ISSN 2395-6216 (PRINT VERSION)
ISSN 2395-6224 (ONLINE VERSION)
Volume 10 Number 2 Nov 2020

Centurion Journal of Multidisciplinary Research

Special issue :
Proceedings of
National Conference on Computational Composite: Power of Synthia
15-17 November 2020

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Centurion Journal of Multidisciplinary Research
ISSN 2395-6216 (PRINT VERSION) ISSN 2395-6224 (ONLINE VERSION)

Centurion Journal of Multidisciplinary Research is published by Centurion University of Technology and Management, Odisha, bi-annually.

Annual Subscription: Rs 300 (within India) excluding postage charges. Outside India USD 30, excluding postage charges.

Published by:
Registrar, Centurion University of Technology and Management
R. Sitapur, Parlakhemundi, Gajapati, Odisha
Pin – 761211

Printer:
Srimandira Publication
EPF Colony, E-Block, Saheed Nagar, Bhubaneswar, Odisha 751007

Volume 10 Number 2
Novemver 2020

Centurion Journal of Multidisciplinary Research

Special issue : Proceedings of National Conference on Computational Composite: Power of Synthia
15-17 November 2020
organized by: Cemistry and Physics Departments
Centurion University of Technology and management, Odisha, India

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CENTURION UNIVERSITY PRESS, ODISHA, INDIA

THE VISION

The objective of the conference was to encourage mainly the students to use computational tools in composite design.

Composites contain more than one material mixed in a way that the constituent materials can contribute to the property of the composite. Thus, by blending different materials one can save the cost of developing a new material with the desired properties.

In this conference papers different properties of polymeric composite materials were presented. The properties were calculated using the Synthia module of Biovia Materials Studio. Synthia uses empirical and semiempirical methods based on connectivity indices to predict various properties of composites.

The following properties were predicted:

A. Permeability related properties:

1. Glass transition temperature: It is defined as the temperature at which the amorphous region of a polymer shows transition from rigid state to flexible state (solid state to rubbery state).

2. Density: Density of a polymer represents the mass of the polymer per unit volume.

3. Oxygen permeability: The permeability of oxygen represents the ease of mass transfer of oxygen through the polymer. It gives an idea of the porosity and pore size of the polymer.

4. Nitrogen permeability: The permeability of nitrogen represents the ease of mass transfer of nitrogen through the polymer. It gives an idea of the porosity and pore size of the polymer.

5. Carbon-di-oxide permeability: The permeability of carbon-di-oxide represents the ease of mass transfer of carbon-di-oxide through the polymer. It gives an idea of the porosity and pore size of the polymer.

B. Optical, electric and thermal properties:

1. Refractive index: It is an important optical property of the polymer. It gives an idea about the transparency and optical density of the polymer.

2. Volume resistivity: It presents the resistance offered to an electric current by a cubical sample of a polymer. Higher resistance implies lower electrical conductivity.

3. Dielectric constant: It is the factor by which the electric field between charges decreases with respect to vacuum. It gives an idea of the electrical susceptibility of the polymer.

4. Coefficient of volumetric thermal expansion: It represents increase in volume of a polymer per unit original volume per degree rise in temperature. It gives an idea of dimensional change of the polymer with change in temperature.

5. Thermal conductivity: It represents the rate at which heat is transferred by conduction through unit cross-section area of the polymer, due to a temperature gradient existing perpendicular to the area.

C. Mechanical properties:

1. Bulk modulus: Bulk modulus indicates the increase in volume of a polymer for infinitesimal decrease in applied pressure.

2. Young's modulus: It gives an idea of the relative change in length of the polymer due to applied force. It is the ration of stress and strain for a polymer.

3. Shear modulus: It is a measure of the rigidity of a polymer, and is presented as the ratio of shear stress to shear strain.

4. Poisson's ratio: It is a dimensionless quantity represented as the ratio of transverse strain to longitudinal strain.

5. Cohesive energy (Fedors) at 298K: It represents the energy required to separate the molecules of a polymer. A higher value indicates greater strength of the polymer.

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Prediction of Permeability for a composite of bisphen_dimeth_carbonate and ethylene

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

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	191.974	305.230	414.398
Density	kg per	0.872	1.001	1.174

	cubic metre			
Oxygen permeability	Perm	745.304	547.020	288.203
Nitrogen permeability	Perm	216.848	155.250	77.690
Carbon dioxide permeability	Perm	3915.815	2795.767	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 226.5 oC per unit weight fraction	increases at rate 218.3 oC per unit weight fraction
Density	increases at rate 0.257 kg per cubic metre per unit weight fraction	increases at rate 0.347 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 396.6 Perm per unit weight fraction	decreases at rate 517.6 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 123.2 Perm per unit weight fraction	decreases at rate 155.1 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 2240.1 Perm per unit weight fraction	decreases at rate 2809.4 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and ethylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and ethylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and ethylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 ethylene

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
Refractive index	0	1.465	1.516	1.587
Volume resistivity	Ohm-metre	22153760000000000000.000	720375900000000000.000	155017300000000000.000

Dielectric constant	0	2.327	2.571	2.905
Coefficient of volumetric thermal expansion	/K	900.860	313.625	236.835
Thermal conductivity	W/(m·K)	0.172	0.182	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.101 0 per unit weight fraction	increases at rate 0.143 0 per unit weight fraction
Volume resistivity	decreases at rate 2990000200000000000 Ohm-metre per unit weight fraction	decreases at rate 1130717200000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.488 0 per unit weight fraction	increases at rate 0.667 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 1174.5 /K per unit weight fraction	decreases at rate 153.6 /K per unit weight fraction
Thermal conductivity	increases at rate 0.021 W/(m·K) per unit weight fraction	increases at rate 0.02 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and ethylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and ethylene

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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 ethylene. 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 ethylene 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 ethylene

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	2466.650	2550.975	4031.244

Young's modulus	newtons per square metre	2.566	1227.433	2212.361
Shear modulus	newtons per square metre	0.855	432.254	785.343
Poisson's ratio	0	0.500	0.420	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	9.883	18.147	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 168.7 newtons per square metre per unit weight fraction	increases at rate 2960.5 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 2449.733 newtons per square metre per unit weight fraction	increases at rate 1969.856 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 862.796 newtons per square metre per unit weight fraction	increases at rate 706.178 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.16 0 per unit weight fraction	decreases at rate 0.0225 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 16.529 kiloJoule per mole per unit weight fraction	increases at rate 149.826 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and ethylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and 1_butene

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of bisphen_dimeth_carbonate and 1_butene. 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 1_butene 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 1_butene

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	212.969	314.759	414.398
Density	kg per	0.855	0.990	1.174

	cubic metre			
Oxygen permeability	Perm	1026.874	665.300	288.203
Nitrogen permeability	Perm	306.565	191.812	77.690
Carbon dioxide permeability	Perm	5551.752	3460.222	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 203.6 oC per unit weight fraction	increases at rate 199.3 oC per unit weight fraction
Density	increases at rate 0.269 kg per cubic metre per unit weight fraction	increases at rate 0.369 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 723.1 Perm per unit weight fraction	decreases at rate 754.2 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 229.5 Perm per unit weight fraction	decreases at rate 228.2 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 4183.1 Perm per unit weight fraction	decreases at rate 4138.3 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and 1_butene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and 1_butene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and 1_butene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of bisphen_dimeth_carbonate and 1_butene on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 1_butene

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
Refractive index	0	1.467	1.516	1.587
Volume resistivity	Ohm-metre	2706390000000000000.000	816608300000000000.000	155017300000000000.000

Dielectric constant	0	2.284	2.544	2.905
Coefficient of volumetric thermal expansion	/K	834.125	304.993	236.835
Thermal conductivity	W/(m·K)	0.134	0.164	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.099 0 per unit weight fraction	increases at rate 0.142 0 per unit weight fraction
Volume resistivity	decreases at rate 3779563400000000000 Ohm-metre per unit weight fraction	decreases at rate 1323182000000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.52 0 per unit weight fraction	increases at rate 0.722 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 1058.3 /K per unit weight fraction	decreases at rate 136.3 /K per unit weight fraction
Thermal conductivity	increases at rate 0.06 W/(m·K) per unit weight fraction	increases at rate 0.057 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and 1_butene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and 1_butene

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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 1_butene. 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 1_butene 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 1_butene

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	2297.805	2652.235	4031.244

Young's modulus	newtons per square metre	1.083	1614.827	2212.361
Shear modulus	newtons per square metre	0.361	577.333	785.343
Poisson's ratio	0	0.500	0.399	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	19.092	32.462	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 708.9 newtons per square metre per unit weight fraction	increases at rate 2758 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 3227.488 newtons per square metre per unit weight fraction	increases at rate 1195.068 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1153.943 newtons per square metre per unit weight fraction	increases at rate 416.02 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.2028 0 per unit weight fraction	increases at rate 0.02 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 26.742 kiloJoule per mole per unit weight fraction	increases at rate 121.195 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and 1_butene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and isobutene

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

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	183.823	300.389	414.398
Density	kg per	0.856	0.990	1.174

	cubic metre			
Oxygen permeability	Perm	2438.329	1094.444	288.203
Nitrogen permeability	Perm	780.327	328.415	77.690
Carbon dioxide permeability	Perm	14240.660	5950.816	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 233.1 oC per unit weight fraction	increases at rate 228 oC per unit weight fraction
Density	increases at rate 0.269 kg per cubic metre per unit weight fraction	increases at rate 0.368 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 2687.8 Perm per unit weight fraction	decreases at rate 1612.5 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 903.8 Perm per unit weight fraction	decreases at rate 501.5 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 16579.7 Perm per unit weight fraction	decreases at rate 9119.5 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and isobutene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and isobutene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and isobutene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity 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. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 isobutene

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
Refractive index	0	1.479	1.524	1.587
Volume resistivity	Ohm-metre	3608102000000000000.000	929159900000000000.000	155017300000000000.000

Dielectric constant	0	2.221	2.516	2.905
Coefficient of volumetric thermal expansion	/K	929.737	318.200	236.835
Thermal conductivity	W/(m·K)	0.131	0.162	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.089 0 per unit weight fraction	increases at rate 0.127 0 per unit weight fraction
Volume resistivity	decreases at rate 5357884200000000000 Ohm-metre per unit weight fraction	decreases at rate 1548285200000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.589 0 per unit weight fraction	increases at rate 0.778 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 1223.1 /K per unit weight fraction	decreases at rate 162.7 /K per unit weight fraction
Thermal conductivity	increases at rate 0.063 W/(m·K) per unit weight fraction	increases at rate 0.06 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and isobutene. Experimental study is required to validate the results.

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 bisphen_dimeth_carbonate and isobutene

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	1332.498	2129.723	4031.244

Young's modulus	newtons per square metre	1.019	1277.192	2212.361
Shear modulus	newtons per square metre	0.340	456.124	785.343
Poisson's ratio	0	0.500	0.400	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	16.870	30.643	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 1594.5 newtons per square metre per unit weight fraction	increases at rate 3803 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 2552.346 newtons per square metre per unit weight fraction	increases at rate 1870.338 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 911.568 newtons per square metre per unit weight fraction	increases at rate 658.438 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.1996 0 per unit weight fraction	increases at rate 0.017 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 27.545 kiloJoule per mole per unit weight fraction	increases at rate 124.834 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and isobutene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and propylene

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

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	229.892	323.166	414.398
Density	kg per	0.858	0.992	1.174

	cubic metre			
Oxygen permeability	Perm	1316.654	766.539	288.203
Nitrogen permeability	Perm	401.007	223.530	77.690
Carbon dioxide permeability	Perm	7278.144	4037.496	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 186.5 oC per unit weight fraction	increases at rate 182.5 oC per unit weight fraction
Density	increases at rate 0.267 kg per cubic metre per unit weight fraction	increases at rate 0.365 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 1100.2 Perm per unit weight fraction	decreases at rate 956.7 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 355 Perm per unit weight fraction	decreases at rate 291.7 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 6481.3 Perm per unit weight fraction	decreases at rate 5292.8 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and propylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and propylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and propylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 propylene

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
Refractive index	0	1.471	1.519	1.587
Volume resistivity	Ohm-metre	2955856000000000000.000	849388600000000000.000	155017300000000000.000

Dielectric constant	0	2.265	2.535	2.905
Coefficient of volumetric thermal expansion	/K	787.126	297.762	236.835
Thermal conductivity	W/(m·K)	0.143	0.168	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.095 0 per unit weight fraction	increases at rate 0.136 0 per unit weight fraction
Volume resistivity	decreases at rate 4212934800000000000 Ohm-metre per unit weight fraction	decreases at rate 1388742600000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.542 0 per unit weight fraction	increases at rate 0.739 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 978.7 /K per unit weight fraction	decreases at rate 121.9 /K per unit weight fraction
Thermal conductivity	increases at rate 0.051 W/(m·K) per unit weight fraction	increases at rate 0.048 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and propylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and propylene

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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 propylene. 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 propylene 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 propylene

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	1976.690	2706.830	4031.244

Young's modulus	newtons per square metre	1.770	1502.795	2212.361
Shear modulus	newtons per square metre	0.590	533.864	785.343
Poisson's ratio	0	0.500	0.407	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	13.775	25.032	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 1460.3 newtons per square metre per unit weight fraction	increases at rate 2648.8 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 3002.051 newtons per square metre per unit weight fraction	increases at rate 1419.132 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1066.549 newtons per square metre per unit weight fraction	increases at rate 502.957 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.1848 0 per unit weight fraction	increases at rate 0.0021 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 22.515 kiloJoule per mole per unit weight fraction	increases at rate 136.055 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and propylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and acrylonitrile

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

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	361.527	388.227	414.398
Density	kg per	1.177	1.176	1.174

	cubic metre			
Oxygen permeability	Perm	0.082	4.748	288.203
Nitrogen permeability	Perm	0.012	0.920	77.690
Carbon dioxide permeability	Perm	0.192	15.886	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 53.4 oC per unit weight fraction	increases at rate 52.3 oC per unit weight fraction
Density	decreases at rate 0.003 kg per cubic metre per unit weight fraction	decreases at rate 0.003 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 9.3 Perm per unit weight fraction	increases at rate 566.9 Perm per unit weight fraction
Nitrogen permeability	increases at rate 1.8 Perm per unit weight fraction	increases at rate 153.5 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 31.4 Perm per unit weight fraction	increases at rate 2750.4 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and acrylonitrile. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and acrylonitrile

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and acrylonitrile. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 acrylonitrile

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
Refractive index	0	1.542	1.565	1.587
Volume resistivity	Ohm-metre	1041069000000000.000	10691120000000000.000	155017300000000000.000

Dielectric constant	0	3.991	3.485	2.905
Coefficient of volumetric thermal expansion	/K	268.697	251.603	236.835
Thermal conductivity	W/(m·K)	0.178	0.185	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.044 0 per unit weight fraction	increases at rate 0.045 0 per unit weight fraction
Volume resistivity	increases at rate 19300102000000000 Ohm-metre per unit weight fraction	increases at rate 288652360000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 1.012 0 per unit weight fraction	decreases at rate 1.161 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 34.2 /K per unit weight fraction	decreases at rate 29.5 /K per unit weight fraction
Thermal conductivity	increases at rate 0.014 W/(m·K) per unit weight fraction	increases at rate 0.014 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and acrylonitrile. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and acrylonitrile

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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 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 bisphen_dimeth_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 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 acrylonitrile

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	6497.867	5343.638	4031.244

Young's modulus	newtons per square metre	3736.424	3005.345	2212.361
Shear modulus	newtons per square metre	1330.481	1068.556	785.343
Poisson's ratio	0	0.404	0.406	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	34.157	44.326	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 2308.5 newtons per square metre per unit weight fraction	decreases at rate 2624.8 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 1462.158 newtons per square metre per unit weight fraction	decreases at rate 1585.968 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 523.85 newtons per square metre per unit weight fraction	decreases at rate 566.427 newtons per square metre per unit weight fraction
Poisson's ratio	increases at rate 0.0042 0 per unit weight fraction	increases at rate 0.0045 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 20.339 kiloJoule per mole per unit weight fraction	increases at rate 97.467 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and acrylonitrile. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and dichloro_ethylene

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

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	277.943	365.429	414.398
Density	kg per	1.689	1.386	1.174

	cubic metre			
Oxygen permeability	Perm	0.982	33.913	288.203
Nitrogen permeability	Perm	0.168	7.698	77.690
Carbon dioxide permeability	Perm	2.853	135.229	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 175 oC per unit weight fraction	increases at rate 97.9 oC per unit weight fraction
Density	decreases at rate 0.608 kg per cubic metre per unit weight fraction	decreases at rate 0.422 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 65.9 Perm per unit weight fraction	increases at rate 508.6 Perm per unit weight fraction
Nitrogen permeability	increases at rate 15.1 Perm per unit weight fraction	increases at rate 140 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 264.8 Perm per unit weight fraction	increases at rate 2511.7 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and dichloro_ethylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and dichloro_ethylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and dichloro_ethylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 dichloro_ethylene

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
Refractive index	0	1.608	1.596	1.587
Volume resistivity	Ohm-metre	193061000000000000.000	170370700000000000.000	155017300000000000.000

Dielectric constant	0	2.857	2.884	2.905
Coefficient of volumetric thermal expansion	/K	678.564	266.055	236.835
Thermal conductivity	W/(m·K)	0.151	0.178	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.025 0 per unit weight fraction	decreases at rate 0.017 0 per unit weight fraction
Volume resistivity	decreases at rate 45380600000000000 Ohm-metre per unit weight fraction	decreases at rate 30706800000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.054 0 per unit weight fraction	increases at rate 0.041 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 825 /K per unit weight fraction	decreases at rate 58.4 /K per unit weight fraction
Thermal conductivity	increases at rate 0.053 W/(m·K) per unit weight fraction	increases at rate 0.029 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and dichloro_ethylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and dichloro_ethylene

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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 dichloro_ethylene. 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 dichloro_ethylene 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 dichloro_ethylene

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	5226.046	4030.623	4031.244

Young's modulus	newtons per square metre	3361.917	2356.651	2212.361
Shear modulus	newtons per square metre	1206.906	840.129	785.343
Poisson's ratio	0	0.393	0.403	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	29.784	47.249	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 2390.8 newtons per square metre per unit weight fraction	increases at rate 1.2 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 2010.532 newtons per square metre per unit weight fraction	decreases at rate 288.58 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 733.553 newtons per square metre per unit weight fraction	decreases at rate 109.574 newtons per square metre per unit weight fraction
Poisson's ratio	increases at rate 0.0195 0 per unit weight fraction	increases at rate 0.012 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 34.93 kiloJoule per mole per unit weight fraction	increases at rate 91.622 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and dichloro_ethylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and difluoro_ethylene

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

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	240.041	336.676	414.398
Density	kg per	1.606	1.357	1.174

	cubic metre			
Oxygen permeability	Perm	1485.349	571.860	288.203
Nitrogen permeability	Perm	456.789	162.880	77.690
Carbon dioxide permeability	Perm	8299.482	2934.333	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 193.3 oC per unit weight fraction	increases at rate 155.4 oC per unit weight fraction
Density	decreases at rate 0.499 kg per cubic metre per unit weight fraction	decreases at rate 0.365 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 1827 Perm per unit weight fraction	decreases at rate 567.3 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 587.8 Perm per unit weight fraction	decreases at rate 170.4 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 10730.3 Perm per unit weight fraction	decreases at rate 3086.5 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and difluoro_ethylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and difluoro_ethylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and difluoro_ethylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 difluoro_ethylene

