*Dedicated to Professor Mircea Diudea*
*on the Occasion of His 65th Anniversary*

# QSPR STUDY ON TRANSITION TEMPERATURE OF TETRAPHENYLETHENE-DERIVED COLUMNAR LIQUID CRYSTALS

## ZOITA BERINDE[a,*], THOMAS DIPPONG[a], CLAUDIA BUTEAN[a]

**ABSTRACT.** The paper presents a study regarding the correlation of the transition temperature for nine derivatives of the tetraphenylethene, a class of columnar liquid crystals, with 35 molecular descriptors (22 topological indices and 13 Van der Waals parameters), calculated for these compounds. Their transition temperature was modelled in mono- and multivariate linear regression equations. In linear, simple correlations, 19 out of the 22 topological indices and 3 out of the 13 Van der Waals parameters show a correlation coefficient higher than 0,8; in multivariate linear correlations the results are even better, with correlation coefficients larger than 0,9.

*Keywords: correlation, columnar crystals, topological indices*

## INTRODUCTION

Derivatives of the tetraphenylethene are chemical compounds whose molecules have structural characteristics and features that include them in the columnar liquid crystals [1]. The transition temperature is an important physical property of liquid crystals in general and of thermotropic liquid crystals in particular, the derivatives of tetraphenylethene belonging to the latter category. Study of liquid crystals begun back in 1888, when Reinitzer [2] and Lehman [3] discovered that the cholesteryl benzoate presents, between solid and liquid phases, several intermediary stable phases, which are: anisotropic, just like

---

[a] *Technical University of Cluj-Napoca, Faculty of Sciences North University Center at Baia Mare, Department of Chemistry and Biology, 76 Victoriei Street, 430122 Baia Mare, Romania*
* *Corresponding Author: zoita_berinde@yahoo.com*

the solid crystals, and fluid, just like liquids. These intermediary stable phases have been called the "liquid crystal state". The liquid crystals, are, therefore, condensed fluid states with spontaneous anisotropy, also called mesophases while the molecules they discovered have been called mesogenic [4,5].

The number of studies and publications dealing with the mesogens and mesophases had continuously increased, especially after 1964, when Fergason [6] draws the attention upon the practical applications of liquid crystals: in the fabrication of alphanumeric and analog displayers, for the conversion of pictures to matrix type screens for showing the pictures [7,8], in the skin thermography and diagnosis, as solvents in UV, VIZ, RMN, RES spectroscopy, giving information about the bond length of the dissolved molecules [9,10] and many other uses.

By studying the relationship between the chemical structure and mesophases, Vorländer found that liquid crystal phases often occur within compounds with elongated and relatively rigid molecules, along their longitudinal axis [11], such as the tetraphenylethenes. Taking into account only the symmetry of their structure, Friedel [12,13] classified the liquid crystals into three important categories: nematic liquid crystals, cholesteric liquid crystals and smectic liquid crystals. By the shape of molecules, the liquid crystals can be divided into: calamitic liquid crystals (with fusiform molecules) and discotic liquid crystals (with disc-shaped molecules), as discovered by Chandrasekhar [14]. According to Friedel și Lawrance [15,16], liquid crystals may be: thermotropic (formed by temperature alteration) and lyotropic (formed by the alteration of their concentration in a solution). Thermotropic liquid crystals are important in fundamental research and technological applications while lyotropic crystals play an important role in biological systems [17]. The tetraphenylethene derivatives are thermotropic liquid crystals and belong to the disc-shaped molecules, for which the mesophase is characterized by the superposition of the discs in columns, wherefrom the name of columnar liquid crystals [18].

The temperature at which the transition, from the crystal state to the mesophase, is produced is often called melting point, and that of the transition, from the mesophase to the isotropic liquid, is called clarification point or clarification temperature [19]. The transition temperature is that at which the number of ordered subsystems equal the number of disordered ones.

This aim of present QSPR study is to find the best regression equations for predicting the transition temperature of columnar liquid crystals of the tetraphenylethene derivatives. In this respect, we calculated and tested 35 molecular descriptors: 22 topological indices and, respectively, 13 Van der Waals parameters. Next, the used descriptors were defined, the work methods described and the results discussed; at the end, conclusions were drawn.

