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**Quantitative Correlation of Randić Indices and Adjacency Matrixes With  
Dewar Resonance Energy of Annulene Compounds**

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**ABSTRACT**

Topological indices are the numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. Graph theory is a delightful playground for the exploration of proof techniques in Discrete Mathematics and its results have applications in many areas of sciences. One of the useful indices for examination of structure-property relationship is Randić index. In this study, is represented the relationship between the Randić index and the determinants of the adjacency matrix to the Dewar resonance energy (DRE) of annulene compounds by using ab-initio calculations (B3LYP/6-31G\*). The alternative double bonds and conjugation are one of the main properties in annulene compounds. DRE is the quantity which allows one to account for the effects of cyclic electron delocalization and thus serves as a measure of the aromatic stabilization of an annulene molecular entity. For calculation the Dewar resonance energy (DRE) of the compounds could use the equation of DRE. The interesting results of concerning among DRE and the above indices are presented.

**Keywords:** Molecular topology; Randić index; Annulene Compounds; Dewar resonance energy; Adjacency matrix ;Ab-initio calculation.

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## INTRODUCTION

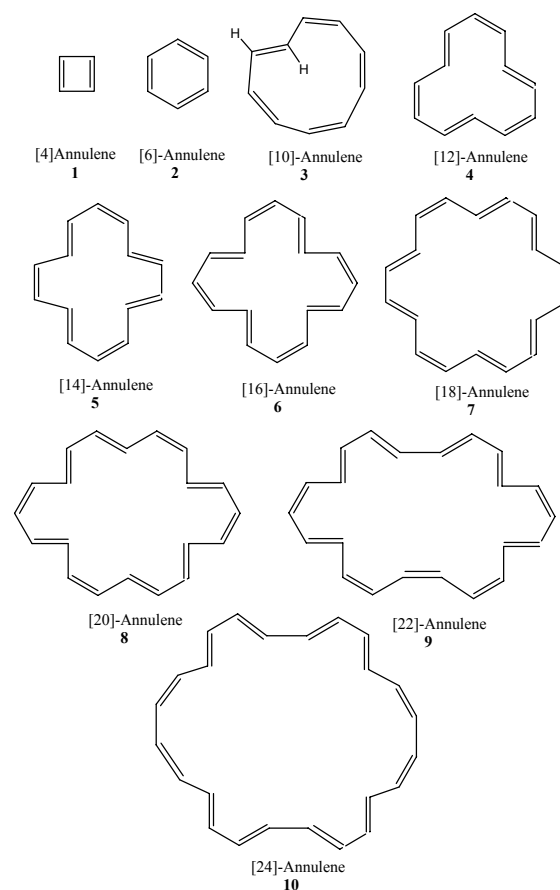
Topological resonance energy (TRE) scheme rests on the formalism of Graph theory. This theory provides the useful natural mathematical frameworks for the quantitative codification of classical chemical bonding ideas. Graph theory is an attractive field for the exploration of proof techniques in Discrete Mathematics and its results have applications in many areas of sciences. A graph is a topological concept rather than a geometrical concept of fixed geometry, and hence Euclidean metric lengths, angles and three-dimensional spatial configurations have no meaning. Graph theory provides many different methods of characterizing chemical structures numerically. Graph theory has been found to be a useful tool in QSAR (Quantitative Structure Activity Relationship) and QSPR (Quantitative Structure Property Relationship).<sup>1-6</sup> One of the stages of topological indices (TI) started in 1975, when M. Randić introduced the molecular branching index that has become one of the most widely used in both QSAR and QSPR studies.<sup>7</sup> QSAR are mathematical models designed for the correlation of various types of physicochemical properties with electronic and other factors of a molecular structure of a given series of compounds. The TIs are based on the original idea of Randić of molecular branching but extended to account for contributions coming from path clusters, clusters and chains of different lengths.<sup>8-15</sup>

It needs to use the effective and useful mathematical methods for making good concern between several data properties of chemicals. One of the indices in graph theory is adjacency matrix,<sup>1,16-20</sup> the determinants of which can serve as TIs. The numerical basis for topological indices is provided (depending on how a molecular graph is converted into a numerical value) by either Randić indices and the adjacency matrixes.

