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Bicyclic olefins polymerization kinetic and Mechanism with symmetrical ansa-metallocene catalysts associative with Active Centers count: Relationships between Activities and their Structure and Activation path

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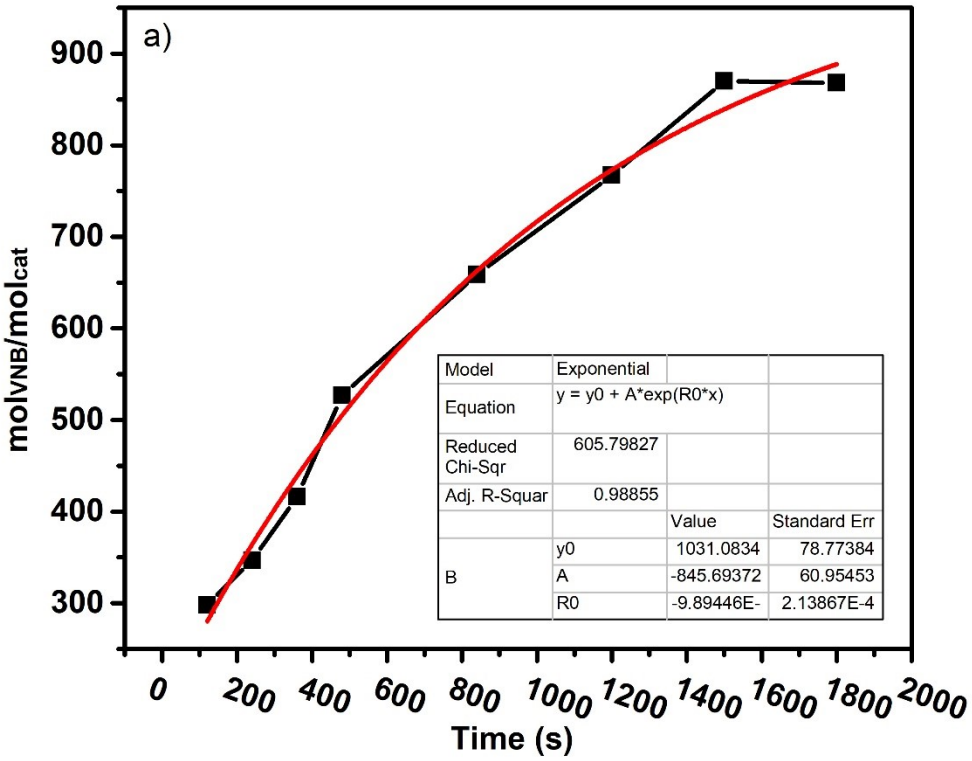
Supporting information

RUN	Time	VNB	VNB in Pol	mol_{VNB}/mol_{cat}	R_P^{ENB}/mol_{cat}	*C	[VNB]	kp VNB
	see	In polymer	wt%		molVNB/molcat s	%	mol/L	L/mol s
1.1	120	10.92	0.345	298	0.7	5.71	0.0525	233
1.2	240	9.33	0.306	347	0.67	7.55	0.0513	173
1.3	360	8.46	0.284	416	0.58	10.1	0.0496	116
1.4	480	8.05	0.273	527	0.52	14.08	0.0468	78.9
1.5	840	7.85	0.268	659	0.36	19.68	0.0435	42.04
1.6	1200	7.22	0.250	767	0.25	26.17	0.0408	23.395
1.7	1500	7.09	0.247	870	0.18	29.93	0.0382	15.727
1.8	1800	5.73	0.207	868	0.14	31.67	0.0383	11.5397

Table S1 Calculation of R_P^{VNB} and K_P^{VNB} in the ethylene-VNB copolymerization.



