

POE very highly branched polyethylene

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	very highly branched polyethylene, ultralow density ethylene copolymer	
CAS name	-	1-octene, polymer with ethene	
Acronym	-	POE	
CAS number	-	26221-73-8	
HISTORY			
Person to discover	-	Finlayson, M F; Garrison, C C; Guerra, R E; Guest, M J; Kolthammer, B W S; Parikh, D R; Ueligger, S M	Finlayson, M F; Garrison, C C; Guerra, R E; Guest, M J; Kolthammer, B W S; Parikh, D R; Ueligger, S M, US Patent 6,723,810, Dow Chemical, Apr. 20, 2004.
Date	-	2004	
Details	-	process of making ultralow density PE	
SYNTHESIS			
Monomer(s) structure	-	$\text{H}_2\text{C}=\text{CH}_2$ $\text{H}_2\text{C}=\text{CH}(\text{CH}_2)_5\text{CH}_3$	
Monomer(s) CAS number(s)	-	74-85-1; 111-66-0	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	28.05; 112.21	
Monomer(s) expected purity(ies)	%	99.99; 97-99	
Ethylene content	%	75-98	
C3-C12 alpha-olefin content	%	1-25	
C4-C20 diene content	%	0-2	
Octene content	%	5.9-25	Yang, K; Yu, W; Zhou, C, J. Appl. Polym. Sci., 105, 846-52, 2007.
Catalyst	-	metallocene (Insite technology)	
Number average molecular weight, M_n	dalton, g/mol, amu	36,000-77,000	Shan, H; White, J L; deGroot, A W, Int. J. Polym. Anal. Charact., 12, 231-49, 2007.
Mass average molecular weight, M_w	dalton, g/mol, amu	76,000-192,000	Shan, H; White, J L; deGroot, A W, Int. J. Polym. Anal. Charact., 12, 231-49, 2007.
Polydispersity, M_w/M_n	-	1.5-2.5	
Degree of branching	per 1000 carbons	13.7-32	Parkinson, M; Klimke, K; Spiess, H W; Wilhelm, M, Macromol. Chem. Phys., 208, 2128-33, 2007; Yang, K; Yu, W; Zhou, C, J. Appl. Polym. Sci., 105, 846-52, 2007; Crosby, B J; Mangnus, M; de Groot, W; Daniels, R; McLeish, T C B; J. Rheol., 46, 2, 401-26, 2002.
Type of branching	-	octene	
STRUCTURE			
Crystallinity	%	12-40	
Entanglement molecular weight	dalton, g/mol, amu	calc.=2,200	
Lamellae thickness	nm	3.2-5.3; 40-100 (lamellar length)	
Heat of crystallization	kJ kg ⁻¹	33-82	
Rapid crystallization temperature	°C	40-54	Shan, H; White, J L; deGroot, A W, Int. J. Polym. Anal. Charact., 12, 231-49, 2007.

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COMMERCIAL POLYMERS			
Some manufacturers	-	DuPont	
Trade names	-	Engage	
PHYSICAL PROPERTIES			
Density at 20°C	g cm ⁻³	0.863-0.885	
Color	-	white	
Melting temperature, DSC	°C	49-76	
Decomposition temperature	°C	300	
Glass transition temperature	°C	-29 to -52	
Heat of fusion	kJ mol ⁻¹	0.35-1.1	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Mooney viscosity	-	5-35	
Melt index, 190°C/2.16 kg	g/10 min	0.5-30	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	very good	
Alcohols	-	good	
Alkalis	-	very good	
Aliphatic hydrocarbons	-	poor	
Aromatic hydrocarbons	-	poor	
Esters	-	poor	
Greases & oils	-	good to poor	
Halogenated hydrocarbons	-	poor	
Ketones	-	poor	
Effect of EtOH sterilization (tensile strength retention)	%	86-131	Navarrete, L; Hermanson, N, Antec, 2807-18, 1996.
FLAMMABILITY			
Autoignition temperature	°C	330-410	
Heat of combustion	J g ⁻¹	47,740	
WEATHER STABILITY			
Spectral sensitivity	nm	<300	
Activation wavelengths	nm	300, 330-360	
Important initiators and accelerators	-	unsaturations, aromatic carbonyl compounds (deoxyanisoin, dibenzocycloheptadienone, flavone, 4-methoxybenzophenone, 10-thioxanthone), hydrogen bound to tertiary carbon at branching points, aromatic amines, groups formed on oxidation (hydroperoxides, carbonyl, carboxyl, hydroxyl) substituted benzophenones, complexes with ground-state oxygen, quinones (anthraquinone, 2-chloroanthraquinone, 2-tert-butyl-athraquinone, 1-methoxyanthraquinone, 2-ethylanthraquinone, 2-methylanthraquinone), transition metal compounds (Ni < Zn < Fe < Co), ferrocene derivatives, titanium dioxide (anatase), ferric stearate, polynuclear aromatic compounds (anthracene, phenanthrene, pyrene, naphthalene)	
Products of degradation	-	free radicals, hydroperoxides, carbonyl groups, chain scission, crosslinking	

