

## Prediction of Permeability for a composite of bisphen\_dimeth\_carbonate and oxyphenyl

Nirnimesh Dalai<sup>1</sup>, Dr Nibedita Nayak<sup>2</sup>

<sup>1</sup>180705120046@cutm.ac.in, <sup>2</sup>nibeditanayak@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 oxyphenyl. 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 oxyphenyl 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 oxyphenyl

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	357.304	385.589	414.398
Density	kg per	1.222	1.198	1.174