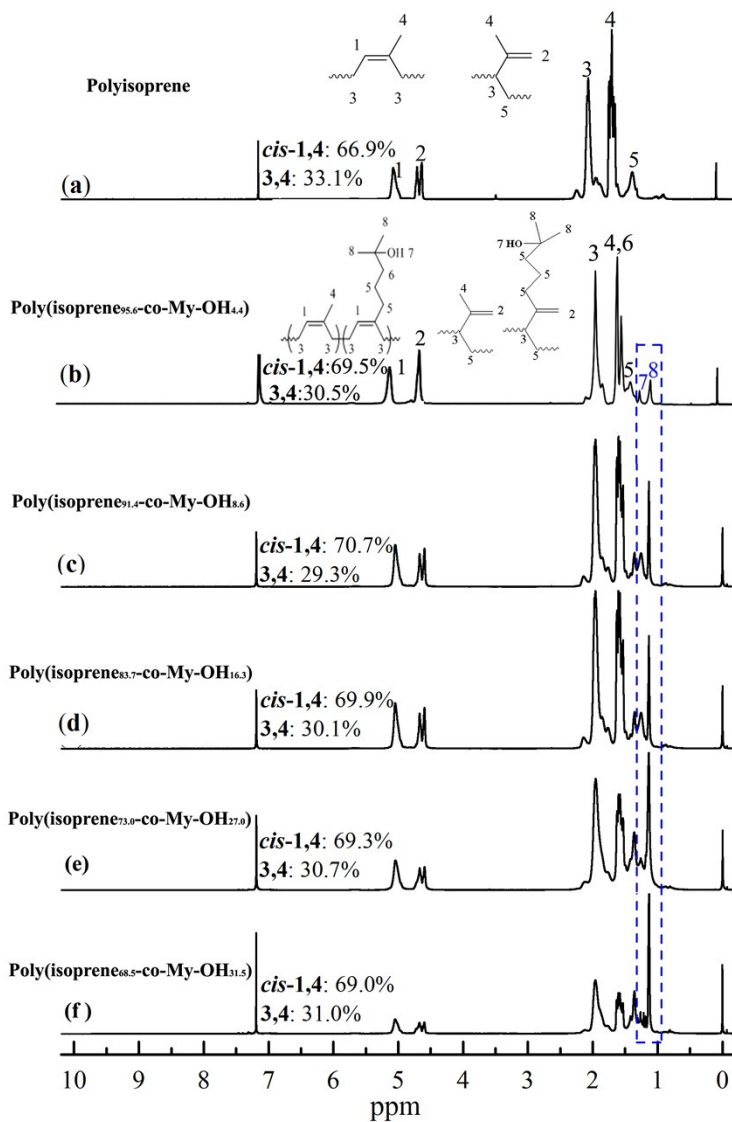


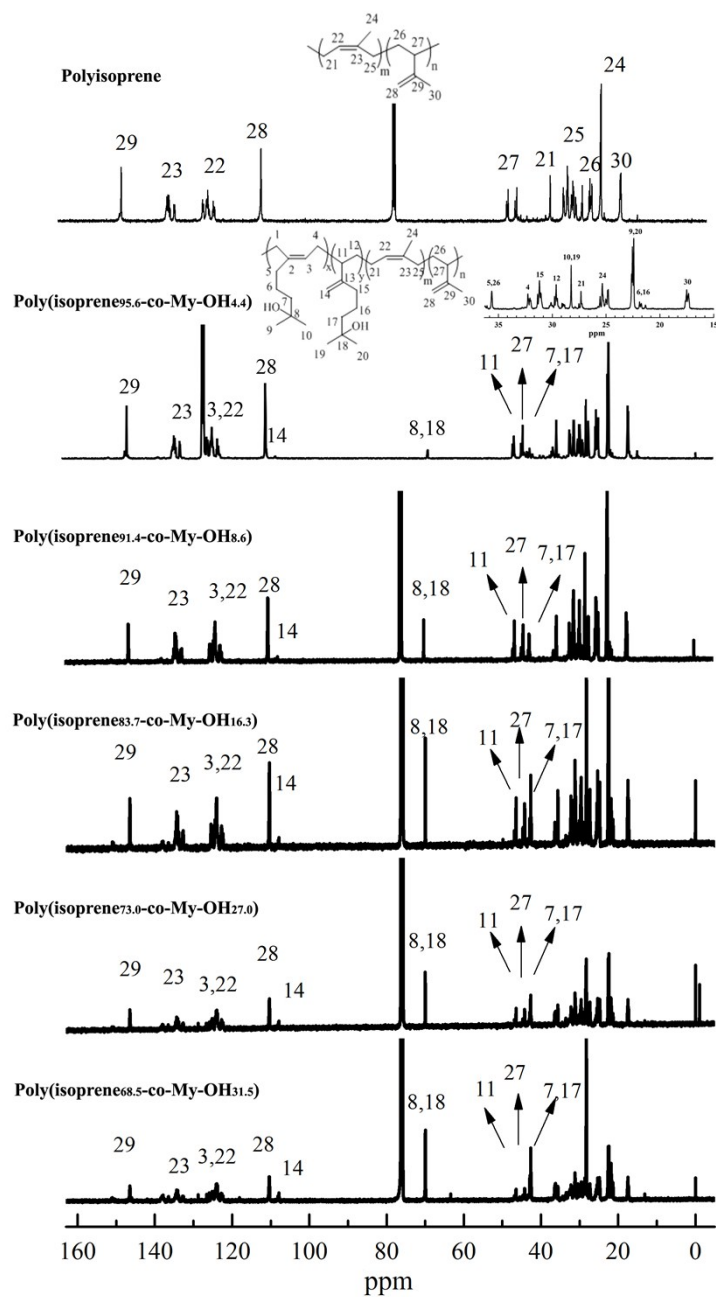
Figure 5S The mass spectra of the Co1 complex