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Stabilizers	-	<p>UVA: 2-hydroxy-4-octyloxybenzophenone; phenol, 2-(5-chloro-2H-benzotriazole-2-yl)-6-(1,1-dimethylethyl)-4-methyl-; 2,2'-methylenebis(6-(2H-benzotriazol-2-yl)-4-1,1,3,3-tetramethylbutyl)phenol; 2,4-di-tert-butyl-6-(5-chloro-2H-benzotriazole-2-yl)-phenol; reaction product of methyl 3-(2H-benzotriazole-2-yl)-5-tert-butyl-4-hydroxyphenyl propionate/ PEG 300; 2-[4,6-bis(2,4-dimethylphenyl)-1,3,5-triazin-2-yl]-5-(octyloxy) phenol; Screener: titanium dioxide; zinc oxide; carbon black; Acid scavenger: hydrotalcite; Fiber: carbon nanotube; HAS: 1,3,5-triazine-2,4,6-triamine, N,N''[1,2-ethane-diyl-bis[[[4,6-bis[butyl(1,2,6,6-pentamethyl-4-piperidinyloxy)amino]-1,3,5-triazine-2-yl]imino]-3,1-propanediyl] bis[N',N''-dibutyl-N',N''-bis(1,2,2,6,6-pentamethyl-4-piperidinyloxy)-; bis(1,2,2,6,6-pentamethyl-4-piperidinyloxy)sebacate + methyl-1,2,2,6,6-pentamethyl-4-piperidyl sebacate; 2,2,6,6-tetramethyl-4-piperidinyloxy stearate; reaction products of N,N'-ethane-1,2-diylbis(1,3-propanediamine), cyclohexane, peroxidized 4-butylamino-2,2,6,6-tetramethylpiperidine and trichloro-1,3,5-triazine; poly[[[6-(1,1,3,3-tetramethylbutyl)amino]-1,3,5-triazine-2,4-diyl][2,2,6,6-tetramethyl-4-piperidinyloxy]imino]-1,6-hexanediyloxy[2,2,6,6-tetramethyl-4-piperidinyloxy]imino]; 1,6-hexanediamine- N,N'-bis(2,2,6,6-tetramethyl-4-piperidinyloxy)- polymer with 2,4,6-trichloro-1,3,5-triazine, reaction products with N-butyl-1-butanamine an N-butyl-2,2,6,6-tetramethyl-4-piperidinyloxyamine; butanedioic acid, dimethylester, polymer with 4-hydroxy-2,2,6,6-tetramethyl-1-piperidine ethanol; alkenes, C20-24-.alpha.-, polymers with maleic anhydride, reaction products with 2,2,6,6-tetramethyl-4-piperidinyloxyamine; 1,6-hexanediamine, N,N'-bis(2,2,6,6-tetramethyl-4-piperidinyloxy)-, polymers with morpholine-2,4,6-trichloro-1,3,5-triazine reaction products, methylated; Phenolic antioxidant: 2,6-di-tert-butyl-4-(4,6-bis(octylthio)-1,3,5-triazine-2-ylamino) phenol; pentaerythritol tetrakis(3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate); octadecyl-3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate; 3,3',3',5,5',5'-hexa-tert-butyl-a,a',a'- (mesitylene-2,4,6-triyl)tri-p-cresol; 2-(1,1-dimethylethyl)-6-[[3-(1,1-dimethylethyl)-2-hydroxy-5-methylphenyl]methyl-4-methylphenyl acrylate; 1,3,5-tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6-(1H,3H,5H)-trione; 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-ol; 2',3-bis[[3-[3,5-di-tert-butyl-4-hydroxyphenyl]propionyl]]propionohydrazide; isotridecyl-3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate; 2,2'-ethylidenebis(4,6-di-tert-butylphenol); ethylene bis[3,3-bis[3-(1,1-dimethylethyl)-4-hydroxyphenyl]butanoate]; 1,3,5-tris(4-tert-butyl-3-hydroxy-2,6-dimethylbenzyl)-1,3,5-triazine-2,4,6-(1H,3H,5H)-trione; 2,2'-methylenebis(4-methyl-6-tertbutylphenol); 3,5-bis(1,1-dimethylethyl)-4-hydroxy-benzenepropanoic acid, C13-15 alkyl esters; 2,2'-isobutylidenebis(2,4-dimethylphenol); 1,1,3-tris(2'-methyl-4'-hydroxy-5'-tert-butylphenyl)butane; Phosphite: bis-(2,4-di-tert-butylphenol) pentaerythritol diphosphite; tris(2,4-di-tert-butylphenyl)phosphite; trinonylphenol phosphite; distearyl pentaerythritol diphosphite; trilauryl triphosphite; Thiosynergist: didodecyl-3,3'-thiodipropionate; dioctadecyl 3,3'-thiodipropionate; 2,2'-thiodiethylene bis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate]; 4,4'-thiobis(2-tert-butyl-5-methylphenol); 2,2'-thiobis(6-tert-butyl-4-methylphenol); pentaerythritol tetrakis(b-laurylthiopropionate); Quencher: (2,2'-thiobis(4-tert-octyl-phenolato))-N-butylamine-nickel(II); Optical brightener: 2,2'-(2,5-thiophenediyl)bis(5-tert-butylbenzoxazole)</p>	
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	1/1/0	

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PARAMETER	UNIT	VALUE	REFERENCES
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
OSHA	mg m ⁻³	5 (respirable), 15 (total)	
PROCESSING			
Applications	-	adhesives, caulks, fibers, inks, oil modifiers, processing aids, sealants, viscosity modifiers, wax substitutes	
BLENDS			
Suitable polymers	-	HDPE, PP, PS	Li, X; Wu, H; Wang, Y; Bai, H; Liu, L; Huang, T, Mater. Sci. Eng., 527A, 3, 531-38, 2010.
ANALYSIS			
NMR (chemical shifts)	ppm	peak assignments for ¹³ C NMR spectra in ref.	Qiu, X H; Redwine, D; Gobbi, G; Naumthanom, A; Rinaldi, P L, Macromolecules, 40, 6879-84, 2007.