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
Refractive index	0	1.371	1.491	1.587
Volume resistivity	Ohm-metre	4526299000000000000.000	667346400000000000.000	155017300000000000.000

Dielectric constant	0	2.172	2.588	2.905
Coefficient of volumetric thermal expansion	/K	761.397	286.835	236.835
Thermal conductivity	W/(m·K)	0.151	0.174	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.241 0 per unit weight fraction	increases at rate 0.191 0 per unit weight fraction
Volume resistivity	decreases at rate 7717905200000000000 Ohm-metre per unit weight fraction	decreases at rate 1024658200000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.831 0 per unit weight fraction	increases at rate 0.634 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 949.1 /K per unit weight fraction	decreases at rate 100 /K per unit weight fraction
Thermal conductivity	increases at rate 0.045 W/(m·K) per unit weight fraction	increases at rate 0.038 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and difluoro_ethylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and difluoro_ethylene

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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 difluoro_ethylene. 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 difluoro_ethylene 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 difluoro_ethylene

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	3417.759	3102.468	4031.244

Young's modulus	newtons per square metre	2.842	1648.363	2212.361
Shear modulus	newtons per square metre	0.947	583.926	785.343
Poisson's ratio	0	0.500	0.411	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	12.566	28.759	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 630.6 newtons per square metre per unit weight fraction	increases at rate 1857.6 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 3291.042 newtons per square metre per unit weight fraction	increases at rate 1127.996 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1165.957 newtons per square metre per unit weight fraction	increases at rate 402.833 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.1768 0 per unit weight fraction	decreases at rate 0.0058 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 32.385 kiloJoule per mole per unit weight fraction	increases at rate 128.603 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and difluoro_ethylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and styrene

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

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	379.529	395.504	414.398
Density	kg per	1.074	1.122	1.174

	cubic metre			
Oxygen permeability	Perm	363.687	323.572	288.203
Nitrogen permeability	Perm	99.887	88.039	77.690
Carbon dioxide permeability	Perm	1792.261	1578.028	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 32 oC per unit weight fraction	increases at rate 37.8 oC per unit weight fraction
Density	increases at rate 0.096 kg per cubic metre per unit weight fraction	increases at rate 0.105 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 80.2 Perm per unit weight fraction	decreases at rate 70.7 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 23.7 Perm per unit weight fraction	decreases at rate 20.7 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 428.5 Perm per unit weight fraction	decreases at rate 373.9 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and styrene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and styrene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and styrene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 styrene

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
Refractive index	0	1.604	1.596	1.587
Volume resistivity	Ohm-metre	734331000000000000.000	357122900000000000.000	155017300000000000.000

Dielectric constant	0	2.567	2.724	2.905
Coefficient of volumetric thermal expansion	/K	256.928	247.315	236.835
Thermal conductivity	W/(m·K)	0.135	0.163	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.016 0 per unit weight fraction	decreases at rate 0.017 0 per unit weight fraction
Volume resistivity	decreases at rate 754416200000000000 Ohm-metre per unit weight fraction	decreases at rate 404211200000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.313 0 per unit weight fraction	increases at rate 0.362 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 19.2 /K per unit weight fraction	decreases at rate 21 /K per unit weight fraction
Thermal conductivity	increases at rate 0.057 W/(m·K) per unit weight fraction	increases at rate 0.058 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and styrene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and styrene

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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 styrene. 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 styrene 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 styrene

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	3585.198	3794.473	4031.244

Young's modulus	newtons per square metre	3014.022	2520.268	2212.361
Shear modulus	newtons per square metre	1108.189	907.028	785.343
Poisson's ratio	0	0.360	0.389	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	39.197	54.848	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 418.6 newtons per square metre per unit weight fraction	increases at rate 473.5 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 987.508 newtons per square metre per unit weight fraction	decreases at rate 615.814 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 402.323 newtons per square metre per unit weight fraction	decreases at rate 243.37 newtons per square metre per unit weight fraction
Poisson's ratio	increases at rate 0.0588 0 per unit weight fraction	increases at rate 0.0385 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 31.302 kiloJoule per mole per unit weight fraction	increases at rate 76.424 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and styrene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and tetrafluoro_ethylene

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

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	251.763	345.868	414.398
Density	kg per	2.053	1.494	1.174

	cubic metre			
Oxygen permeability	Perm	1275.484	497.945	288.203
Nitrogen permeability	Perm	387.477	140.258	77.690
Carbon dioxide permeability	Perm	7030.605	2523.689	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 188.2 oC per unit weight fraction	increases at rate 137.1 oC per unit weight fraction
Density	decreases at rate 1.118 kg per cubic metre per unit weight fraction	decreases at rate 0.639 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 1555.1 Perm per unit weight fraction	decreases at rate 419.5 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 494.4 Perm per unit weight fraction	decreases at rate 125.1 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 9013.8 Perm per unit weight fraction	decreases at rate 2265.2 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and tetrafluoro_ethylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and tetrafluoro_ethylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and tetrafluoro_ethylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 tetrafluoro_ethylene

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
Refractive index	0	1.335	1.490	1.587
Volume resistivity	Ohm-metre	6581058000000000000.000	651245200000000000.000	155017300000000000.000

Dielectric constant	0	2.091	2.593	2.905
Coefficient of volumetric thermal expansion	/K	733.699	279.848	236.835
Thermal conductivity	W/(m·K)	0.146	0.172	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.309 0 per unit weight fraction	increases at rate 0.194 0 per unit weight fraction
Volume resistivity	decreases at rate 1185962560000000000 Ohm-metre per unit weight fraction	decreases at rate 992455800000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 1.005 0 per unit weight fraction	increases at rate 0.623 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 907.7 /K per unit weight fraction	decreases at rate 86 /K per unit weight fraction
Thermal conductivity	increases at rate 0.051 W/(m·K) per unit weight fraction	increases at rate 0.041 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and tetrafluoro_ethylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and tetrafluoro_ethylene

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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 tetrafluoro_ethylene. 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 tetrafluoro_ethylene 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 tetrafluoro_ethylene

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	5941.105	3268.825	4031.244

Young's modulus	newtons per square metre	2.223	1834.550	2212.361
Shear modulus	newtons per square metre	0.741	652.186	785.343
Poisson's ratio	0	0.500	0.406	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	16.097	37.823	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 5344.6 newtons per square metre per unit weight fraction	increases at rate 1524.8 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 3664.654 newtons per square metre per unit weight fraction	increases at rate 755.622 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1302.89 newtons per square metre per unit weight fraction	increases at rate 266.313 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.187 0 per unit weight fraction	increases at rate 0.0041 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 43.451 kiloJoule per mole per unit weight fraction	increases at rate 110.474 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and tetrafluoro_ethylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and vinyl_acetate

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

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	302.653	359.667	414.398
Density	kg per	1.219	1.196	1.174

	cubic metre			
Oxygen permeability	Perm	90.468	164.071	288.203
Nitrogen permeability	Perm	22.219	42.270	77.690
Carbon dioxide permeability	Perm	393.760	753.092	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 114 oC per unit weight fraction	increases at rate 109.5 oC per unit weight fraction
Density	decreases at rate 0.045 kg per cubic metre per unit weight fraction	decreases at rate 0.043 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 147.2 Perm per unit weight fraction	increases at rate 248.3 Perm per unit weight fraction
Nitrogen permeability	increases at rate 40.1 Perm per unit weight fraction	increases at rate 70.8 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 718.7 Perm per unit weight fraction	increases at rate 1276 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and vinyl_acetate. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and vinyl_acetate

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and vinyl_acetate. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 vinyl_acetate

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
Refractive index	0	1.481	1.534	1.587
Volume resistivity	Ohm-metre	340495100000000000.000	728340600000000000.000	1550173000000000000.000

Dielectric constant	0	3.234	3.069	2.905
Coefficient of volumetric thermal expansion	/K	316.043	269.975	236.835
Thermal conductivity	W/(m·K)	0.175	0.184	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.105 0 per unit weight fraction	increases at rate 0.106 0 per unit weight fraction
Volume resistivity	increases at rate 77569100000000000 Ohm-metre per unit weight fraction	increases at rate 164366480000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.33 0 per unit weight fraction	decreases at rate 0.328 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 92.1 /K per unit weight fraction	decreases at rate 66.3 /K per unit weight fraction
Thermal conductivity	increases at rate 0.018 W/(m·K) per unit weight fraction	increases at rate 0.017 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and vinyl_acetate. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and vinyl_acetate

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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 vinyl_acetate. 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 vinyl_acetate 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 vinyl_acetate

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	3101.366	3718.834	4031.244

Young's modulus	newtons per square metre	2163.179	2272.808	2212.361
Shear modulus	newtons per square metre	781.636	812.797	785.343
Poisson's ratio	0	0.384	0.398	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	31.136	46.799	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 1234.9 newtons per square metre per unit weight fraction	increases at rate 624.8 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 219.258 newtons per square metre per unit weight fraction	decreases at rate 120.894 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 62.322 newtons per square metre per unit weight fraction	decreases at rate 54.909 newtons per square metre per unit weight fraction
Poisson's ratio	increases at rate 0.0288 0 per unit weight fraction	increases at rate 0.0208 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 31.324 kiloJoule per mole per unit weight fraction	increases at rate 92.523 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and vinyl_acetate. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and vinyl_chloride

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

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	291.873	372.354	404.316
Density	kg per	1.383	1.259	1.191

	cubic metre			
Oxygen permeability	Perm	8.277	81.721	229.047
Nitrogen permeability	Perm	1.677	19.907	60.614
Carbon dioxide permeability	Perm	29.100	352.474	1083.115

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 161 oC per unit weight fraction	increases at rate 63.9 oC per unit weight fraction
Density	decreases at rate 0.249 kg per cubic metre per unit weight fraction	decreases at rate 0.136 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 146.9 Perm per unit weight fraction	increases at rate 294.7 Perm per unit weight fraction
Nitrogen permeability	increases at rate 36.5 Perm per unit weight fraction	increases at rate 81.4 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 646.7 Perm per unit weight fraction	increases at rate 1461.3 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and vinyl_chloride. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and vinyl_chloride

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and vinyl_chloride. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 vinyl_chloride

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
Refractive index	0	1.556	1.574	1.585
Volume resistivity	Ohm-metre	138712800000000000.000	147895700000000000.000	153576800000000000.000

Dielectric constant	0	2.929	2.915	2.907
Coefficient of volumetric thermal expansion	/K	652.476	261.493	242.314
Thermal conductivity	W/(m·K)	0.157	0.180	0.190

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.037 0 per unit weight fraction	increases at rate 0.02 0 per unit weight fraction
Volume resistivity	increases at rate 18365800000000000 Ohm-metre per unit weight fraction	increases at rate 11362200000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.028 0 per unit weight fraction	decreases at rate 0.016 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 782 /K per unit weight fraction	decreases at rate 38.4 /K per unit weight fraction
Thermal conductivity	increases at rate 0.048 W/(m·K) per unit weight fraction	increases at rate 0.02 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and vinyl_chloride. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and vinyl_chloride

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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 vinyl_chloride. 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 vinyl_chloride 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 vinyl_chloride

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	4019.120	3827.010	3983.959

Young's modulus	newtons per square metre	2250.873	2118.197	2190.081
Shear modulus	newtons per square metre	800.077	752.333	777.518
Poisson's ratio	0	0.407	0.408	0.408
Cohesive energy (Fedors) at 298K	kiloJoule per mole	20.231	37.348	71.998

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 384.2 newtons per square metre per unit weight fraction	increases at rate 313.9 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 265.352 newtons per square metre per unit weight fraction	increases at rate 143.768 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 95.488 newtons per square metre per unit weight fraction	increases at rate 50.37 newtons per square metre per unit weight fraction
Poisson's ratio	increases at rate 0.0022 0 per unit weight fraction	increases at rate 0.0013 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 34.233 kiloJoule per mole per unit weight fraction	increases at rate 69.301 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and vinyl_chloride. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and vinyl_ether

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

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	263.627	341.573	414.398
Density	kg per	1.048	1.108	1.174

	cubic metre			
Oxygen permeability	Perm	925.452	562.600	288.203
Nitrogen permeability	Perm	273.987	160.032	77.690
Carbon dioxide permeability	Perm	4957.183	2882.615	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 155.9 oC per unit weight fraction	increases at rate 145.6 oC per unit weight fraction
Density	increases at rate 0.119 kg per cubic metre per unit weight fraction	increases at rate 0.133 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 725.7 Perm per unit weight fraction	decreases at rate 548.8 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 227.9 Perm per unit weight fraction	decreases at rate 164.7 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 4149.1 Perm per unit weight fraction	decreases at rate 2983.1 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and vinyl_ether. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and vinyl_ether

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and vinyl_ether. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 vinyl_ether

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
Refractive index	0	1.470	1.524	1.587
Volume resistivity	Ohm-metre	309217600000000000.000	221784100000000000.000	155017300000000000.000

Dielectric constant	0	2.755	2.827	2.905
Coefficient of volumetric thermal expansion	/K	707.642	283.070	236.835
Thermal conductivity	W/(m·K)	0.168	0.181	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.107 0 per unit weight fraction	increases at rate 0.126 0 per unit weight fraction
Volume resistivity	decreases at rate 174867000000000000 Ohm-metre per unit weight fraction	decreases at rate 133533600000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.144 0 per unit weight fraction	increases at rate 0.156 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 849.1 /K per unit weight fraction	decreases at rate 92.5 /K per unit weight fraction
Thermal conductivity	increases at rate 0.025 W/(m·K) per unit weight fraction	increases at rate 0.023 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and vinyl_ether. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and vinyl_ether

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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 vinyl_ether. 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 vinyl_ether 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 vinyl_ether

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	1335.147	3024.643	4031.244

Young's modulus	newtons per square metre	1.823	1712.858	2212.361
Shear modulus	newtons per square metre	0.608	609.291	785.343
Poisson's ratio	0	0.500	0.406	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	17.298	31.385	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 3379 newtons per square metre per unit weight fraction	increases at rate 2013.2 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 3422.071 newtons per square metre per unit weight fraction	increases at rate 999.006 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1217.366 newtons per square metre per unit weight fraction	increases at rate 352.103 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.1883 0 per unit weight fraction	increases at rate 0.0058 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 28.174 kiloJoule per mole per unit weight fraction	increases at rate 123.35 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and vinyl_ether. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and vinyl_amide

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

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	364.481	392.271	414.398
Density	kg per	1.265	1.218	1.174

	cubic metre			
Oxygen permeability	Perm	0.143	7.264	288.203
Nitrogen permeability	Perm	0.021	1.457	77.690
Carbon dioxide permeability	Perm	0.350	25.242	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 55.6 oC per unit weight fraction	increases at rate 44.3 oC per unit weight fraction
Density	decreases at rate 0.094 kg per cubic metre per unit weight fraction	decreases at rate 0.087 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 14.2 Perm per unit weight fraction	increases at rate 561.9 Perm per unit weight fraction
Nitrogen permeability	increases at rate 2.9 Perm per unit weight fraction	increases at rate 152.5 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 49.8 Perm per unit weight fraction	increases at rate 2731.7 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and vinyl_amide. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and vinyl_amide

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and vinyl_amide. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 vinyl_amide

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
Refractive index	0	1.525	1.557	1.587
Volume resistivity	Ohm-metre	196654000000000.000	5238320000000000.000	155017300000000000.000

Dielectric constant	0	4.353	3.640	2.905
Coefficient of volumetric thermal expansion	/K	266.692	249.202	236.835
Thermal conductivity	W/(m·K)	0.186	0.189	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.063 0 per unit weight fraction	increases at rate 0.06 0 per unit weight fraction
Volume resistivity	increases at rate 10083332000000000 Ohm-metre per unit weight fraction	increases at rate 299557960000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 1.425 0 per unit weight fraction	decreases at rate 1.471 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 35 /K per unit weight fraction	decreases at rate 24.7 /K per unit weight fraction
Thermal conductivity	increases at rate 0.007 W/(m·K) per unit weight fraction	increases at rate 0.006 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and vinyl_amide. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and vinyl_amide

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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 vinyl_amide. 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 vinyl_amide 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 vinyl_amide

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	6800.892	5460.358	4031.244

Young's modulus	newtons per square metre	4363.514	3227.872	2212.361
Shear modulus	newtons per square metre	1566.156	1151.598	785.343
Poisson's ratio	0	0.393	0.401	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	44.297	54.949	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 2681.1 newtons per square metre per unit weight fraction	decreases at rate 2858.2 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 2271.284 newtons per square metre per unit weight fraction	decreases at rate 2031.022 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 829.116 newtons per square metre per unit weight fraction	decreases at rate 732.511 newtons per square metre per unit weight fraction
Poisson's ratio	increases at rate 0.0168 0 per unit weight fraction	increases at rate 0.0141 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 21.306 kiloJoule per mole per unit weight fraction	increases at rate 76.221 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and vinyl_amide. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and vinyl_fluoride

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

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	273.265	348.814	414.398
Density	kg per	1.310	1.238	1.174

	cubic metre			
Oxygen permeability	Perm	799.842	467.126	288.203
Nitrogen permeability	Perm	234.040	130.904	77.690
Carbon dioxide permeability	Perm	4228.931	2354.024	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 151.1 oC per unit weight fraction	increases at rate 131.2 oC per unit weight fraction
Density	decreases at rate 0.143 kg per cubic metre per unit weight fraction	decreases at rate 0.128 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 665.4 Perm per unit weight fraction	decreases at rate 357.8 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 206.3 Perm per unit weight fraction	decreases at rate 106.4 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 3749.8 Perm per unit weight fraction	decreases at rate 1925.9 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and vinyl_fluoride. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and vinyl_fluoride

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and vinyl_fluoride. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 vinyl_fluoride

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
Refractive index	0	1.404	1.497	1.587
Volume resistivity	Ohm-metre	2752753000000000000.000	624291700000000000.000	155017300000000000.000

Dielectric constant	0	2.280	2.602	2.905
Coefficient of volumetric thermal expansion	/K	687.800	277.680	236.835
Thermal conductivity	W/(m·K)	0.157	0.176	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.187 0 per unit weight fraction	increases at rate 0.18 0 per unit weight fraction
Volume resistivity	decreases at rate 4256922600000000000 Ohm-metre per unit weight fraction	decreases at rate 938548800000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.644 0 per unit weight fraction	increases at rate 0.605 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 820.2 /K per unit weight fraction	decreases at rate 81.7 /K per unit weight fraction
Thermal conductivity	increases at rate 0.039 W/(m·K) per unit weight fraction	increases at rate 0.034 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and vinyl_fluoride. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and vinyl_fluoride

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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 vinyl_fluoride. 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 vinyl_fluoride 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 vinyl_fluoride

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	3362.694	3200.054	4031.244

Young's modulus	newtons per square metre	1604.039	1634.482	2212.361
Shear modulus	newtons per square metre	564.604	577.608	785.343
Poisson's ratio	0	0.420	0.415	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	11.622	24.108	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 325.3 newtons per square metre per unit weight fraction	increases at rate 1662.4 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 60.886 newtons per square metre per unit weight fraction	increases at rate 1155.758 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 26.006 newtons per square metre per unit weight fraction	increases at rate 415.47 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0113 0 per unit weight fraction	decreases at rate 0.0127 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 24.971 kiloJoule per mole per unit weight fraction	increases at rate 137.904 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and vinyl_fluoride. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and ethyl_urethane

