

Electronic Supplementary Information (ESI) for RSC Advances.

Silyl diol ester as a new selectivity control agent in $MgCl_2$ -supported Ziegler-Natta systems for Propylene polymerization: catalyst structure and polymer properties

Fatemeh Poorsank,^a Hassan Arabi^{*a} and Nona Ghasemi Hamedani^a

Department of Polymerization Engineering, Iran Polymer and Petrochemical Institute,

P.O. Box: 14965/115, Tehran, Iran

E-mail: h.arabi@ippi.ac.ir

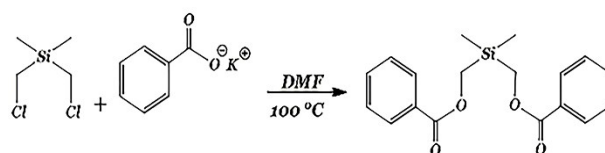


Figure S1 Synthetic route of silyl diol ester

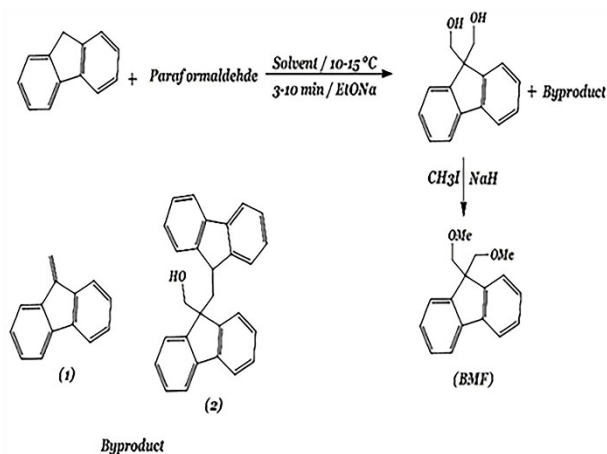


Figure S2 Synthetic route of 9, 9-bis (methoxymethyl) fluorene

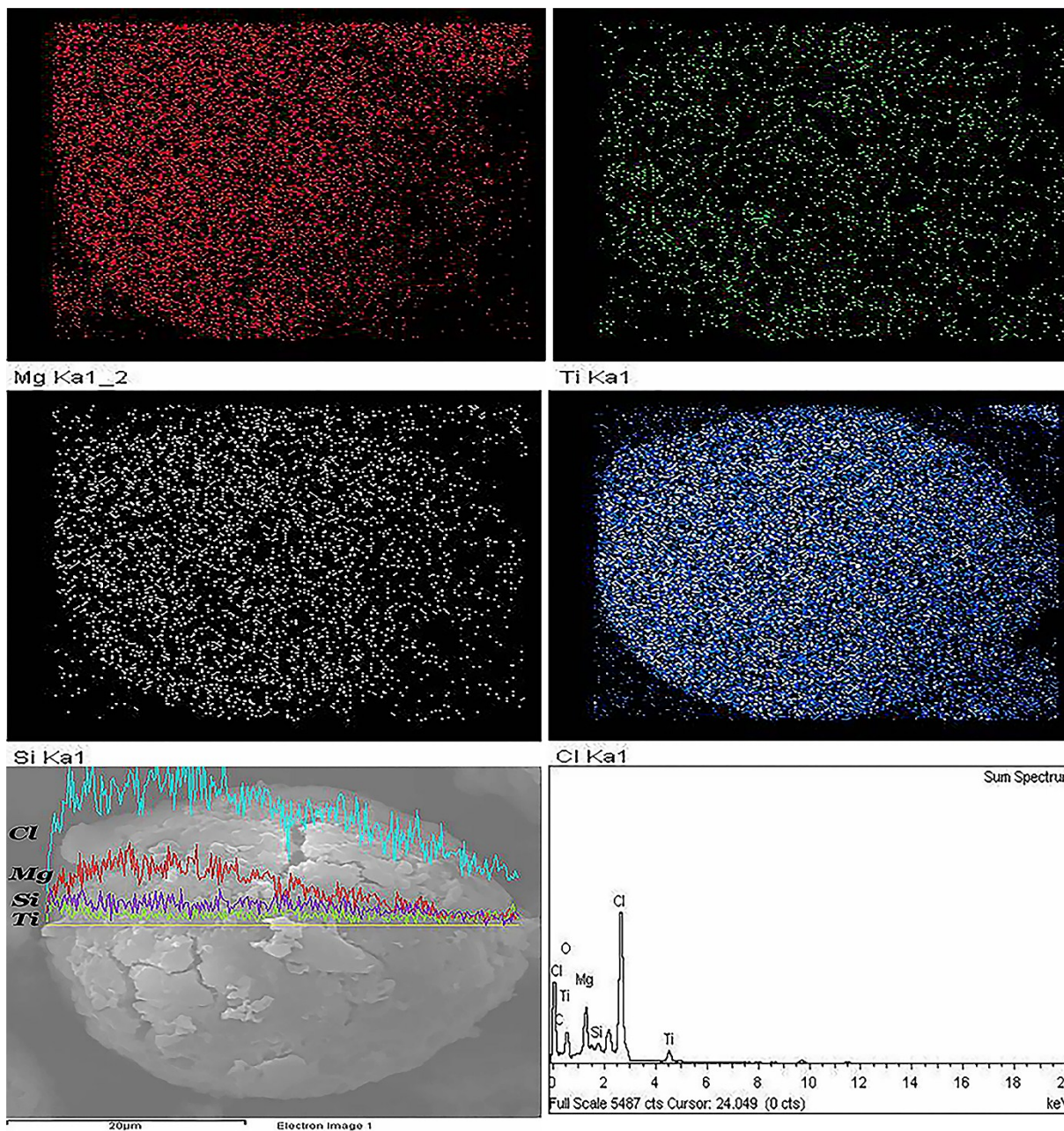


Figure S3 SEM photograph of cross-section of catalyst A3 particle and the element distribution data. The curves on the particle are the element distributions along the line (top to bottom): Cl, Mg, Si and Ti

