

Analysis of the Absorption Spectra of Styrene-butadiene in Toluene

*Mahasin F. Hadi Al-Kadhemy, Raad Hussein and Ali A. Dawood Al-Zuky

Physics Department, College of Science,
Al-Mustansiriyah University Baghdad, Iraq

*Corresponding author: drmahasinf@yahoo.com

Abstract: *The absorption spectra of styrene-butadiene in toluene at varying concentrations (0.1–0.6 wt%) were studied, and a theoretical model for these spectra was estimated. A blue shift towards a shorter wavelength of approximately 31.64 nm was observed as the concentration was increased. A theoretical model of the effect of concentration on the absorption spectra of styrene-butadiene in toluene was estimated utilising the "Table Curve 2D, version 5.01" program. This theoretical model was then applied to the test concentration of 0.45 wt% styrene-butadiene in toluene, which had not been measured experimentally. A good agreement for the wavelength values and appearance of the overall spectra was observed between the experimental and predicted spectra.*

Keywords: Styrene-butadiene, absorption spectrum, concentration effect, theoretical model

1. INTRODUCTION

In recent years, the polymer industry has been interested in improving the cost-effectiveness of techniques that convert waste and used rubber into a form that can be processed.^{1–4} One general-purpose synthetic rubber is the copolymer of styrene and butadiene. A great quantity of styrene-butadiene rubber (SBR) is utilised in automobile and truck tires, generally as an abrasion-resistant replacement for natural rubber (produced from polyisoprene). SBR is a mixture of approximately 75% butadiene ($\text{CH}_2=\text{CH}-\text{CH}=\text{CH}_2$) and 25% styrene ($\text{CH}_2=\text{CHC}_6\text{H}_5$). In most cases, these two compounds are copolymerised (their single-unit molecules are linked to form long, multiple-unit molecules) through an emulsion process in which a soap-like surfactant disperses, or emulsifies, the materials in an aqueous solution.⁵

Styrene-butadiene is the most widely used synthetic rubber in the world. Tires manufactured with styrene-butadiene show better tread-wear and aging properties than natural rubber, as well as good aberration and crack-initiation resistance. However, they have poor tack and heat build-up properties. Their

physical properties are also poor in the absence of reinforcing fillers. The major applications are tires (~15%), shoes and other footwear, mechanical goods, sponge and foam products, waterproof materials, belting and adhesives.⁶

Feller et al.⁷ studied the sensitivity of polystyrene/carbon black conductivity in toluene and other solvents. Rubber materials generally behave as electrical insulators, so most reports concern the conductivity of rubber.^{8,9}

The present work clarifies the effect of the concentration of styrene-butadiene solutions in toluene on the absorption spectrum and estimates a theoretical model for these effects.

2. EXPERIMENTAL

Particular weights of styrene-butadiene were dissolved in toluene, and a magnetic stirrer was used to dissolve the polymer quickly. The concentrations were chosen to be 0.2–0.6 wt%. The absorption spectra were recorded with a UV-160/visible recording spectrophotometer.

The estimated theoretical model was obtained by taking a curve fitting for all of the absorption spectra and determining the best fit equation with "Table Curve 2D, version 5.01" software.

3. RESULTS AND DISCUSSIONS

Our results are divided into experimental and theoretical parts as below.

3.1 Experimental Part

The absorption spectra for styrene-butadiene at different concentrations in toluene (0.2–0.6 wt%) are shown in Figures 1 and 2. A blue shift towards shorter wavelengths (lower energies) is observed. This result is clearly shown in Figure 3; the absorbance wavelength was 328.67 nm at $C = 0.2$ wt% and decreased to 297.03 nm at $C = 0.6$ wt%. The increased concentration results in a 31.64 nm shift in the absorption wavelength towards a shorter wavelength.