### Topological molecular descriptors

#### *Wiener (W) and Polarity (P) indices:*

The Wiener index (W) can be defined as the half-sum of the entries $d_{ij}$ in the distance matrix associated to the molecular graph [20]:

$$W = \frac{1}{2} \cdot \sum_{i=1}^{n} \sum_{j=1}^{n} d_{ij} \tag{1}$$

The polarity index (P) has also been defined by Wiener in the same pioneering paper [20] and is obtained by summing up the number of atom pairs, separated by three edges, in a molecule:

$$P = \frac{1}{2} \cdot \sum_{i} d_{3,i} \tag{2}$$

#### *Gordon-Scantlebury Index ($N_2$):*

This index counts the number of two-edges paths $P_2$ in a molecular graph [21]:

$$N_2 = \sum_{i} (P_2)_i \tag{3}$$

#### *Zagreb ($M_1$ and $M_2$) Indices:*

Gutman and collabs. [22,23] proposed two indices based on the vertex degrees $\delta_i$, $\delta_j$:

$$M_1 = \sum_{i=1}^{n} (\delta_i)^2 \tag{4}$$

$$M_2 = \sum_{(i,j) \in E(G)} (\delta_i \cdot \delta_j) \tag{5}$$

#### *Connectivity indices:*

The original connectivity index was propodes by *Randić* [24] as:

$$^1\chi = \sum_{i,j} (\delta_i \cdot \delta_j)^{-\frac{1}{2}} \tag{6}$$

Balaban [25] extended the above definition by changing the vertex degree with the distance sum $D_i$, $D_j$:

$$J = \frac{q}{\mu+1} \cdot \sum (D_i \cdot D_j) \tag{7}$$

where q represents the number of edges, and μ is the cyclomatic number (μ=q-n+1, and n= no. atoms). By multiplying the local invariants ($D_i$) by the covalent radii, Mulliken's electronegativities and by Van der Waals radii, some extended indices $J^{rc}$, $J^{el}$, $J^{Rw}$ are obtained.

### *Kier and Hall Indices*

Kier and Hall [26] further generalized the *Randić*-type index:

$$^m\chi = \sum_r (\delta_1 \cdot \delta_2 \cdot ... \cdot \delta_{m+1})^{-\frac{1}{2}} \tag{8}$$

where *r* represents all the possible *m* lenght ways in the molecular graph.

In the following, we used, for the Kier-Hall versions only sequences containing at most 3 bonds, as shown below:

$$^2\chi = \sum_{r=2} (\delta_i \cdot \delta_j \cdot \delta_k)^{-\frac{1}{2}} \tag{9}$$

$$^3\chi = \sum_{r=3} (\delta_i \cdot \delta_j \cdot \delta_k \cdot \delta_l)^{-\frac{1}{2}} \tag{10}$$

$$^2J_p = \frac{q}{\mu+1}\sum_{r=2} (d_i \cdot d_j \cdot d_k)^{-\frac{1}{2}} \tag{11}$$

$$^3J_p = \frac{q}{\mu+1}\sum_{r=3} (d_i \cdot d_j \cdot d_k \cdot d_l)^{-\frac{1}{2}} \tag{12}$$

The D index (average square distance) was also calculated:

$$D = (\sum_i \sum_j d_{ij}^{\,2})^{-\frac{1}{2}} \tag{13}$$

Based on these data, the indices $\chi D^{el}$, $JD^{el}$ were calculated for Mulliken's electronegativities, the indices $\chi D^{rc}$ şi $JD^{rc}$ for the covalent radii, and, respectively, the indices $\chi D^{Rw}$, $JD^{Rw}$ for van der Waals radii.

### *Van der Waals parameters*

The volume and surface of the molecules may be computed based on the 3D cartesian coordinates and they bring information regarding the dimension and shape of three-dimensional molecules. The most frequently used Van der Waals parameters are van der Waals radius ($R^w$), van der Waals volume ($V^w$) and van der Waals surface ($S^w$). The 2 latter parameters are obtained using the Monte Carlo method [27,28], but can also be calculated analytically [29]. The atoms are considered to be spherical, incompressible, with a radius equal to Van der Waals radius [30] while de molecules are assimilated to spheres having the same radii as Van der Waals radii of the constitutive atoms.