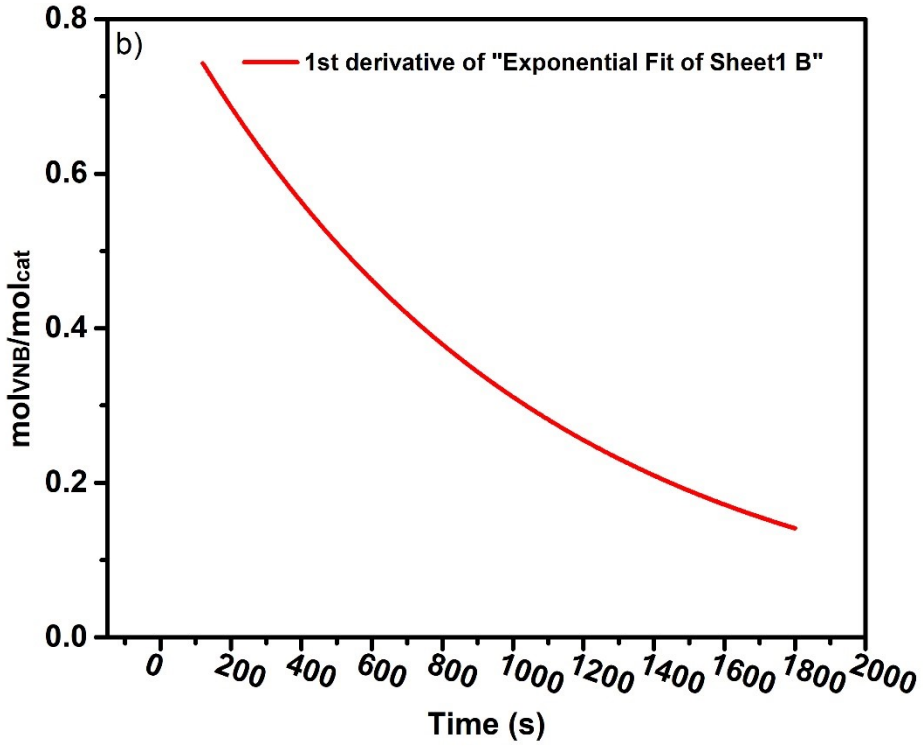
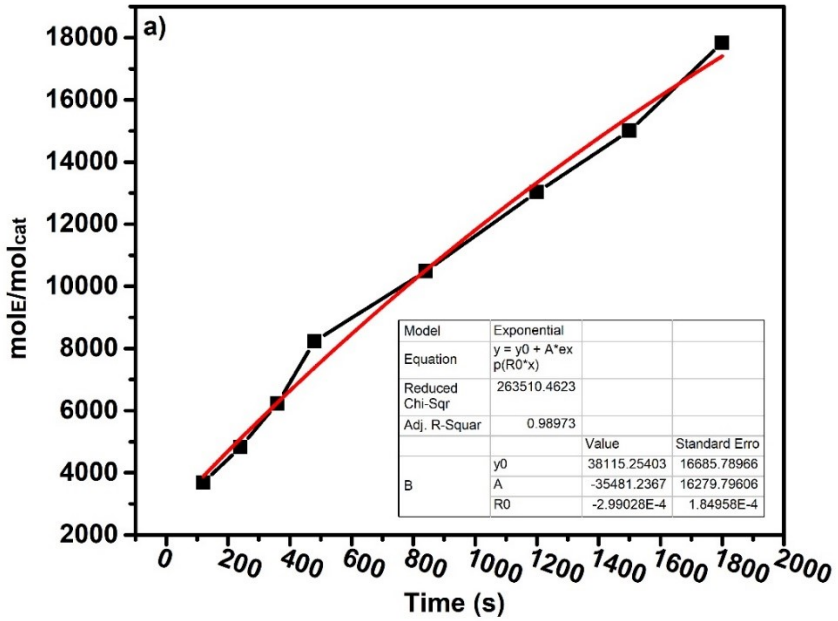


Figure S1.The plot of mol_{VNB}/mol_{cat} vs. time, and Differentiate.

Table S2. Calculation of R_P^E and K_P^E in the ethylene-VNB copolymerization.

RUN	Time	VNB	VNB in Pol	*C	mE	mol_E/mol_{cat}	R_P^E	kp E
	see	In polymer	wt%	%	g		molE/molcat s	L/mol s
1.1	120	10.92	0.345	5.71	0.129	3686	10.23	4266
1.2	240	9.33	0.306	7.55	0.169	4829	9.87	3113
1.3	360	8.46	0.284	10.1	0.218	6229	9.52	2244
1.4	480	8.05	0.273	14.08	0.288	8229	9.18	1552
1.5	840	7.85	0.268	19.68	0.367	10486	8.25	998
1.6	1200	7.22	0.250	26.17	0.456	13029	7.41	674
1.7	1500	7.09	0.247	29.93	0.525	15000	6.77	539
1.8	1800	5.73	0.207	31.67	0.624	17829	6.19	465



