INFLUENCE OF STRUCTURAL AND TOPOGICAL CONNECTIVITY INDICES ON DIELECTRIC PROPERTIES OF BLENDS BASED ON QUATERNIZED POLYSULFONES: THEORETICAL APPROACH

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Abstract

Cationic polysulfones containing quaternary ammonium side groups (PSFQ), synthesized by reaction of the chloromethylated polysulfone (CMPSF) with a tertiary amine, N,N-dimethylbutylamine (DMBA), are considered to be suitable for a wide range of applications from the electronic field. Additionally, quaternized polysulfone-based composites with optical and electrical properties represent a challenge for researchers. Therefore, it is of interest to find out whether PSFQ can be designed for specific applications in blends with polyvinyl alcohol (PVA) and to establish their impact on the different properties. Thus, in the present study the cationic polysulfone PSFQ was analyzed in combination with PVA, which is supposed to improve among the other properties, such as hydrophylicity, flexibility, and the optical ones [1].In this context, the thermoplastic characteristics (*e.g.*,the refractive index and dielectric constant)were evaluated using the structural and topological techniques of spatial arrangement of the constituent atoms from analyzed polymer [2], by means the zero-order connectivity indices and first-order connectivity indices (Table 1).

Table 1. Zero-order connectivity indices, ${}^0\chi$,and ${}^0\chi^v$, and first-orderconnectivity indices, ${}^1\chi$and ${}^1\chi^v$, as well as the theoretical values of the refractive index, n_{th}, and dielectric constant, ε_{th}, for different mixing ratio of PSFQ/PVA blend

Sample	Parameters					
	${}^0\chi$	${}^0\chi^v$	${}^1\chi$	${}^1\chi^v$	n_{th}	ε_{th}
PSFQ	52.054	43.439	34.680	24.785	1.580	2.496
PVA	2.284	1.732	0.986	0.666	1.500	2.250
PSFQ/PVA						
75/25	39.612	33.012	26.256	18.755	1.5600	2.434
50/50	27.169	22.585	17.833	12.725	1.5400	2.372
25/75	14.726	12.158	9.409	6.695	1.5200	2.310

Data obtained emphasize the effects generated by the molecular structure, electrostatic repulsions between charge groups, and/or intermolecular interactions; a slightly decrease of n and ε with increasing of the PVA content was observed, this being useful for certain applications that involves a lower polarizability for the final products. Consequently, results will be useful in predicting of the special properties of these polymers in order to obtain high performance materials with applications both in electronic and optical field.

References

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