The distance at which the antagonist attraction and rejection foreces are balanced is called *van der Waals ($R^w$) radius.* The steric effects are usually ascribed to the repulsive forces that occur when direct, non-bound atoms get close to a shorter distance than the sum of the Van der Waals radii ($R^w$), which leads to the appearance of a compression.

*The Van der Waals Molecular Volume ($V^W$)* represents the volume sum of the spheres of constitutive atoms of the considered molecule. The van der Waals molecular volume ($V^W$) is a useful parameter in the studies regarding the packing density of organic compounds in crystal structures and in many other studies that describe the molecule structure [30]. *The van der Waals surface* ($S^w$), represents the molecular surface related to a Van der Waals volume ($V^W$).

Sometimes it is helpful to analyse the ratio $V^w/S^w$, which has the measurement units of a length; also, the parameters of the ellipsoid about which the molecule is circumscribed. The semi-axes of such an ellipsoid defined within the approximation of hard spheres, characterize the globularity of the molecule:

$$GL1 = V^{SF}/V^W \tag{14}$$
$$GL2 = V^{SF}/V^{EL} \tag{15}$$

The ellipsoid and the three parameters that describe it (i.e., its semi-axes, $E_X$, $E_Y$, $E_Z$) represent indices of the molecular shape and can be used in QSAR studies [30].

Two other parameters, that define the molecular geometry can be calculated: (i) the ellipsoidal globularity degree ($GL_{EL}$), as the ratio of the volume of the ellipsoid ($V^{EL}$) that cirscumscribes about the molecule to the volume of the sphere ($V^{SF}$) with the same radius as the longest semi-axis of the ellipsoid (relation 16); and (ii) the degree of volume globularity (GLOB), as the ratio of the Van der Waals volume ($V^W$) to the sphere volume ($V^{SF}$) (relation 17).

$$GL_{EL} = V^{EL}/V^{SF} \tag{16}$$
$$GLOB = V^W/V^{SF} \tag{17}$$

## RESULTS AND DISCUSSION

The values of Pearson`s correlation coefficient R, resulted from the linear correlation tests, between the transition temperature $T_z$ and each of the 35 molecular descriptors are shown in Table 1. The positive value of the correlation coefficient R, in all cases, shows that the transition temperature increases when the value of the molecular descriptor increases.

In case of topological indices, most of them are correlated to the transition temperature, having the correlation coefficient R about 0.82 (excepting only Balaban's index [2]J, with R=0.5189, Wiener's index, where R=0.7392 and Balaban's [3]J with R= 0.7148 – not included in Table 1). The best correlation, R = 0.8712, was found in case of Balaban's index, weighted by the Mulliken electronegativities, symbolized by $J^{el}$.

The values of the correlation coefficient R > 0,8 in case of the Van der Waals molecular volume ($V^W$) and Van der Waals surface (Sw), proves the existence of a correlation between the transition temperature and these parameters, correlation that is improved when using the ratio $V^w/S^w$. The bigger the volume of the molecule is, the higher its transition temperature. It is interesting that amongst the three semi-axes of the ellipsoid circumscribed about the molecular aggregate, only the semi-axis EY has a correlation coefficient > R=0.7609, which shoes a significant relationship with the transition temperature.

The best statistical parameters were obtained in the case of the transition temperature modelling by a simple linear equation using the ratio of Van der Waals volume to the corresponding surface (relation 18). It should be noted that using this ratio we get an improvement of the quality of regression using the Van der Waals volume (0.8261) or surface (0.8258) as independent variables. The best thre monovariate linear equations that model the transition temperature are as follows:

