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Supplementary information

¹³C spectrum of NPN-OH oligomer



FT-IR spectra of NPN-OH oligomers





Typical calculation for extent of phthalonitrilation and cyanation in NPN-OCN1 is done as follows :

Nitrogen content for NPN-OH1 (from CHN analysis) = 3 %

Composition of NPN-OH1 can be represented as [[(Ph-CH₂) OH]_(1-x)(OPN)_x]_n

Where Ph stands for phenyl and degree of substitution of phenolic OH by phthalonitrile (OPN) group is represented as 'x'

Molecular weight of repeat unit of NPN-OH1 = 91 + 17(1-x) + 143x = 108+126x

Nitrogen fraction=28x/(108+126x) = 0.03

Solving this, x is obtained as 0.13, i.e degree of phthalonitrile substitution is 13 %

Precursor composition is therefore [(Ph-CH₂) OH]_{0.87}(OPN)_{0.13}]_n

Upon cyanation, NPN-OH1 is transformed to NPN-OCN1 and the composition of this copolymer can be represented as $[(Ph-CH_2) (OPN)_{0.13}(OCN)_yOH_{(0.87-y)}]_n$ where 'y' is degree of cyanation of free -OH groups in NPN-OH1

Nitrogen content for NPN-OCN1 (from CHN analysis) = 11.3 %

Molecular weight of repeat unit of NPN-OCN1 = 91 + 143*0.13 + 42y + 17(0.87-y) = 124.38 + 25y

(Contribution to molecular weight by OCN group is 14y)

Nitrogen content contributed by –OPN groups= 3 %

Therefore, nitrogen content contributed by -OCN groups = 11.3 - 3 = 8.3 %

i.e 14y/(124.38 + 25y) = 0.083

Solving this, y is obtained as 0.87. This shows completion of cyanation reaction too

Therefore, in NPN-OCN1, the mole fraction of OPN = 0.13 and that of OCN = 0.87