Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and isobutene

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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 isobutene. 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 isobutene 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 bisph	nen dimeth	carbonate and isobutene

Property		Results for				
Name	Unit	0.0 weight fraction of	0.5 weight fraction of	1.0 weight fraction of		
		bisphen_dimeth_carbon	bisphen_dimeth_carbon	bisphen_dimeth_carbon		
		ate	ate	ate		
Bulk	newton	1332.498	2129.723	4031.244		
modulu	s per					
S	square					
	metre					

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