**Table 1.** Statistics of the monovariate regression equations

| X | Statistics | | | X | Statistics | | |
|---|---|---|---|---|---|---|---|
| | R | F | s | | R | F | s |
| $V^W$ | 0.826 | 15.044 | 25.6 | $\chi^{el}$ | 0.826 | 15.143 | 25.6 |
| $S^W$ | 0.825 | 15.018 | 25.6 | $\chi^{Rw}$ | 0.836 | 16.332 | 24.9 |
| $E_Y$ | 0.760 | 9.630 | 29.5 | $\chi D^{rc}$ | 0.844 | 17.477 | 24.3 |
| $V^W/S^W$ | 0.885 | 25.421 | 21.1 | $\chi D^{el}$ | 0.836 | 16.255 | 24.9 |
| N2 | 0.849 | 18.189 | 24.0 | $\chi D^{Rw}$ | 0.832 | 15.811 | 25.2 |
| P | 0.864 | 20.792 | 22.8 | $J^{rc}$ | 0.850 | 18.319 | 23.9 |
| M1 | 0.843 | 17.300 | 24.4 | $J^{el}$ | 0.871 | 22.064 | 22.3 |
| M2 | 0.852 | 18.600 | 23.8 | $J^{Rw}$ | 0.852 | 18.625 | 23.8 |
| $^1\chi$ | 0.835 | 16.119 | 25.0 | $JD^{rc}$ | 0.830 | 15.543 | 25.3 |
| $^2\chi$ | 0.840 | 16.781 | 24.7 | $JD^{el}$ | 0.853 | 18.856 | 23.7 |
| $^3\chi$ | 0.832 | 15.811 | 25.2 | $JD^{Rw}$ | 0.861 | 20.115 | 23.1 |
| $\chi^{rc}$ | 0.837 | 16.445 | 24.8 | X = Independent variable | | | |

$$T_z = -4424.59 + 5576.456\ V^W/S^W \tag{18}$$
$$R = 0.885\ \ s = 21.1\ \ F = 25.422$$

$$T_z = 462.232 - 3011.261\ J^{el} \tag{19}$$
$$R = 0.871\ \ s = 22.3\ \ F = 22.064$$

$$T_z = 456.366 + 869.326\ JD^{RW} \tag{20}$$
$$R = 0.861\ \ s = 23.144\ \ F = 20.116$$

In general, an improvement of the correlation coefficient may be found as the number of predictor variables increases. However, if the number of predictor variables is larger than the number of observations, chance correlations may occur. In our study, we considered two, three and four predictor variables. When the two predictor variables are topological indices, the correlation coefficient does not exceed 0.9:

$$T_z = 351.214 + 2815.676\ ^2J - 2730.661\ J^{el} \qquad (21)$$
$$R = 0.891\ \ s = 22.3\ \ F = 11.55$$

In case of Van der Waals parameters, in several combinations, the correlation coefficient exceeds 0,92. From a statistical point of view, the best bi-variable regression equation is:

$$T_z = -7997.780 + 9897.055\ V^W/S^W + 0.009\ V^{EL} \qquad (22)$$
$$R = 0.950\ \ s = 15.4\ \ F = 27.55$$

This correlation coefficient is slightly improved when three predictor variables are used, especially those belonging to the category of Van der Waals parameters:

$$T_z = -9303.279 + 1139.967 V^W/S^W + 0.007 V^{EL} + 5.811 E_Y \qquad (23)$$
$$R = 0.954\ \ s = 16.07\ \ F = 17.068$$

When we use the predictor variables from the topological indices category, the highest correlation coefficient is 0.9474, lower than in the previous case, but higher than in the case of topological indices bi-variable correlation:

$$T_z = 1444.9 + 11.3 \cdot {}^1\chi + 7291.9 \cdot J^{rc} - 98426.5 \cdot J^{el} \qquad (24)$$
$$R = 0.947\ \ s = 17.24\ \ F = 14.615$$

Adding another predictor variable, from both the Van der Waals parameter category and the topological indices category, leads to a very slight increase of the correlation coefficient value:

$$T_z = 1054.997 + 18600.248 \cdot {}^2J - 12.971 N_2 - 25482.873 \cdot J^{el} + 19.128\ P \qquad (25)$$
$$R = 0.958\ \ s = 17.23\ \ F = 11.221$$

$$T_z = -10615.02 + 12848.2 V^W/S^W + 6.39 \cdot E_Y + 0.011 V^{EL} + 837.8\ GLOB \qquad (26)$$
$$R = 0.960\ \ s = 16.89\ \ F = 11.72$$

The correlation coefficient $R$ increases when using more independent variables but the system could become over-estimated. In such situations, Topliss and Costello [31] recommend the use of two independent variables for a small number of values for the dependent variable, e.g., $T_z$. In order to exclude the chance correlation, in the case of equations 25 and 26 (with four variables), we applied the "random test" which assumes the random mixture of the values of $T_z$ and then the computation of the corresponding correlation coefficients, which are given in Table 1a.