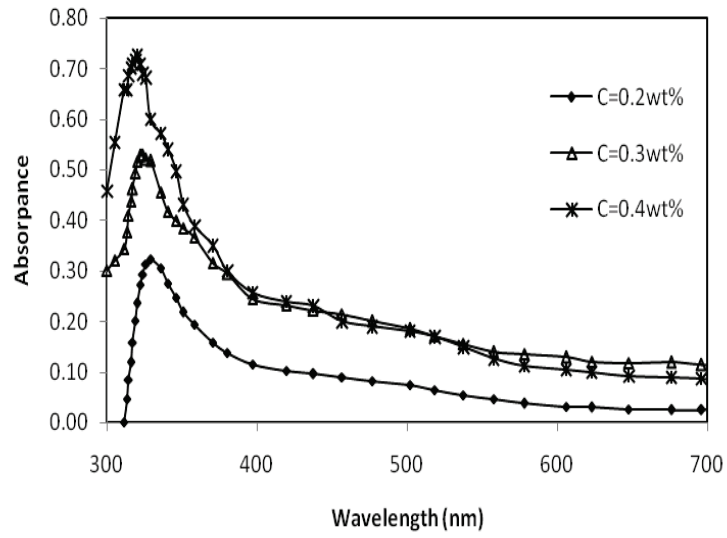


Figure 1: The absorption spectra of styrene-butadiene in toluene at varying concentrations (0.2, 0.3, 0.4 wt%).

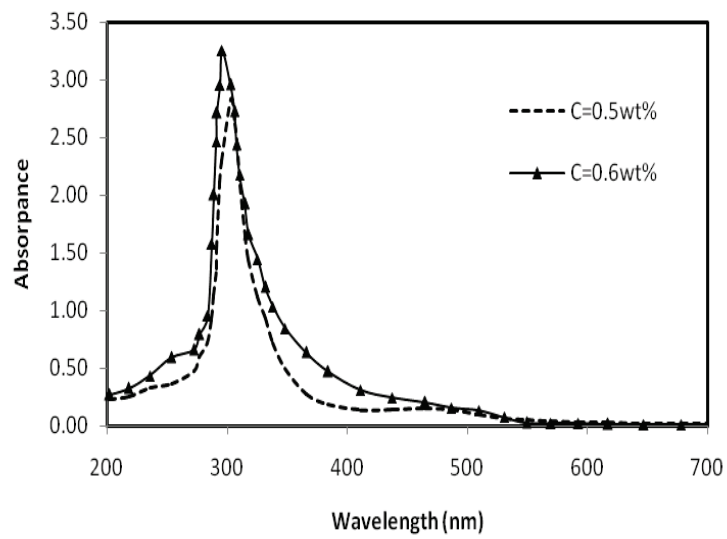


Figure 2: The absorption spectra of styrene-butadiene in toluene at concentrations of 0.5 and 0.6 wt%.

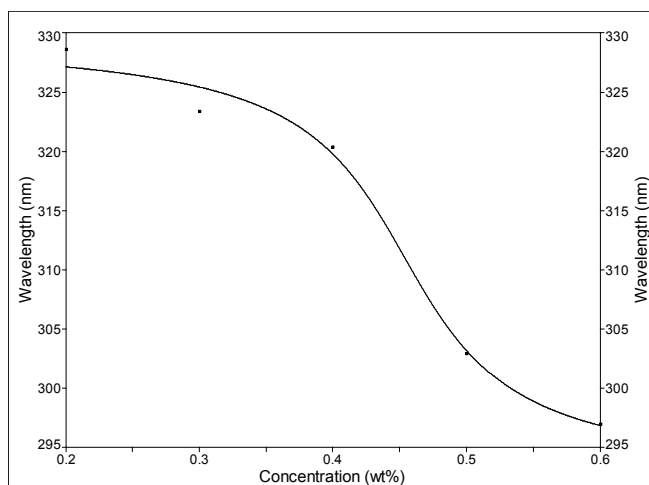


Figure 3: The relationship between absorption wavelength and concentration.

