

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and 25_thiazole

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Abstract: A computational study has been done to predict Mechanical properties of a polymer composite consisting of bisphen_dimeth_carbonate and 25_thiazole. Synthia module of Biovia Materials Studio software was used to predict Bulk modulus, Young's modulus, Shear modulus, Poisson's ratio and Cohesive energy (Fedors) at 298K of the composite.

Objective: In this study the effect of mixing of bisphen_dimeth_carbonate and 25_thiazole on the following properties have been predicted.

- a. Bulk modulus
- b. Young's modulus
- c. Shear modulus
- d. Poisson's ratio
- e. Cohesive energy (Fedors) at 298K

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 Mechanical properties 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 25_thiazole

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
Bulk modulus	newtons per square metre	6467.823	5086.531	4031.244