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# Determination of Molecular Radius of Glycerol Molecule By Using R Software

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**Abstract:** Our study focuses on using R computer programming techniques to analyze and interpret wet Practical data in chemical science laboratories. In this research for determination of radius of Glycerol molecule with the help of Statistical R-Software. The flexibility and scope of the R programming environment has made it a popular choice for statistical modeling and scientific prototyping in a number of fields. In the field of chemistry, R provides several tools for a variety of problems related to statistical modeling of chemical information. However, one aspect common to these tools is that they do not have direct access to the information that is available from chemical structures, such as contained in molecular descriptors. R-Software is freely available from various sources on the internet. It is easy to understand for non-statistical background researchers. It reduces complicated calculations (deriving, developing and implementing statistical analysis algorithms in various programming languages and computer architectures) and save ones time, resources, and chemical cost. Computational practical methods are also ecofriendly. In this study solution of Glycerol in different concentration are used and the viscosities are determined from the run times of the various solutions passing through a capillary. The same experiment is simulated by using an in-house developed R program. An R-program is also developed to analyze the results of experimental wet chemistry data. Parameters are analyzed and investigated based on a Parametric Design of Statistical Experiment to determine the functional dependence of viscosity and absolute polymer radius as a function of solvent, temperature, pH, ionic strength. The objective of this work is to record absolute radius of the Glycerol molecule(s) and viscosity as a function of various process parameters by both methods and compared the results using the R-programming language to document the use of the R-programming language for design of process parameters and statistical analyzes of experiment and simulations results. We have also study Dextrose (monosaccharide) and Sucrose (Polysaccharide) molecule. So this method successfully applicable for larger molecule (Polymer)

**Keywords:** Glycerol, Experimental data, Radius, R-Software, Program.

## 1. INTRODUCTION

The purpose of study is to check different property of Glycerol i.e. molecular mass, viscosity, radius of polymer molecule by using Ostwald viscometer method. Glucose, Sucrose, Lactose, manitol, cellulose acetate, polystyrene, crap rubber, polyvinyl alcohols etc. are successfully study. Experimental method run in chemical laboratory. It requires chemical, glassware and space. After completion of experiment waste Glycerol solution released in eco system. Its create pollution in water. So our intention is to find another method to find radius of Glycerol molecule instead of experimental method and save chemicals as well as time. Now a days many experiments by simulation techniques for better results. Computerized programming experiments save many thinks like as chemical cost, nature, related disease and time. Our objective is to measure radius of Glycerol molecule by Ostwald method, this is experimental technique. We are interested to made computer program to know radius. This program help to reduce time, lengthy calculation and chemical cost, by using statistical software like R- Software. R is a language and environment for statistical computing and graphics. R provides a wide variety of statistical (linear and nonlinear modeling, classical statistical tests, time-series analysis, classification, clustering, programming etc.) and graphical techniques, and is highly extensible. It is easy to understand for non-statistical background researchers. In this work, we develop program to find radius of glycerol molecules without using chemical lab.

The R language is a platform for mathematical and statistical computations designed to turn ideas into software, quickly and faithfully. It is free in two senses: R can be obtained free of cost (although commercial versions exist) and anyone is free to examine or modify the source code. R is released under the General Public License, which outlines how the program can be redistributed. As a statistical computing environment with a wide variety of functionality, R is very suitable for chemo informatics and statistical modeling problems.The R language has seen considerable use in a variety a fields because it offers many advantages over other computing languages and mathematical programs. Many innovative modeling techniques are implemented as packages. Packages are collections of R functions, data, and compiled code. R comes with a standard set of packages.

