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## Densities From Fundamental Parameters

V.R.Murthy<sup>1</sup> and A.Raghavendra Rao<sup>2</sup>.

Prof. & Head of the Department of Physics , P.G .Department of Physics , T.J.P.S College (PG Courses),Guntur ,  
Andhra Pradesh, India<sup>1</sup>.

Lecturer in Physics , P.G. Department of Physics, T.J.P.S College (PG Courses), Guntur ,Andhra Pradesh , India<sup>2</sup>.

**Abstract:** The valuable data on fundamental parameters like bond energies are very useful in estimating the physical quantities such as Densities, Refractive index...etc. An algebraic relationship is developed to correlate the densities with the bond energies with the help to few other relevant parameters like covalence factor . The relation reads as

$$\rho = 0.0095 \xi q^{\frac{1}{2}} p \left[ \sum_i \left( \frac{E_i r_i}{\sigma_i s_i} \right) m \right]$$

**Keywords:** Density, Bond energy, covalence factor, alcohols, halides

### I. INTRODUCTION

The valuable data on fundamental parameters like bond energies are very useful in estimating the physical parameters such as Densities The densities of molecules are usually constituted on the vectorial basis of addition of densities of individual atoms, Which in turn has been shown to be dependent on Bond Energies For ex; C = C has bond strength of 146.8 K.cal/mol, Where as c-c has the strength 83.2K.Cal/mol. The bond strength of CCl is less than that of CBr and the density of CCl<sub>4</sub> is less than that of CBr<sub>4</sub>. This shows that density varies directly as bond strengths

The densities have an indirect bearing on the percentage covalency which depend on electro negativity of constituent atom For ex; C-Cl has bondstrength of 78K.Cal/mol where as C-Br has bond strength 66K.cai/mol . The density of CCl<sub>4</sub> is less than of CBr<sub>4</sub>.

The density, refractive index ,melting point and boiling point are a few impotent parameters characterising the state of molecule or atoms.An estimation of density also surves as a litmus proof for measuring the purity of the molecule .For example an Analor sample of benzene is purer than the lab reagent in that ,the latter contains a few other ingredients other than the main .Similarly spec pure samples are supposed to 99.99% pure.The density of spec pure sample aggress with the ideal sample near to the fourth decimal place. Thus measurement of density of a molecule can be taken to be a test for a purity of a sample . So determination of densities is very important parameter characterising the state of the molecule.

### II . Method:

An algebraic relationship is developed to correlate the densities with the bond energies with the help of few other relevant parameters like covalence factor. The relation reads as.

$$\rho = 0.0095 \xi q^{\frac{1}{2}} p \left[ \sum_i \left( \frac{E_i r_i}{\sigma_i s_i} \right) m \right]$$

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Where  $\rho$  = density in gm/cc  
 $E_b$  = Bond energy in Kcal/mole.  
 $m$  = fraction of valance electrons participating in bonding to the total number of valence electrons in that atom .  
 $\xi$  = characteristic parameter, I (aliphatic), 0.8 (aromatic and hydroxides).  
 $q, p$  are the row numbers of electrons in the bond.  
 $\frac{r}{s}$  = fraction of bonds of  $i^{th}$  type of the total no of bonds.

Aromatic and Aliphatic alkenes as well as their hydroxides and halogen substituent have been chosen as samples . There relevant data on the bond strength ( $E_b$ ) and densities ( $\rho$ ) are taken from reference 1. The covalence factor( $\sigma$ ) calculated from the Pauling electro nativity are taken from reference 2. These values are reported in table 1. The calculated densities (in gm/cc) are presented in table 2 along with a reported values . The constant is chosen as 0.0095.

**Table – 1**

Bond energy and Pauling covalence values.

Name	Bond Energy ( $E_b$ ) K cal/mol	Pauling covalence factor $\sigma$
C – C	83.2	1
C = C	146.8	1
C – H	98.8	0.9698
N – H	93	0.8347
O – H	110.6	0.6340
C – O	85.5	0.7788
C – Cl	78	0.9394
C – Br	66	0.9777
N – Cl	48	1
N – N	38	1
C = O	178	0.7788

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Table – 2

Density values calculated and standard In gm/cc.

Name	Calculated density	Standard density
CH <sub>3</sub> Cl	0.923	0.920
CH <sub>3</sub> Br	1.154	1.732
CH <sub>3</sub> OH	0.7853	0.7914
Propenol	0.8036	0.7881
Butanol	0.7871	0.8098
C <sub>6</sub> H <sub>6</sub>	0.8242	0.8787
C <sub>7</sub> H <sub>8</sub>	0.8369	0.8669
C <sub>8</sub> H <sub>10</sub>	0.8454	0.8968
CHCl <sub>3</sub>	1.4438	1.483
C <sub>3</sub> H <sub>7</sub> Cl	0.9144	0.8923
CCl <sub>4</sub>	1.5775	1.5943
C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	1.2621	1.2881
C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub>	1.9717	1.9523
C <sub>6</sub> H <sub>5</sub> OH	1.7634	0.7893

## III. RESULTS AND DISCUSSION

With the value of the content equal to 0.0095, maximum deviation is found to be not more than 3 %.T he error is found to increase in higher homologous of alcohols ( propyl alcohol , butyl alcohol).

The values of densities obtained from the expression shows a near coincidence with the experimentally determined  $\rho$ 's .Hence this suggests a direct relationship between bond energies and a constant characteristic bonds and densities .With the increase in the bond strength involving heavier atoms the densities show promising increase . In case where the constituent element repeat the densities are not showing a pronounced increase.

Ex :Methyl Alcohol , Propyl alcohol ,ethyl alcohol ,butyl alcohol the same behavior is observed in aryl halides also. This work is continued for polymers also.

## IV. SAMPLE CALCULATION

CH<sub>3</sub>Cl

$$\rho = 0.0095 * 1 \left[ \left( \frac{98.8}{0.9693} * \frac{3}{4} \right) + \left( \frac{78}{0.9394} * \frac{1}{4} \right) \right]$$

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=0.923(calculated)

=0.920 (standard)

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## BIOGRAPHY

VEDAM RAMA MURTHY.



Former Prof of physics in S.K. University, Ananthapur, till 2003, and at present Prof & Head of the Dept of Physics T.J.P.S College (PG Courses) Guntur. Since 2003. So far supervised 15 Ph.D's and 28 M.Phils and Published 125 research papers in International and National Journals

Interested in guiding in Medical Physics, Semiconducting Physics and Polymer Physics & Lowcost instrumentation.

1. Visited and worked as a "Resource Person in school of Bio-Physics Organized by International Centre for Theoretical Physics". Trieste, Italy during 30<sup>th</sup> August to 4<sup>th</sup> October in 1994.
2. Recipient of Andhra Pradesh State government "Best Teacher Award" for the Year 1987-1988 Recipient of "K.R.Rama Nathan's Award for Best Teaching Aid in Physics", Organised by Institute of Physics Bombay in 1994.

ANKAM. RAGHAVENDRA RAO



Qualification: M.Sc, M.Phil..(Ph.D)

**Designation:** Lecturer in physics T.J.P.S College (PG Courses).

Working for the Ph.D in "PHYSICAL STUDYS IN OLIGOMERS&POLYMERS",

Since July – 2012. Under the supervision of Prof . V.R.Murthy.

Published Four Research papers in reputed Journals of physics.