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Aromatic Polyamides Containing Trityl Substituted Triphenylamine: Gas Transport Properties and Molecular Dynamics Simulations

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Abstract: A series of fully aromatic polyamides (PAs) was prepared by the polycondensation reaction of 4,4'-diamino-4-tritylaniline with four commercial diacids. The polymers were well-characterized using different analytical tools and membranes were prepared from the PAs using a solution cast method. The resulting PAs exhibited good mechanical properties, with a tensile strength up to 74 MPa, thermal stability, and a high glass transition temperature. The gas permeation properties of different gases through the PA membranes were investigated using a constant-volume method. The incorporation of a trityl group into the polymer backbone offers a successful approach to improve the gas permeabilitiy with P_{CO2} and P_{O2} values as high as 141.0 and 33.4 Barrer, respectively. The PA membranes also exhibited a reasonably high permselectivity for the separation of important gas pairs CO_2/CH_4 and O_2/N_2. The effect of a trityl-substituted triphenylamine (TPA) and its spatial arrangement and size-distribution function of the free-volume on gas transport properties were calculated using molecular dynamics (MD) simulation. Gas diffusivity is supported by individual penetrant molecule trajectories and mean-square displacements in a polymer matrix. MD simulations were consistent with the experimental data.

Keywords: Polyamides; Trityl moiety; Gas transport properties; Molecular dynamics simulation.

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