The best fit equation for this curve (Figure 3) is shown below.

$$y = 292.11264 + 37.862641 \left(\operatorname{atan} \left(\frac{x - .45398612}{-0.060704644} + \frac{\pi}{2} \right) / \pi \right) \quad (1)$$

This equation indicates that increasing the concentration of styrene-butadiene leads to a decrease in the absorption wavelength. The broadening of the absorption bands occurs due to fluctuations in the structure of the solvation shell around a solute. This effect is called inhomogeneous broadening; it supersedes homogeneous broadening because of the existence of a continuous set of vibrational sublevels. In addition, shifts in the absorption bands can be stimulated by altering the nature or composition of the solvent. These solvatochromic shifts are evidence of the changes in solvation energy. In an instance during which a solute is surrounded by solvent molecules, its ground and excited states are either more or less stabilised by solute–solvent interactions. The chemical nature of both the solute and solvent molecules will influence this interaction. Solute–solvent interactions are usually described as Van der Waals interactions or possibly as more specific interactions such as hydrogen bonding.¹⁰

3.2 Theoretical Part

To estimate a theoretical model for the effect of concentration on the absorption spectra of styrene-butadiene in toluene, we must initially match the shift of the absorption curves for concentrations of 0.3–0.6 wt% with the absorption wavelength at 628.67 nm for the 0.2 wt% concentration (Figure 4) and

subsequently take the fitting curves for these spectra as illustrated in Figures 5 to 8.

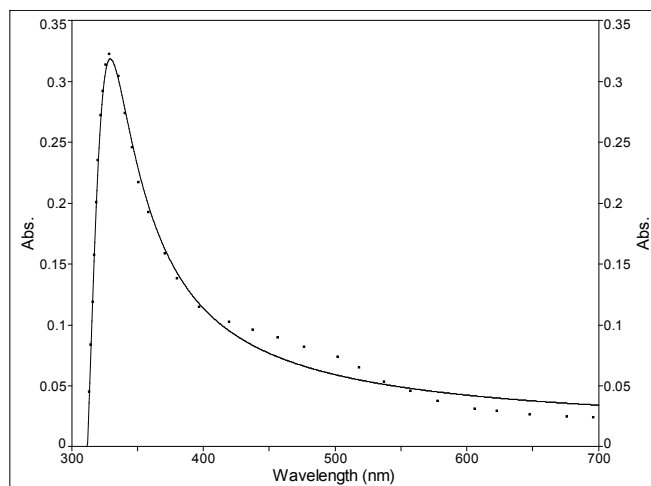


Figure 4: Fitting curve for the absorption spectrum at $C = 0.2$ wt%.

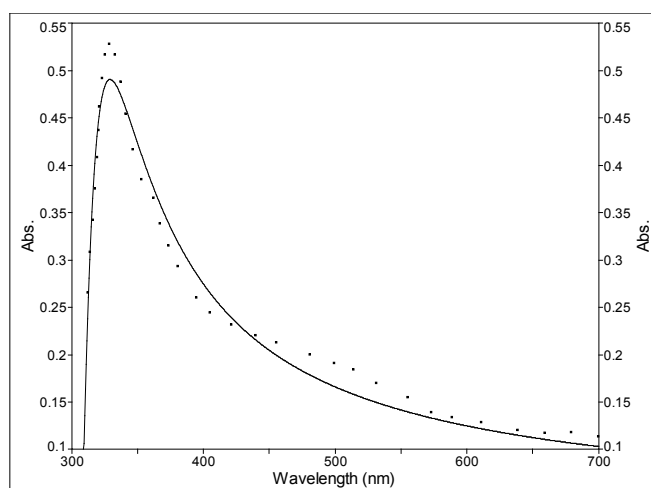


Figure 5: Fitting curve for the absorption spectrum at $C = 0.3$ wt%.

