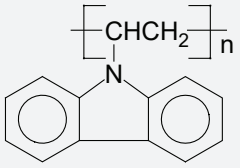
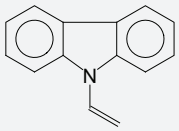
PVK poly(N-vinyl carbazole)

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	poly(N-vinyl carbazole)	
CAS name	-	9H-carbazole, 9-ethenyl-, homopolymer	
Acronym	-	PVK	
CAS number	-	25067-59-8	
RTECS number	-	FE6225480	
Formula			
HISTORY			
Person to discover	-	Reppe, W, Keyssner, E; Dorrer, E	Reppe, W, Keyssner, E; Dorrer, E, US Patent 2,072,465, IG Farben, Mar. 2, 1937.
Date	-	1937	
Details	-	production of polymeric N-vinyl compounds	
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	1484-13-5	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	193.24	
Monomer(s) expected purity(ies)	%	less than 100 ppm impurities	
Monomer ratio	-	100% (can also be copolymerized with various monomers, see ref.)	Fink, J K, High Performance Polymers, William Andrew, 2008.
Method of synthesis	-	free radical polymerization, using AIBN as initiator	
Catalyst	-	Ziegler-Natta	
Activation energy of polymerization	J mol^{-1}	22.8-27.4 (propagation)	
Number average molecular weight, M_n	dalton, g/mol, amu	9,900-151,400	
Mass average molecular weight, M_w	dalton, g/mol, amu	40,000-3,230,000	
Polydispersity, M_w/M_n	-	2.06-3.30	
STRUCTURE			
Crystallinity	%	28-38	
Cell type (lattice)	-	hexagonal, orthorhombic	
Cell dimensions	nm	a:b:c=1.23:1.23:0.744 (hexagonal); 2.16:1.25:0.744 (orthorhombic)	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.18-1.20; 1.84 (amorphous)	

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Color	-	white to off-white to yellow	
Refractive index, 20°C	-	1.683-1.696	
Odor	-	odorless	
Melting temperature, DSC	°C	>320	
Softening point	°C	>175	
Thermal expansion coefficient, 23-80°C	$^{o}C^{-1}$	5E-5	
Glass transition temperature	°C	200-227; 126 (isotactic); 227 (amorphous); 276 (syndiotactic)	
Specific heat capacity	J K^{-1} kg^{-1}	1260	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile modulus	MPa	4,120; 4,000 (amorphous)	
Elongation	%	1.1	
Water absorption, equilibrium in water at 23°C	%	<0.1	
CHEMICAL RESISTANCE			
Alcohols	-	resistant	
Aliphatic hydrocarbons	-	resistant	
Aromatic hydrocarbons	-	non-resistant	
Esters	-	resistant	
Halogenated hydrocarbons	-	non-resistant	
Ketones	-	non-resistant	
Θ solvent, Θ-temp.=-37.5, -21.5, 37°C	-	chlorobenzene, nitrobenzene, toluene	
Good solvent	-	aromatic hydrocarbons, chloroform, chlorobenzene, methylene tetrachloride, THF	
Non-solvent	-	alcohols, aliphatic hydrocarbons, carbon tetrachloride, esters	
WEATHER STABILITY			
Absorption bands	nm	261, 295, 331, 344	Wu, H-X; Qiu, X-Q; Cai, R-F; Qian, S-X, Appl. Surface Sci., 253, 5122-28, 2007.
Excitation wavelengths	nm	256	Baibarac, M; Lira-Cantu, M; Sol, J O; Baltog, I; Casan-Pastor, N; Gomez-Romero, P, Composites Sci. Technol., 67, 2556-63, 2007.
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	0/1/0	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
Oral rat, LD_{50}	mg kg^{-1}	>5,000	
PROCESSING			
Typical processing methods	-	spin coating, screen-printing, vacuum deposition	Fink, J K, High Performance Polymers, William Andrew, 2008.
Additives used in final products	-	Plasticizers: N-methylcarbazole, N-ethylcarbazole, N-butylcarbazole, N-hexylcarbazole, N-phenylcarbazole, 1,3-biscarbazolylpropane, o-nitroanisole, m-nitroanisole, p-nitroanisole, triphenylamine; Release: amorphous silica, PVDF	

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PARAMETER	UNIT	VALUE	REFERENCES
Applications	-	electrophotography, light emitting diodes, photorefractive materials, photovoltaic devices	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	aromatic ring – 722; tail-to-tail – 744; aromatic ring – 1220; vinylidene group – 1320; vinyl carbazole – 1450	Baibarac, M; Lira-Cantu, M; Sol, J O; Baltog, I; Casan-Pastor, N; Gomez-Romero, P, Composites Sci. Technol., 67, 2556-63, 2007.
Raman (wavenumber-assignment)	cm^{-1}/-	C-H – 1128, 1156, 1316, 1451; C-C – 1388, 1618; benzene ring – 1514, 1570; C=C – 1594	Baibarac, M; Gomez-Romero, P; Lira-Cantu, M; Casan-Pastor, N; Mestres, N; Lefrant, S, Eur. Polym. J., 42, 2302-12, 2006.