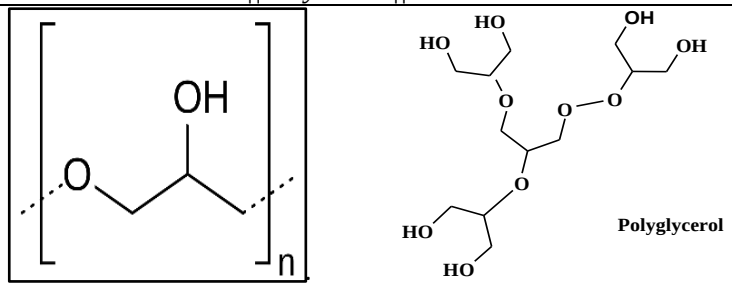


Fig.1.Linear chain Glycerol molecule and non Linear Glycerol molecule

R- Software

R is a free software environment for statistical computing and graphics. It available on https://cran.r-project.org/bin/windows/base/ and www.r-project.org.The R programming language (R Development Core Team 2006) has been used for the purposes of statistical analyses in a variety of fields. Numerous examples of its use in chemistry can be found (Versteeg, Richardson, and Rowe 2006; Vidal, Thormann, and Pons 2005; Guha, Dutta, and Jurs 2006). However, the feature common to these applications is that R is use for the purposes of modeling data that has been generate outside the R environment. Examples of such data are the results of spectroscopic or chromatographic analyzes and molecular descriptor values calculated using a variety of software. Why is R, a statistical programming language, of value to medicinal chemistry today? At the heart of medicinal chemistry, decision-making is determining which compounds to make during the next round of synthesis. Naturally, it is often found useful to look at what past structure-activity trends tell us. To this end, medicinal and computational chemists have made significant advances in how to best describe molecules in terms of numerical vectors that can then be correlated to a biological activity or other med-chem related property. However, the field of correlative statistics is very rich and spans many different fields.

## 2. METHODS

### 2.1. Experimental Method

In experimental method, we have prepare Glycerol solution in suitable solvent ($H_2O$). Here we use standard Ostwald viscometer having capillary length 6 cm and capillary diameter 0.5 mm. In clean viscometer, solvent inserted from clamp side and the solution suck from capillary side by rubber bulb above the upper mark. After passing solvent through capillary time recorded. This is time required for flow of solvent from upper to lower mark. Same procedure repeated for various concentrations of Glycerol solution. Concentration affects on the density, viscosity and resistance of Glycerol solution. Viscosity and time are inversely proportional. Using Mark-Houwink equation, the molecular mass of Glycerol is calculated. The graph of (ŋsp/C) Vs. Concentration, gave intrinsic viscosity [$\eta_{inv}$]. This equation valid only for dilute solution

$$\frac{\eta_{sp}}{C} = KM^{\alpha}$$ **Or** $$\eta = KM^{\alpha}$$

**K andαare constant, M-Molecular mass**

Radius of molecule derived from flow time of various concentration of Glycerol solution, using given equation. Specific Viscosity obtained by following equation

$$\frac{\eta}{\eta_o} = \left(\frac{t}{t_o}\right)\left(\frac{d}{d_o}\right)$$ [1]

$\eta sp = (\eta/\eta o)-1$ [2]

Where t and $t_o$ are flow time of Solution and solvent.d and $d_o$ are density of solution and solvent.

$$r = \left(\frac{\eta_{sp}-1}{6.3*10^{21}*C}\right)^{1/3}$$ [3]

Tabel1. Experimental data (298K Temperature)

| Conc. C | Time in sec. t | | | Mean time in sec. t | t/to | d/do | η/ηo | Radius r in $A^0$ |
|---|---|---|---|---|---|---|---|---|
| solvent | 64 | 64 | 64 | 64 | 1 | 1.0210 | 1.0210 | --- |
| 0.2M | 66 | 66 | 66 | 66 | 1.031 | 1.0042 | 1.0353 | 3.037 |
| 0.4M | 68 | 68 | 68 | 68 | 1.062 | 1.0084 | 1.0709 | 3.041 |
| 0.6M | 70 | 70 | 70 | 70 | 1.093 | 1.0126 | 1.1067 | 3.044 |
| 0.8M | 72 | 72 | 72 | 72 | 1.125 | 1.0168 | 1.1439 | 3.056 |
| 1.0M | 75 | 75 | 75 | 75 | 1.171 | 1.0210 | 1.1955 | 3.095 |