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

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	294.359	356.866	414.398
Density	kg per	1.361	1.261	1.174

	cubic metre			
Oxygen permeability	Perm	1.537	24.328	288.203
Nitrogen permeability	Perm	0.272	5.377	77.690
Carbon dioxide permeability	Perm	4.650	94.175	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 125 oC per unit weight fraction	increases at rate 115.1 oC per unit weight fraction
Density	decreases at rate 0.2 kg per cubic metre per unit weight fraction	decreases at rate 0.173 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 45.6 Perm per unit weight fraction	increases at rate 527.7 Perm per unit weight fraction
Nitrogen permeability	increases at rate 10.2 Perm per unit weight fraction	increases at rate 144.6 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 179 Perm per unit weight fraction	increases at rate 2593.8 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and ethyl_urethane. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and ethyl_urethane

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and ethyl_urethane. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 ethyl_urethane

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
Refractive index	0	1.514	1.553	1.587
Volume resistivity	Ohm-metre	1050938000000000.000	14860390000000000.000	155017300000000000.000

Dielectric constant	0	3.989	3.414	2.905
Coefficient of volumetric thermal expansion	/K	648.030	271.923	236.835
Thermal conductivity	W/(m·K)	0.227	0.209	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.078 0 per unit weight fraction	increases at rate 0.069 0 per unit weight fraction
Volume resistivity	increases at rate 27618904000000000 Ohm-metre per unit weight fraction	increases at rate 280313820000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 1.15 0 per unit weight fraction	decreases at rate 1.018 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 752.2 /K per unit weight fraction	decreases at rate 70.2 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.036 W/(m·K) per unit weight fraction	decreases at rate 0.033 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and ethyl_urethane. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and ethyl_urethane

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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 ethyl_urethane. 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 ethyl_urethane 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 ethyl_urethane

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	3386.431	4160.685	4031.244

Young's modulus	newtons per square metre	1367.995	1941.417	2212.361
Shear modulus	newtons per square metre	477.427	682.525	785.343
Poisson's ratio	0	0.433	0.422	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	35.772	50.386	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 1548.5 newtons per square metre per unit weight fraction	decreases at rate 258.9 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 1146.844 newtons per square metre per unit weight fraction	increases at rate 541.888 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 410.195 newtons per square metre per unit weight fraction	increases at rate 205.635 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0209 0 per unit weight fraction	decreases at rate 0.0274 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 29.227 kiloJoule per mole per unit weight fraction	increases at rate 85.348 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and ethyl_urethane. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and urethane

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

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	299.416	357.417	414.398
Density	kg per	1.171	1.173	1.174

	cubic metre			
Oxygen permeability	Perm	26.197	87.506	288.203
Nitrogen permeability	Perm	5.824	21.434	77.690
Carbon dioxide permeability	Perm	102.082	379.739	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 116 oC per unit weight fraction	increases at rate 114 oC per unit weight fraction
Density	increases at rate 0.003 kg per cubic metre per unit weight fraction	increases at rate 0.003 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 122.6 Perm per unit weight fraction	increases at rate 401.4 Perm per unit weight fraction
Nitrogen permeability	increases at rate 31.2 Perm per unit weight fraction	increases at rate 112.5 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 555.3 Perm per unit weight fraction	increases at rate 2022.7 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and urethane. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and urethane

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and urethane. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 urethane

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
Refractive index	0	1.506	1.546	1.587
Volume resistivity	Ohm-metre	24988100000000000.000	60035010000000000.000	155017300000000000.000

Dielectric constant	0	3.301	3.111	2.905
Coefficient of volumetric thermal expansion	/K	319.135	271.537	236.835
Thermal conductivity	W/(m·K)	0.209	0.200	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.08 0 per unit weight fraction	increases at rate 0.083 0 per unit weight fraction
Volume resistivity	increases at rate 70093820000000000 Ohm-metre per unit weight fraction	increases at rate 189964580000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.381 0 per unit weight fraction	decreases at rate 0.412 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 95.2 /K per unit weight fraction	decreases at rate 69.4 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.017 W/(m·K) per unit weight fraction	decreases at rate 0.016 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and urethane. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and urethane

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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 urethane. 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 urethane 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 urethane

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	3971.734	3918.367	4031.244

Young's modulus	newtons per square metre	1710.314	1874.103	2212.361
Shear modulus	newtons per square metre	598.753	659.763	785.343
Poisson's ratio	0	0.428	0.420	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	108.366	100.653	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 106.7 newtons per square metre per unit weight fraction	increases at rate 225.8 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 327.578 newtons per square metre per unit weight fraction	increases at rate 676.516 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 122.02 newtons per square metre per unit weight fraction	increases at rate 251.159 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0159 0 per unit weight fraction	decreases at rate 0.0235 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	decreases at rate 15.427 kiloJoule per mole per unit weight fraction	decreases at rate 15.186 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and urethane. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and 1_butene

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of tetmeth_bisphen_carbonate and 1_butene. 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 1_butene 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 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 1_butene

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	212.969	341.392	466.509
Density	kg per	0.855	0.954	1.080

	cubic metre			
Oxygen permeability	Perm	1026.874	1406.619	1595.547
Nitrogen permeability	Perm	306.565	430.688	493.508
Carbon dioxide permeability	Perm	5551.752	7821.462	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 256.8 oC per unit weight fraction	increases at rate 250.2 oC per unit weight fraction
Density	increases at rate 0.198 kg per cubic metre per unit weight fraction	increases at rate 0.251 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 759.5 Perm per unit weight fraction	increases at rate 377.9 Perm per unit weight fraction
Nitrogen permeability	increases at rate 248.2 Perm per unit weight fraction	increases at rate 125.6 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 4539.4 Perm per unit weight fraction	increases at rate 2301.8 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and 1_butene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and 1_butene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and 1_butene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and 1_butene on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 1_butene

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
Refractive index	0	1.467	1.512	1.572
Volume resistivity	Ohm-metre	2706390000000000000.000	1081328000000000000.000	324667800000000000.000

Dielectric constant	0	2.284	2.483	2.744
Coefficient of volumetric thermal expansion	/K	834.125	283.207	212.051
Thermal conductivity	W/(m·K)	0.134	0.155	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.091 0 per unit weight fraction	increases at rate 0.119 0 per unit weight fraction
Volume resistivity	decreases at rate 3250124000000000000 Ohm-metre per unit weight fraction	decreases at rate 1513320400000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.398 0 per unit weight fraction	increases at rate 0.523 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 1101.8 /K per unit weight fraction	decreases at rate 142.3 /K per unit weight fraction
Thermal conductivity	increases at rate 0.041 W/(m·K) per unit weight fraction	increases at rate 0.039 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and 1_butene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and 1_butene

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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 1_butene. 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 1_butene 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 1_butene

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	2297.805	2716.670	3812.095

Young's modulus	newtons per square metre	1.083	1891.989	2839.722
Shear modulus	newtons per square metre	0.361	683.558	1031.991
Poisson's ratio	0	0.500	0.384	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	19.092	32.901	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 837.7 newtons per square metre per unit weight fraction	increases at rate 2190.9 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 3781.812 newtons per square metre per unit weight fraction	increases at rate 1895.466 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1366.394 newtons per square metre per unit weight fraction	increases at rate 696.866 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.232 0 per unit weight fraction	decreases at rate 0.0162 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 27.618 kiloJoule per mole per unit weight fraction	increases at rate 152.787 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and 1_butene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and ethylene

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

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	191.974	331.903	466.509
Density	kg per	0.872	0.965	1.080

	cubic metre			
Oxygen permeability	Perm	745.304	1169.480	1595.547
Nitrogen permeability	Perm	216.848	352.806	493.508
Carbon dioxide permeability	Perm	3915.815	6396.562	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 279.9 oC per unit weight fraction	increases at rate 269.2 oC per unit weight fraction
Density	increases at rate 0.185 kg per cubic metre per unit weight fraction	increases at rate 0.229 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 848.4 Perm per unit weight fraction	increases at rate 852.1 Perm per unit weight fraction
Nitrogen permeability	increases at rate 271.9 Perm per unit weight fraction	increases at rate 281.4 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 4961.5 Perm per unit weight fraction	increases at rate 5151.6 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and ethylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and ethylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and ethylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and ethylene on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 ethylene

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
Refractive index	0	1.465	1.512	1.572
Volume resistivity	Ohm-metre	2215376000000000000.000	958874000000000000.000	3246678000000000000.000

Dielectric constant	0	2.327	2.509	2.744
Coefficient of volumetric thermal expansion	/K	900.860	290.603	212.051
Thermal conductivity	W/(m·K)	0.172	0.173	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.093 0 per unit weight fraction	increases at rate 0.12 0 per unit weight fraction
Volume resistivity	decreases at rate 2513004000000000000 Ohm-metre per unit weight fraction	decreases at rate 1268412400000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.364 0 per unit weight fraction	increases at rate 0.47 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 1220.5 /K per unit weight fraction	decreases at rate 157.1 /K per unit weight fraction
Thermal conductivity	increases at rate 0.003 W/(m·K) per unit weight fraction	increases at rate 0.002 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and ethylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and ethylene

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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 ethylene. 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 ethylene 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 ethylene

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	2466.650	2734.074	3812.095

Young's modulus	newtons per square metre	2.566	1445.472	2839.722
Shear modulus	newtons per square metre	0.855	511.894	1031.991
Poisson's ratio	0	0.500	0.412	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	9.883	18.123	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 534.8 newtons per square metre per unit weight fraction	increases at rate 2156 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 2885.811 newtons per square metre per unit weight fraction	increases at rate 2788.5 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1022.077 newtons per square metre per unit weight fraction	increases at rate 1040.194 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.1759 0 per unit weight fraction	decreases at rate 0.0721 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 16.481 kiloJoule per mole per unit weight fraction	increases at rate 182.343 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and ethylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and isobutene

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

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	183.823	327.119	466.509
Density	kg per	0.856	0.955	1.080

	cubic metre			
Oxygen permeability	Perm	2438.329	2282.123	1595.547
Nitrogen permeability	Perm	780.327	726.462	493.508
Carbon dioxide permeability	Perm	14240.660	13249.830	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 286.6 oC per unit weight fraction	increases at rate 278.8 oC per unit weight fraction
Density	increases at rate 0.198 kg per cubic metre per unit weight fraction	increases at rate 0.25 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 312.4 Perm per unit weight fraction	decreases at rate 1373.2 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 107.7 Perm per unit weight fraction	decreases at rate 465.9 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 1981.7 Perm per unit weight fraction	decreases at rate 8554.9 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and isobutene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and isobutene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and isobutene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and isobutene on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 isobutene

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
Refractive index	0	1.479	1.519	1.572
Volume resistivity	Ohm-metre	36081020000000000000.000	1236246000000000000.000	324667800000000000.000

Dielectric constant	0	2.221	2.454	2.744
Coefficient of volumetric thermal expansion	/K	929.737	294.480	212.051
Thermal conductivity	W/(m·K)	0.131	0.153	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.08 0 per unit weight fraction	increases at rate 0.105 0 per unit weight fraction
Volume resistivity	decreases at rate 4743712000000000000 Ohm-metre per unit weight fraction	decreases at rate 1823156400000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.465 0 per unit weight fraction	increases at rate 0.581 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 1270.5 /K per unit weight fraction	decreases at rate 164.9 /K per unit weight fraction
Thermal conductivity	increases at rate 0.044 W/(m·K) per unit weight fraction	increases at rate 0.043 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and isobutene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and isobutene

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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 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 tetmeth_bisphen_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 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 isobutene

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	1332.498	2478.280	3812.095

Young's modulus	newtons per square metre	1.019	1701.372	2839.722
Shear modulus	newtons per square metre	0.340	613.956	1031.991
Poisson's ratio	0	0.500	0.386	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	16.870	31.020	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 2291.6 newtons per square metre per unit weight fraction	increases at rate 2667.6 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 3400.706 newtons per square metre per unit weight fraction	increases at rate 2276.7 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1227.233 newtons per square metre per unit weight fraction	increases at rate 836.069 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.2286 0 per unit weight fraction	decreases at rate 0.0195 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 28.298 kiloJoule per mole per unit weight fraction	increases at rate 156.549 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and isobutene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and propylene

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

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	229.892	349.940	466.509
Density	kg per	0.858	0.956	1.080

	cubic metre			
Oxygen permeability	Perm	1316.654	1615.423	1595.547
Nitrogen permeability	Perm	401.007	500.153	493.508
Carbon dioxide permeability	Perm	7278.144	9094.171	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 240.1 oC per unit weight fraction	increases at rate 233.1 oC per unit weight fraction
Density	increases at rate 0.196 kg per cubic metre per unit weight fraction	increases at rate 0.247 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 597.5 Perm per unit weight fraction	decreases at rate 39.8 Perm per unit weight fraction
Nitrogen permeability	increases at rate 198.3 Perm per unit weight fraction	decreases at rate 13.3 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 3632.1 Perm per unit weight fraction	decreases at rate 243.6 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and propylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and propylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and propylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and propylene on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 propylene

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
Refractive index	0	1.471	1.515	1.572
Volume resistivity	Ohm-metre	2955856000000000000.000	1126650000000000000.000	3246678000000000000.000

Dielectric constant	0	2.265	2.474	2.744
Coefficient of volumetric thermal expansion	/K	787.126	276.860	212.051
Thermal conductivity	W/(m·K)	0.143	0.159	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.087 0 per unit weight fraction	increases at rate 0.114 0 per unit weight fraction
Volume resistivity	decreases at rate 3658412000000000000 Ohm-metre per unit weight fraction	decreases at rate 1603964400000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.419 0 per unit weight fraction	increases at rate 0.54 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 1020.5 /K per unit weight fraction	decreases at rate 129.6 /K per unit weight fraction
Thermal conductivity	increases at rate 0.032 W/(m·K) per unit weight fraction	increases at rate 0.031 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and propylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and propylene

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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 propylene. 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 propylene 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 propylene

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	1976.690	2721.361	3812.095

Young's modulus	newtons per square metre	1.770	1698.328	2839.722
Shear modulus	newtons per square metre	0.590	608.289	1031.991
Poisson's ratio	0	0.500	0.396	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	13.775	25.179	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 1489.3 newtons per square metre per unit weight fraction	increases at rate 2181.5 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 3393.117 newtons per square metre per unit weight fraction	increases at rate 2282.788 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1215.398 newtons per square metre per unit weight fraction	increases at rate 847.404 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.2077 0 per unit weight fraction	decreases at rate 0.0403 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 22.808 kiloJoule per mole per unit weight fraction	increases at rate 168.232 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and propylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and acrylonitrile

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of tetmeth_bisphen_carbonate and acrylonitrile. 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 acrylonitrile 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 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 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
Glass transition temperature	oC	361.527	413.320	466.509
Density	kg per	1.177	1.126	1.080

	cubic metre			
Oxygen permeability	Perm	0.082	12.859	1595.547
Nitrogen permeability	Perm	0.012	2.700	493.508
Carbon dioxide permeability	Perm	0.192	47.025	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 103.6 oC per unit weight fraction	increases at rate 106.4 oC per unit weight fraction
Density	decreases at rate 0.101 kg per cubic metre per unit weight fraction	decreases at rate 0.093 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 25.6 Perm per unit weight fraction	increases at rate 3165.4 Perm per unit weight fraction
Nitrogen permeability	increases at rate 5.4 Perm per unit weight fraction	increases at rate 981.6 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 93.7 Perm per unit weight fraction	increases at rate 17850.7 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and acrylonitrile. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and acrylonitrile

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and acrylonitrile. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity 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. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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
Refractive index	0	1.542	1.558	1.572
Volume resistivity	Ohm-metre	1041069000000000.000	16337880000000000.000	324667800000000000.000

Dielectric constant	0	3.991	3.393	2.744
Coefficient of volumetric thermal expansion	/K	268.697	237.409	212.051
Thermal conductivity	W/(m·K)	0.178	0.176	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.03 0 per unit weight fraction	increases at rate 0.028 0 per unit weight fraction
Volume resistivity	increases at rate 30593622000000000 Ohm-metre per unit weight fraction	increases at rate 616659840000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 1.196 0 per unit weight fraction	decreases at rate 1.298 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 62.6 /K per unit weight fraction	decreases at rate 50.7 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.004 W/(m·K) per unit weight fraction	decreases at rate 0.004 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and acrylonitrile. Experimental study is required to validate the results.

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

Young's modulus	newtons per square metre	3736.424	3371.657	2839.722
Shear modulus	newtons per square metre	1330.481	1210.223	1031.991
Poisson's ratio	0	0.404	0.393	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	34.157	45.127	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 2493.2 newtons per square metre per unit weight fraction	decreases at rate 2878.4 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 729.534 newtons per square metre per unit weight fraction	decreases at rate 1063.87 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 240.516 newtons per square metre per unit weight fraction	decreases at rate 356.464 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0223 0 per unit weight fraction	decreases at rate 0.0343 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 21.94 kiloJoule per mole per unit weight fraction	increases at rate 128.335 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and acrylonitrile. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and dichloro_ethylene

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

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	277.943	398.243	466.509
Density	kg per	1.689	1.317	1.080

	cubic metre			
Oxygen permeability	Perm	0.982	101.111	1595.547
Nitrogen permeability	Perm	0.168	25.056	493.508
Carbon dioxide permeability	Perm	2.853	444.475	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 240.6 oC per unit weight fraction	increases at rate 136.5 oC per unit weight fraction
Density	decreases at rate 0.744 kg per cubic metre per unit weight fraction	decreases at rate 0.475 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 200.3 Perm per unit weight fraction	increases at rate 2988.9 Perm per unit weight fraction
Nitrogen permeability	increases at rate 49.8 Perm per unit weight fraction	increases at rate 936.9 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 883.2 Perm per unit weight fraction	increases at rate 17055.8 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and dichloro_ethylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and dichloro_ethylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and dichloro_ethylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and dichloro_ethylene on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 dichloro_ethylene

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
Refractive index	0	1.608	1.586	1.572
Volume resistivity	Ohm-metre	193061000000000000.000	261442800000000000.000	324667800000000000.000

Dielectric constant	0	2.857	2.791	2.744
Coefficient of volumetric thermal expansion	/K	678.564	245.739	212.051
Thermal conductivity	W/(m·K)	0.151	0.166	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.045 0 per unit weight fraction	decreases at rate 0.028 0 per unit weight fraction
Volume resistivity	increases at rate 136763600000000000 Ohm-metre per unit weight fraction	increases at rate 126450000000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.132 0 per unit weight fraction	decreases at rate 0.094 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 865.6 /K per unit weight fraction	decreases at rate 67.4 /K per unit weight fraction
Thermal conductivity	increases at rate 0.03 W/(m·K) per unit weight fraction	increases at rate 0.017 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and dichloro_ethylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and dichloro_ethylene

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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 dichloro_ethylene. 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 dichloro_ethylene 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 dichloro_ethylene

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	5226.046	3974.772	3812.095

Young's modulus	newtons per square metre	3361.917	2772.901	2839.722
Shear modulus	newtons per square metre	1206.906	1001.967	1031.991
Poisson's ratio	0	0.393	0.384	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	29.784	48.707	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 2502.5 newtons per square metre per unit weight fraction	decreases at rate 325.4 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 1178.032 newtons per square metre per unit weight fraction	increases at rate 133.642 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 409.878 newtons per square metre per unit weight fraction	increases at rate 60.048 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0181 0 per unit weight fraction	decreases at rate 0.0158 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 37.846 kiloJoule per mole per unit weight fraction	increases at rate 121.175 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and dichloro_ethylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and difluoro_ethylene

