

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and benz_imidazoles

Manorama Bastia¹, Dr. Ashish Kumar Sahoo²

¹180705100016@cutm.ac.in, ²ashish.sahoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of tetmeth_bisphen_carbonate and benz_imidazoles. Synthia module of Biovia Materials Studio software was used to predict Glass transition temperature, Density, Oxygen permeability, Nitrogen permeability and Carbon dioxide permeability of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and benz_imidazoles on the following properties have been predicted.

- a. Glass transition temperature
- b. Density
- c. Oxygen permeability
- d. Nitrogen permeability
- e. Carbon dioxide permeability

The weight fractions of the monomers were varied in the range of 0 to 1.

Software used: Synthia module of Biovia Materials Studio software (Dassault Systemes, France) was used for the study.

Results and Discussion: The effect of weight fraction of tetmeth_bisphen_carbonate (Monomer 1) on the Permeability of the composite has been presented in Table 1. The predicted properties of the composite for 0, 0.5 and 1.0 weight fractions of tetmeth_bisphen_carbonate have been summarized in Table 1. The rate of change for the properties have been summarized in Table 2.

Table 1. Properties of composite of tetmeth_bisphen_carbonate and benz_imidazoles

Property		Results for		
Name	Unit	0.0 weight fraction of tetmeth_bisphen_carbonate	0.5 weight fraction of tetmeth_bisphen_carbonate	1.0 weight fraction of tetmeth_bisphen_carbonate
Glass transition temperature	oC	645.418	557.479	466.509
Density	kg per	1.349	1.199	1.080