**Table 1a.** Random mixed Y values

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | (25) | (26) |
|---|---|---|---|---|---|---|---|---|------|------|
| 37 | 29 | 139 | 40 | 34 | 47 | 126 | 55 | 101 | 0.665 | 0.806 |
| 55 | 29 | 101 | 37 | 34 | 40 | 126 | 139 | 47 | 0.415 | 0.787 |
| 40 | 29 | 37 | 139 | 55 | 126 | 101 | 34 | 47 | 0.652 | 0.503 |
| 40 | 34 | 37 | 47 | 126 | 55 | 29 | 139 | 101 | 0.598 | 0.869 |
| 55 | 47 | 29 | 40 | 126 | 34 | 101 | 37 | 139 | 0.559 | 0.724 |
| 29 | 40 | 55 | 101 | 47 | 126 | 34 | 37 | 139 | 0.578 | 0.449 |
| 37 | 34 | 29 | 101 | 139 | 40 | 126 | 47 | 55 | 0.617 | 0.591 |
| 40 | 34 | 37 | 139 | 47 | 55 | 101 | 126 | 29 | 0.571 | 0.648 |
| 126 | 55 | 34 | 139 | 40 | 37 | 29 | 101 | 47 | 0.520 | 0.675 |

In our study, we determined a number of lienar regression relations: among these, the best statistics is provided by equation (22), with: R = 0.950; s = 15.4; F = 27.55. This equation shows the lowest standard error of estimate, s, that is a strong requirement for a statistical model.

## CONCLUSIONS

The results herein reported show that, a part of the tested Van der Waals parameters and all topological descriptors considered, are correlated with the transition temperature of the derivatives of tetra-phenylethene of the columnar liquid crystals.

The statistical quality of the simple or multiple regression models, recommends the used descriptors (Van der Waals- type descriptors and topological indices, respectively) to predict the transition temperature of columnar liquid crystals.

Including the descriptors concerning the molecular flexibility, electronegativities of the constitutive atoms or the atom size, by covalent radii or Van der Waals radii, led to the improvement of statistical parameters of the models.

## EXPERIMENTAL SECTION

In our study we had in mind four main directions:

1. Drawing, by means of the Hyperchem software, of the 9 structures (S1-S9), standing for the tetraphenylethene derivatives which belong to the category of columnar liquid crystals. Figure 1 illustrates the general structure of this category of liquid crystals, detailed in Table 2.
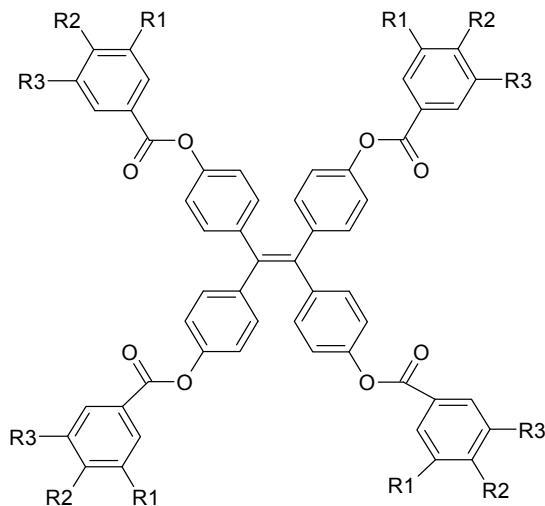