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

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	240.041	365.473	466.509
Density	kg per	1.606	1.291	1.080

	cubic metre			
Oxygen permeability	Perm	1485.349	1470.861	1595.547
Nitrogen permeability	Perm	456.789	451.977	493.508
Carbon dioxide permeability	Perm	8299.482	8211.345	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 250.9 oC per unit weight fraction	increases at rate 202.1 oC per unit weight fraction
Density	decreases at rate 0.629 kg per cubic metre per unit weight fraction	decreases at rate 0.423 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 29 Perm per unit weight fraction	increases at rate 249.4 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 9.6 Perm per unit weight fraction	increases at rate 83.1 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 176.3 Perm per unit weight fraction	increases at rate 1522 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and difluoro_ethylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and difluoro_ethylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and difluoro_ethylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and difluoro_ethylene on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 difluoro_ethylene

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
Refractive index	0	1.371	1.487	1.572
Volume resistivity	Ohm-metre	4526299000000000000.000	979231100000000000.000	324667800000000000.000

Dielectric constant	0	2.172	2.505	2.744
Coefficient of volumetric thermal expansion	/K	761.397	266.026	212.051
Thermal conductivity	W/(m·K)	0.151	0.164	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.233 0 per unit weight fraction	increases at rate 0.169 0 per unit weight fraction
Volume resistivity	decreases at rate 7094135800000000000 Ohm-metre per unit weight fraction	decreases at rate 1309126600000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.665 0 per unit weight fraction	increases at rate 0.479 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 990.7 /K per unit weight fraction	decreases at rate 107.9 /K per unit weight fraction
Thermal conductivity	increases at rate 0.025 W/(m·K) per unit weight fraction	increases at rate 0.021 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and difluoro_ethylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and difluoro_ethylene

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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 difluoro_ethylene. 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 difluoro_ethylene 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 difluoro_ethylene

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	3417.759	3059.917	3812.095

Young's modulus	newtons per square metre	2.842	1889.146	2839.722
Shear modulus	newtons per square metre	0.947	676.094	1031.991
Poisson's ratio	0	0.500	0.397	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	12.566	29.109	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 715.7 newtons per square metre per unit weight fraction	increases at rate 1504.4 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 3772.608 newtons per square metre per unit weight fraction	increases at rate 1901.152 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1350.293 newtons per square metre per unit weight fraction	increases at rate 711.794 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.2055 0 per unit weight fraction	decreases at rate 0.0425 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 33.085 kiloJoule per mole per unit weight fraction	increases at rate 160.372 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and difluoro_ethylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and meth_styrene

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

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	407.893	435.016	466.509
Density	kg per	1.036	1.057	1.080

	cubic metre			
Oxygen permeability	Perm	617.633	980.372	1595.547
Nitrogen permeability	Perm	177.009	291.594	493.508
Carbon dioxide permeability	Perm	3191.058	5278.457	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 54.2 oC per unit weight fraction	increases at rate 63 oC per unit weight fraction
Density	increases at rate 0.043 kg per cubic metre per unit weight fraction	increases at rate 0.044 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 725.5 Perm per unit weight fraction	increases at rate 1230.4 Perm per unit weight fraction
Nitrogen permeability	increases at rate 229.2 Perm per unit weight fraction	increases at rate 403.8 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 4174.8 Perm per unit weight fraction	increases at rate 7387.8 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and meth_styrene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and meth_styrene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and meth_styrene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and meth_styrene on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 meth_styrene

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
Refractive index	0	1.591	1.582	1.572
Volume resistivity	Ohm-metre	975460300000000000.000	578870000000000000.000	324667800000000000.000

Dielectric constant	0	2.505	2.619	2.744
Coefficient of volumetric thermal expansion	/K	240.342	226.367	212.051
Thermal conductivity	W/(m·K)	0.130	0.152	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.019 0 per unit weight fraction	decreases at rate 0.02 0 per unit weight fraction
Volume resistivity	decreases at rate 793180600000000000 Ohm-metre per unit weight fraction	decreases at rate 508404400000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.227 0 per unit weight fraction	increases at rate 0.251 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 27.9 /K per unit weight fraction	decreases at rate 28.6 /K per unit weight fraction
Thermal conductivity	increases at rate 0.043 W/(m·K) per unit weight fraction	increases at rate 0.044 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and meth_styrene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and meth_styrene

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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 meth_styrene. 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 meth_styrene 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 meth_styrene

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	3471.108	3636.804	3812.095

Young's modulus	newtons per square metre	3138.433	2975.224	2839.722
Shear modulus	newtons per square metre	1162.980	1090.903	1031.991
Poisson's ratio	0	0.349	0.364	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	42.616	61.003	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 331.4 newtons per square metre per unit weight fraction	increases at rate 350.6 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 326.418 newtons per square metre per unit weight fraction	decreases at rate 271.004 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 144.154 newtons per square metre per unit weight fraction	decreases at rate 117.824 newtons per square metre per unit weight fraction
Poisson's ratio	increases at rate 0.0287 0 per unit weight fraction	increases at rate 0.0244 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 36.773 kiloJoule per mole per unit weight fraction	increases at rate 96.583 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and meth_styrene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and styrene

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

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	379.529	420.782	466.509
Density	kg per	1.074	1.077	1.080

	cubic metre			
Oxygen permeability	Perm	363.687	749.378	1595.547
Nitrogen permeability	Perm	99.887	218.129	493.508
Carbon dioxide permeability	Perm	1792.261	3939.137	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 82.5 oC per unit weight fraction	increases at rate 91.5 oC per unit weight fraction
Density	increases at rate 0.006 kg per cubic metre per unit weight fraction	increases at rate 0.006 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 771.4 Perm per unit weight fraction	increases at rate 1692.3 Perm per unit weight fraction
Nitrogen permeability	increases at rate 236.5 Perm per unit weight fraction	increases at rate 550.8 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 4293.8 Perm per unit weight fraction	increases at rate 10066.4 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and styrene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and styrene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and styrene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and styrene on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 styrene

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
Refractive index	0	1.604	1.588	1.572
Volume resistivity	Ohm-metre	734331000000000000.000	497376800000000000.000	324667800000000000.000

Dielectric constant	0	2.567	2.652	2.744
Coefficient of volumetric thermal expansion	/K	256.928	233.492	212.051
Thermal conductivity	W/(m·K)	0.135	0.154	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.032 0 per unit weight fraction	decreases at rate 0.032 0 per unit weight fraction
Volume resistivity	decreases at rate 473908400000000000 Ohm-metre per unit weight fraction	decreases at rate 345418000000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.169 0 per unit weight fraction	increases at rate 0.185 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 46.9 /K per unit weight fraction	decreases at rate 42.9 /K per unit weight fraction
Thermal conductivity	increases at rate 0.039 W/(m·K) per unit weight fraction	increases at rate 0.04 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and styrene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and styrene

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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 styrene. 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 styrene 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 styrene

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	3585.198	3712.690	3812.095

Young's modulus	newtons per square metre	3014.022	2936.816	2839.722
Shear modulus	newtons per square metre	1108.189	1073.270	1031.991
Poisson's ratio	0	0.360	0.368	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	39.197	56.809	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 255 newtons per square metre per unit weight fraction	increases at rate 198.8 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 154.412 newtons per square metre per unit weight fraction	decreases at rate 194.188 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 69.838 newtons per square metre per unit weight fraction	decreases at rate 82.558 newtons per square metre per unit weight fraction
Poisson's ratio	increases at rate 0.0166 0 per unit weight fraction	increases at rate 0.0154 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 35.223 kiloJoule per mole per unit weight fraction	increases at rate 104.971 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and styrene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and tetrafluoro_ethylene

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

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	251.763	375.211	466.509
Density	kg per	2.053	1.415	1.080

	cubic metre			
Oxygen permeability	Perm	1275.484	1381.171	1595.547
Nitrogen permeability	Perm	387.477	422.276	493.508
Carbon dioxide permeability	Perm	7030.605	7667.452	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 246.9 oC per unit weight fraction	increases at rate 182.6 oC per unit weight fraction
Density	decreases at rate 1.276 kg per cubic metre per unit weight fraction	decreases at rate 0.671 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 211.4 Perm per unit weight fraction	increases at rate 428.8 Perm per unit weight fraction
Nitrogen permeability	increases at rate 69.6 Perm per unit weight fraction	increases at rate 142.5 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 1273.7 Perm per unit weight fraction	increases at rate 2609.8 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and tetrafluoro_ethylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and tetrafluoro_ethylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and tetrafluoro_ethylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and tetrafluoro_ethylene on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 tetrafluoro_ethylene

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
Refractive index	0	1.335	1.486	1.572
Volume resistivity	Ohm-metre	6581058000000000000.000	987949500000000000.000	324667800000000000.000

Dielectric constant	0	2.091	2.503	2.744
Coefficient of volumetric thermal expansion	/K	733.699	259.656	212.051
Thermal conductivity	W/(m·K)	0.146	0.162	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.301 0 per unit weight fraction	increases at rate 0.172 0 per unit weight fraction
Volume resistivity	decreases at rate 1118621700000000000 Ohm-metre per unit weight fraction	decreases at rate 1326563400000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.824 0 per unit weight fraction	increases at rate 0.483 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 948.1 /K per unit weight fraction	decreases at rate 95.2 /K per unit weight fraction
Thermal conductivity	increases at rate 0.031 W/(m·K) per unit weight fraction	increases at rate 0.025 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and tetrafluoro_ethylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and tetrafluoro_ethylene

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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 tetrafluoro_ethylene. 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 tetrafluoro_ethylene 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 tetrafluoro_ethylene

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	5941.105	3195.183	3812.095

Young's modulus	newtons per square metre	2.223	2147.526	2839.722
Shear modulus	newtons per square metre	0.741	773.615	1031.991
Poisson's ratio	0	0.500	0.388	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	16.097	38.809	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 5491.8 newtons per square metre per unit weight fraction	increases at rate 1233.8 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 4290.606 newtons per square metre per unit weight fraction	increases at rate 1384.392 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1545.748 newtons per square metre per unit weight fraction	increases at rate 516.752 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.2239 0 per unit weight fraction	decreases at rate 0.0243 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 45.424 kiloJoule per mole per unit weight fraction	increases at rate 140.97 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and tetrafluoro_ethylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and vinyl_acetate

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

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	302.653	386.461	466.509
Density	kg per	1.219	1.145	1.080

	cubic metre			
Oxygen permeability	Perm	90.468	403.423	1595.547
Nitrogen permeability	Perm	22.219	111.728	493.508
Carbon dioxide permeability	Perm	393.760	2006.568	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 167.6 oC per unit weight fraction	increases at rate 160.1 oC per unit weight fraction
Density	decreases at rate 0.147 kg per cubic metre per unit weight fraction	decreases at rate 0.131 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 625.9 Perm per unit weight fraction	increases at rate 2384.2 Perm per unit weight fraction
Nitrogen permeability	increases at rate 179 Perm per unit weight fraction	increases at rate 763.6 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 3225.6 Perm per unit weight fraction	increases at rate 13931.6 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and vinyl_acetate. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and vinyl_acetate

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and vinyl_acetate. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and vinyl_acetate on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 vinyl_acetate

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
Refractive index	0	1.481	1.529	1.572
Volume resistivity	Ohm-metre	34049510000000000.000	108908800000000000.000	324667800000000000.000

Dielectric constant	0	3.234	2.981	2.744
Coefficient of volumetric thermal expansion	/K	316.043	252.667	212.051
Thermal conductivity	W/(m·K)	0.175	0.175	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.094 0 per unit weight fraction	increases at rate 0.086 0 per unit weight fraction
Volume resistivity	increases at rate 149718580000000000 Ohm-metre per unit weight fraction	increases at rate 431518000000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.505 0 per unit weight fraction	decreases at rate 0.474 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 126.8 /K per unit weight fraction	decreases at rate 81.2 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.001 W/(m·K) per unit weight fraction	decreases at rate 0.001 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and vinyl_acetate. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and vinyl_acetate

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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 vinyl_acetate. 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 vinyl_acetate 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 vinyl_acetate

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	3101.366	3668.181	3812.095

Young's modulus	newtons per square metre	2163.179	2644.366	2839.722
Shear modulus	newtons per square metre	781.636	958.207	1031.991
Poisson's ratio	0	0.384	0.380	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	31.136	48.107	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 1133.6 newtons per square metre per unit weight fraction	increases at rate 287.8 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 962.374 newtons per square metre per unit weight fraction	increases at rate 390.712 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 353.142 newtons per square metre per unit weight fraction	increases at rate 147.568 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0078 0 per unit weight fraction	decreases at rate 0.008 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 33.942 kiloJoule per mole per unit weight fraction	increases at rate 122.374 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and vinyl_acetate. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and vinyl_chloride

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

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	291.873	397.535	466.509
Density	kg per	1.383	1.213	1.080

	cubic metre			
Oxygen permeability	Perm	8.277	183.446	1595.547
Nitrogen permeability	Perm	1.677	47.688	493.508
Carbon dioxide permeability	Perm	29.100	850.455	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 211.3 oC per unit weight fraction	increases at rate 137.9 oC per unit weight fraction
Density	decreases at rate 0.341 kg per cubic metre per unit weight fraction	decreases at rate 0.266 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 350.3 Perm per unit weight fraction	increases at rate 2824.2 Perm per unit weight fraction
Nitrogen permeability	increases at rate 92 Perm per unit weight fraction	increases at rate 891.6 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 1642.7 Perm per unit weight fraction	increases at rate 16243.8 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and vinyl_chloride. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and vinyl_chloride

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and vinyl_chloride. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and vinyl_chloride on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 vinyl_chloride

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
Refractive index	0	1.556	1.565	1.572
Volume resistivity	Ohm-metre	138712800000000000.000	218728000000000000.000	324667800000000000.000

Dielectric constant	0	2.929	2.830	2.744
Coefficient of volumetric thermal expansion	/K	652.476	246.144	212.051
Thermal conductivity	W/(m·K)	0.157	0.167	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.018 0 per unit weight fraction	increases at rate 0.014 0 per unit weight fraction
Volume resistivity	increases at rate 160030400000000000 Ohm-metre per unit weight fraction	increases at rate 211879600000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.198 0 per unit weight fraction	decreases at rate 0.172 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 812.7 /K per unit weight fraction	decreases at rate 68.2 /K per unit weight fraction
Thermal conductivity	increases at rate 0.022 W/(m·K) per unit weight fraction	increases at rate 0.014 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and vinyl_chloride. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and vinyl_chloride

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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 vinyl_chloride. 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 vinyl_chloride 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 vinyl_chloride

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	4019.120	3746.577	3812.095

Young's modulus	newtons per square metre	2250.873	2403.413	2839.722
Shear modulus	newtons per square metre	800.077	862.623	1031.991
Poisson's ratio	0	0.407	0.393	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	20.231	35.159	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 545.1 newtons per square metre per unit weight fraction	increases at rate 131 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 305.08 newtons per square metre per unit weight fraction	increases at rate 872.618 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 125.092 newtons per square metre per unit weight fraction	increases at rate 338.736 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0272 0 per unit weight fraction	decreases at rate 0.0345 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 29.855 kiloJoule per mole per unit weight fraction	increases at rate 148.271 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and vinyl_chloride. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and butylene_isophthalate

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

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	308.194	362.127	414.398
Density	kg per	1.237	1.205	1.174

	cubic metre			
Oxygen permeability	Perm	14.676	66.646	288.203
Nitrogen permeability	Perm	3.114	15.971	77.690
Carbon dioxide permeability	Perm	54.304	282.271	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 107.9 oC per unit weight fraction	increases at rate 104.5 oC per unit weight fraction
Density	decreases at rate 0.064 kg per cubic metre per unit weight fraction	decreases at rate 0.061 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 103.9 Perm per unit weight fraction	increases at rate 443.1 Perm per unit weight fraction
Nitrogen permeability	increases at rate 25.7 Perm per unit weight fraction	increases at rate 123.4 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 455.9 Perm per unit weight fraction	increases at rate 2217.6 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and butylene_isophthalate. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and butylene_isophthalate

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and butylene_isophthalate. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 butylene_isophthalate

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
Refractive index	0	1.544	1.566	1.587
Volume resistivity	Ohm-metre	59131880000000000.000	96048610000000000.000	155017300000000000.000

Dielectric constant	0	3.114	3.009	2.905
Coefficient of volumetric thermal expansion	/K	310.887	268.288	236.835
Thermal conductivity	W/(m·K)	0.205	0.199	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.043 0 per unit weight fraction	increases at rate 0.042 0 per unit weight fraction
Volume resistivity	increases at rate 73833460000000000 Ohm-metre per unit weight fraction	increases at rate 117937380000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.211 0 per unit weight fraction	decreases at rate 0.208 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 85.2 /K per unit weight fraction	decreases at rate 62.9 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.013 W/(m·K) per unit weight fraction	decreases at rate 0.012 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and butylene_isophthalate. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and butylene_isophthalate

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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 butylene_isophthalate. 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 butylene_isophthalate 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 butylene_isophthalate

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	3450.766	3865.436	4031.244

Young's modulus	newtons per square metre	1719.804	2018.442	2212.361
Shear modulus	newtons per square metre	606.874	714.255	785.343
Poisson's ratio	0	0.417	0.413	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	83.969	88.188	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 829.3 newtons per square metre per unit weight fraction	increases at rate 331.6 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 597.276 newtons per square metre per unit weight fraction	increases at rate 387.838 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 214.762 newtons per square metre per unit weight fraction	increases at rate 142.175 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0079 0 per unit weight fraction	decreases at rate 0.0089 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 8.438 kiloJoule per mole per unit weight fraction	increases at rate 9.743 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and butylene_isophthalate. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and butylene_terepthalate

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

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	345.485	380.463	414.398
Density	kg per	1.237	1.205	1.174

	cubic metre			
Oxygen permeability	Perm	14.676	66.646	288.203
Nitrogen permeability	Perm	3.114	15.971	77.690
Carbon dioxide permeability	Perm	54.304	282.271	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 70 oC per unit weight fraction	increases at rate 67.9 oC per unit weight fraction
Density	decreases at rate 0.064 kg per cubic metre per unit weight fraction	decreases at rate 0.061 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 103.9 Perm per unit weight fraction	increases at rate 443.1 Perm per unit weight fraction
Nitrogen permeability	increases at rate 25.7 Perm per unit weight fraction	increases at rate 123.4 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 455.9 Perm per unit weight fraction	increases at rate 2217.6 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and butylene_terepthalate. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and butylene_terepthalate

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and butylene_terepthalate. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 butylene_terepthalate

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
Refractive index	0	1.544	1.566	1.587
Volume resistivity	Ohm-metre	59131880000000000.000	96048610000000000.000	155017300000000000.000

Dielectric constant	0	3.114	3.009	2.905
Coefficient of volumetric thermal expansion	/K	280.133	256.345	236.835
Thermal conductivity	W/(m·K)	0.205	0.199	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.043 0 per unit weight fraction	increases at rate 0.042 0 per unit weight fraction
Volume resistivity	increases at rate 73833460000000000 Ohm-metre per unit weight fraction	increases at rate 117937380000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.211 0 per unit weight fraction	decreases at rate 0.208 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 47.6 /K per unit weight fraction	decreases at rate 39 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.013 W/(m·K) per unit weight fraction	decreases at rate 0.012 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and butylene_terepthalate. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and butylene_terepthalate

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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 butylene_terepthalate. 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 butylene_terepthalate 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 butylene_terepthalate

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	3912.751	3999.145	4031.244

Young's modulus	newtons per square metre	1869.451	2040.907	2212.361
Shear modulus	newtons per square metre	658.086	721.197	785.343
Poisson's ratio	0	0.420	0.415	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	83.969	88.188	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 172.8 newtons per square metre per unit weight fraction	increases at rate 64.2 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 342.912 newtons per square metre per unit weight fraction	increases at rate 342.908 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 126.222 newtons per square metre per unit weight fraction	increases at rate 128.291 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0109 0 per unit weight fraction	decreases at rate 0.0128 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 8.438 kiloJoule per mole per unit weight fraction	increases at rate 9.743 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and butylene_terepthalate. Experimental study is required to validate the results.