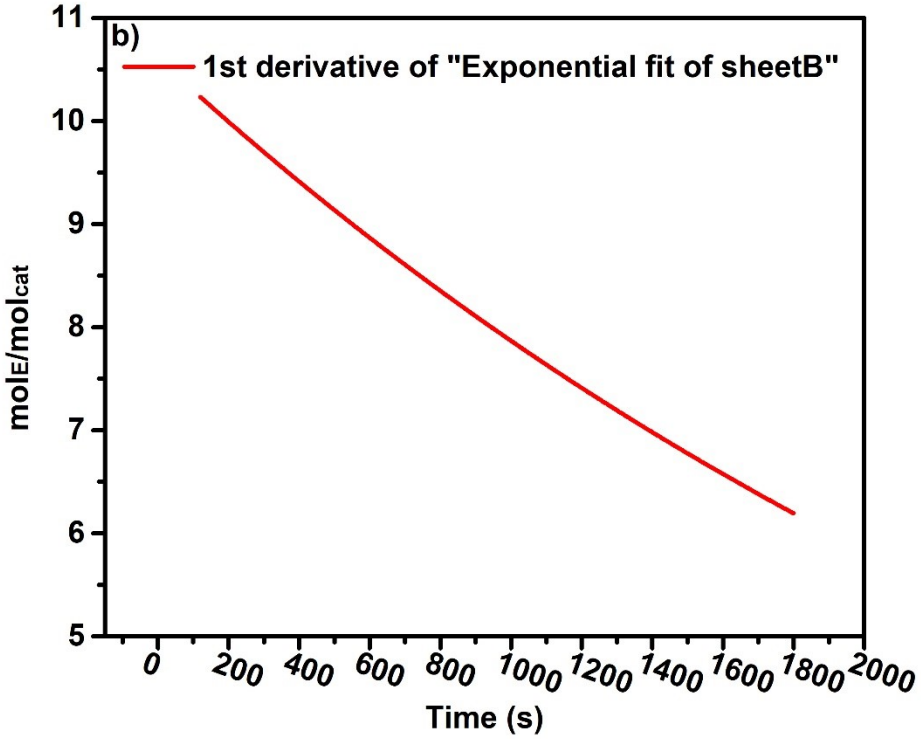


Figure S2.Plot of mol_{VNB}/mol_{cat} vs time, and Differentiate.

