

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

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**Abstract:** A computational study has been done to predict Permeability of a polymer composite consisting of bisphen\_dimeth\_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 bisphen\_dimeth\_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 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 benz\_imidazoles

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	645.418	532.187	414.398
Density	kg per	1.349	1.255	1.174