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.

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 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

	cubic metre			
Oxygen permeability	Perm	14.676	164.832	1595.547
Nitrogen permeability	Perm	3.114	42.482	493.508
Carbon dioxide permeability	Perm	54.304	756.895	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 160.4 oC per unit weight fraction	increases at rate 156.3 oC per unit weight fraction
Density	decreases at rate 0.168 kg per cubic metre per unit weight fraction	decreases at rate 0.146 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 300.3 Perm per unit weight fraction	increases at rate 2861.4 Perm per unit weight fraction
Nitrogen permeability	increases at rate 78.7 Perm per unit weight fraction	increases at rate 902.1 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 1405.2 Perm per unit weight fraction	increases at rate 16430.9 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and butylene_isophthalate. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and butylene_isophthalate

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and butylene_isophthalate. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity 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.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 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
Refractive index	0	1.544	1.559	1.572
Volume resistivity	Ohm-metre	59131880000000000.000	142694700000000000.000	324667800000000000.000

Dielectric constant	0	3.114	2.923	2.744
Coefficient of volumetric thermal expansion	/K	310.887	251.510	212.051
Thermal conductivity	W/(m·K)	0.205	0.189	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.029 0 per unit weight fraction	increases at rate 0.026 0 per unit weight fraction
Volume resistivity	increases at rate 167125640000000000 Ohm-metre per unit weight fraction	increases at rate 363946200000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.383 0 per unit weight fraction	decreases at rate 0.357 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 118.8 /K per unit weight fraction	decreases at rate 78.9 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.031 W/(m·K) per unit weight fraction	decreases at rate 0.03 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and butylene_isophthalate. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and butylene_isophthalate

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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 butylene_isophthalate. 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 butylene_isophthalate 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 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
Bulk modulus	newtons per square metre	3450.766	3807.407	3812.095

Young's modulus	newtons per square metre	1719.804	2260.186	2839.722
Shear modulus	newtons per square metre	606.874	806.597	1031.991
Poisson's ratio	0	0.417	0.401	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	83.969	94.480	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 713.3 newtons per square metre per unit weight fraction	increases at rate 9.4 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 1080.764 newtons per square metre per unit weight fraction	increases at rate 1159.072 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 399.447 newtons per square metre per unit weight fraction	increases at rate 450.787 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0317 0 per unit weight fraction	decreases at rate 0.0504 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 21.021 kiloJoule per mole per unit weight fraction	increases at rate 29.628 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and butylene_isophthalate. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and butylene_terepthalate

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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_terepthalate. 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_terepthalate 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 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_terepthalate

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	345.485	406.766	466.509
Density	kg per	1.237	1.153	1.080

	cubic metre			
Oxygen permeability	Perm	14.676	164.832	1595.547
Nitrogen permeability	Perm	3.114	42.482	493.508
Carbon dioxide permeability	Perm	54.304	756.895	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 122.6 oC per unit weight fraction	increases at rate 119.5 oC per unit weight fraction
Density	decreases at rate 0.168 kg per cubic metre per unit weight fraction	decreases at rate 0.146 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 300.3 Perm per unit weight fraction	increases at rate 2861.4 Perm per unit weight fraction
Nitrogen permeability	increases at rate 78.7 Perm per unit weight fraction	increases at rate 902.1 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 1405.2 Perm per unit weight fraction	increases at rate 16430.9 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and butylene_terepthalate. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and butylene_terepthalate

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and butylene_terepthalate. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and butylene_terepthalate on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 butylene_terepthalate

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
Refractive index	0	1.544	1.559	1.572
Volume resistivity	Ohm-metre	59131880000000000.000	142694700000000000.000	324667800000000000.000

Dielectric constant	0	3.114	2.923	2.744
Coefficient of volumetric thermal expansion	/K	280.133	240.960	212.051
Thermal conductivity	W/(m·K)	0.205	0.189	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.029 0 per unit weight fraction	increases at rate 0.026 0 per unit weight fraction
Volume resistivity	increases at rate 167125640000000000 Ohm-metre per unit weight fraction	increases at rate 363946200000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.383 0 per unit weight fraction	decreases at rate 0.357 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 78.3 /K per unit weight fraction	decreases at rate 57.8 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.031 W/(m·K) per unit weight fraction	decreases at rate 0.03 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and butylene_terepthalate. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and butylene_terepthalate

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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 butylene_terepthalate. 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 butylene_terepthalate 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 butylene_terepthalate

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	3912.751	3920.721	3812.095

Young's modulus	newtons per square metre	1869.451	2264.620	2839.722
Shear modulus	newtons per square metre	658.086	806.642	1031.991
Poisson's ratio	0	0.420	0.404	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	83.969	94.480	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 15.9 newtons per square metre per unit weight fraction	decreases at rate 217.3 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 790.338 newtons per square metre per unit weight fraction	increases at rate 1150.204 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 297.112 newtons per square metre per unit weight fraction	increases at rate 450.697 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0333 0 per unit weight fraction	decreases at rate 0.0558 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 21.021 kiloJoule per mole per unit weight fraction	increases at rate 29.628 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and butylene_terepthalate. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and ethylene_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 ethylene_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 ethylene_isophthalate 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 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 ethylene_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	325.591	396.759	466.509
Density	kg per	1.317	1.187	1.080

	cubic metre			
Oxygen permeability	Perm	6.631	117.842	1595.547
Nitrogen permeability	Perm	1.320	29.564	493.508
Carbon dioxide permeability	Perm	22.857	525.154	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 142.3 oC per unit weight fraction	increases at rate 139.5 oC per unit weight fraction
Density	decreases at rate 0.261 kg per cubic metre per unit weight fraction	decreases at rate 0.214 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 222.4 Perm per unit weight fraction	increases at rate 2955.4 Perm per unit weight fraction
Nitrogen permeability	increases at rate 56.5 Perm per unit weight fraction	increases at rate 927.9 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 1004.6 Perm per unit weight fraction	increases at rate 16894.4 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and ethylene_isophthalate. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and ethylene_isophthalate

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and ethylene_isophthalate. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and ethylene_isophthalate on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 ethylene_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
Refractive index	0	1.556	1.565	1.572
Volume resistivity	Ohm-metre	27194300000000000.000	101655700000000000.000	324667800000000000.000

Dielectric constant	0	3.283	2.996	2.744
Coefficient of volumetric thermal expansion	/K	295.740	246.590	212.051
Thermal conductivity	W/(m·K)	0.210	0.192	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.017 0 per unit weight fraction	increases at rate 0.014 0 per unit weight fraction
Volume resistivity	increases at rate 148922800000000000 Ohm-metre per unit weight fraction	increases at rate 446024200000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.573 0 per unit weight fraction	decreases at rate 0.504 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 98.3 /K per unit weight fraction	decreases at rate 69.1 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.036 W/(m·K) per unit weight fraction	decreases at rate 0.035 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and ethylene_isophthalate. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and ethylene_isophthalate

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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 ethylene_isophthalate. 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 ethylene_isophthalate 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 ethylene_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
Bulk modulus	newtons per square metre	4022.684	3995.934	3812.095

Young's modulus	newtons per square metre	2275.292	2575.435	2839.722
Shear modulus	newtons per square metre	809.292	924.698	1031.991
Poisson's ratio	0	0.406	0.393	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	74.087	87.550	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 53.5 newtons per square metre per unit weight fraction	decreases at rate 367.7 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 600.286 newtons per square metre per unit weight fraction	increases at rate 528.574 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 230.814 newtons per square metre per unit weight fraction	increases at rate 214.585 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0263 0 per unit weight fraction	decreases at rate 0.0335 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 26.925 kiloJoule per mole per unit weight fraction	increases at rate 43.489 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and ethylene_isophthalate. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and ethylene_terepthalate

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

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	368.161	417.783	466.509
Density	kg per	1.317	1.187	1.080

	cubic metre			
Oxygen permeability	Perm	6.631	117.842	1595.547
Nitrogen permeability	Perm	1.320	29.564	493.508
Carbon dioxide permeability	Perm	22.857	525.154	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 99.2 oC per unit weight fraction	increases at rate 97.5 oC per unit weight fraction
Density	decreases at rate 0.261 kg per cubic metre per unit weight fraction	decreases at rate 0.214 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 222.4 Perm per unit weight fraction	increases at rate 2955.4 Perm per unit weight fraction
Nitrogen permeability	increases at rate 56.5 Perm per unit weight fraction	increases at rate 927.9 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 1004.6 Perm per unit weight fraction	increases at rate 16894.4 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and ethylene_terepthalate. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and ethylene_terepthalate

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and ethylene_terepthalate. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and ethylene_terepthalate on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 ethylene_terepthalate

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
Refractive index	0	1.556	1.565	1.572
Volume resistivity	Ohm-metre	27194300000000000.000	101655700000000000.000	324667800000000000.000

Dielectric constant	0	3.283	2.996	2.744
Coefficient of volumetric thermal expansion	/K	264.237	235.050	212.051
Thermal conductivity	W/(m·K)	0.210	0.192	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.017 0 per unit weight fraction	increases at rate 0.014 0 per unit weight fraction
Volume resistivity	increases at rate 148922800000000000 Ohm-metre per unit weight fraction	increases at rate 446024200000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.573 0 per unit weight fraction	decreases at rate 0.504 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 58.4 /K per unit weight fraction	decreases at rate 46 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.036 W/(m·K) per unit weight fraction	decreases at rate 0.035 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and ethylene_terepthalate. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and ethylene_terepthalate

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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 ethylene_terepthalate. 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 ethylene_terepthalate 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 ethylene_terepthalate

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	4411.336	4125.155	3812.095

Young's modulus	newtons per square metre	2294.199	2528.705	2839.722
Shear modulus	newtons per square metre	811.634	904.508	1031.991
Poisson's ratio	0	0.413	0.398	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	74.087	87.550	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 572.4 newtons per square metre per unit weight fraction	decreases at rate 626.1 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 469.012 newtons per square metre per unit weight fraction	increases at rate 622.034 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 185.75 newtons per square metre per unit weight fraction	increases at rate 254.965 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.031 0 per unit weight fraction	decreases at rate 0.044 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 26.925 kiloJoule per mole per unit weight fraction	increases at rate 43.489 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and ethylene_terepthalate. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and oxyethylene

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

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	204.934	314.573	414.398
Density	kg per	1.127	1.150	1.174

	cubic metre			
Oxygen permeability	Perm	658.412	454.819	288.203
Nitrogen permeability	Perm	189.668	127.182	77.690
Carbon dioxide permeability	Perm	3421.221	2286.551	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 219.3 oC per unit weight fraction	increases at rate 199.6 oC per unit weight fraction
Density	increases at rate 0.046 kg per cubic metre per unit weight fraction	increases at rate 0.048 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 407.2 Perm per unit weight fraction	decreases at rate 333.2 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 125 Perm per unit weight fraction	decreases at rate 99 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 2269.3 Perm per unit weight fraction	decreases at rate 1790.9 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and oxyethylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and oxyethylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and oxyethylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 oxyethylene

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
Refractive index	0	1.465	1.523	1.587
Volume resistivity	Ohm-metre	292826500000000000.000	212942100000000000.000	155017300000000000.000

Dielectric constant	0	2.767	2.836	2.905
Coefficient of volumetric thermal expansion	/K	858.465	305.157	236.835
Thermal conductivity	W/(m·K)	0.217	0.204	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.117 0 per unit weight fraction	increases at rate 0.128 0 per unit weight fraction
Volume resistivity	decreases at rate 159768800000000000 Ohm-metre per unit weight fraction	decreases at rate 115849600000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.138 0 per unit weight fraction	increases at rate 0.138 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 1106.6 /K per unit weight fraction	decreases at rate 136.6 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.026 W/(m·K) per unit weight fraction	decreases at rate 0.023 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and oxyethylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and oxyethylene

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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 oxyethylene. 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 oxyethylene 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 oxyethylene

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	1255.800	2844.313	4031.244

Young's modulus	newtons per square metre	2.885	1352.166	2212.361
Shear modulus	newtons per square metre	0.962	475.857	785.343
Poisson's ratio	0	0.500	0.421	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	13.030	24.848	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 3177 newtons per square metre per unit weight fraction	increases at rate 2373.9 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 2698.563 newtons per square metre per unit weight fraction	increases at rate 1720.39 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 949.791 newtons per square metre per unit weight fraction	increases at rate 618.97 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.1577 0 per unit weight fraction	decreases at rate 0.0245 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 23.635 kiloJoule per mole per unit weight fraction	increases at rate 136.425 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and oxyethylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and oxymethylene

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

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	213.273	320.020	414.398
Density	kg per	1.306	1.236	1.174

	cubic metre			
Oxygen permeability	Perm	619.548	410.486	288.203
Nitrogen permeability	Perm	177.602	113.843	77.690
Carbon dioxide permeability	Perm	3201.837	2044.865	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 213.5 oC per unit weight fraction	increases at rate 188.8 oC per unit weight fraction
Density	decreases at rate 0.138 kg per cubic metre per unit weight fraction	decreases at rate 0.124 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 418.1 Perm per unit weight fraction	decreases at rate 244.6 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 127.5 Perm per unit weight fraction	decreases at rate 72.3 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 2313.9 Perm per unit weight fraction	decreases at rate 1307.6 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and oxymethylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and oxymethylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and oxymethylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 oxymethylene

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
Refractive index	0	1.465	1.528	1.587
Volume resistivity	Ohm-metre	60918530000000000.000	101674300000000000.000	155017300000000000.000

Dielectric constant	0	3.108	2.996	2.905
Coefficient of volumetric thermal expansion	/K	833.233	300.428	236.835
Thermal conductivity	W/(m·K)	0.240	0.215	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.126 0 per unit weight fraction	increases at rate 0.119 0 per unit weight fraction
Volume resistivity	increases at rate 81511540000000000 Ohm-metre per unit weight fraction	increases at rate 106686000000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.222 0 per unit weight fraction	decreases at rate 0.183 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 1065.6 /K per unit weight fraction	decreases at rate 127.2 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.05 W/(m·K) per unit weight fraction	decreases at rate 0.044 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and oxymethylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and oxymethylene

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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 oxymethylene. 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 oxymethylene 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 oxymethylene

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	789.159	3068.272	4031.244

Young's modulus	newtons per square metre	4.045	1367.095	2212.361
Shear modulus	newtons per square metre	1.349	479.433	785.343
Poisson's ratio	0	0.499	0.426	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	8.089	17.063	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 4558.2 newtons per square metre per unit weight fraction	increases at rate 1925.9 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 2726.1 newtons per square metre per unit weight fraction	increases at rate 1690.532 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 956.169 newtons per square metre per unit weight fraction	increases at rate 611.819 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.1468 0 per unit weight fraction	decreases at rate 0.0344 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 17.948 kiloJoule per mole per unit weight fraction	increases at rate 151.994 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and oxymethylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and oxyphenyl

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

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	357.304	385.589	414.398
Density	kg per	1.222	1.198	1.174

	cubic metre			
Oxygen permeability	Perm	201.679	242.316	288.203
Nitrogen permeability	Perm	52.828	64.416	77.690
Carbon dioxide permeability	Perm	942.923	1151.636	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 56.6 oC per unit weight fraction	increases at rate 57.6 oC per unit weight fraction
Density	decreases at rate 0.049 kg per cubic metre per unit weight fraction	decreases at rate 0.047 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 81.3 Perm per unit weight fraction	increases at rate 91.8 Perm per unit weight fraction
Nitrogen permeability	increases at rate 23.2 Perm per unit weight fraction	increases at rate 26.5 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 417.4 Perm per unit weight fraction	increases at rate 478.9 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and oxyphenyl. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and oxyphenyl

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and oxyphenyl. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 oxyphenyl

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
Refractive index	0	1.621	1.604	1.587
Volume resistivity	Ohm-metre	182508600000000000.000	168206500000000000.000	155017300000000000.000

Dielectric constant	0	2.869	2.887	2.905
Coefficient of volumetric thermal expansion	/K	271.616	253.195	236.835
Thermal conductivity	W/(m·K)	0.206	0.199	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.035 0 per unit weight fraction	decreases at rate 0.033 0 per unit weight fraction
Volume resistivity	decreases at rate 28604200000000000 Ohm-metre per unit weight fraction	decreases at rate 26378400000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.035 0 per unit weight fraction	increases at rate 0.035 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 36.8 /K per unit weight fraction	decreases at rate 32.7 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.013 W/(m·K) per unit weight fraction	decreases at rate 0.013 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and oxyphenyl. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and oxyphenyl

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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 oxyphenyl. 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 oxyphenyl 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 oxyphenyl

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	3848.015	3951.783	4031.244

Young's modulus	newtons per square metre	1868.283	2033.714	2212.361
Shear modulus	newtons per square metre	658.273	719.019	785.343
Poisson's ratio	0	0.419	0.414	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	34.090	49.769	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 207.5 newtons per square metre per unit weight fraction	increases at rate 158.9 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 330.862 newtons per square metre per unit weight fraction	increases at rate 357.294 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 121.493 newtons per square metre per unit weight fraction	increases at rate 132.646 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0097 0 per unit weight fraction	decreases at rate 0.0114 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 31.358 kiloJoule per mole per unit weight fraction	increases at rate 86.582 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and oxyphenyl. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and oxypropylene

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

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	227.650	324.207	414.398
Density	kg per	1.023	1.093	1.174

	cubic metre			
Oxygen permeability	Perm	1188.898	652.441	288.203
Nitrogen permeability	Perm	359.139	187.810	77.690
Carbon dioxide permeability	Perm	6512.338	3387.435	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 193.1 oC per unit weight fraction	increases at rate 180.4 oC per unit weight fraction
Density	increases at rate 0.141 kg per cubic metre per unit weight fraction	increases at rate 0.162 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 1072.9 Perm per unit weight fraction	decreases at rate 728.5 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 342.7 Perm per unit weight fraction	decreases at rate 220.2 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 6249.8 Perm per unit weight fraction	decreases at rate 3992.7 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and oxypropylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and oxypropylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and oxypropylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 oxypropylene

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
Refractive index	0	1.467	1.521	1.587
Volume resistivity	Ohm-metre	779896700000000000.000	362030700000000000.000	155017300000000000.000

Dielectric constant	0	2.554	2.721	2.905
Coefficient of volumetric thermal expansion	/K	793.048	296.891	236.835
Thermal conductivity	W/(m·K)	0.184	0.188	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.109 0 per unit weight fraction	increases at rate 0.131 0 per unit weight fraction
Volume resistivity	decreases at rate 835732000000000000 Ohm-metre per unit weight fraction	decreases at rate 414026800000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.333 0 per unit weight fraction	increases at rate 0.368 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 992.3 /K per unit weight fraction	decreases at rate 120.1 /K per unit weight fraction
Thermal conductivity	increases at rate 0.009 W/(m·K) per unit weight fraction	increases at rate 0.008 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and oxypropylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and oxypropylene

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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 oxypropylene. 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 oxypropylene 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 oxypropylene