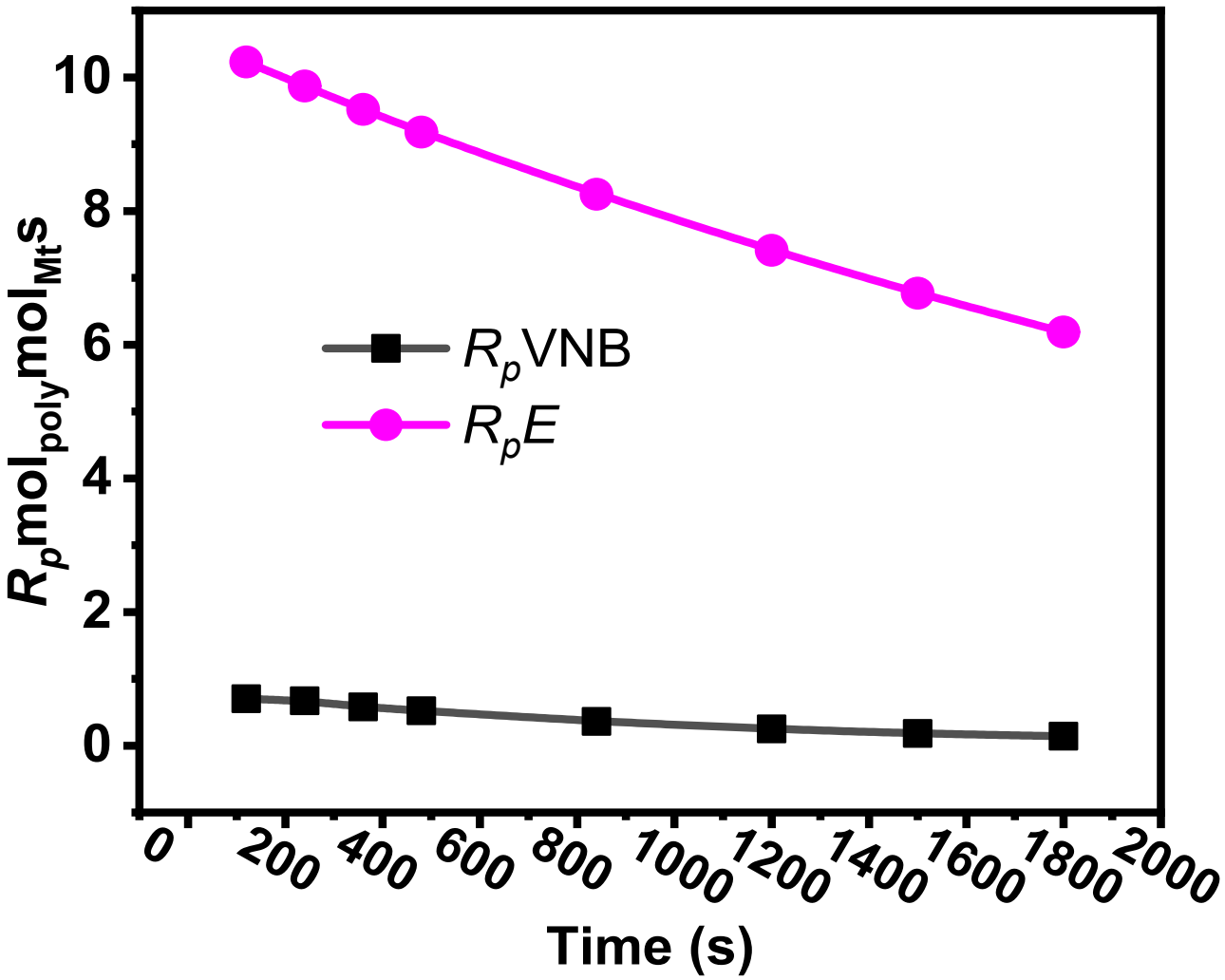


Figure S3. Variation of chain propagation rate R_pE and k_pVNB with polymerization time (t_p) in E/VNB copolymerization.

