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Excess molar enthalpies for acetylene tetrachloride with cyclohexanone, pyrralidin 2-one and methyl ethyl ketone at 308.15 K

Abstract
Excess molar enthalpies, H^E, at 308.15K were determined calorimetrically for binary liquid mixtures of acetylene tetrachloride ($CHCl_2CHCl_2$) with cyclohexanone, pyrralidin-2-one and methyl ethyl ketone. Exothermic behavior is shown by all the systems. The values of H^E are fitted with suitable equation with the help of the least squares method. The results point to the presence of specific interactions.

Keywords: Microcalorimeter, cyclohexanone, mixtures, charge-transer complex, mole fraction

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Introduction

The research of excess properties are of massive hobby in knowledge the heteroatom interactions within the multi-constituent liquid mixtures. Consequently, assessment and calculation of these excess values as functions of mole fraction are of academic and realistic significance. Our aim is gathering of the facts for physical properties of of n-donor or π-donor and σ-acceptors organic liquid mixtures to observe the probable interactions happening in the combined liquid systems. As a part of our uninterrupted attempts to achieve nonthermodynamic and thermodynamic parameters on binary liquid mixtures of various organic compounds (Tripathi AD,2010,2018,2020,2021), determination of excess molar enthalpies of acetylene tetrachloride ($CHCl_2CHCl_2$)(AT) with cyclohexanone ($C_6H_{10}O$), pyrralidin-2-one (C_4H_7NO) and methyl ethyl ketone($CH_3COC_2H_5$) have been undertaken in the current work at the temperature 308.15K. Binary systems of $CHCl_2CHCl_2$ with $C_6H_{10}O$, C_4H_7NO and $CH_3COC_2H_5$ are of significant interest because of interactions among these components .This is due to the presence of four Chlorine and two Hydrogen atoms in $CHCl_2CHCl_2$, which can consequently carry out as σ-acceptors in the path of, and be engazed in the H- bond creation with cyclohexanone, pyrralidin-2-one and methyl ethyl ketone . The later compounds will carry out as n-donors. A literature inspection disclosed that vast research on such systems have not been undertaken till now. The data obtained for H^E have been explained in this paper.

Experimental Section

Acetylene Tetrachloride (Fluka) has been purified with the aid of fractional distillation, only the center fraction turned into used for experiments.

Cyclohexanone (B.D.H.), and Methyl ethyl ketone (A.R.) were dried over freshly activated molecular sieves before use for removing moisture . All the chemicals have a purity of 99.0 mol% as obtained by GLC. Chemical purities , as measured by GLC for the samples of acetylene tetrachloride ($CHCl_2CHCl_2$) , cyclohexanone, pyrralidin-2-one and methyl ethyl ketone are found to be 99.8, 99.8, 99.3 and 99.0 mol%, respectively. The excess enthalpies were determined using the microcalorimeter. The mean error in the experimental data of H^E are envisioned to be within 1 per cent.

Result and Discussion

Experimental data for H^E, at 308.15K for all binary mixtures, in terms of the $CHCl_2CHCl_2$ mole fraction x_1 are listed in Table 1. Experimental values were fitted to the following equation:

$$\frac{H^E}{J.mol^{-1}} = x_1 x_2 \sum_{i=0}^{m} A_i \, (x_1 - x_2)^i \qquad (1)$$

The constants Ai, along with the standard deviations, σ , are collected in Table 2 . The expression used to evaluate the standard deviation, σ , was

$$\sigma = [\sum (H^E_{exp} - H^E_{calc})^2/(m-n)]^{½} \qquad (2)$$

Wherein n is the quantity of parameters and m is the wide variety of information geared up. Graphical presentations of experimental values of H^E information for all binary mixtures are supplied in figure 1. As may be discovered, the values of H^E are negative throughout the whole mole fraction variety for whole combination.