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	1339.108	2836.692	4031.244

Young's modulus	newtons per square metre	1.861	1520.993	2212.361
Shear modulus	newtons per square metre	0.621	539.116	785.343
Poisson's ratio	0	0.500	0.411	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	16.922	31.079	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 2995.2 newtons per square metre per unit weight fraction	increases at rate 2389.1 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 3038.263 newtons per square metre per unit weight fraction	increases at rate 1382.736 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1076.991 newtons per square metre per unit weight fraction	increases at rate 492.453 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.1783 0 per unit weight fraction	decreases at rate 0.0042 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 28.314 kiloJoule per mole per unit weight fraction	increases at rate 123.962 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and oxypropylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and oxyethylene

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

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	204.934	341.523	466.509
Density	kg per	1.127	1.103	1.080

	cubic metre			
Oxygen permeability	Perm	658.412	1053.777	1595.547
Nitrogen permeability	Perm	189.668	315.251	493.508
Carbon dioxide permeability	Perm	3421.221	5710.365	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 273.2 oC per unit weight fraction	increases at rate 250 oC per unit weight fraction
Density	decreases at rate 0.049 kg per cubic metre per unit weight fraction	decreases at rate 0.047 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 790.7 Perm per unit weight fraction	increases at rate 1083.5 Perm per unit weight fraction
Nitrogen permeability	increases at rate 251.2 Perm per unit weight fraction	increases at rate 356.5 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 4578.3 Perm per unit weight fraction	increases at rate 6524 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and oxyethylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and oxyethylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and oxyethylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and oxyethylene on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 oxyethylene

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
Refractive index	0	1.465	1.518	1.572
Volume resistivity	Ohm-metre	292826500000000000.000	308807900000000000.000	324667800000000000.000

Dielectric constant	0	2.767	2.755	2.744
Coefficient of volumetric thermal expansion	/K	858.465	283.108	212.051
Thermal conductivity	W/(m·K)	0.217	0.195	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.107 0 per unit weight fraction	increases at rate 0.107 0 per unit weight fraction
Volume resistivity	increases at rate 31962800000000000 Ohm-metre per unit weight fraction	increases at rate 31719800000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.023 0 per unit weight fraction	decreases at rate 0.022 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 1150.7 /K per unit weight fraction	decreases at rate 142.1 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.045 W/(m·K) per unit weight fraction	decreases at rate 0.041 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and oxyethylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and oxyethylene

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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 oxyethylene. 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 oxyethylene 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 oxyethylene

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	1255.800	2938.895	3812.095

Young's modulus	newtons per square metre	2.885	1560.944	2839.722
Shear modulus	newtons per square metre	0.962	552.947	1031.991
Poisson's ratio	0	0.500	0.411	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	13.030	24.995	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 3366.2 newtons per square metre per unit weight fraction	increases at rate 1746.4 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 3116.119 newtons per square metre per unit weight fraction	increases at rate 2557.556 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1103.97 newtons per square metre per unit weight fraction	increases at rate 958.089 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.1763 0 per unit weight fraction	decreases at rate 0.0713 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 23.929 kiloJoule per mole per unit weight fraction	increases at rate 168.599 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and oxyethylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and oxymethylene

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

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	213.273	347.173	466.509
Density	kg per	1.306	1.182	1.080

	cubic metre			
Oxygen permeability	Perm	619.548	996.439	1595.547
Nitrogen permeability	Perm	177.602	296.760	493.508
Carbon dioxide permeability	Perm	3201.837	5372.755	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 267.8 oC per unit weight fraction	increases at rate 238.7 oC per unit weight fraction
Density	decreases at rate 0.247 kg per cubic metre per unit weight fraction	decreases at rate 0.205 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 753.8 Perm per unit weight fraction	increases at rate 1198.2 Perm per unit weight fraction
Nitrogen permeability	increases at rate 238.3 Perm per unit weight fraction	increases at rate 393.5 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 4341.8 Perm per unit weight fraction	increases at rate 7199.2 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and oxymethylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and oxymethylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and oxymethylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and oxymethylene on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 oxymethylene

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
Refractive index	0	1.465	1.522	1.572
Volume resistivity	Ohm-metre	60918530000000000.000	156067200000000000.000	324667800000000000.000

Dielectric constant	0	3.108	2.903	2.744
Coefficient of volumetric thermal expansion	/K	833.233	278.884	212.051
Thermal conductivity	W/(m·K)	0.240	0.205	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.115 0 per unit weight fraction	increases at rate 0.099 0 per unit weight fraction
Volume resistivity	increases at rate 190297340000000000 Ohm-metre per unit weight fraction	increases at rate 337201200000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.409 0 per unit weight fraction	decreases at rate 0.318 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 1108.7 /K per unit weight fraction	decreases at rate 133.7 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.069 W/(m·K) per unit weight fraction	decreases at rate 0.062 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and oxymethylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and oxymethylene

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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 oxymethylene. 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 oxymethylene 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 oxymethylene

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	789.159	3058.648	3812.095

Young's modulus	newtons per square metre	4.045	1523.336	2839.722
Shear modulus	newtons per square metre	1.349	537.524	1031.991
Poisson's ratio	0	0.499	0.417	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	8.089	17.016	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 4539 newtons per square metre per unit weight fraction	increases at rate 1506.9 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 3038.582 newtons per square metre per unit weight fraction	increases at rate 2632.772 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1072.351 newtons per square metre per unit weight fraction	increases at rate 988.933 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.1643 0 per unit weight fraction	decreases at rate 0.0823 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 17.853 kiloJoule per mole per unit weight fraction	increases at rate 184.557 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and oxymethylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and oxyphenyl

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

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	357.304	411.131	466.509
Density	kg per	1.222	1.147	1.080

	cubic metre			
Oxygen permeability	Perm	201.679	591.618	1595.547
Nitrogen permeability	Perm	52.828	168.968	493.508
Carbon dioxide permeability	Perm	942.923	3044.933	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 107.7 oC per unit weight fraction	increases at rate 110.8 oC per unit weight fraction
Density	decreases at rate 0.151 kg per cubic metre per unit weight fraction	decreases at rate 0.134 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 779.9 Perm per unit weight fraction	increases at rate 2007.9 Perm per unit weight fraction
Nitrogen permeability	increases at rate 232.3 Perm per unit weight fraction	increases at rate 649.1 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 4204 Perm per unit weight fraction	increases at rate 11854.9 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and oxyphenyl. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and oxyphenyl

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and oxyphenyl. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and oxyphenyl on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 oxyphenyl

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
Refractive index	0	1.621	1.595	1.572
Volume resistivity	Ohm-metre	182508600000000000.000	245365900000000000.000	324667800000000000.000

Dielectric constant	0	2.869	2.805	2.744
Coefficient of volumetric thermal expansion	/K	271.616	238.583	212.051
Thermal conductivity	W/(m·K)	0.206	0.190	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.053 0 per unit weight fraction	decreases at rate 0.046 0 per unit weight fraction
Volume resistivity	increases at rate 125714600000000000 Ohm-metre per unit weight fraction	increases at rate 158603800000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.129 0 per unit weight fraction	decreases at rate 0.122 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 66.1 /K per unit weight fraction	decreases at rate 53.1 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.031 W/(m·K) per unit weight fraction	decreases at rate 0.032 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and oxyphenyl. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and oxyphenyl

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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 oxyphenyl. 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 oxyphenyl 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 oxyphenyl

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	3848.015	3865.140	3812.095

Young's modulus	newtons per square metre	1868.283	2252.796	2839.722
Shear modulus	newtons per square metre	658.273	802.931	1031.991
Poisson's ratio	0	0.419	0.403	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	34.090	51.298	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 34.3 newtons per square metre per unit weight fraction	decreases at rate 106.1 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 769.026 newtons per square metre per unit weight fraction	increases at rate 1173.852 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 289.316 newtons per square metre per unit weight fraction	increases at rate 458.121 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0324 0 per unit weight fraction	decreases at rate 0.054 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 34.416 kiloJoule per mole per unit weight fraction	increases at rate 115.993 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and oxyphenyl. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and oxypropylene

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

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	227.650	351.178	466.509
Density	kg per	1.023	1.050	1.080

	cubic metre			
Oxygen permeability	Perm	1188.898	1452.578	1595.547
Nitrogen permeability	Perm	359.139	445.911	493.508
Carbon dioxide permeability	Perm	6512.338	8100.227	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 247.1 oC per unit weight fraction	increases at rate 230.7 oC per unit weight fraction
Density	increases at rate 0.055 kg per cubic metre per unit weight fraction	increases at rate 0.059 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 527.4 Perm per unit weight fraction	increases at rate 285.9 Perm per unit weight fraction
Nitrogen permeability	increases at rate 173.5 Perm per unit weight fraction	increases at rate 95.2 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 3175.8 Perm per unit weight fraction	increases at rate 1744.3 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and oxypropylene. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and oxypropylene

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and oxypropylene. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and oxypropylene on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 oxypropylene

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
Refractive index	0	1.467	1.517	1.572
Volume resistivity	Ohm-metre	779896700000000000.000	508094200000000000.000	324667800000000000.000

Dielectric constant	0	2.554	2.647	2.744
Coefficient of volumetric thermal expansion	/K	793.048	275.964	212.051
Thermal conductivity	W/(m·K)	0.184	0.179	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.1 0 per unit weight fraction	increases at rate 0.11 0 per unit weight fraction
Volume resistivity	decreases at rate 543605000000000000 Ohm-metre per unit weight fraction	decreases at rate 366852800000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.186 0 per unit weight fraction	increases at rate 0.195 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 1034.2 /K per unit weight fraction	decreases at rate 127.8 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.01 W/(m·K) per unit weight fraction	decreases at rate 0.009 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and oxypropylene. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and oxypropylene

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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 oxypropylene. 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 oxypropylene 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 oxypropylene

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	1339.108	2838.307	3812.095

Young's modulus	newtons per square metre	1.861	1725.383	2839.722
Shear modulus	newtons per square metre	0.621	616.788	1031.991
Poisson's ratio	0	0.500	0.399	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	16.922	31.482	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 2998.4 newtons per square metre per unit weight fraction	increases at rate 1947.6 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 3447.043 newtons per square metre per unit weight fraction	increases at rate 2228.678 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 1232.335 newtons per square metre per unit weight fraction	increases at rate 830.406 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.2022 0 per unit weight fraction	decreases at rate 0.0457 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 29.12 kiloJoule per mole per unit weight fraction	increases at rate 155.624 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and oxypropylene. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and benzamide

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

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	603.481	510.692	414.398
Density	kg per	1.295	1.232	1.174

	cubic metre			
Oxygen permeability	Perm	0.129	6.820	288.203
Nitrogen permeability	Perm	0.019	1.361	77.690
Carbon dioxide permeability	Perm	0.313	23.565	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	decreases at rate 185.6 oC per unit weight fraction	decreases at rate 192.6 oC per unit weight fraction
Density	decreases at rate 0.126 kg per cubic metre per unit weight fraction	decreases at rate 0.114 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 13.4 Perm per unit weight fraction	increases at rate 562.8 Perm per unit weight fraction
Nitrogen permeability	increases at rate 2.7 Perm per unit weight fraction	increases at rate 152.7 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 46.5 Perm per unit weight fraction	increases at rate 2735 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and benzamide. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and benzamide

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and benzamide. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 benzamide

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
Refractive index	0	1.630	1.607	1.587
Volume resistivity	Ohm-metre	1720322000000000.000	16734310000000000.000	155017300000000000.000

Dielectric constant	0	3.882	3.388	2.905
Coefficient of volumetric thermal expansion	/K	166.307	194.770	236.835
Thermal conductivity	W/(m·K)	0.205	0.199	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.046 0 per unit weight fraction	decreases at rate 0.041 0 per unit weight fraction
Volume resistivity	increases at rate 30027976000000000 Ohm-metre per unit weight fraction	increases at rate 276565980000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.988 0 per unit weight fraction	decreases at rate 0.967 0 per unit weight fraction
Coefficient of volumetric thermal expansion	increases at rate 56.9 /K per unit weight fraction	increases at rate 84.1 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.013 W/(m·K) per unit weight fraction	decreases at rate 0.013 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and benzamide. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and benzamide

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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 benzamide. 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 benzamide 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 benzamide

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	7919.206	5868.347	4031.244

Young's modulus	newtons per square metre	3893.074	3042.513	2212.361
Shear modulus	newtons per square metre	1372.669	1076.166	785.343
Poisson's ratio	0	0.418	0.414	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	64.611	73.687	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 4101.7 newtons per square metre per unit weight fraction	decreases at rate 3674.2 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 1701.122 newtons per square metre per unit weight fraction	decreases at rate 1660.304 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 593.006 newtons per square metre per unit weight fraction	decreases at rate 581.647 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.009 0 per unit weight fraction	decreases at rate 0.0101 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 18.151 kiloJoule per mole per unit weight fraction	increases at rate 38.746 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and benzamide. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and nylon6

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of bisphen_dimeth_carbonate and nylon6. 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 nylon6 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 nylon6

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	328.410	373.554	414.398
Density	kg per	1.078	1.124	1.174

	cubic metre			
Oxygen permeability	Perm	6.731	41.653	288.203
Nitrogen permeability	Perm	1.342	9.612	77.690
Carbon dioxide permeability	Perm	23.234	169.166	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 90.3 oC per unit weight fraction	increases at rate 81.7 oC per unit weight fraction
Density	increases at rate 0.092 kg per cubic metre per unit weight fraction	increases at rate 0.1 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 69.8 Perm per unit weight fraction	increases at rate 493.1 Perm per unit weight fraction
Nitrogen permeability	increases at rate 16.5 Perm per unit weight fraction	increases at rate 136.2 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 291.9 Perm per unit weight fraction	increases at rate 2443.8 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and nylon6. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and nylon6

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and nylon6. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of bisphen_dimeth_carbonate and nylon6 on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 nylon6

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
Refractive index	0	1.513	1.548	1.587
Volume resistivity	Ohm-metre	117207500000000000.000	385538800000000000.000	1550173000000000000.000

Dielectric constant	0	3.466	3.207	2.905
Coefficient of volumetric thermal expansion	/K	293.424	260.718	236.835
Thermal conductivity	W/(m·K)	0.197	0.195	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.07 0 per unit weight fraction	increases at rate 0.078 0 per unit weight fraction
Volume resistivity	increases at rate 53666260000000000 Ohm-metre per unit weight fraction	increases at rate 232926840000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.517 0 per unit weight fraction	decreases at rate 0.604 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 65.4 /K per unit weight fraction	decreases at rate 47.8 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.004 W/(m·K) per unit weight fraction	decreases at rate 0.004 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and nylon6. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and nylon6

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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 nylon6. 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 nylon6 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 nylon6

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	4560.567	4420.569	4031.244

Young's modulus	newtons per square metre	2027.928	2147.367	2212.361
Shear modulus	newtons per square metre	711.110	756.627	785.343
Poisson's ratio	0	0.426	0.419	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	60.003	70.183	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 280 newtons per square metre per unit weight fraction	decreases at rate 778.7 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 238.878 newtons per square metre per unit weight fraction	increases at rate 129.988 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 91.034 newtons per square metre per unit weight fraction	increases at rate 57.431 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0137 0 per unit weight fraction	decreases at rate 0.021 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 20.361 kiloJoule per mole per unit weight fraction	increases at rate 45.753 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and nylon6. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and nylon12

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of bisphen_dimeth_carbonate and nylon12. 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 nylon12 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 nylon12

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	268.888	342.721	414.398
Density	kg per	0.980	1.068	1.174

	cubic metre			
Oxygen permeability	Perm	64.683	134.770	288.203
Nitrogen permeability	Perm	15.464	34.177	77.690
Carbon dioxide permeability	Perm	273.225	607.832	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 147.7 oC per unit weight fraction	increases at rate 143.4 oC per unit weight fraction
Density	increases at rate 0.177 kg per cubic metre per unit weight fraction	increases at rate 0.212 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 140.2 Perm per unit weight fraction	increases at rate 306.9 Perm per unit weight fraction
Nitrogen permeability	increases at rate 37.4 Perm per unit weight fraction	increases at rate 87 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 669.2 Perm per unit weight fraction	increases at rate 1566.5 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and nylon12. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and nylon12

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and nylon12. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of bisphen_dimeth_carbonate and nylon12 on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 nylon12

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
Refractive index	0	1.492	1.535	1.587
Volume resistivity	Ohm-metre	134359100000000000.000	143162900000000000.000	155017300000000000.000

Dielectric constant	0	2.936	2.922	2.905
Coefficient of volumetric thermal expansion	/K	696.671	282.201	236.835
Thermal conductivity	W/(m·K)	0.186	0.189	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.084 0 per unit weight fraction	increases at rate 0.105 0 per unit weight fraction
Volume resistivity	increases at rate 17607600000000000 Ohm-metre per unit weight fraction	increases at rate 23708800000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.028 0 per unit weight fraction	decreases at rate 0.035 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 828.9 /K per unit weight fraction	decreases at rate 90.7 /K per unit weight fraction
Thermal conductivity	increases at rate 0.007 W/(m·K) per unit weight fraction	increases at rate 0.006 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and nylon12. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and nylon12

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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 nylon12. 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 nylon12 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 nylon12

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	3509.426	3613.141	4031.244

Young's modulus	newtons per square metre	1546.425	1738.828	2212.361
Shear modulus	newtons per square metre	542.013	612.353	785.343
Poisson's ratio	0	0.427	0.420	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	89.650	91.140	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 207.4 newtons per square metre per unit weight fraction	increases at rate 836.2 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 384.806 newtons per square metre per unit weight fraction	increases at rate 947.066 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 140.681 newtons per square metre per unit weight fraction	increases at rate 345.979 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0135 0 per unit weight fraction	decreases at rate 0.0225 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 2.979 kiloJoule per mole per unit weight fraction	increases at rate 3.84 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and nylon12. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and nylon66

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of bisphen_dimeth_carbonate and nylon66. 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 nylon66 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 nylon66

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	326.725	371.975	414.398
Density	kg per	1.078	1.124	1.174

	cubic metre			
Oxygen permeability	Perm	6.731	41.653	288.203
Nitrogen permeability	Perm	1.342	9.612	77.690
Carbon dioxide permeability	Perm	23.234	169.166	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 90.5 oC per unit weight fraction	increases at rate 84.8 oC per unit weight fraction
Density	increases at rate 0.092 kg per cubic metre per unit weight fraction	increases at rate 0.1 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 69.8 Perm per unit weight fraction	increases at rate 493.1 Perm per unit weight fraction
Nitrogen permeability	increases at rate 16.5 Perm per unit weight fraction	increases at rate 136.2 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 291.9 Perm per unit weight fraction	increases at rate 2443.8 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and nylon66. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and nylon66

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and nylon66. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of bisphen_dimeth_carbonate and nylon66 on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 nylon66

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
Refractive index	0	1.513	1.548	1.587
Volume resistivity	Ohm-metre	117207500000000000.000	385538800000000000.000	1550173000000000000.000

Dielectric constant	0	3.466	3.207	2.905
Coefficient of volumetric thermal expansion	/K	294.804	261.739	236.835
Thermal conductivity	W/(m·K)	0.197	0.195	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.07 0 per unit weight fraction	increases at rate 0.078 0 per unit weight fraction
Volume resistivity	increases at rate 53666260000000000 Ohm-metre per unit weight fraction	increases at rate 232926840000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.517 0 per unit weight fraction	decreases at rate 0.604 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 66.1 /K per unit weight fraction	decreases at rate 49.8 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.004 W/(m·K) per unit weight fraction	decreases at rate 0.004 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and nylon66. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and nylon66