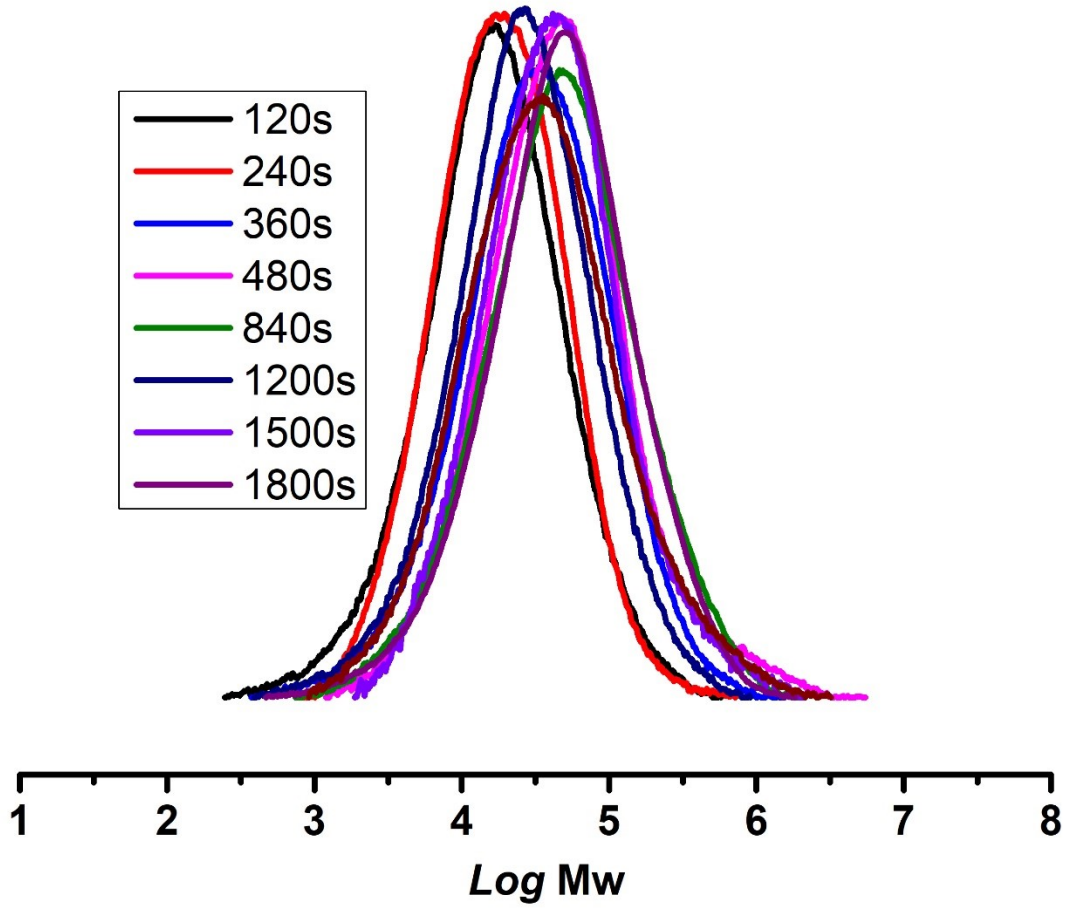
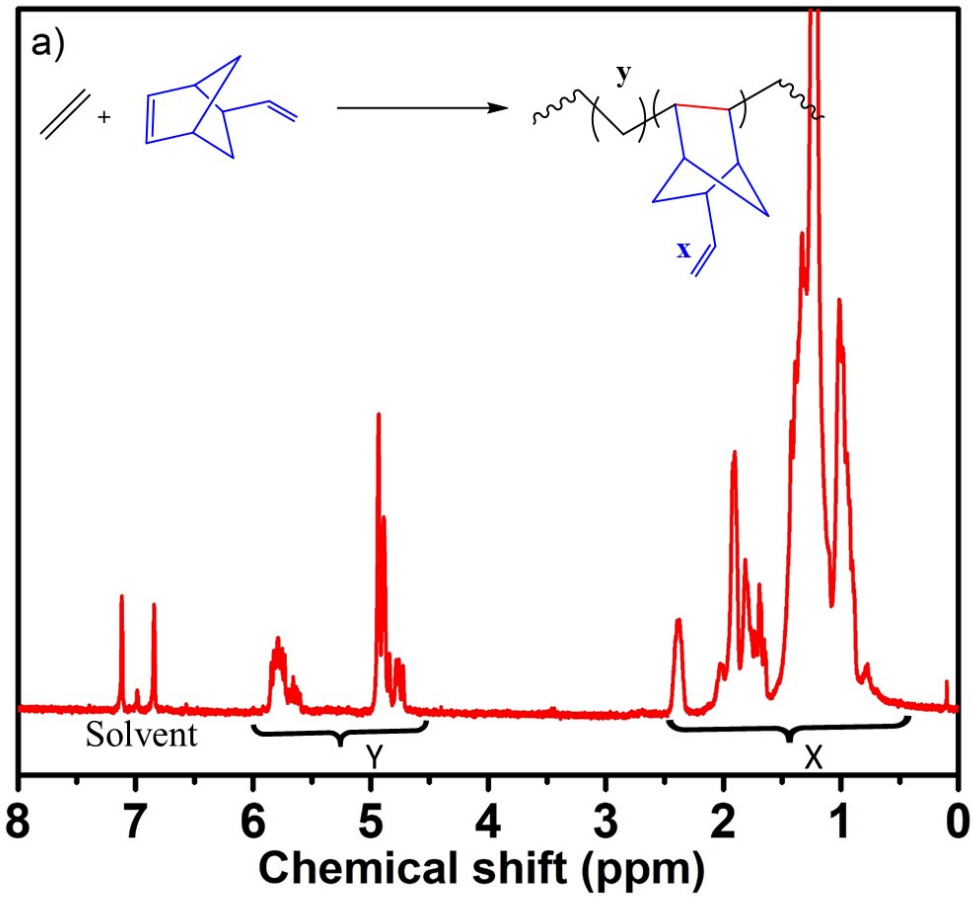


Figure S4 Molecular weight distribution of E-VNB copolymers with polymerization time.


a)
y
x
Solvent
Y
X
8
7
6
5
4
3
2
1
0
Chemical shift (ppm)