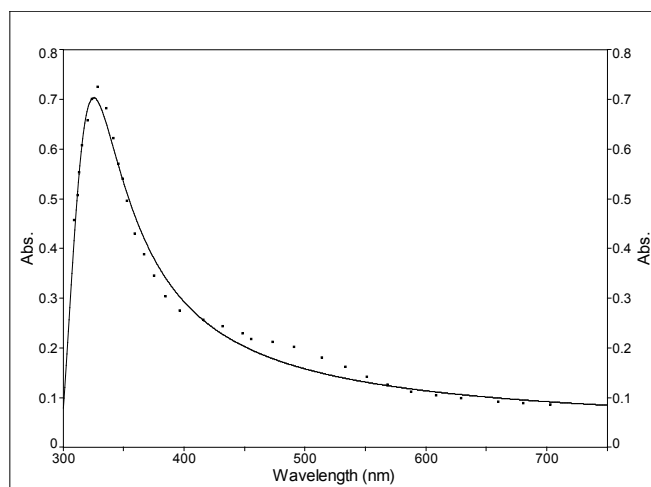


Figure 6: Fitting curve for the absorption spectrum at $C = 0.4$ wt%.

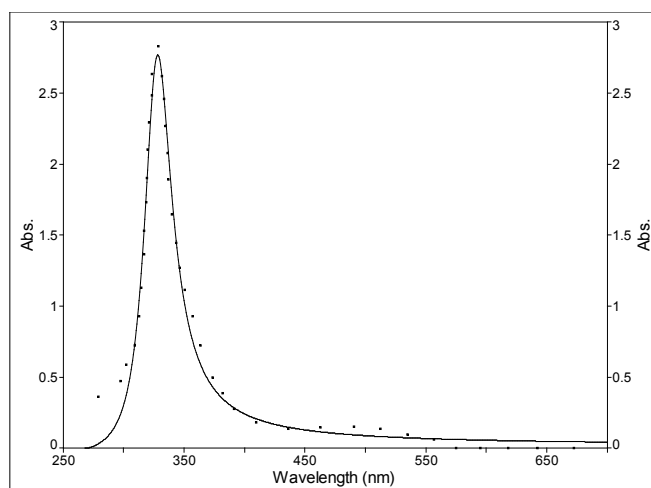


Figure 7: Fitting curve for the absorption spectrum at $C = 0.5$ wt%.

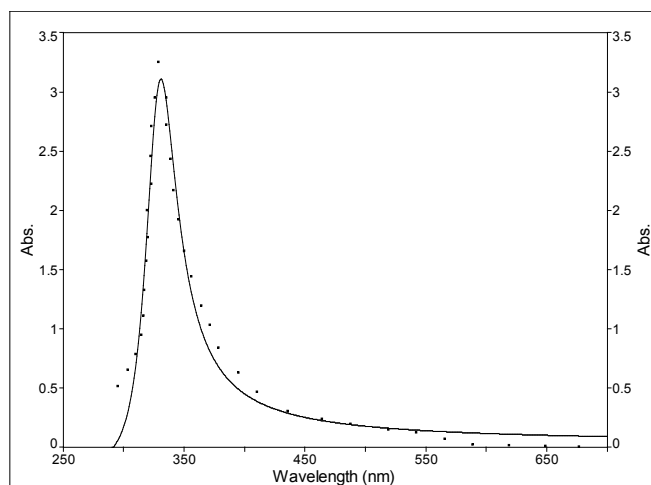


Figure 8: Fitting curve for the absorption spectrum at C = 0.6 wt%.

The best fit equation is

$$y = \frac{a + c \ln x}{1 + b \ln x + d (\ln x)^2} \quad (2)$$

where x describes the wavelength of absorption band, y represents the absorbance, and the value of the parameters a , b , c , and d are given in Table 1 for each concentration.

Table 1: The values of the parameters of the theoretical equation.