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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 nylon66. 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 nylon66 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 nylon66

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	4541.758	4407.768	4031.244

Young's modulus	newtons per square metre	2015.515	2138.488	2212.361
Shear modulus	newtons per square metre	706.684	753.445	785.343
Poisson's ratio	0	0.426	0.419	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	120.006	107.317	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 268 newtons per square metre per unit weight fraction	decreases at rate 753 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 245.946 newtons per square metre per unit weight fraction	increases at rate 147.746 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 93.523 newtons per square metre per unit weight fraction	increases at rate 63.794 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0138 0 per unit weight fraction	decreases at rate 0.0212 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	decreases at rate 25.378 kiloJoule per mole per unit weight fraction	decreases at rate 28.514 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and nylon66. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and benzamide

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

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	603.481	535.581	466.509
Density	kg per	1.295	1.177	1.080

	cubic metre			
Oxygen permeability	Perm	0.129	18.460	1595.547
Nitrogen permeability	Perm	0.019	3.990	493.508
Carbon dioxide permeability	Perm	0.313	69.720	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	decreases at rate 135.8 oC per unit weight fraction	decreases at rate 138.1 oC per unit weight fraction
Density	decreases at rate 0.234 kg per cubic metre per unit weight fraction	decreases at rate 0.195 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 36.7 Perm per unit weight fraction	increases at rate 3154.2 Perm per unit weight fraction
Nitrogen permeability	increases at rate 7.9 Perm per unit weight fraction	increases at rate 979 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 138.8 Perm per unit weight fraction	increases at rate 17805.3 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and benzamide. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and benzamide

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and benzamide. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and benzamide on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 benzamide

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
Refractive index	0	1.630	1.598	1.572
Volume resistivity	Ohm-metre	1720322000000000.000	26159650000000000.000	324667800000000000.000

Dielectric constant	0	3.882	3.291	2.744
Coefficient of volumetric thermal expansion	/K	166.307	186.221	212.051
Thermal conductivity	W/(m·K)	0.205	0.190	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.064 0 per unit weight fraction	decreases at rate 0.053 0 per unit weight fraction
Volume resistivity	increases at rate 48878656000000000 Ohm-metre per unit weight fraction	increases at rate 597016300000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 1.182 0 per unit weight fraction	decreases at rate 1.094 0 per unit weight fraction
Coefficient of volumetric thermal expansion	increases at rate 39.8 /K per unit weight fraction	increases at rate 51.7 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.031 W/(m·K) per unit weight fraction	decreases at rate 0.031 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and benzamide. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and benzamide

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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 benzamide. 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 benzamide 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 benzamide

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	7919.206	5647.614	3812.095

Young's modulus	newtons per square metre	3893.074	3325.973	2839.722
Shear modulus	newtons per square metre	1372.669	1186.282	1031.991
Poisson's ratio	0	0.418	0.402	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	64.611	77.004	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 4543.2 newtons per square metre per unit weight fraction	decreases at rate 3671 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 1134.202 newtons per square metre per unit weight fraction	decreases at rate 972.502 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 372.774 newtons per square metre per unit weight fraction	decreases at rate 308.582 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0324 0 per unit weight fraction	decreases at rate 0.052 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 24.785 kiloJoule per mole per unit weight fraction	increases at rate 64.581 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and benzamide. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and nylon12

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of tetmeth_bisphen_carbonate and nylon12. 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 nylon12 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 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 nylon12

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	268.888	368.176	466.509
Density	kg per	0.980	1.027	1.080

	cubic metre			
Oxygen permeability	Perm	64.683	312.790	1595.547
Nitrogen permeability	Perm	15.464	84.874	493.508
Carbon dioxide permeability	Perm	273.225	1520.835	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 198.6 oC per unit weight fraction	increases at rate 196.7 oC per unit weight fraction
Density	increases at rate 0.095 kg per cubic metre per unit weight fraction	increases at rate 0.105 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 496.2 Perm per unit weight fraction	increases at rate 2565.5 Perm per unit weight fraction
Nitrogen permeability	increases at rate 138.8 Perm per unit weight fraction	increases at rate 817.3 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 2495.2 Perm per unit weight fraction	increases at rate 14903.1 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and nylon12. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and nylon12

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and nylon12. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and nylon12 on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 nylon12

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
Refractive index	0	1.492	1.530	1.572
Volume resistivity	Ohm-metre	134359100000000000.000	201188200000000000.000	324667800000000000.000

Dielectric constant	0	2.936	2.848	2.744
Coefficient of volumetric thermal expansion	/K	696.671	264.227	212.051
Thermal conductivity	W/(m·K)	0.186	0.180	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.074 0 per unit weight fraction	increases at rate 0.084 0 per unit weight fraction
Volume resistivity	increases at rate 133658200000000000 Ohm-metre per unit weight fraction	increases at rate 246959200000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.175 0 per unit weight fraction	decreases at rate 0.208 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 864.9 /K per unit weight fraction	decreases at rate 104.4 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.012 W/(m·K) per unit weight fraction	decreases at rate 0.011 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and nylon12. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and nylon12

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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 nylon12. 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 nylon12 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 nylon12

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	3509.426	3598.356	3812.095

Young's modulus	newtons per square metre	1546.425	1912.420	2839.722
Shear modulus	newtons per square metre	542.013	677.480	1031.991
Poisson's ratio	0	0.427	0.411	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	89.650	97.285	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 177.9 newtons per square metre per unit weight fraction	increases at rate 427.5 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 731.99 newtons per square metre per unit weight fraction	increases at rate 1854.604 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 270.935 newtons per square metre per unit weight fraction	increases at rate 709.022 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0303 0 per unit weight fraction	decreases at rate 0.0712 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 15.269 kiloJoule per mole per unit weight fraction	increases at rate 24.019 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and nylon12. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and nylon6

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of tetmeth_bisphen_carbonate and nylon6. 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 nylon6 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 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 nylon6

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	328.410	398.978	466.509
Density	kg per	1.078	1.079	1.080

	cubic metre			
Oxygen permeability	Perm	6.731	104.029	1595.547
Nitrogen permeability	Perm	1.342	25.838	493.508
Carbon dioxide permeability	Perm	23.234	458.465	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 141.1 oC per unit weight fraction	increases at rate 135.1 oC per unit weight fraction
Density	increases at rate 0.001 kg per cubic metre per unit weight fraction	increases at rate 0.001 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 194.6 Perm per unit weight fraction	increases at rate 2983 Perm per unit weight fraction
Nitrogen permeability	increases at rate 49 Perm per unit weight fraction	increases at rate 935.3 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 870.5 Perm per unit weight fraction	increases at rate 17027.8 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and nylon6. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and nylon6

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and nylon6. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and nylon6 on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 nylon6

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
Refractive index	0	1.513	1.542	1.572
Volume resistivity	Ohm-metre	11720750000000000.000	56776750000000000.000	324667800000000000.000

Dielectric constant	0	3.466	3.123	2.744
Coefficient of volumetric thermal expansion	/K	293.424	245.319	212.051
Thermal conductivity	W/(m·K)	0.197	0.185	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.058 0 per unit weight fraction	increases at rate 0.059 0 per unit weight fraction
Volume resistivity	increases at rate 90112000000000000 Ohm-metre per unit weight fraction	increases at rate 535782100000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.685 0 per unit weight fraction	decreases at rate 0.757 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 96.2 /K per unit weight fraction	decreases at rate 66.5 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.023 W/(m·K) per unit weight fraction	decreases at rate 0.022 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and nylon6. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and nylon6

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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 nylon6. 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 nylon6 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 nylon6

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	4560.567	4361.418	3812.095

Young's modulus	newtons per square metre	2027.928	2352.673	2839.722
Shear modulus	newtons per square metre	711.110	834.225	1031.991
Poisson's ratio	0	0.426	0.410	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	60.003	73.172	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 398.3 newtons per square metre per unit weight fraction	decreases at rate 1098.6 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 649.49 newtons per square metre per unit weight fraction	increases at rate 974.098 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 246.229 newtons per square metre per unit weight fraction	increases at rate 395.533 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0316 0 per unit weight fraction	decreases at rate 0.0685 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 26.338 kiloJoule per mole per unit weight fraction	increases at rate 72.245 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and nylon6. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and nylon66

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of tetmeth_bisphen_carbonate and nylon66. 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 nylon66 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 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 nylon66

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	326.725	396.911	466.509
Density	kg per	1.078	1.079	1.080

	cubic metre			
Oxygen permeability	Perm	6.731	104.029	1595.547
Nitrogen permeability	Perm	1.342	25.838	493.508
Carbon dioxide permeability	Perm	23.234	458.465	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 140.4 oC per unit weight fraction	increases at rate 139.2 oC per unit weight fraction
Density	increases at rate 0.001 kg per cubic metre per unit weight fraction	increases at rate 0.001 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 194.6 Perm per unit weight fraction	increases at rate 2983 Perm per unit weight fraction
Nitrogen permeability	increases at rate 49 Perm per unit weight fraction	increases at rate 935.3 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 870.5 Perm per unit weight fraction	increases at rate 17027.8 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and nylon66. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and nylon66

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and nylon66. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and nylon66 on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 nylon66

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
Refractive index	0	1.513	1.542	1.572
Volume resistivity	Ohm-metre	11720750000000000.000	56776750000000000.000	324667800000000000.000

Dielectric constant	0	3.466	3.123	2.744
Coefficient of volumetric thermal expansion	/K	294.804	246.503	212.051
Thermal conductivity	W/(m·K)	0.197	0.185	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.058 0 per unit weight fraction	increases at rate 0.059 0 per unit weight fraction
Volume resistivity	increases at rate 90112000000000000 Ohm-metre per unit weight fraction	increases at rate 535782100000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.685 0 per unit weight fraction	decreases at rate 0.757 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 96.6 /K per unit weight fraction	decreases at rate 68.9 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.023 W/(m·K) per unit weight fraction	decreases at rate 0.022 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and nylon66. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and nylon66

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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 nylon66. 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 nylon66 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 nylon66

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	4541.758	4347.097	3812.095

Young's modulus	newtons per square metre	2015.515	2341.591	2839.722
Shear modulus	newtons per square metre	706.684	830.220	1031.991
Poisson's ratio	0	0.426	0.410	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	120.006	115.489	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 389.3 newtons per square metre per unit weight fraction	decreases at rate 1070 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 652.152 newtons per square metre per unit weight fraction	increases at rate 996.262 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 247.072 newtons per square metre per unit weight fraction	increases at rate 403.543 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0316 0 per unit weight fraction	decreases at rate 0.0688 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	decreases at rate 9.034 kiloJoule per mole per unit weight fraction	decreases at rate 12.389 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and nylon66. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and 25_thiazole

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of bisphen_dimeth_carbonate and 25_thiazole. 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 25_thiazole 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 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
Glass transition temperature	oC	544.571	472.868	414.398
Density	kg per	1.508	1.321	1.174

	cubic metre			
Oxygen permeability	Perm	17.428	84.434	288.203
Nitrogen permeability	Perm	3.750	20.622	77.690
Carbon dioxide permeability	Perm	65.483	365.242	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	decreases at rate 143.4 oC per unit weight fraction	decreases at rate 116.9 oC per unit weight fraction
Density	decreases at rate 0.376 kg per cubic metre per unit weight fraction	decreases at rate 0.292 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 134 Perm per unit weight fraction	increases at rate 407.5 Perm per unit weight fraction
Nitrogen permeability	increases at rate 33.7 Perm per unit weight fraction	increases at rate 114.1 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 599.5 Perm per unit weight fraction	increases at rate 2051.7 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and 25_thiazole. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and 25_thiazole

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and 25_thiazole. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity 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. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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
Refractive index	0	1.743	1.653	1.587
Volume resistivity	Ohm-metre	1910580000000000.000	21479110000000000.000	155017300000000000.000

Dielectric constant	0	3.859	3.334	2.905
Coefficient of volumetric thermal expansion	/K	183.315	209.378	236.835
Thermal conductivity	W/(m·K)	0.217	0.203	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.18 0 per unit weight fraction	decreases at rate 0.132 0 per unit weight fraction
Volume resistivity	increases at rate 39137060000000000 Ohm-metre per unit weight fraction	increases at rate 267076380000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 1.051 0 per unit weight fraction	decreases at rate 0.858 0 per unit weight fraction
Coefficient of volumetric thermal expansion	increases at rate 52.1 /K per unit weight fraction	increases at rate 54.9 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.027 W/(m·K) per unit weight fraction	decreases at rate 0.022 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and 25_thiazole. Experimental study is required to validate the results.

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

Young's modulus	newtons per square metre	3263.424	2684.191	2212.361
Shear modulus	newtons per square metre	1152.415	950.459	785.343
Poisson's ratio	0	0.416	0.412	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	32.982	47.781	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 2762.6 newtons per square metre per unit weight fraction	decreases at rate 2110.6 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 1158.466 newtons per square metre per unit weight fraction	decreases at rate 943.66 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 403.911 newtons per square metre per unit weight fraction	decreases at rate 330.234 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0077 0 per unit weight fraction	decreases at rate 0.007 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 29.597 kiloJoule per mole per unit weight fraction	increases at rate 90.558 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and 25_thiazole. Experimental study is required to validate the results.

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

	cubic metre			
Oxygen permeability	Perm	46.209	125.661	288.203
Nitrogen permeability	Perm	10.752	31.688	77.690
Carbon dioxide permeability	Perm	189.415	563.220	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	decreases at rate 226.5 oC per unit weight fraction	decreases at rate 235.6 oC per unit weight fraction
Density	decreases at rate 0.186 kg per cubic metre per unit weight fraction	decreases at rate 0.162 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 158.9 Perm per unit weight fraction	increases at rate 325.1 Perm per unit weight fraction
Nitrogen permeability	increases at rate 41.9 Perm per unit weight fraction	increases at rate 92 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 747.6 Perm per unit weight fraction	increases at rate 1655.7 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and benz_imidazoles. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and benz_imidazoles

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and benz_imidazoles. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity 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. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 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
Refractive index	0	1.712	1.644	1.587
Volume resistivity	Ohm-metre	4915633000000000.000	29620090000000000.000	155017300000000000.000

Dielectric constant	0	3.654	3.264	2.905
Coefficient of volumetric thermal expansion	/K	156.004	187.343	236.835
Thermal conductivity	W/(m·K)	0.216	0.205	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.136 0 per unit weight fraction	decreases at rate 0.113 0 per unit weight fraction
Volume resistivity	increases at rate 49408914000000000 Ohm-metre per unit weight fraction	increases at rate 250794420000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.78 0 per unit weight fraction	decreases at rate 0.719 0 per unit weight fraction
Coefficient of volumetric thermal expansion	increases at rate 62.7 /K per unit weight fraction	increases at rate 99 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.023 W/(m·K) per unit weight fraction	decreases at rate 0.024 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and benz_imidazoles. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and benz_imidazoles

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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 benz_imidazoles. 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 benz_imidazoles 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 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
Bulk modulus	newtons per square metre	6368.798	5196.780	4031.244

Young's modulus	newtons per square metre	3112.864	2690.613	2212.361
Shear modulus	newtons per square metre	1097.208	951.615	785.343
Poisson's ratio	0	0.419	0.414	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	47.393	61.709	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 2344 newtons per square metre per unit weight fraction	decreases at rate 2331.1 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 844.502 newtons per square metre per unit weight fraction	decreases at rate 956.504 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 291.186 newtons per square metre per unit weight fraction	decreases at rate 332.545 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0097 0 per unit weight fraction	decreases at rate 0.0104 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 28.633 kiloJoule per mole per unit weight fraction	increases at rate 62.701 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and benz_imidazoles. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and benzimid

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

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	793.792	607.698	414.398
Density	kg per	1.478	1.309	1.174

	cubic metre			
Oxygen permeability	Perm	11.843	72.273	288.203
Nitrogen permeability	Perm	2.470	17.433	77.690
Carbon dioxide permeability	Perm	42.991	308.327	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	decreases at rate 372.2 oC per unit weight fraction	decreases at rate 386.6 oC per unit weight fraction
Density	decreases at rate 0.338 kg per cubic metre per unit weight fraction	decreases at rate 0.269 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 120.9 Perm per unit weight fraction	increases at rate 431.9 Perm per unit weight fraction
Nitrogen permeability	increases at rate 29.9 Perm per unit weight fraction	increases at rate 120.5 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 530.7 Perm per unit weight fraction	increases at rate 2165.5 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and benzimid. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and benzimid

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and benzimid. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 benzimid

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
Refractive index	0	1.724	1.646	1.587
Volume resistivity	Ohm-metre	467113600000000.000	10344250000000000.000	155017300000000000.000

Dielectric constant	0	4.165	3.493	2.905
Coefficient of volumetric thermal expansion	/K	127.956	165.210	236.835
Thermal conductivity	W/(m·K)	0.230	0.211	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.156 0 per unit weight fraction	decreases at rate 0.118 0 per unit weight fraction
Volume resistivity	increases at rate 19754272800000000 Ohm-metre per unit weight fraction	increases at rate 289346100000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 1.345 0 per unit weight fraction	decreases at rate 1.176 0 per unit weight fraction
Coefficient of volumetric thermal expansion	increases at rate 74.5 /K per unit weight fraction	increases at rate 143.3 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.036 W/(m·K) per unit weight fraction	decreases at rate 0.037 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and benzimid. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and benzimid

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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 benzimid. 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 benzimid 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 benzimid

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	7673.034	5811.118	4031.244

Young's modulus	newtons per square metre	3659.985	2975.530	2212.361
Shear modulus	newtons per square metre	1288.273	1051.677	785.343
Poisson's ratio	0	0.421	0.415	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	65.471	75.967	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 3723.8 newtons per square metre per unit weight fraction	decreases at rate 3559.7 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 1368.91 newtons per square metre per unit weight fraction	decreases at rate 1526.338 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 473.192 newtons per square metre per unit weight fraction	decreases at rate 532.669 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0117 0 per unit weight fraction	decreases at rate 0.0123 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 20.992 kiloJoule per mole per unit weight fraction	increases at rate 34.186 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and benzimid. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and benzothiazol

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

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	791.880	588.714	414.398
Density	kg per	1.639	1.368	1.174

	cubic metre			
Oxygen permeability	Perm	9.095	69.766	288.203
Nitrogen permeability	Perm	1.857	16.781	77.690
Carbon dioxide permeability	Perm	32.247	296.695	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	decreases at rate 406.3 oC per unit weight fraction	decreases at rate 348.6 oC per unit weight fraction
Density	decreases at rate 0.541 kg per cubic metre per unit weight fraction	decreases at rate 0.388 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 121.3 Perm per unit weight fraction	increases at rate 436.9 Perm per unit weight fraction
Nitrogen permeability	increases at rate 29.8 Perm per unit weight fraction	increases at rate 121.8 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 528.9 Perm per unit weight fraction	increases at rate 2188.8 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and benzothiazol. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and benzothiazol

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and benzothiazol. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 benzothiazol

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
Refractive index	0	1.812	1.676	1.587
Volume resistivity	Ohm-metre	1041786000000000.000	18273720000000000.000	155017300000000000.000