The calculated average radius of Glycerol molecule is $3.0546A^0$

Using equation [3] , from table 1

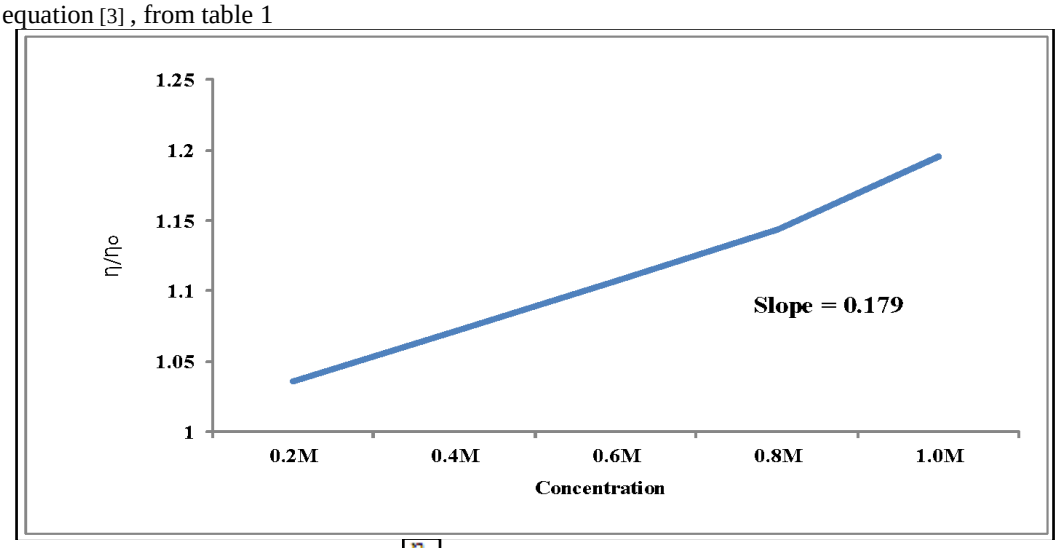


Fig.2 Graph Plotted $\frac{\eta}{\eta_o}$ Vs. Conc.

$$r = \left(\frac{Slope}{6.3*10^{21}*C}\right)^{1/3}$$ [4]

In addition, radius of Glycerol molecule is measure from Graph (Fig.2) using equation [4].

Slope 0.179 and Radius By graph r = $3.05098\ A^0$

**2.2Computer programming**

In computer programming, we have developed formula based program by using R-software. This is simple technique used for calculation of Glycerol molecule radius. R-software program code is providing below.

```
c=rbind(0.2,0.4,0.6,0.8,1,1);c
t=rbind(66,68,70,72,75,64);t
T=data.frame(c,t)
T
n=length(t)
n
t0=64
t1=t/t0
t1
d1=1+0.021*c
d1
n1=d1*t1
n1
n0=n1[-6,]
```

```
c0=c[-6,]
ConcTime=data.frame(c,t,t1,d1,n1)
ConcTime
rcube=((n1-1)/(6.3*(10^21)*c))
rcube
r1=rcube^(1/3)
r1
r=r1[-6,]
r
ave=mean(r)
ave
slope=(n1[2,]-n1[1,])/(c[2,]-c[1,])
slope
r_cub=slope/(6.3*(10^21))
r_cub
r3=r_cub^(1/3)
r3
plot(c0,n0,"l",main="RADIUS OF GLYCEROL MOLECULE", xlab="concentration",ylab="Specific
Viscosity")
```

**2.2.1 Output of Glycerol molecule**

by R program
>ave=mean(r)
>ave ( Average of radius by calculation)
[1] 3.07019e-08 cm, or R= 3.07 $A^0$
>r3(radius by slope)
[1] 3.052678e-08 cm, or R= 3.05 $A^0$

**2.2.2 Molecular Radius of Dextrose and Sucrose**

Using same technique, we analyzes dextrose and sucrose molecule. Table2. Give the detailed about slope and molecular radius. Here we compared monosaccharide and polysaccharide sugar molecule at 298K temperature.