Parameter	0.2 wt%	0.3 wt%	0.4 wt%	0.5 wt%	0.6 wt%
r^2	0.9932946998	0.9773373116	0.9894033602	0.9869050557	0.9702025866
A	-0.00466655	-0.01591647	-0.01261929	-0.00442461	-0.01018270
B	-0.34753767	-0.35060022	-0.34881596	-0.34549804	-0.34530042
C	0.000812643	0.002778575	0.002215512	0.000790366	0.001794787
D	0.030198148	0.030733882	0.030424132	0.029843864	0.029810212

The correlation factor between the experimental and theoretical curves is represented by r^2 . Each parameter was plotted against the concentration as shown in Figures 9 to 12. The best fit equations are shown above each curve.

$$y = a_1 + b_1 x^2 + c_1 e^x + \frac{d_1 x}{\ln x} \quad (3)$$

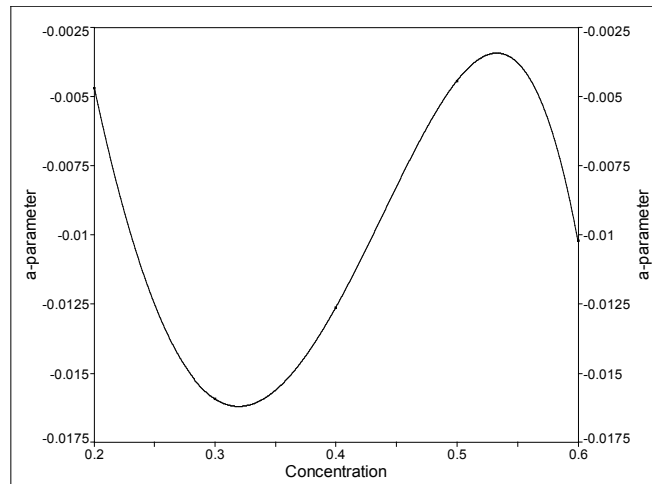


Figure 9: The relationship between parameter a and the concentration.

$$y = a_1 + b_1 x^2 + \frac{c_1 x}{\ln x} + d_1 \ln x \quad (4)$$

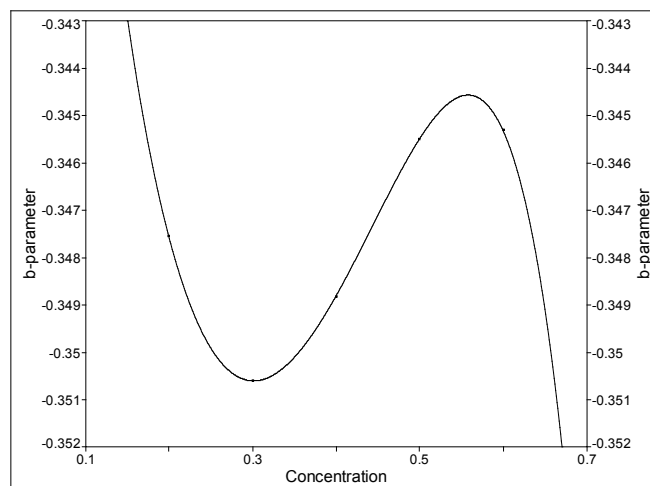


Figure 10: The relation between b-parameter and concentration.

$$y = a_1 + b_1 x^{2.5} + \frac{c_1 x}{\ln x} + \frac{d_1}{x^{0.5}} \quad (5)$$

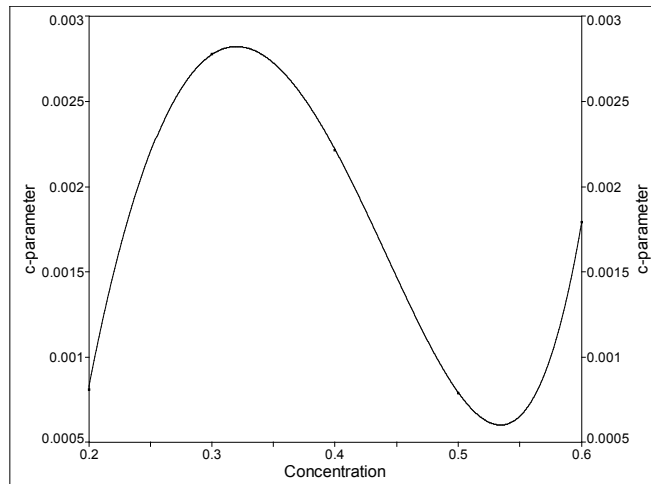


Figure 11: The relationship between parameter c and the concentration.