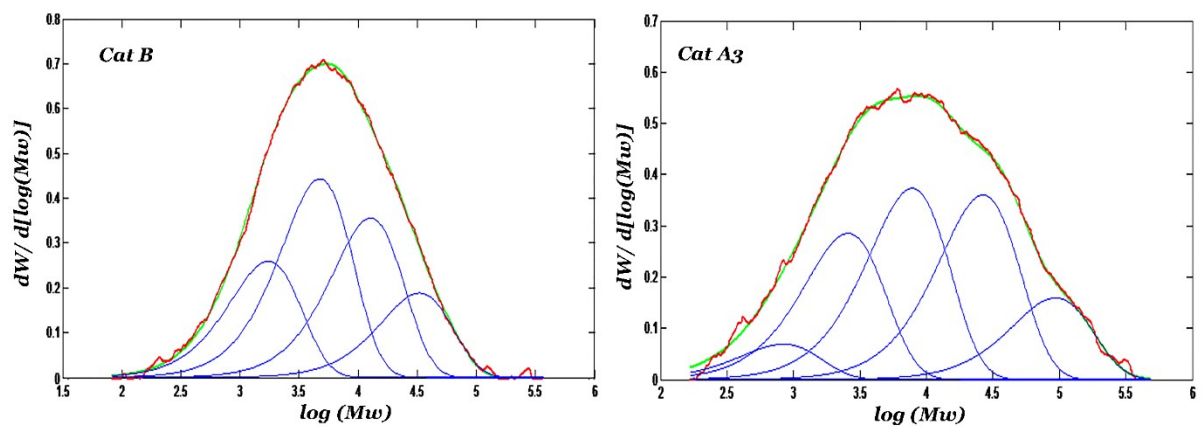


Figure S4 Molecular weight distribution of catalysts: B and A₃

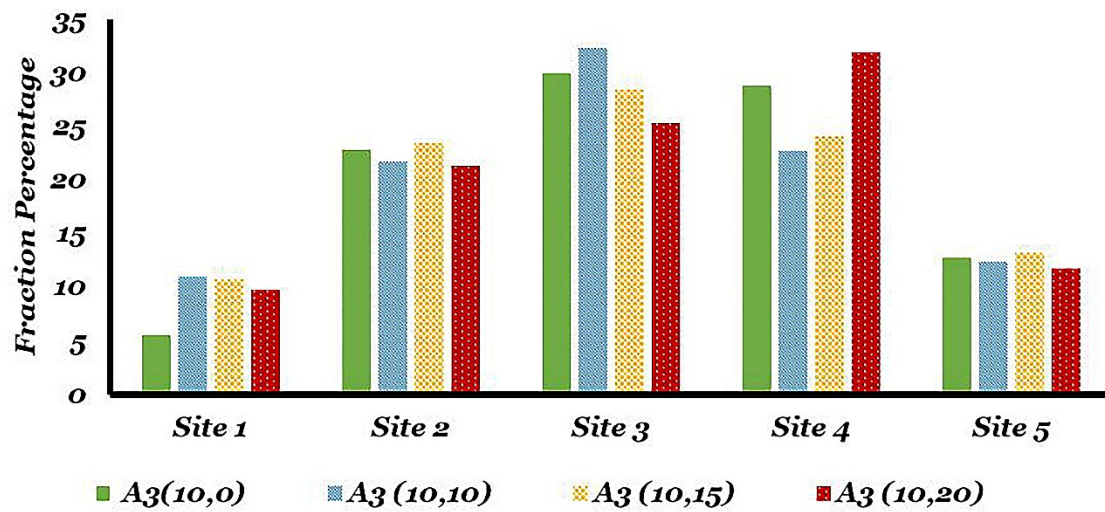


Figure S5 Effect of ED/cat ratio on fraction percentage of different sites

Table S1. Effect of the ED/cat ratio on the performances of the catalyst catalyst A₃

ED ^a /Cat	0	0.5	0.66	1
Activity ^b	2.06	1.3	1.53	1.48
I.I (%) ^c	97.6	96.3	97.4	96.3
M _n	84000	141000	152000	134600
M _w	647000	964000	943000	887000
PDI	7.71	6.85	6.22	6.59

^aexternal donor: C-donor; ^b polymerization conditions: 20 mg catalyst, TEA/cat: 10, ^c xylene solubility.

Table S2. Effect of the TEA/cat ratios on the performances of the catalyst A₃

TEA/Cat	5	10	20
Activity	0.98	1.53	1.39
I.I (%) ^b	95.6	97.4	96.72
M _n	133000	152000	76000
M _w	943000	943000	758000
PDI	7.07	6.22	10.00

^aPolymerization conditions: 20 mg catalyst, ED/cat= 0.66, external donor: C-donor, ^b xylene solubility.

Table S3. Hydrogen response of catalysts: A₃, D and B

Catalyst	H ₂ (mmol)	Activity	I.I	MFR
D	2.25	2.69	98.7	16.91
D	4.5	4.32	99.3	24.1
D	9	3.94	98.74	57.88
D	13.5	2.11	98.74	117.38
A ₃	1.12	2.45	98.78	4.55
A ₃	2.25	3.48	96.66	7.18
A ₃	4.5	2.02	96.03	14.9
