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Application of the vectors in the determination of the miscibility of the substances

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Abstract

The molecular bonds formed in the two different atoms having different electro negativities, develop a dipole in the molecule. In mathematical point of view, each bond can be considered as a vector and the resultant vector is the molecular dipole. In the present studies, the miscibility of the substances is correlated with resultant vector value i.e. the dipole moment.

Keywords: dipole, vectors, miscibility, solvents

1. Introduction

The vector is defined as a quantity which has magnitude as well as direction ^[1]. In a molecule, there is an existence of dipole moment due to their electro negativities. Therefore, each bond among the two different atoms is considered as a vector. The total dipole moment of the molecule is the magnitude of the resultant vector of the all the bond moments in the molecule ^[2, 3]. This value fairly matches with the experimentally determined dipole moment ^[2]. Hence, it is a good application of mathematical concept in the determination of a chemical property of a molecule. Dipole moment tells about the polar and nonpolar nature of the molecule which also gives an idea about the miscibility of a molecule in a given solvent ^[4]. Further it helps in understanding the intermolecular forces ^[5].

Present study deals with the preparation of calibration plots regarding the miscibility of the two substances.

2. Experimental

The dipole moments of various substances are determined theoretically considering the bond moments of the molecules as shown in Figure 1. The calibration curve was plotted and accordingly the miscibility of the compounds is confirmed experimentally.

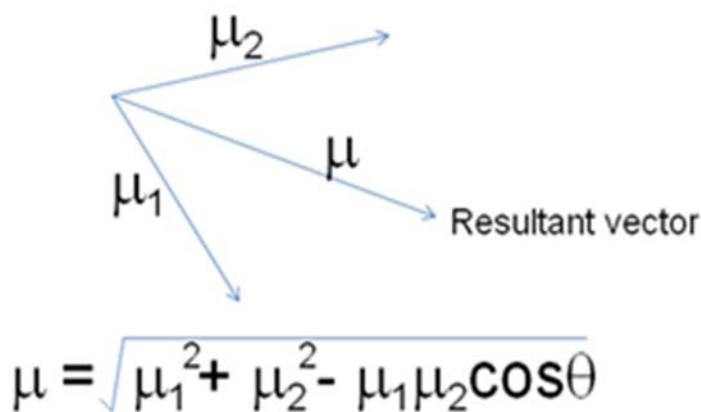


Fig 1: Determination of resultant vector of the two vectors.

3. Results and Discussion

The dipole moments of protic solvents, aprotic solvents and substituted benzenes have been calculated and recorded (Table 1 to 4). The bond moments are taken from the literature. ^[6] The trend and calibration has been shown graphically in Figure 2.

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3.1 Protic solvents

Table 1

Sr no.	Protic solvent	Dipole moment (μ) in Debye
1	Ethanol	1.69
2	Methanol	1.70
3	Acetic acid	1.74
4	Water	78.5

In Figure 2, represented by blue line

3.2 Aprotic Solvents

Table 2

Sr no.	Aprotic solvent	Dipole moment (μ) in Debye
1	Tetrahydrofuran (THF)	1.75
2	Ethyl acetate	1.78
3	Acetone	2.88
4	Dimethyl Sulfoxide (DMSO)	3.96

In Figure 2, represented by red line

From Figure 2, it is clear that the substances with higher dipole moments i.e. above the solvent line are having more solubility in those solvents.

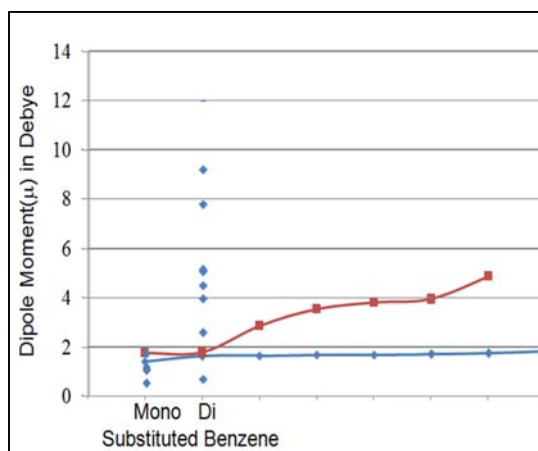


Fig 2: Plot of comparison of dipole moments. Line plots are of protic (-♦-) and aprotic (-♦-) solvent where as dots (♦) are of mono and di substituted benzenes.

3.3 Substituted Benzenes

Table 3

Sr no	Monosubstituted Benzene	Dipole moment (μ) in Debye
1	Aniline	0.524
2	Toluene	1.06
3	Acetophenone	1.06
4	Benzaldehyde	1.06
5	Benzoic acid	1.06
6	Phenol	1.19
7	Nitrobenzene	1.739

Represented In Figure 2

Table 4

Sr no	Dinosubstituted Benzene	Dipole moment (μ) in Debye
1	para-Bromotoluene	0.68
2	para-Chlorobenzaldehyde	2.59
3	meta-Chlorotoluene	3.9536
4	meta-Dimethylbenzene	4.49
5	Acetylsalicylic acid	5.071
6	ortho- Dichlorobenzene	5.1268
7	ortho-Xylene	7.7769
8	Salicylic acid	9.1867

Represented In Figure 2

From the calibration curve, just by knowing the dipole moment, its miscibility can be found out.

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