**Figure 1.** General structure of columnar crystals

**Table 2.** R1, R2 and R3 radicals for 9 compounds (S1-S9)

| Compound | R1 | R2 | R3 | $T_z$ (℃) |
|---|---|---|---|---|
| S1 | H | $OC_{10}H_{21}$ | H | 139 |
| S2 | $OC_{10}H_{21}$ | $OC_{10}H_{21}$ | H | 101 |
| S3 | $OC_5H_{11}$ | $OC_5H_{11}$ | $OC_5H_{11}$ | 126 |
| S4 | $OC_6H_{11}$ | $OC_6H_{13}$ | $OC_6H_{13}$ | 55 |
| S5 | $OC_7H_{15}$ | $OC_7H_{15}$ | $OC_7H_{15}$ | 37 |
| S6 | $OC_8H_{17}$ | $OC_8H_{17}$ | $OC_8H_{17}$ | 47 |
| S7 | $OC_9H_{19}$ | $OC_9H_{19}$ | $OC_9H_{19}$ | 40 |
| S8 | $OC_{10}H_{21}$ | $OC_{10}H_{21}$ | $OC_{10}H_{21}$ | 29 |
| S9 | $OC_{12}H_{25}$ | $OC_{12}H_{25}$ | $OC_{12}H_{25}$ | 34 |

The transition temperatures $T_z$ (℃) of the 9 tetraphenylethene derivatives, were taken from Schultz's work2001 [32].

2. The values of the calculated 35 molecular descriptors (22 topological indices and 13 Van der Waals parameters), for each of the considered 9 structures are given in Tables 3, 3a and 3b and Tables 4 and 4a.

**Table 3.** Topological indices

| Sample | W | N2 | P | M1 | M2 | $^1\chi$ | $^2\chi$ | $^3\chi$ |
|--------|-----|-----|-----|-----|------|---------|---------|---------|
| S1 | 95417 | 130 | 152 | 510 | 573 | 48.100 | 36.412 | 21.967 |
| S2 | 220861 | 178 | 208 | 694 | 769 | 69.895 | 52.183 | 32.952 |
| S3 | 145589 | 166 | 204 | 638 | 725 | 61.690 | 46.886 | 28.612 |
| S4 | 183473 | 178 | 216 | 686 | 773 | 67.690 | 51.129 | 31.612 |
| S5 | 227209 | 190 | 228 | 734 | 821 | 73.690 | 55.371 | 34.612 |
| S6 | 277205 | 202 | 240 | 782 | 869 | 79.690 | 59.614 | 37.612 |
| S7 | 333869 | 214 | 252 | 830 | 917 | 85.690 | 63.856 | 40.612 |
| S8 | 397609 | 226 | 264 | 878 | 965 | 91.690 | 68.099 | 43.612 |
| S9 | 547949 | 250 | 288 | 974 | 1061 | 103.690 | 76.584 | 49.612 |

**Table 3a.** Topological indices (continuation)

| Sample | $\chi^{rc}$ | $\chi^{el}$ | $\chi^{Rw}$ | $\chi D^{rc}$ | $\chi D^{el}$ | $\chi D^{Rw}$ |
|--------|---------|--------|---------|---------|---------|---------|
| S1 | 64.720 | 2.234 | 26.959 | 16.619 | -45.866 | -21.141 |
| S2 | 93.442 | 4.849 | 39.902 | 23.546 | -65.046 | -29.992 |
| S3 | 83.203 | 3.704 | 35.199 | 21.513 | -57.985 | -26.491 |
| S4 | 90.995 | 4.456 | 38.728 | 23.305 | -63.233 | -28.961 |
| S5 | 98.787 | 5.208 | 42.257 | 25.097 | -68.481 | -31.432 |
| S6 | 106.58 | 5.960 | 45.787 | 26.889 | -73.729 | -33.902 |
| S7 | 114.372 | 6.712 | 49.316 | 28.681 | -78.978 | -36.373 |
| S8 | 122.164 | 7.464 | 52.846 | 30.474 | -84.226 | -38.844 |
| S9 | 137.748 | 8.967 | 59.905 | 34.058 | -94.722 | -43.785 |

