

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and butylene_isophthalate

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of tetmeth_bisphen_carbonate and butylene_isophthalate. 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 butylene_isophthalate 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 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 butylene_isophthalate

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	308.194	388.383	466.509
Density	kg per	1.237	1.153	1.080