In this study, the relationship of Randić index and the determinants of the adjacency matrixes

det(A) with the Dewar resonance energy (DRE) will be considered for the annulene compounds "C<sub>n</sub>H<sub>n</sub>" (1-10) by the use of ab-initio calculations. See Fig.-1.

The general name annulene is sometimes given to rings that contain alternating single and double bonds in a single Lewis structure. The alternative double bonds and conjugation in the compounds 1-10 make some of the main properties in these compounds such as anisotropic magnetic field in explanation of chemical shifts in NMR spectroscopy of annulene compounds and Hückel aromaticity properties.



**Fig.1.** The structural shapes of [4]- to [24]-Annulenes. Compounds 1-10.

[4]Annulene is the smallest member of this group. It has  $4\pi$  electrons in its structure. It is a Möbius system ( $4n$ ). The famous member of annulenes is benzene with 6 electrons in its conjugated  $\pi$ -system. This molecule is a Hückel aromatic system ( $4n+2$ ). Although, [8]annulene has alternative C=C bonds, but because of the non planar form, in this study was ignored. [10]Annulene has three configuration and one of them that has a trans C=C, is more stable than the other structural forms. [14]Annulene has 14 electrons in its conjugated  $\pi$ -system, so it should have some aromatic character. The hydrogens on the outside of the ring appear downfield in the NMR spectrum at 7.6 ppm, whereas the hydrogens inside the ring appear at 0.0 ppm. Steric interactions among the endo hydrogen atoms destabilize this compound and make it quite reactive. View a space-filling model to see the steric restraint caused by these Hs. It has many characteristics of an aromatic compound, including an aromatic ring current. [18]Annulene fits the  $4n+2$  rule and should have some aromatic character. It has an aromatic ring current. The exo Hs appear at 9 ppm in its NMR spectrum, whereas the endo Hs appear at the high field position of -3 ppm. [24]Annulene similar to [16]annulene has no any Hückel aromatic characters. The bonds in both two annulenes are alternate with different bond length of C-C and C=C.<sup>21-23</sup>

Hückel theory to predict that aromatic  $C_nH_n$  [n]-annulenes ( $4n+2$  systems) exhibit novel properties, starting with  $n=34$  was used by Longuet-Higgins and Salem.<sup>22,23</sup> Choi and Kertesz used the density functional theory (DFT) for demonstration that the delocalization of aromatic  $C_nH_n$  annulene ( $4n+2$ ) remains.<sup>22,24</sup> Larger aromatic annulenes have an increasing bond alternation which converges to 0.06 Å.<sup>22</sup> Möbius system annulenes ( $4n$ ), have bond-alternated structures from  $C_4H_4$  in the series of these compounds. One of the properties could be computed using the various types of resonance energy methods is delocalization energy of electrons. For calculation of the delocalization energy of compounds (**1-10**) was utilized the

concepts of the Dewar resonance energy (DRE) and its equation. (See Eq.-4).<sup>26-35</sup>

### MATHEMATICAL METHODS:

The basis of the Topological Resonance Energy (TRE) rests on the formalism of graph theory. A characteristic polynomial is constructed for the reference structure with the graphs for the given molecule taken into account. The branching index that was introduced by M. Randić is defined as the sum of certain bond contributions calculated from the degree of the bonds suppressed molecular graphs. These bond contributions, named  $C_{ij}$  are calculated as:

$$C_{ij} = (\delta_i \delta_j)^{-0.5} \quad (\text{Eq.-1})$$

Here,  $\delta_i$  is the degree of the vertex representing atom "i", i.e., the number of bonds incident to this atom. Accordingly, the Randić index is defined as<sup>1,7,36</sup>:

$$\chi = \sum C_{ij} = \sum (\delta_i \delta_j)^{-0.5} \quad (\text{Eq.-2})$$

Where the summation is carried out over all the bonds of simply conjugated annulenes (**1-10**). The inverse squared-root of the vertex degree is identified here as a measure of the relative accessible perimeter of an atom from the outside. These perimeters, which have length units, are proposed to be measured in a new unit called the Randić index ( $\chi$ ). On this basis, the bond contributions to the Randić index are relative areas of bond accessibility from the environment.

