

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and benzothiazol

Pranab Prayesh Rout¹, Dr Padmaja Pattanayak²

¹180705120038@cutm.ac.in, ²padmaja.patnaik@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 bisphen_dimeth_carbonate and benzothiazol. 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 bisphen_dimeth_carbonate and benzothiazol on the following properties have been predicted.

- Glass transition temperature
- Density
- Oxygen permeability
- Nitrogen permeability
- 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 bisphen_dimeth_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 bisphen_dimeth_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 bisphen_dimeth_carbonate and benzothiazol

Property		Results for		
Name	Unit	0.0 weight fraction of bisphen_dimeth_carbonate	0.5 weight fraction of bisphen_dimeth_carbonate	1.0 weight fraction of bisphen_dimeth_carbonate
Glass transition temperature	oC	791.880	588.714	414.398
Density	kg per	1.639	1.368	1.174