

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and acrylonitrile

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Abstract: A computational study has been done to predict Mechanical properties of a polymer composite consisting of tetmeth_bisphen_carbonate and acrylonitrile. 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 tetmeth_bisphen_carbonate and acrylonitrile 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 tetmeth_bisphen_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 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 acrylonitrile

| 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 |
| Bulk modulus | newtons per square metre | 6497.867 | 5251.292 | 3812.095 |