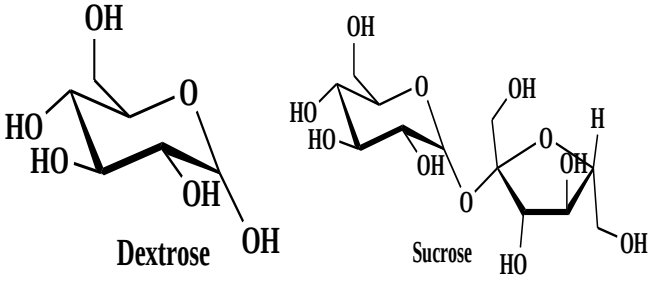


Fig.3 Dextrose and Sucrose molecule

**Table 2**

| Molecule | Slope | | Radius in $A^0$ | |
|---|---|---|---|---|
| | Exp. | Programme | Exp. | Programme |
| Dextrose | 0.195 | 0.195 | 3.32 | 3.32 |
| Sucrose | 0.6045 | 0.602 | 4.66 | 4.68 |

## 3. RESULT AND DISCUSSION

Using R-software, the radius of glycerol molecule obtain 3.07019 e-08 cm or 3.07 $A^0$ Computational value are equivalent to experimental result i.e. 3.0546 $A^0$. Similarly, radius of dextrose and sucrose molecule 3.32 and 4.68 $A^0$ respectively obtained and compare. It is observed that increase in monomer number molecular radius also increase. So computational method can be used for determine molecule radius of polymer system. Due to programming, we save chemical and time. Without chemical no waste produced that is why its ecofriendly.

## 4. CONCLUSION

The study has shown many of the highlights of R use in the Physical chemistry literature. These include modeling from to Determine Molecular Radius of Glycerol Molecule. Therefore, R Software Program gives the same value of Molecular Radius of Glycerol Molecule similar like experimental method. R software can use for the Determine Molecular Radius of various Molecule in Physical Chemistry. So This technique help for study of Molecular Radius of Glucose, Lactose, Sucrose, cellulose acetate, polystyrene, crap rubber, polyvinyl alcohol etc.

## REFERENCES

[1] Chambers, J. M., Programming with Data: a Guide to the S Languange. 3rd ed.; Springer-Verlag: New York, 1998; p 469
[2] Scot Mente , and Max Kuhn, The Use of the R Language for Medicinal Chemistry ApplicationsCurrent Topics in Medicinal Chemistry, 2012, 12, 1957-1964.
[3] Ertl P, Rhode B, Selzer P (2000). Fast Calculation of Molecular Polar Surface Area as a Sumof Fragment-Based Contributions and Its Application to the Prediction of Drug Transport Properties. Journal of Medicinal Chemistry, 43(20), 37143717.
[4] Grant, B. J.; Rodrigues, A. P. C.; ElSawy, K. M.; McCammon, J. A.; Caves, L. S. D., Bio3d: an R package for the comparative analysis of protein structures. Bioinformatics**2006,** 22 (21), 2695-2696.
[5] Guha, R., Generating, Using and Visualizing Molecular Information in R. R News **2006,** 6 (3), 28-33
[6] Stanley g. Schultz and a. K. Solomon. The journal of general physiology, 1191-1199.december 2, 1960.
[7] V.A.Bloomfield and R.K.DewanJ. Phys. Chem. 1971, 75, 20, 3113-3119
[8] S. Lorefice, F. Saba, The Italian primary kinematic viscosity standard: the viscosity scale, Measurement **112**, 18 (2017)