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The Deformity Vibrations of Carbon Tetrachloride in Alcoholic Environment

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Abstract: Raman spectra of Carbon Tetrachloride and Methanol solutions were measured. Spectral lines ν_2(symmetric Deformity vibrations), ν_4(asymmetric Deformity vibrations) of Carbon Tetrachloride were analyzed. The Raman spectra were fitted by using Peak-Fit software by a sum of Gaussian and Lorentzian components. Results indicate that, there is a clear similarity in the behavior of peak position and width of the two type of vibration with varying the structural composition of the surrounding environment due to varying of the methanol concentration. On the other hand we found a similarity in the dependence of the intensity of spectral lines on the concentration of methanol, with a high degree of non-linearity.
Keywords: Raman – Carbon Tetrachloride – Methanol – Deformity Vibrations.

1. Introduction

CCl_4 is considered to be a non-polar solvent as it doesn't express any permanent molecular dipole moment. This feature is very important in the spectral studies in the cases of using Carbon Tetrachloride as a dilute for some polar substances such as Methanol and Acetone [1-3], because it is possible to study the interactions between the molecules of the dissolved substances without having a strong influence of the Carbon Tetrachloride molecules.

Methanol/Carbon Tetrachloride mixture gained the attention of many research groups[2-6], where the attention was focused on developing an ideation for the microscopic structure of the mixture, and the changes that happen as a result of concentration alteration. Some of these studies relied on the use of Raman spectroscopy, which is the appropriate way to study the structure as a function of concentration, because in liquid mixtures, the band shape of a reference vibrational mode of the molecule is influenced by the concentration fluctuations of the environment [7–9].

The dependence of the bandwidth and frequency of Raman bands on the environment provides useful information regarding the solute–solvent interactions and intermolecular forces[7].

In Methanol/Carbon Tetrachloride mixture, the Methanol molecules are linked together in hydrogen bonds forming winding chains in the range of the high concentrations level, and cyclic structures in the range of the low concentrations level[9]. The mutual influence between Methanol molecules and CCL_4 molecules increased up to the solvent cage effect at the high concentrations of Methanol, where the molecules of Carbon Tetrachloride are confined in a potential well created by Methanol molecules[7]. Some researches[10]suggest that solvent cage effect may be accompanied with forming HO..Cl bonds, although there is no structural evidence to support this prediction.

This study is considered as a part of a series of studies which are interested in vibrating spectrum of Carbon Tetrachloride mixed with Methanol[1,2]. In this work, we compare the spectrum influences on symmetric and asymmetric deformity vibrations as a result of adding Methanol. this study results shall enrich the available information on the mutual influences between Methanol and Carbon Tetrachloride especially that most of the studies that were interested in following up the structural composition of such mixture through Raman spectrum study, has not taken into consideration the Carbon Tetrachloride spectrum, but it was interested in Methanol spectrum as it is the substance that has a chemical efficiency in the considered mixture

2. Experimental procedure

CCL_4 and CH_3OH solutions were prepared in different concentrations of Methanol ranged from 0 to 1 (v/v).The compounds (Aldrich) are commercial products which were used without further purification. The FT-IR and Raman spectra were measured as a function of concentration at room temperature with a Nicolet-6700/NXR-Raman, provided with laser source He/Ne at 632.8 nm, with resolution of 4 cm^{-1}. The Raman spectra were fitted by using Peak-Fit program by a sum of Gaussian and Lorentzian components. We paid attention to the fact that the Methanol concentration should not exceed a certain level in order to avoid formatting any kind of link between the Methanol molecule and Carbon Tetrachloride carbon[2].

3. Results and Discussion

Figure (1) illustrates a sample of the spectra obtained which regards the sample prepared at the concentration of C=0 v/v of the Methanol.

