Thus, it can be concluded that the overall fatty acid distribution profile of the seed oils and polar lipids differed widely, but the fatty acids remained the same. The phospholipids and glycolipids have several biological functions.[6] This study aims to understand these functions in a better way and to give a quantitative dimension to them. The study agrees well with earlier studies on Kenaf,[5] Ritha[2] and Palm[6] oils.

ACKNOWLEDGEMENT

All the authors are thankful to Dr. B.R. Gaikwad, Bombay, for his help in carrying out GLC analysis of the methyl ester samples.

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Estimation of Solubility Parameter and Molar Volume Through Computer Programming

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Received 13 November 1995

A computer programme for calculation of solubility parameter and molar volume of liquids and solids is given. The programme written in BASIC is based on Fedors constants. It is user friendly and interactive.

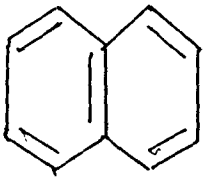
SOLUBILITY parameter, δ, is an intrinsic physicochemical property of a substance. In pharmacy, it has been used to explain drug action,[1] structure-activity relationship,[2,3] drug transport kinetics[4] and *in situ* release of theophyline.[5] Solubility parameters are used in polarity index scales for the solubilization of drugs in solvents and their mixtures[6] and are extensively in the selection of solvents for elution of drugs in HPLC.[7]

Note :Programme Package can be obtained by contacting the authors.

***For Correspondence**

The solubility parameter has been introduced to explain the behaviour of regular solutions.[8] The evaluation of solubility parameter for different substances has been reviewed.[9] A widely used indirect method for estimating the solubility parameter is based on the additive property of substituent constants.[10] Fedors method is the recent one and was evolved after extensive analysis of the earlier methods.[11,12] The advantage is that the method requires only a knowledge of the structural formula of the compound. As new drug molecules are being constantly introduced, there is a need for a simple computer programme for quick calculation of their solubility parameters and molar volumes. This paper describes one such effort.

According to the Fedors method a molecule is considered as a collection of different fragments (atoms/groups). Two parameters such as energy of vaporisation substituent constant (Δe) and molar volume (Δv) were assigned for each fragment. A total of 84 atom/group values were reported including several metals in organometalic compounds.[10] The computation method can be illustrated using naphthalene.[9] The Fedors approach to cyclic compounds was to open the rings, treat the resulting structure as an open chain compound, and then apply correction for ring closure.



Ring Opens to give

= HC–C–CH=CH–CH =
CH–CH–=CH–C–CH =

The solubility parameter is calculated as given in **Table 1**. The error estimated in this calculation is generally less than 10 percent. A programme is written in GWBASIC using a simple menu driven approach in which the user is guided through the options at every stage. The menu options are number coded. The user has only to enter the specific number code or a number to execute the programme at all stages. The programme can be run on any IBM PC- Clone (XT and above) loaded with MS - DOS 4.01 and above and A GWBASIC interpreter.

The programme is functional without spectacular display and frills of commercial packages. This programe was validated by taking a series of compounds having different functional groups. The calculated values using this packages agree well with the literature data **Table. 2**. Minor differences, if any, may be due to the inappropriate selection of fragments by the users of the package. Some groups such as in organometallics, could not be tested with this package due to lack of literature data for comparison. Since the algorithm is same for all groups, such compounds should also give appropriate values.

The input-output routine for computation begins with a Main Menu. The menu displays different groups such as hydrocarbon, aromatic and other common fragments made-up of one or more of oxygen, halogen, nitrogen, sulphur, phosphorus and metals. Choosing a particular group provides access for different fragments. For example, hydrocarbon group consists of fragments such as CH_3, CH_2, CH, C, = CH- etc. The group numbers and number of such groups available in the structure are the input for the calculation. The constants (heat of vaporisation and molar volume) for the groups/atoms were built in the programme. After the input of data for every fragment is completed, the solubility parameter value is displayed (output) with an option for printout. The printout for naphthalene is given below.

Name of the compound being studied: Naphthalene

GROUP	NO OF GROUP
-CH=	8
C=	2
Ring Clos (5 or 6)	2
Conjugation (each)	5

Sum of Energy of Vaporisation Substituent Constant: 12800 cal./mol.

Molar Volume: 118 cm3/mol.

Solubility Parameter :10.42 H

Table 1: Group Contribution Method for Calculating Molar Volume and Solubility Parameter of Naphthalene

Atom/Group	No. of[a] Groups, n	Δe^b	nXΔe	ΔV^b	nXΔV
(- CH =)	8	1030	8240	13.5	108.0
(- C =)	2	1030	2060	-5.5	-11.0
Ring closure (6 membered)	2	250	500	16.0	32.0
Conjugated double bonds	5	200	1000	-2.2	-11.0
			12800		118.0

[a]Obtained from open structure. [b] Taken from the Ref. 10. Solubility parameter $\delta = \sqrt{\frac{12800}{118.0}} = 10.42H$

Table 2: Solubility Parameter and Molar Volume of Different Compounds obtained using the Present Programme

Name of the compound	Solubility parameter, H Calc. (Lit.)	Molar volume ml/mole Calc. (Lit.)	Ref. No.
n - Phenylpiperazine	10.29 (10.3)	147.3 (147.3)	10
p - Hydroxybenzoic acid	15.33 (15.3)	90.4 (94.35)	13
Sulfadiazine	13.17 (13.17)	154.2 (154.2)	14
Sulfisomidine	12.58 (12.6)	183.2 (183.2)	14
Sulfathiazole	13.15 (13.1)	149.9 (150.1)	14
Sulfamethoxypyridazine	12.89 (12.9)	172.5 (172.5)	15
Physostigmine	10.65 (10.7)	215.9 (215.9)	16
Tolbutamide	10.78 (10.98)	211.2 (209.9)	16
Acetohexamide	11.46 (11.64)	237.5 (234.4)	16

The facilities of the present programme are as follows;

1. Specific instruction are available in the package explaining the system of breaking up of the structural formula into different atoms/groups, needed for the calculation.

2. A demonstration programme with six model compounds is included in the package, to make the use familiar with the package.

3. The display of the final result along with the input data on the screen permits quick verification and detection of errors in input.

4. The programme provides for a printout of the input data, solubility parameter and molar volume of the substance.

ACKNOWLEDGEMENTS

The authors thank Dr. C.V.S. Subrahmanyam, Professor, College of Pharmaceutical Sciences, Manipal for the help extended in this work.

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