A ₃	6.75	2.16	95.68	21.1
A ₃	13.5	3.40	93.97	67.1
B	2.25	4.34	99.7	17.85
B	4.5	3.75	99.2	35.37
B	9	4.04	98.46	120.44

Table S4. Result of deconvolution the MWD curve of catalysts: A₃ and B

Catalyst	Site 1		Site 2		Site 3		Site 4		Site 5		Site 6	
	F _r ^a	M _w ^b	F _r	M _w	F _r	M _w	F _r	M _w	F _r	M _w	F _r	M _w
B	20.8	2.43	35.56	6.64	28.53	17.89	15.11	46.29				

A₃ 5.53 1.18 22.88 3.61 29.93 10.97 28.87 37.32 12.79 130.98

^aF_r was the weight percentage of the fraction produced by a certain active centre in catalyst.

^b Weight average molecular weight, in 10⁴ g/mol.

Table S5. Effect of ED/cat ratio on active centers of catalyst A₃

		Site 1		Site 2		Site 3		Site 4		Site 5	
TEA/Cat	TEA/ED	F _r ^a	M _w ^b	F _r	M _w	F _r	M _w	F _r	M _w	F _r	M _w
10	0	5.53	1.18	22.88	3.61	29.93	10.97	28.87	37.32	12.79	130.98
10	10	10.96	2.61	21.67	7.97	32.3	26.69	22.72	62.67	12.34	157.26
10	15	10.81	3.03	23.45	8.73	28.43	26.45	24.11	61.84	13.2	171.22
10	20	9.74	2.79	21.30	7.9	25.37	21.77	31.89	59.71	11.69	190.95

^aF_r was the weight percentage of the fraction produced by a certain active center in catalyst.

^b Weight average molecular weight, in 10⁴ g/mol.