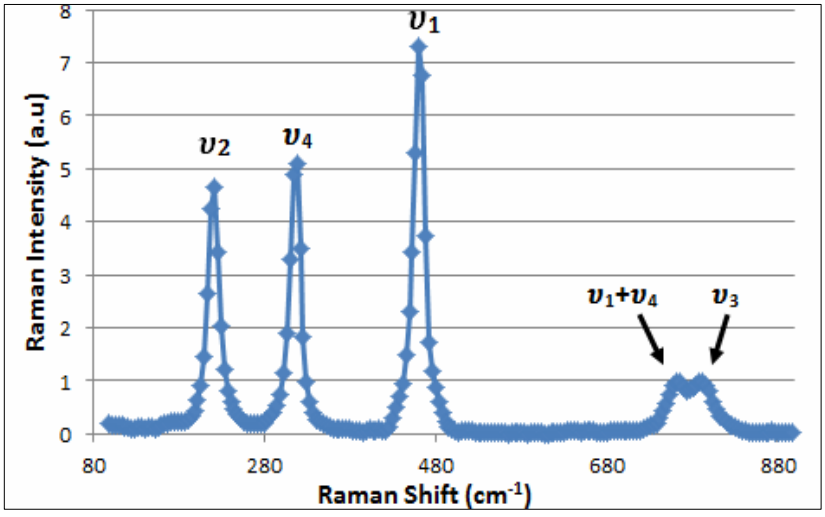
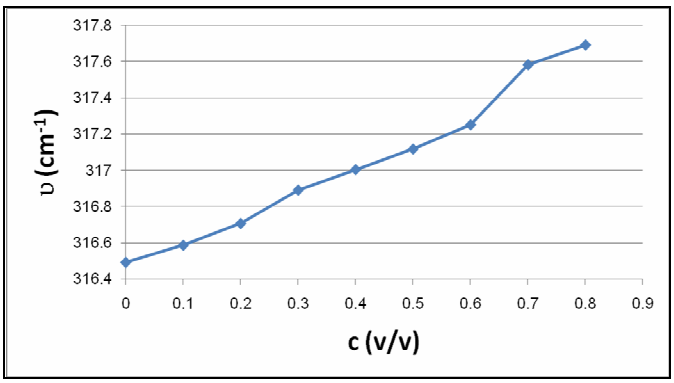


Fig. (1) Raman spectra of the mixture at c=0 v/v.

We notice that spectrum contains the peaks υ_1 (symmetric stretch vibrations) and υ_2 (symmetric deformity vibrations) and υ_3 (asymmetric stretch vibrations) and υ_4 (asymmetric deformity vibrations),we also notice the emergence of the peak $\nu_1+\nu_4$ which resulting from combining υ_1 and υ_4.
Figure (2) illustrates the peak position dependency on the concentration for peaks ν_2, ν_4.

(a)



(b)

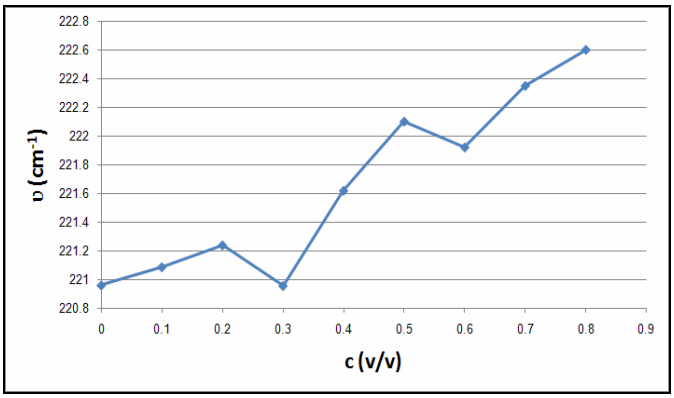


Fig. (2) Variation of Raman shift as a function of concentration
(a) line υ_2 (b) line υ_4

We notice that the increase in concentration Leads to the shift toward higher wave numbers. This results refers to that fact that the link C-Cl is subjected to centrifuge force which its influence increases with the increase of Methanol concentration. We notice the same thing for to the asymmetric vibration (curve b) where shifts occur towards the high wave numbers But with a higher numerical values.