**Figure 6S** The  $^1\text{H}$  NMR spectra of Poly(IP-co-My-OH)s (a): run 1, table 1, (b) run 6, table 1, (c) run 8, table 1 and (d) run 7, table 1

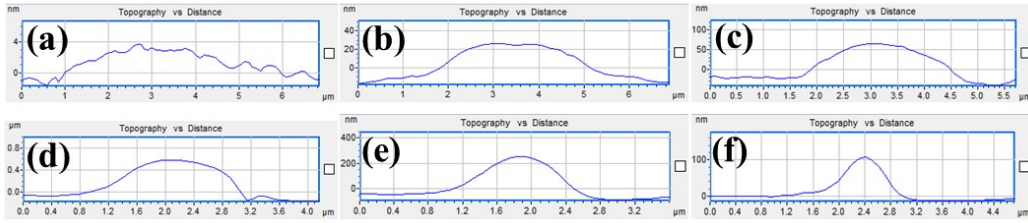


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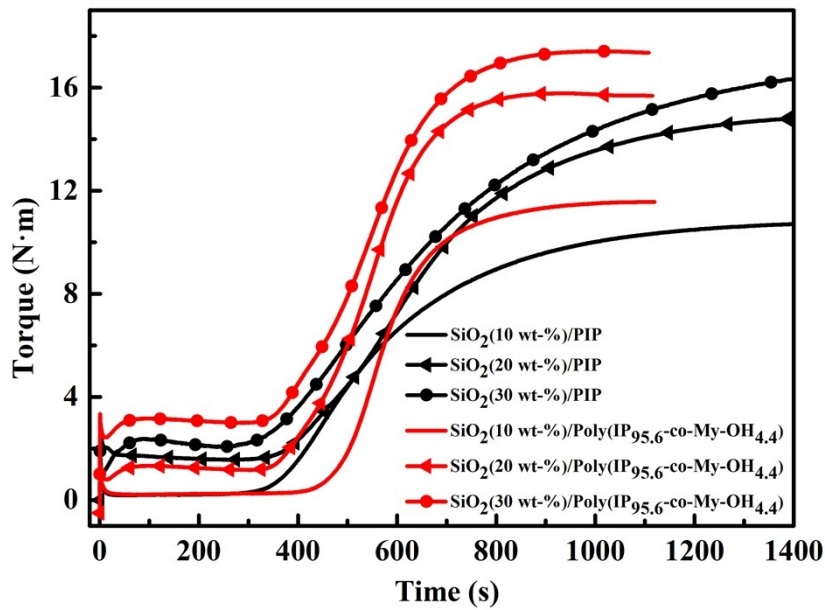