Dielectric constant	0	3.991	3.369	2.905
Coefficient of volumetric thermal expansion	/K	128.253	170.267	236.835
Thermal conductivity	W/(m·K)	0.214	0.202	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.272 0 per unit weight fraction	decreases at rate 0.178 0 per unit weight fraction
Volume resistivity	increases at rate 34463868000000000 Ohm-metre per unit weight fraction	increases at rate 273487160000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 1.244 0 per unit weight fraction	decreases at rate 0.929 0 per unit weight fraction
Coefficient of volumetric thermal expansion	increases at rate 84 /K per unit weight fraction	increases at rate 133.1 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.023 W/(m·K) per unit weight fraction	decreases at rate 0.019 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and benzothiazol. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and benzothiazol

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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 benzothiazol. 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 benzothiazol 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 benzothiazol

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	8050.285	5828.530	4031.244

Young's modulus	newtons per square metre	3951.617	3042.254	2212.361
Shear modulus	newtons per square metre	1393.191	1076.518	785.343
Poisson's ratio	0	0.418	0.413	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	75.514	83.023	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 4443.5 newtons per square metre per unit weight fraction	decreases at rate 3594.6 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 1818.726 newtons per square metre per unit weight fraction	decreases at rate 1659.786 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 633.346 newtons per square metre per unit weight fraction	decreases at rate 582.351 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0104 0 per unit weight fraction	decreases at rate 0.0089 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 15.018 kiloJoule per mole per unit weight fraction	increases at rate 20.074 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and benzothiazol. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and cyclopentylm

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

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	392.616	403.355	414.398
Density	kg per	1.037	1.101	1.174

	cubic metre			
Oxygen permeability	Perm	312.797	304.419	288.203
Nitrogen permeability	Perm	84.876	82.423	77.690
Carbon dioxide permeability	Perm	1520.871	1476.556	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 21.5 oC per unit weight fraction	increases at rate 22.1 oC per unit weight fraction
Density	increases at rate 0.129 kg per cubic metre per unit weight fraction	increases at rate 0.146 kg per cubic metre per unit weight fraction
Oxygen permeability	decreases at rate 16.8 Perm per unit weight fraction	decreases at rate 32.4 Perm per unit weight fraction
Nitrogen permeability	decreases at rate 4.9 Perm per unit weight fraction	decreases at rate 9.5 Perm per unit weight fraction
Carbon dioxide permeability	decreases at rate 88.6 Perm per unit weight fraction	decreases at rate 170.9 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and cyclopentylm. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and cyclopentylm

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and cyclopentylm. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 cyclopentylm

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
Refractive index	0	1.537	1.560	1.587
Volume resistivity	Ohm-metre	5385898000000000000.000	1092652000000000000.000	155017300000000000.000

Dielectric constant	0	2.134	2.481	2.905
Coefficient of volumetric thermal expansion	/K	248.999	242.850	236.835
Thermal conductivity	W/(m·K)	0.176	0.185	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.046 0 per unit weight fraction	increases at rate 0.054 0 per unit weight fraction
Volume resistivity	decreases at rate 8586492000000000000 Ohm-metre per unit weight fraction	decreases at rate 1875269400000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.693 0 per unit weight fraction	increases at rate 0.848 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 12.3 /K per unit weight fraction	decreases at rate 12 /K per unit weight fraction
Thermal conductivity	increases at rate 0.016 W/(m·K) per unit weight fraction	increases at rate 0.016 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and cyclopentylm. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and cyclopentylm

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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 cyclopentylm. 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 cyclopentylm 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 cyclopentylm

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	3364.420	3676.825	4031.244

Young's modulus	newtons per square metre	1903.341	2051.485	2212.361
Shear modulus	newtons per square metre	677.002	729.024	785.343
Poisson's ratio	0	0.406	0.407	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	24.373	38.886	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 624.8 newtons per square metre per unit weight fraction	increases at rate 708.8 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 296.288 newtons per square metre per unit weight fraction	increases at rate 321.752 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 104.043 newtons per square metre per unit weight fraction	increases at rate 112.637 newtons per square metre per unit weight fraction
Poisson's ratio	increases at rate 0.0026 0 per unit weight fraction	increases at rate 0.003 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 29.025 kiloJoule per mole per unit weight fraction	increases at rate 108.348 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and cyclopentylm. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and ethylene_terepthalate

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

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	368.161	391.540	414.398
Density	kg per	1.317	1.242	1.174

	cubic metre			
Oxygen permeability	Perm	6.631	46.292	288.203
Nitrogen permeability	Perm	1.320	10.773	77.690
Carbon dioxide permeability	Perm	22.857	189.789	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 46.8 oC per unit weight fraction	increases at rate 45.7 oC per unit weight fraction
Density	decreases at rate 0.151 kg per cubic metre per unit weight fraction	decreases at rate 0.135 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 79.3 Perm per unit weight fraction	increases at rate 483.8 Perm per unit weight fraction
Nitrogen permeability	increases at rate 18.9 Perm per unit weight fraction	increases at rate 133.8 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 333.9 Perm per unit weight fraction	increases at rate 2402.6 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and ethylene_terepthalate. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and ethylene_terepthalate

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and ethylene_terepthalate. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 ethylene_terepthalate

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
Refractive index	0	1.556	1.572	1.587
Volume resistivity	Ohm-metre	27194300000000000.000	66971170000000000.000	155017300000000000.000

Dielectric constant	0	3.283	3.087	2.905
Coefficient of volumetric thermal expansion	/K	264.237	249.633	236.835
Thermal conductivity	W/(m·K)	0.210	0.201	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.033 0 per unit weight fraction	increases at rate 0.03 0 per unit weight fraction
Volume resistivity	increases at rate 79553740000000000 Ohm-metre per unit weight fraction	increases at rate 176092260000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.391 0 per unit weight fraction	decreases at rate 0.364 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 29.2 /K per unit weight fraction	decreases at rate 25.6 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.017 W/(m·K) per unit weight fraction	decreases at rate 0.017 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and ethylene_terepthalate. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and ethylene_terepthalate

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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 ethylene_terepthalate. 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 ethylene_terepthalate 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 ethylene_terepthalate

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	4411.336	4223.801	4031.244

Young's modulus	newtons per square metre	2294.199	2257.379	2212.361
Shear modulus	newtons per square metre	811.634	799.963	785.343
Poisson's ratio	0	0.413	0.411	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	74.087	82.254	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 375.1 newtons per square metre per unit weight fraction	decreases at rate 385.1 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 73.64 newtons per square metre per unit weight fraction	decreases at rate 90.036 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 23.341 newtons per square metre per unit weight fraction	decreases at rate 29.242 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0048 0 per unit weight fraction	decreases at rate 0.0048 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 16.333 kiloJoule per mole per unit weight fraction	increases at rate 21.613 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and ethylene_terepthalate. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and 25_thiazole

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of tetmeth_bisphen_carbonate and 25_thiazole. 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 25_thiazole 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 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 25_thiazole

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	544.571	501.338	466.509
Density	kg per	1.508	1.258	1.080

	cubic metre			
Oxygen permeability	Perm	17.428	238.674	1595.547
Nitrogen permeability	Perm	3.750	63.371	493.508
Carbon dioxide permeability	Perm	65.483	1132.794	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	decreases at rate 86.5 oC per unit weight fraction	decreases at rate 69.7 oC per unit weight fraction
Density	decreases at rate 0.5 kg per cubic metre per unit weight fraction	decreases at rate 0.358 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 442.5 Perm per unit weight fraction	increases at rate 2713.7 Perm per unit weight fraction
Nitrogen permeability	increases at rate 119.2 Perm per unit weight fraction	increases at rate 860.3 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 2134.6 Perm per unit weight fraction	increases at rate 15679.1 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and 25_thiazole. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and 25_thiazole

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and 25_thiazole. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 25_thiazole

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
Refractive index	0	1.743	1.640	1.572
Volume resistivity	Ohm-metre	1910580000000000.000	34630330000000000.000	324667800000000000.000

Dielectric constant	0	3.859	3.230	2.744
Coefficient of volumetric thermal expansion	/K	183.315	198.190	212.051
Thermal conductivity	W/(m·K)	0.217	0.193	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.205 0 per unit weight fraction	decreases at rate 0.137 0 per unit weight fraction
Volume resistivity	increases at rate 65439500000000000 Ohm-metre per unit weight fraction	increases at rate 580074940000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 1.258 0 per unit weight fraction	decreases at rate 0.972 0 per unit weight fraction
Coefficient of volumetric thermal expansion	increases at rate 29.7 /K per unit weight fraction	increases at rate 27.7 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.047 W/(m·K) per unit weight fraction	decreases at rate 0.038 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and 25_thiazole. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_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 tetmeth_bisphen_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 tetmeth_bisphen_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 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 25_thiazole

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	6467.823	4900.931	3812.095

Young's modulus	newtons per square metre	3263.424	2985.880	2839.722
Shear modulus	newtons per square metre	1152.415	1067.561	1031.991
Poisson's ratio	0	0.416	0.398	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	32.982	49.099	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 3133.8 newtons per square metre per unit weight fraction	decreases at rate 2177.7 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 555.088 newtons per square metre per unit weight fraction	decreases at rate 292.316 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 169.708 newtons per square metre per unit weight fraction	decreases at rate 71.14 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0349 0 per unit weight fraction	decreases at rate 0.0452 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 32.234 kiloJoule per mole per unit weight fraction	increases at rate 120.39 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and 25_thiazole. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and benz_imidazoles

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of tetmeth_bisphen_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 tetmeth_bisphen_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 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 benz_imidazoles

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	645.418	557.479	466.509
Density	kg per	1.349	1.199	1.080

	cubic metre			
Oxygen permeability	Perm	46.209	325.493	1595.547
Nitrogen permeability	Perm	10.752	88.604	493.508
Carbon dioxide permeability	Perm	189.415	1588.233	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	decreases at rate 175.9 oC per unit weight fraction	decreases at rate 181.9 oC per unit weight fraction
Density	decreases at rate 0.299 kg per cubic metre per unit weight fraction	decreases at rate 0.239 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 558.6 Perm per unit weight fraction	increases at rate 2540.1 Perm per unit weight fraction
Nitrogen permeability	increases at rate 155.7 Perm per unit weight fraction	increases at rate 809.8 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 2797.6 Perm per unit weight fraction	increases at rate 14768.3 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and benz_imidazoles. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and benz_imidazoles

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and benz_imidazoles. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and benz_imidazoles on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 benz_imidazoles

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
Refractive index	0	1.712	1.632	1.572
Volume resistivity	Ohm-metre	4915633000000000.000	46131940000000000.000	324667800000000000.000

Dielectric constant	0	3.654	3.168	2.744
Coefficient of volumetric thermal expansion	/K	156.004	179.297	212.051
Thermal conductivity	W/(m·K)	0.216	0.196	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	decreases at rate 0.159 0 per unit weight fraction	decreases at rate 0.121 0 per unit weight fraction
Volume resistivity	increases at rate 82432614000000000 Ohm-metre per unit weight fraction	increases at rate 557071720000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.972 0 per unit weight fraction	decreases at rate 0.847 0 per unit weight fraction
Coefficient of volumetric thermal expansion	increases at rate 46.6 /K per unit weight fraction	increases at rate 65.5 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.041 W/(m·K) per unit weight fraction	decreases at rate 0.043 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and benz_imidazoles. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and benz_imidazoles

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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 benz_imidazoles. 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 benz_imidazoles 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 benz_imidazoles

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	6368.798	4976.199	3812.095

Young's modulus	newtons per square metre	3112.864	2937.704	2839.722
Shear modulus	newtons per square metre	1097.208	1047.976	1031.991
Poisson's ratio	0	0.419	0.402	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	47.393	64.246	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	decreases at rate 2785.2 newtons per square metre per unit weight fraction	decreases at rate 2328.2 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 350.32 newtons per square metre per unit weight fraction	decreases at rate 195.964 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 98.464 newtons per square metre per unit weight fraction	decreases at rate 31.97 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0339 0 per unit weight fraction	decreases at rate 0.0515 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 33.706 kiloJoule per mole per unit weight fraction	increases at rate 90.097 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and benz_imidazoles. Experimental study is required to validate the results.

Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and cyclopentylm

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

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	392.616	429.901	466.509
Density	kg per	1.037	1.058	1.080

	cubic metre			
Oxygen permeability	Perm	312.797	694.969	1595.547
Nitrogen permeability	Perm	84.876	201.070	493.508
Carbon dioxide permeability	Perm	1520.871	3628.635	8972.360

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 74.6 oC per unit weight fraction	increases at rate 73.2 oC per unit weight fraction
Density	increases at rate 0.042 kg per cubic metre per unit weight fraction	increases at rate 0.044 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 764.3 Perm per unit weight fraction	increases at rate 1801.2 Perm per unit weight fraction
Nitrogen permeability	increases at rate 232.4 Perm per unit weight fraction	increases at rate 584.9 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 4215.5 Perm per unit weight fraction	increases at rate 10687.5 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of tetmeth_bisphen_carbonate and cyclopentylm. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of tetmeth_bisphen_carbonate and cyclopentylm

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of tetmeth_bisphen_carbonate and cyclopentylm. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and cyclopentylm on the following properties have been predicted.

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 cyclopentylm

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
Refractive index	0	1.537	1.554	1.572
Volume resistivity	Ohm-metre	5385898000000000000.000	1465310000000000000.000	324667800000000000.000

Dielectric constant	0	2.134	2.417	2.744
Coefficient of volumetric thermal expansion	/K	248.999	228.877	212.051
Thermal conductivity	W/(m·K)	0.176	0.175	0.174

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.034 0 per unit weight fraction	increases at rate 0.036 0 per unit weight fraction
Volume resistivity	decreases at rate 7841176000000000000 Ohm-metre per unit weight fraction	decreases at rate 2281284400000000000 Ohm-metre per unit weight fraction
Dielectric constant	increases at rate 0.565 0 per unit weight fraction	increases at rate 0.654 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 40.2 /K per unit weight fraction	decreases at rate 33.7 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.002 W/(m·K) per unit weight fraction	decreases at rate 0.002 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of tetmeth_bisphen_carbonate and cyclopentylm. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of tetmeth_bisphen_carbonate and cyclopentylm

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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 cyclopentylm. 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 cyclopentylm 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 cyclopentylm

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	3364.420	3599.074	3812.095

Young's modulus	newtons per square metre	1903.341	2277.559	2839.722
Shear modulus	newtons per square metre	677.002	816.604	1031.991
Poisson's ratio	0	0.406	0.395	0.376
Cohesive energy (Fedors) at 298K	kiloJoule per mole	24.373	39.656	109.294

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 469.3 newtons per square metre per unit weight fraction	increases at rate 426 newtons per square metre per unit weight fraction
Young's modulus	increases at rate 748.436 newtons per square metre per unit weight fraction	increases at rate 1124.326 newtons per square metre per unit weight fraction
Shear modulus	increases at rate 279.204 newtons per square metre per unit weight fraction	increases at rate 430.773 newtons per square metre per unit weight fraction
Poisson's ratio	decreases at rate 0.0224 0 per unit weight fraction	decreases at rate 0.0374 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 30.566 kiloJoule per mole per unit weight fraction	increases at rate 139.276 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of tetmeth_bisphen_carbonate and cyclopentylm. Experimental study is required to validate the results.

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and ethylene_isophthalate

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of bisphen_dimeth_carbonate and ethylene_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 bisphen_dimeth_carbonate and ethylene_isophthalate 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 ethylene_isophthalate

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	325.591	370.568	414.398
Density	kg per	1.317	1.242	1.174

	cubic metre			
Oxygen permeability	Perm	6.631	46.292	288.203
Nitrogen permeability	Perm	1.320	10.773	77.690
Carbon dioxide permeability	Perm	22.857	189.789	1391.085

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Glass transition temperature	increases at rate 90 oC per unit weight fraction	increases at rate 87.7 oC per unit weight fraction
Density	decreases at rate 0.151 kg per cubic metre per unit weight fraction	decreases at rate 0.135 kg per cubic metre per unit weight fraction
Oxygen permeability	increases at rate 79.3 Perm per unit weight fraction	increases at rate 483.8 Perm per unit weight fraction
Nitrogen permeability	increases at rate 18.9 Perm per unit weight fraction	increases at rate 133.8 Perm per unit weight fraction
Carbon dioxide permeability	increases at rate 333.9 Perm per unit weight fraction	increases at rate 2402.6 Perm per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Permeability of a composite made of bisphen_dimeth_carbonate and ethylene_isophthalate. Experimental study is required to validate the results.

Prediction of Optical, electrical and thermal properties for a composite of bisphen_dimeth_carbonate and ethylene_isophthalate

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Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and ethylene_isophthalate. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

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

a. Refractive index

b. Volume resistivity

c. Dielectric constant

d. Coefficient of volumetric thermal expansion

e. Thermal conductivity

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 Optical, electrical and thermal 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 ethylene_isophthalate

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
Refractive index	0	1.556	1.572	1.587
Volume resistivity	Ohm-metre	27194300000000000.000	66971170000000000.000	155017300000000000.000

Dielectric constant	0	3.283	3.087	2.905
Coefficient of volumetric thermal expansion	/K	295.740	262.655	236.835
Thermal conductivity	W/(m·K)	0.210	0.201	0.193

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Refractive index	increases at rate 0.033 0 per unit weight fraction	increases at rate 0.03 0 per unit weight fraction
Volume resistivity	increases at rate 79553740000000000 Ohm-metre per unit weight fraction	increases at rate 176092260000000000 Ohm-metre per unit weight fraction
Dielectric constant	decreases at rate 0.391 0 per unit weight fraction	decreases at rate 0.364 0 per unit weight fraction
Coefficient of volumetric thermal expansion	decreases at rate 66.2 /K per unit weight fraction	decreases at rate 51.6 /K per unit weight fraction
Thermal conductivity	decreases at rate 0.017 W/(m·K) per unit weight fraction	decreases at rate 0.017 W/(m·K) per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Optical, electrical and thermal properties of a composite made of bisphen_dimeth_carbonate and ethylene_isophthalate. Experimental study is required to validate the results.

Prediction of Mechanical properties for a composite of bisphen_dimeth_carbonate and ethylene_isophthalate

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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 ethylene_isophthalate. 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 ethylene_isophthalate 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 ethylene_isophthalate

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	4022.684	4071.452	4031.244

Young's modulus	newtons per square metre	2275.292	2266.755	2212.361
Shear modulus	newtons per square metre	809.292	805.408	785.343
Poisson's ratio	0	0.406	0.407	0.409
Cohesive energy (Fedors) at 298K	kiloJoule per mole	74.087	82.254	93.060

Table 2. Rate of change of property

Property	Trend for 0.0 to 0.5 weight fraction of Monomer 1	Trend for 0.5 to 1.0 weight fraction of Monomer 1
Bulk modulus	increases at rate 97.5 newtons per square metre per unit weight fraction	decreases at rate 80.4 newtons per square metre per unit weight fraction
Young's modulus	decreases at rate 17.074 newtons per square metre per unit weight fraction	decreases at rate 108.788 newtons per square metre per unit weight fraction
Shear modulus	decreases at rate 7.767 newtons per square metre per unit weight fraction	decreases at rate 40.13 newtons per square metre per unit weight fraction
Poisson's ratio	increases at rate 0.003 0 per unit weight fraction	increases at rate 0.0026 0 per unit weight fraction
Cohesive energy (Fedors) at 298K	increases at rate 16.333 kiloJoule per mole per unit weight fraction	increases at rate 21.613 kiloJoule per mole per unit weight fraction

Conclusions: The application of Synthia module of Biovia Materials Studio predicted different Mechanical properties of a composite made of bisphen_dimeth_carbonate and ethylene_isophthalate. Experimental study is required to validate the results.

Centurion Journal of Multidisciplinary Research (India)
Volume 10 **Number** 2 November 2020