**Table 3b.** Topological indices (continuation)

| Sample | $^2J$ | $^3J$ | $J^{rc}$ | $J^{el}$ | $J^{Rw}$ | $JD^{rc}$ | $JD^{el}$ | $JD^{Rw}$ |
|--------|-------|--------|-------|-------|-------|-------|--------|--------|
| S1 | 0.027 | 0.0007 | 1.149 | 0.104 | 0.517 | 0.278 | -0.766 | -0.353 |
| S2 | 0.024 | 0.0005 | 1.339 | 0.120 | 0.603 | 0.325 | -0.893 | -0.410 |
| S3 | 0.031 | 0.0007 | 1.457 | 0.128 | 0.655 | 0.359 | -0.969 | -0.442 |
| S4 | 0.029 | 0.0006 | 1.481 | 0.131 | 0.666 | 0.364 | -0.986 | -0.451 |
| S5 | 0.027 | 0.0006 | 1.504 | 0.134 | 0.676 | 0.368 | -1.001 | -0.458 |
| S6 | 0.026 | 0.0005 | 1.525 | 0.136 | 0.686 | 0.372 | -1.016 | -0.466 |
| S7 | 0.024 | 0.0005 | 1.545 | 0.138 | 0.695 | 0.376 | -1.029 | -0.472 |
| S8 | 0.023 | 0.0004 | 1.563 | 0.140 | 0.703 | 0.380 | -1.042 | -0.479 |
| S9 | 0.021 | 0.0003 | 1.595 | 0.144 | 0.718 | 0.386 | -1.064 | -0.490 |

**Table 4.** Van der Waals Parameters

| Sample | $V^W$ | $S^W$ | $V^{SF}$ | $S^{SF}$ | $V^{EL}$ | $E_X$ |
|--------|-------|-------|----------|----------|----------|-------|
| S1 | 1414.894 | 1732.120 | 63806.6 | 7721.965 | 6816.521 | 24.789 |
| S2 | 2115.972 | 2623.446 | 70800.47 | 8276.401 | 11355.38 | 25.663 |
| S3 | 1807.141 | 2222.947 | 30794.91 | 4751.201 | 5956.107 | 19.444 |
| S4 | 2006.938 | 2481.165 | 37366.59 | 5405.133 | 6803.804 | 20.740 |
| S5 | 2209.620 | 2743.427 | 43134.60 | 5947.959 | 7859.230 | 21.756 |
| S6 | 2411.699 | 3003.459 | 51191.36 | 6667.278 | 11290.38 | 23.034 |
| S7 | 2613.578 | 3260.065 | 59358.21 | 7358.760 | 13228.16 | 24.199 |
| S8 | 2806.754 | 3521.798 | 70808.77 | 8277.049 | 14656.55 | 25.665 |
| S9 | 3216.908 | 4036.716 | 92594.17 | 9897.828 | 15677.04 | 28.065 |

**Table 4a.** Van der Waals Parameters (continuation)

| Sample | $E_Y$ | $E_Z$ | GLOB | GL1 | GL2 | $GL_{EL}$ | $V^W/S^W$ |
|--------|-------|-------|------|-----|-----|-----------|-----------|
| S1 | 15.140 | 4.336 | 0.099 | 45.096 | 4.458 | 4.818 | 0.817 |
| S2 | 20.729 | 5.096 | 0.094 | 33.460 | 3.155 | 5.367 | 0.807 |
| S3 | 16.834 | 4.344 | 0.125 | 17.041 | 2.137 | 3.296 | 0.813 |
| S4 | 17.856 | 4.386 | 0.117 | 18.619 | 2.178 | 3.390 | 0.809 |
| S5 | 19.554 | 4.411 | 0.111 | 19.521 | 2.168 | 3.557 | 0.805 |
| S6 | 20.063 | 5.833 | 0.105 | 21.226 | 2.22 | 4.682 | 0.803 |
| S7 | 21.467 | 6.079 | 0.099 | 22.711 | 2.257 | 5.061 | 0.802 |
| S8 | 22.341 | 6.102 | 0.093 | 25.228 | 2.35 | 5.222 | 0.797 |
| S9 | 24.597 | 5.422 | 0.085 | 28.784 | 2.452 | 4.873 | 0.797 |

3. Correlation analysis was performed by Pearson's linear correlation. The results are listed in Tables 1 and 1a and equations (18) to (26), as above discussed.

