Supplementary Materials: Influence of Branching Density in Ethylene-Octene Copolymers on Electron Beam Crosslinkability

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EOC-20 calculation: 20 wt % of octene, M_n = 37,400 g/mol.

$$ethylene = -CH_2 - CH_2 -, \quad M_{ET} = 2C + 4H = 2 \times 12.011 + 4 \times 1.008 = 28.054\ g/mol$$

$$octene = (CH_2 - CH_2)_4, \ M_{OCT} = 8C + 16H = 8 \times 12.011 + 16 \times 1.008 = 112.216\ g/mol$$

$$wt.fraction\ of\ octene\ w_{OCT} = \frac{20}{100} = 0.20$$

$$wt.fraction\ of\ ethylene\ w_{ET} = 1 - w_{OCT} = 1 - 0.20 = 0.80$$

$$Molar\ fraction\ of\ octene = x_{OCT}$$

$$x_{OCT} = \frac{\frac{w_{OCT}}{M_{OCT}}}{\frac{w_{OCT}}{M_{OCT}} + \frac{w_{ET}}{M_{ET}}} = \frac{\frac{0.20}{112.216}}{\frac{0.20}{112.216} + \frac{0.80}{28.054}} = 0.05882 \quad (5)$$

$$Molar\ fraction\ of\ ethylene = x_{ET} = 1 - x_{OCT} = 1 - 0.05882 = 0.94118$$

$$molecular\ weight\ of\ repeating\ unit$$

$$M_{ET-OCT} = x_{ET}M_{ET} + x_{OCT}M_{OCT} = 0.94118 \times 28.054 + 0.05882 \times 112.216 = 33.0047\ g/mol$$

$$Polymerization\ degree = P_n = \frac{M_{nEOC}}{M_{ET-OCT}} = \frac{37400}{33.0047} = 1133$$

Charlesby-Pinner equation

$$s + \sqrt{s} = \frac{p_0}{q_0} + \frac{1}{q_0 P_n D}$$

$$In\ plot \quad s + \sqrt{s} \quad vs.\ \frac{1}{D}: \quad intercept = \frac{p_0}{q_0}, \ slope = \frac{1}{q_0 P_n}$$

$$In\ case\ of\ EOC - 20: \quad intercept = 0.315645, \ slope = 50.3139$$

$$then \quad \frac{p_0}{q_0} = 0.315645 \quad and \quad \frac{1}{q_0 P_n} = 50.3139$$

$$q_0 = \frac{1}{slope \cdot P_n} = \frac{1}{50.3139 \cdot 1133} = 0.00001754$$

$$then \quad p_0 = q_0 \cdot intercept = q_0 \cdot \frac{p_0}{q_0} = 0.00001754 \cdot 0.315645 = 0.000005536$$

Calculation of G parameters according to Charlesby-Pinner equation:

$$s + \sqrt{s} = \frac{G(S)}{2G(X)} + \frac{4.82 \times 10^6}{G(X)M_n D}$$

$$then \quad \frac{G(S)}{2G(X)} = \frac{p_0}{q_0}$$

$$\frac{G(X)}{G(S)} = \frac{1}{2\frac{p_0}{q_0}} = \frac{1}{2 \cdot 0.315645} = 1.5841$$

$$slope = \frac{4.82 \times 10^6}{G(X)M_n}$$

$$G(X) = \frac{4.82 \times 10^6}{slope \cdot M_n} = \frac{4.82 \times 10^6}{50.3139 \cdot 37400} = 2.5615$$

$$intercept = \frac{G(S)}{2G(X)}$$

$$G(S) = 2G(X) \cdot intercept = 2 \times 2.5615 \times 0.315645 = 1.6170$$

Drawing a curve through the points in Gel–Dose graph after evaluation of Charlesby-Pinner parameters

$$s + \sqrt{s} = \frac{p_0}{q_0} + \frac{1}{q_0 P_n D}$$

$$s + \sqrt{s} = A + \frac{B}{D} \tag{6}$$

A = intercept, B = slope

$$s = \frac{2B + D - \sqrt{-D(-4B - D - 4AD)} + 2AD}{2D} \tag{7}$$

For EOC-20 the intercept A = 0.315645 and the slope B = 50.3139

$$s = \frac{2 \cdot 50.3139 + D - \sqrt{-D \cdot (-4 \cdot 50.3139 - D - 4 \cdot 0.315645 \cdot D)} + 2 \cdot 0.315645 \cdot D}{2 \cdot D}$$

Calculation in EXCEL:

$s = (2 \times 50.3139 + D - SQRT((-D) \times (-4 \times 50.3139 - D - 4 \times 0.315645D)) + 2 \times 0.315645D)/(2D)$

$$Gel\ in\ \% = (1 - s) * 100$$

Table S1. Calculation of Charlesby-Pinner parameters.

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
wt % of octene	**wt fraction of octene**	**wt fraction of ethylene**	**molar fraction of octene**	**molar fraction of ethylene**	**$M_{ET\text{-}OCT}$**	**M_n**	**P_n**	**slope**	**p_0/q_0**	**q_0**	**p_0**	**G(X)/G(S)**	**G(X)**	**G(S)**
20	0.20	0.80	0.05882	0.94118	33.0047	37,400	1,133	50.3139	0.315645	1.754×10^{-5}	5.536×10^{-6}	1.5841	2.5615	1.6170
35	0.35	0.65	0.11864	0.88136	38.0393	42,321	1,113	53.9744	0.198488	1.665×10^{-5}	3.305×10^{-6}	2.5190	2.1101	0.8377

A, from DuPont Dow Elastomers; B, A3/100; C, 1−B3; D, (B3/112.216)/((B3/112.216)+(C3/28.054)); E, 1−D3; F, E3*28.054+D3*112.216; G, from GPC; H, G3/F3; I, from Charlesby-Pinner linear plot; J, from Charlesby-Pinner linear plot; K, 1/(I3*H3); L, J3*K3; M, 1/(2*J3); N, 4,820,000/(I3*G3); O, J3*2*N3.