Figure (3) shows the peaks' intensities of ν_2, ν_4, lines as a function of the concentration of Methanol in the mixture.

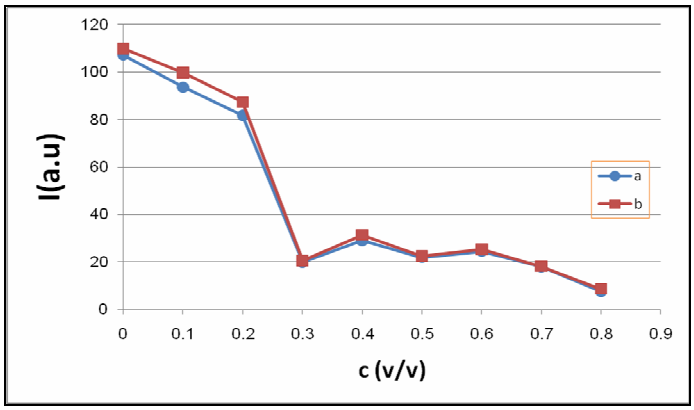


Fig. (3) The variation of Raman intensity as a function of concentration
(a) line υ_1 (b) line υ_4.

We notice that there is a complete compatibility between both curves related to both kinds of vibrations which means an equality of intensity for the whole concentration. We also notice that the intensity is declining to decrease along with an increase of methanol's concentration. The extreme decrease in intensity is happened when moving to the concentration C=0.3 v/v .

If we look at the curves in figure 3 , it is clear that there is no linearity in relation between intensity and concentration , this can be explained by the mutual influences between Carbon Tetrachloride and Methanol molecules. The mutual influences affect the possibility of energy transference which is appear as an decrease in peak intensity, added to the intensity decrease resulted from the decrease of concentration molecules of Carbon Tetrachloride.

The diagram of the spectral width for the three peaks as a function of concentration are plotted in figure (4).

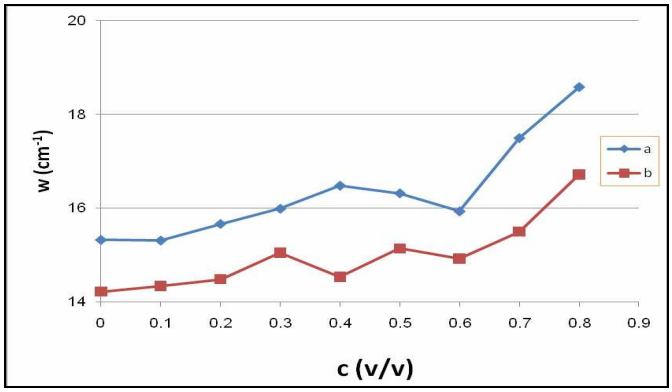


Fig. (4) The variation of Raman bandwidth as a function of concentration
(a) line υ_2 (b) line υ_4

We notice the increasing of spectrum line width for both vibrations with the increasing of Methanol concentration. We also notice that the spectrum width of the spectrum line υ_2 is higher than the one related to line υ_4 for all concentrations.

4. Conclusion

This study includes the spectrum analysis results of Raman spectroscopy for the symmetric and asymmetric deformity vibrations for the pounds C-CI in Carbon Tetrachloride/methanol mixtures. We found that the nature of the affecting forces on the deformity vibrations is not affected with methanol concentration. In addition, the study shows the symmetry of influence of structural composition change of the solution on the intensity curves for both vibrations with a high level of non-linearity attitude in the relationship between the spectrum line intensity and concentration. In addition, we have found that adding methanol will lead to widening the spectrum lines.

Acknowledgments

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