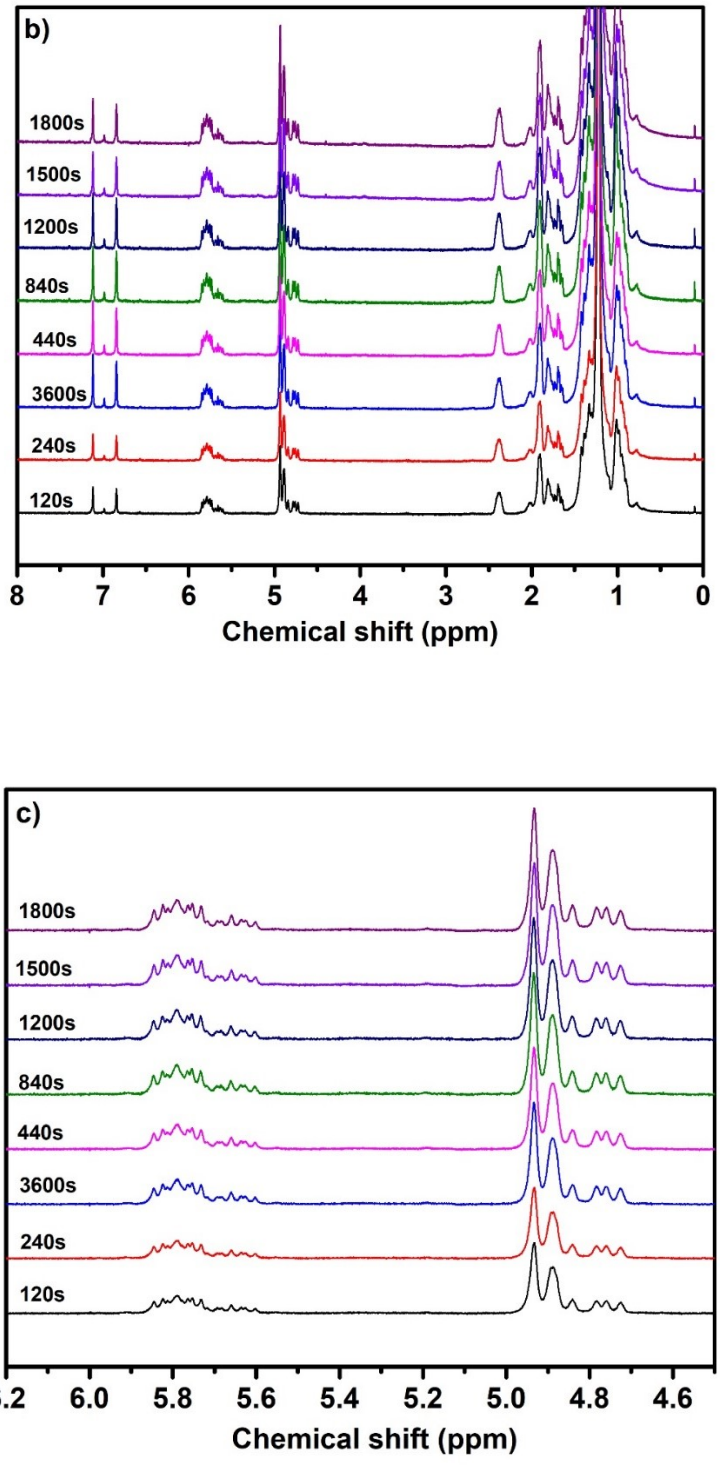
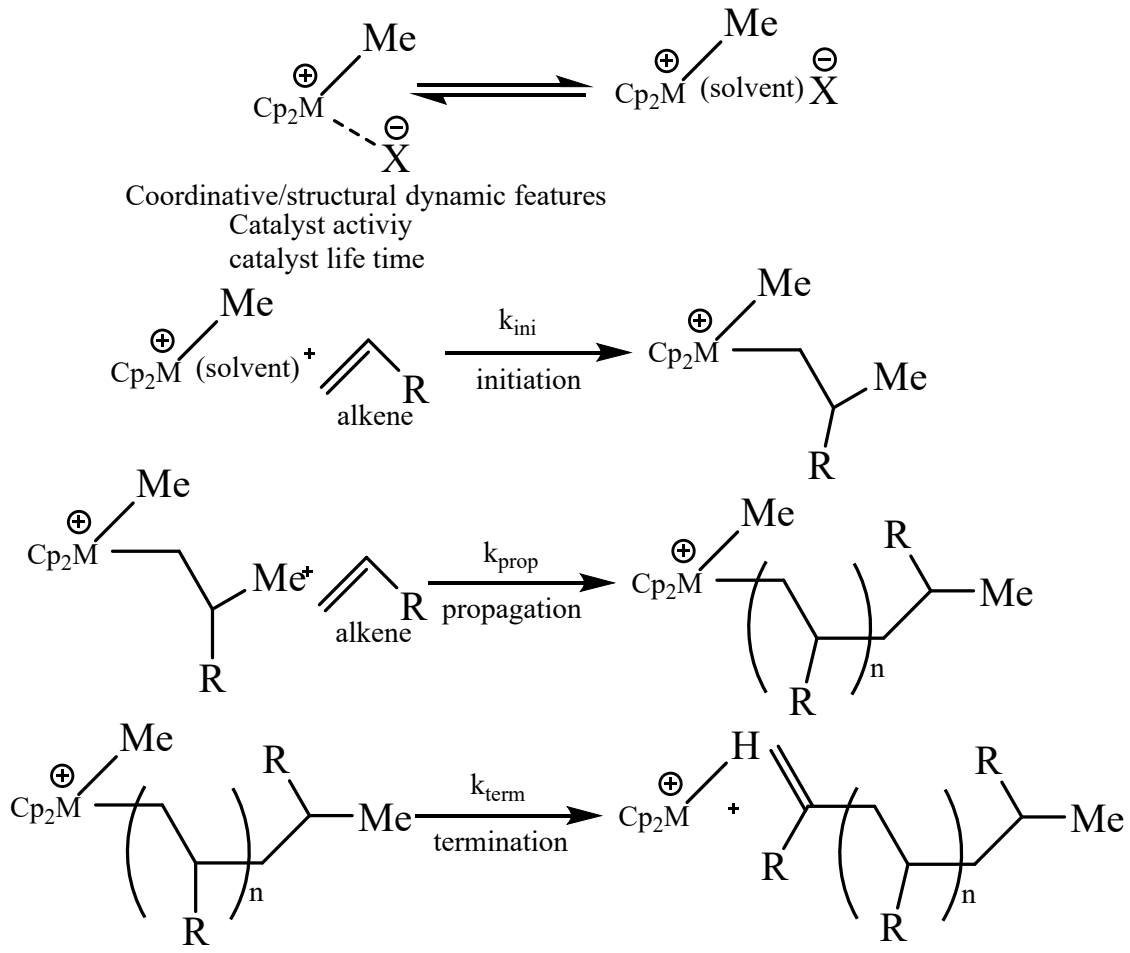
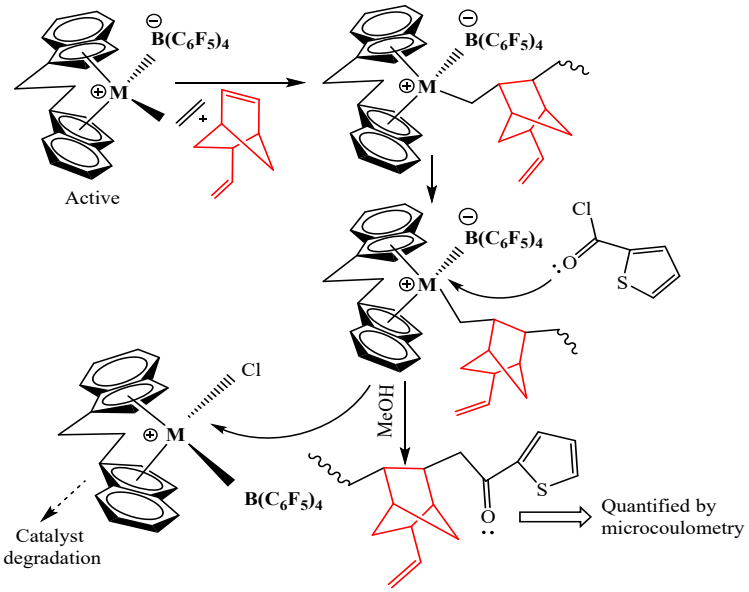


Figure S5 ^{1}HNMR of E-ENB copolymers with polymerization time.



Scheme 1. [20]

Scheme 1 is a simple example of how metallocene-catalyzed polymerization of alkenes might work. It emerged from the work of Richardson, Guo, and Siedle et al.



Scheme S2. TPPC quenched active sites calculated through sulfur (S) content using A YHTS-2000 ultra-violet fluorescence sulfur detector for *rac*-Et(Ind)$_2$ZrCl$_2$ catalyzed E/VNB copolymers.