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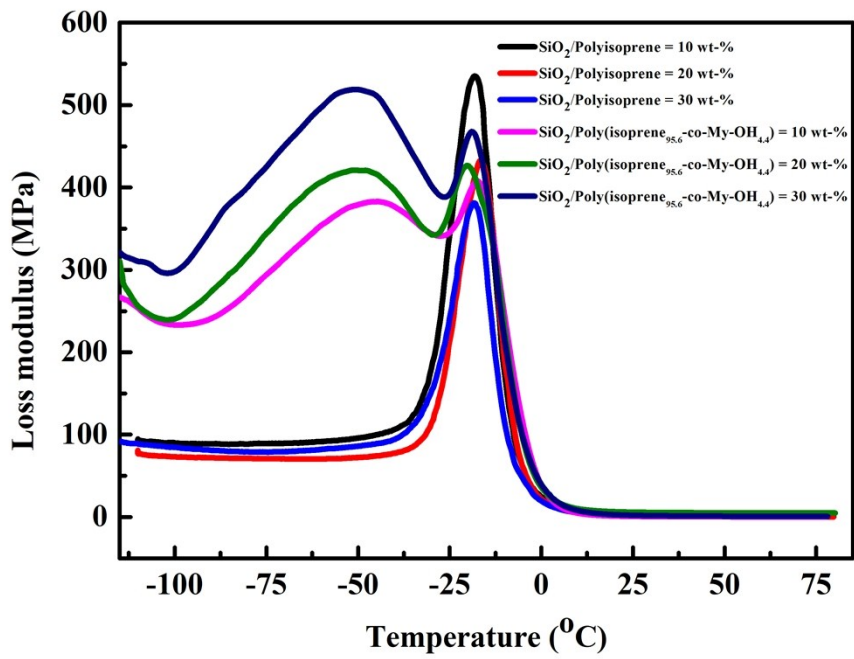




**Figure 9S** AFM topography of poly(IP-co-My-OH)s: (a) polyisoprene, (b) poly(isoprene<sub>95.6</sub>-co-My-OH<sub>4.4</sub>), (c) poly(isoprene<sub>91.4</sub>-co-My-OH<sub>8.6</sub>), (d) poly(isoprene<sub>83.7</sub>-co-My-OH<sub>16.3</sub>), (e) poly(isoprene<sub>73.0</sub>-co-My-OH<sub>27.0</sub>) and (f) poly(isoprene<sub>68.5</sub>-co-My-OH<sub>31.5</sub>)



**Figure 10S** The vulcanization profiles of SiO<sub>2</sub> reinforced SiO<sub>2</sub>/PIP composites and SiO<sub>2</sub>/poly(IP-co-My-OH)s composites



**Figure 11S** The loss storage of SiO<sub>2</sub> reinforced SiO<sub>2</sub>/PIP composites and SiO<sub>2</sub>/poly(IP-co-My-OH)s composites

**Table 1S** Crystal Data and Structure Refinements of Complex **Co1·CH<sub>3</sub>OH**

<b>Co1·MeOH</b>	
Formula	C <sub>17</sub> H <sub>30</sub> Cl <sub>2</sub> CoN <sub>3</sub> O <sub>2</sub>
	P
Molecular Weight	485.24
Crystal system	monoclinic
Space group	P 121/c1
a(Å)	16.5582(3)
b(Å)	8.70090(10)
c(Å)	16.7290(3)
α(deg)	90.00
β(deg)	111.858(2)
γ(deg)	90.00
V(Å <sup>3</sup> )	2236.90(7)
D <sub>calcd</sub> (Mg/m <sup>3</sup> )	1.441
Absorp coeff (mm <sup>-1</sup> )	9.073
F(000)	1012.0
Crystal size(mm)	0.14x0.20x0.33
θ Range (deg)	2.875 to 74.093
No. Of reflns collected	11707 (R <sub>int</sub> = 0.0328)
No. of indep reflns	4399
No. of data/ restraint/params	4399/3/254
GOF on F <sub>2</sub>	1.058
R <sub>1</sub> (I>2sigma(I))	0.0354
wR <sub>2</sub>	0.0881

**Table 2S** The summarized properties of SiO<sub>2</sub> reinforced SiO<sub>2</sub>/PIP composites and SiO<sub>2</sub>/poly(IP-co-My-OH)s composites

Parameter	PIP SiO <sub>2</sub> 10%	PIP SiO <sub>2</sub> 20%	PIP SiO <sub>2</sub> 30%	PIP-MY- OH SiO <sub>2</sub> 10%	PIP-MY- OH SiO <sub>2</sub> 20%	PIP-MY- OH SiO <sub>2</sub> 30%
Optimum cure time, Tc90,(s)	920	1015	1033	729	708	703
Scorch time, Tc10, (s)	433	473	464	515	407	397
Minimum torque, ML, (dNm)	0.18	1.23	2.12	0.26	1.51	3.05
Maximum torque, MH, (dNm)	10.55	14.82	16.33	11.35	15.88	17.48
Cure Rate Index(s <sup>-1</sup> )	0.19	0.17	0.17	0.41	0.31	0.30