$$y = a_1 + b_1x + c_1x^{1.5} + \frac{d_1}{\ln x} \tag{6}$$

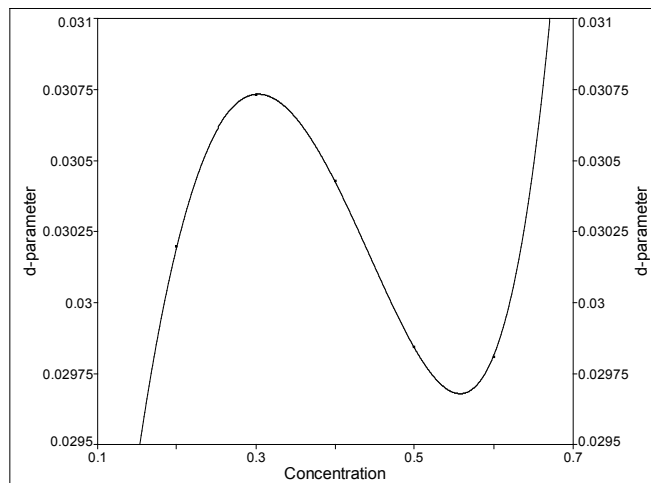


Figure 12: The relation between parameter d and the concentration.

Table 2: The values of the parameters of the best fit equations for the parameters of the theoretical equations.

Parameter	a-parameter	b-parameter	c-parameter	d-parameter
a_1	0.666444581	-0.39056765	0.012948422	0.021301661
b_1	1.912098285	0.279205179	-0.23057938	0.057849515
c_1	-0.58639590	0.057578947	0.05238346	-0.09717187
d_1	0.252432522	-0.02424243	-0.00649381	-0.00968536

The estimated equation for the theoretical model of the absorption spectrum was calculated for the test concentration of 0.45 wt% of styrene-butadiene and is shown below.

$$y = \frac{-0.0081341 + 0.00146662 \ln x}{1 - 0.34711953 \ln x + 0.030130082 (\ln x)^2} \quad (7)$$

The estimated theoretical absorption spectrum is illustrated in Figure 13. We concluded that the behaviour of the theoretical spectrum is similar to the experimental spectra, and the maximum theoretical absorption wavelength is 311.83 nm. This model allows us to plot the absorption spectrum for any concentration ratio of styrene-butadiene to toluene that has not been experimentally taken.

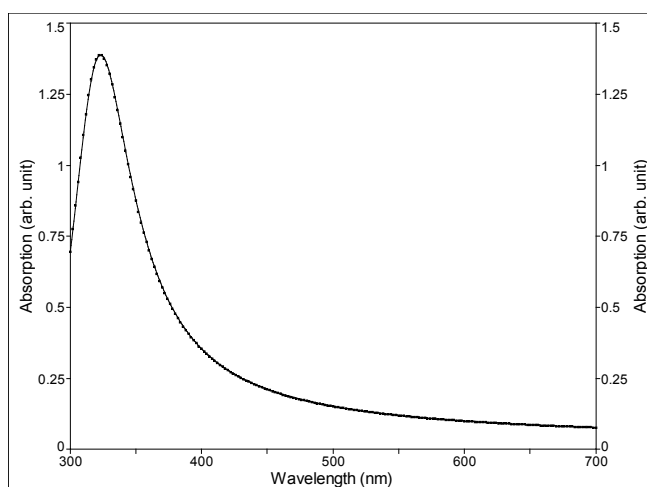


Figure 13: Theoretical absorption spectrum of styrene-butadiene in toluene at test concentration of 0.45 wt%.

4. CONCLUSION

An estimated theoretical model for the absorption spectrum of styrene-butadiene in toluene was investigated. The experimental and theoretical absorption spectra are in good agreement. The estimated theoretical equation is shown below.

$$y = \frac{a + c \ln x}{1 + b \ln x + d(\ln x)^2} \quad (8)$$

This model allows us to plot an absorption spectrum for styrene-butadiene in toluene at a concentration that has not been tested experimentally.

5. REFERENCES

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