# R E F E R E N C E S

1. A. Shulty, S. Diele, S. Laschat, "Novel columnar tetraphenylethenes", Tehnische Universitat Braunschweig, **1998**.
2. S. Laschat, *Beilstein J Org Chem*, **2009**, *5*, 48.
3. I. Sage, *Liquid Crystals*, **2011**, *38*, 1551.
4. A. Dequidt, P. Oswald, *The European Physical Journal E*, **2007**, *24*, 157.
5. Y. Chen, F. Peng, T. Yamaguchi, X. Song, S-T. Wu, *Crystals*, **2013**, *3*, 483.

6. Patent US 3114836 A, **1963**, Inventor: Fergason James.
7. G. Singh, G.V. Prakash, A. Choudhary, *Physica B*, **2010**, *405*, 2118.
8. I. Abdulhalim, R. Moses, R. Sharon, *Acta Physica Polonica A,* **2007**, **112**, 715.
9. B. Stevensson, A.Marini, H. Zimmermann, A. Maliniak, *J. Phys. Chem. B*, **2011**, *115* (23), 7561.
10. E. Westphal, M. Prehm, I.H, Bechtold, C Tschierskeb, H, Gallardo *J. Mater. Chem. C*, **2013**, *1*, 8011.
11. S. Yilmaz, H. Melik, F. Angay, M. Emek, A. Yildirim, *Journal of Modern Physics*, **2011**, *2*, 248.
12. S. Chandrasekhar, "Liquid Crystals", Cambridge University Press, **1992**.
13. D. Demus, J.W.G. Goodby, G.W. Gray, H.W. Spiess, "Handbook of Liquid Crystals", Wiley-VCH, **1998**.
14. S. Chandrasekhar, B.K. Sadashiva, K.A. Suresh, *Pramana,* **1977**, *9*, 471-480
15. D. Jurašin, M. Vinceković, A. Pustak, I. Šmit, M. Bujan, *Soft Matter*, **2013**, *9*, 3349.
16. M.R. Alcantara, E.G. Fernandes, *J. Phys*., **2002**, *2*, 32.
17. I. Dumitraşcu, D.O. Dorohoi, „Proprietăţi optice ale mediilor cu ordonare parţială. Aplicaţii", Editura Tehnopres, Iaşi, **2009**.
18. H. Bock, *Columnar Liquid Crystals*, **2001**, 355.
19. Britannica Concise Encyclopedia, Encyclopædia Britannica Inc., **2006**.
20. H. Wiener, *J. Amer. Chem. Soc.*, **1947**, *69*, 17.
21. M. Gordon, G.R. Scantlebury, *Trans. Faraday Soc.,* **1964**, *60*, 604.
22. I. Gutman, N. Trinajstić, *Chem. Phys. Lett.*, **1972**, *17*, 535.
22. I. Gutman, I. Rusćić, N. Trinajstić, C.F. Wilkox, Jr., *J. Chem. Phys.,* **1975**, *62*, 3339.
23. M. Randić, *J. Amer. Chem. Soc.,* **1975**, *97*, 6609.
25. A.T. Balaban, L.V. Quintas, MATCH *Commun. Math. Comput. Chem.,* **1983**, *14*, 213.
26. L.B. Kier, L.H. Hall, "Molecular Connectivity in Chemistry and Drug Research"*,* Acad. Press, **1976**.
27. A. Tkatchenko, M. Scheffler, *Physical Review Letters*, **2009**, *102*, 073005.
28. A. Schultz S. Laschat, S Diele, M. Nimtz, *European Journal of Organic Chemistry*, **2003**, *15*, 2829.
29. A. Schultz, S. Diele, S. Laschat, M. Nimtz, *Advanced Functional Materials*, **2001**, *11* (6), 441.
30. D. Ciubotariu, M. Medeleanu, V. Vlaia, T. Olariu, C. Ciubotariu, D Dragoş, C. Seiman, *Molecules*, **2004**, *9*, 1053.
31. J.G. Topliss, R.J. Costello, *J. Med. Chem*., **1972**, 1066.
32. A. Schultz, S. Diele, S. Laschat, M. Nimtz, *Adv. Funct. Mater*., **2001**, *11* (6), 441.