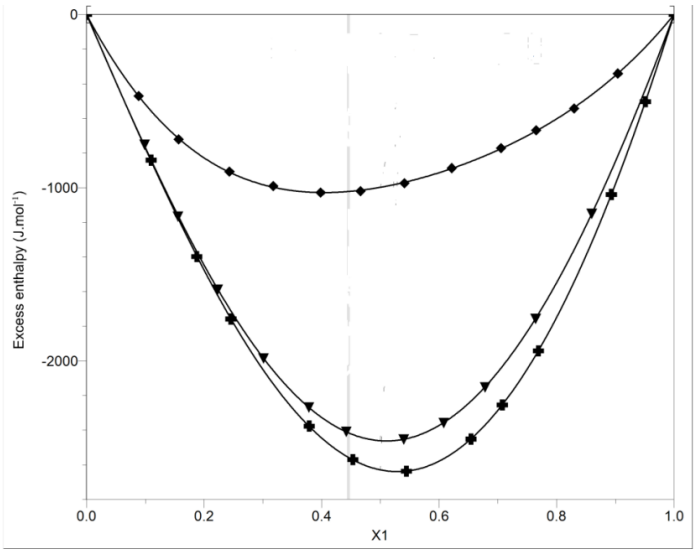

Fig. 1: Excess molar enthalpies of binary liquid mixtures of x1 of acetylene tetrachloride ($CHCl_2CHCl_2$)(1) + cyclohexanone ($C_6H_{10}O$)(2) (✚),+ pyrralidin-2-one (C_4H_7NO)(2))(▼), and +methyl ethyl ketone($CH_3COC_2H_5$ (2)(◆) at the temperature 308.15 K.

Fig. 1 represents that the negative values of the excess molar enthalpies H^E, for all binary liquid mixtures is substantially influenced by means of the electronic surroundings of Oxygen atom. The sign of H^E effects from the disorder of interactions among resembling molecules and the beginning of

recent interactions between contrasting molecules. The remaining end result of both type of interactions. This may be because of contravention of bonds or The scale of H^E for these mixtures is because of the interactions among resembling molecules, and from the creation of new bonds such as H- bonds between contrasting molecules. In case the interaction among resembling molecules are weaker in comparison to contrasting molecules, the negative values of H^E is observed. The high negativity of all these systems signify robust specific interactions connecting the contrasting molecules. If cyclic ketones have saturated rings and it reacts with bromine - or chlorine containing compounds, strong interaction is observed. $C_6H_{10}O$ or C_4H_7NO has saturated ring, consequently they form stronger complexes i.e. high exothermicity is shown in the value of H^E . Since $CH_3COC_2H_5$ does not have ring(saturated or unsaturated) in its structure, thus it has less negativity as compared to other keto compounds.

Table-1 Excess molar enthalpies for acetylene tetrachloride ($CHCl_2CHCl_2$)with cyclohexanone($C_6H_{10}O$), pyrralidin-2-one (C_4H_7NO) and methyl ethyl ketone($CH_3COC_2H_5$) at 308.15K

$CHCl_2CHCl_2$+ cyclohexanone		$CHCl_2CHCl_2$+ pyrrolidin-2one		$CHCl_2CHCl_2$+ methyl ethyl ketone	
x1	H^E ($J.mol^{-1}$)	x1	H^E ($J.mol^{-1}$)	x1	H^E ($J.mol^{-1}$)
0.1098	-841	0.0886	-576	0.0886	-576
0.1876	-1397	0.1567	-748	0.1567	-748
0.2456	-1758	0.2432	-907	0.2432	-907
0.3788	-2376	0.3176	-991	0.3176	-991
0.4532	-2569	0.3984	-1028	0.3984	-1028
0.5444	-2636	0.4662	-1020	0.4662	-1020
0.6542	-2451	0.5409	-974	0.5409	-974
0.7076	-2254	0.6216	-887	0.6216	-887
0.7689	-1942	0.7054	-766	0.7054	-766
0.8932	-1039	0.7651	-668	0.7651	-668
0.9511	-504	0.8298	-555	0.8298	-555
		0.9043	-429	0.9043	-429

Table 2. Least Squares Coefficients of Eq 1 for the Excess Molar Enthalpies , and the standard deviations,σ,of Acetylene tetrachloride ($CHCl_2.CHCl_2$)(1) + cyclohexanone ($C_6H_{10}O$)(2) ,+ pyrralidin-2-one (C_4H_7NO)(2)),+ and +methyl ethyl ketone($CH_3COC_2H_5$)(2) at the temperature 308.15 K.

System	A0	A1	A2	A3	σ (J mol^{-1})
$CHCl_2CHCl_2$ (1) + cyclohexanone (2)	-1.05E+04	-1397	1214	-82.56	2
$CHCl_2CHCl_2$ (1) + pyrralidin-2-one (2)	-9842	-483.5	1337	-135.5	3.3
$CHCl_2CHCl_2$ (1) + methyl ethyl ketone (2)	-3992	1192	-1330	-6692	4.5

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