For the each carbon atoms in the rings of annulene compounds **1-10**, the Randić indices are:  $C = 1/(3 \times 3)^{0.5}$ . On the basis, the final equation for calculating the Randić indices of the [n]-annulenes " $C_nH_n$ " is:

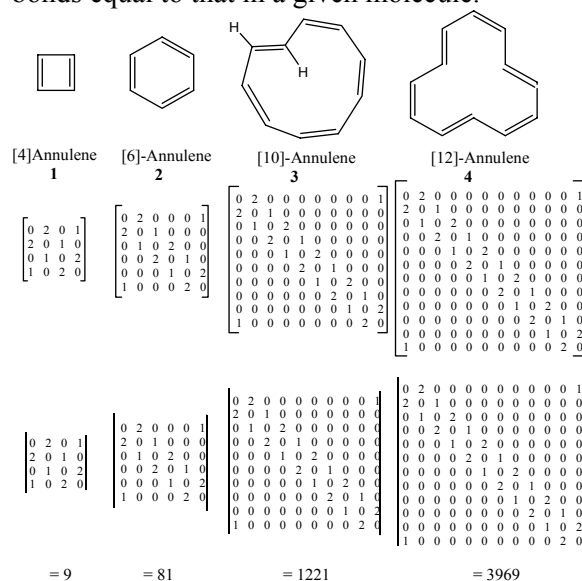
$$\chi = n[1/(3 \times 3)^{0.5}] \quad (\text{Eq.-3})$$

In this equation the number of carbon atoms is introduced by "n".

The adjacency matrixes is defined such that each element  $a_{ij}$  equals "1", if and only if atoms "i" and "j" are adjacent (i.e., bonded to each other) while all other  $a_{ij}$ 's equal zero. In the [n]-annulenes, because of the double bonds between atoms "i" and "j" (adjacent atoms), the  $a_{ij}$  equals to "2".<sup>1,16-20</sup> Some of the adjacency

matrixes for annulenes were identified in Fig.-2. (See Table-1 and Table-2).

The various types of Resonance Energy (RE) methods include the part of the total energy due to electron delocalization. To find the value of the resonance energy (RE), the difference must be calculated between a quantity characterizing experimentally determined energy of a given molecule (such as heat of atomization or heat of formation) and the same characteristic obtained with the aid of an additive scheme, e.g. sum of the bond energies (thermo chemical resonance energy). When the total energy or the heat of formation (atomization) is calculated with use of quantum mechanical methods, the RE value is referred to as the Quantum Mechanical Resonance Energy (QMRE). Various schemes for the determination of QMRE are distinguished by the choice of the reference structure which should have non-interacting  $\square$ -bonds. The Dewar Resonance Energy (DRE) is the quantity which allows one to account for the effects of electron delocalization and thus serves as a measure of the stabilization of an annulene (**1-10**) molecular entity. The model reference structure is not a system of isolated  $\square$ -bonds (as is the case for "Hückel Resonance Energy" HRE ), but a hypothetical annulene with the number of the  $\square$ - and  $\square$ -bonds equal to that in a given molecule.



**Fig.2.** Some of the adjacency matrixes and the solved determinants of annulenes.

The condition of the additivity of bond energies for annulenes (**1-10**) is adopted.<sup>26-35</sup>

For calculation of the Dewar Resonance Energy of compounds (**1-10**) could utilized the Eq.-4 :

$$\text{DRE} = \Delta H_f^{\text{loc.}} - \Delta H_f \quad (\text{Eq.-4})$$

Here,  $\Delta H_f^{\text{loc.}}$  is the calculated heat of formation of a given conjugated molecule and  $\Delta H_f$  is the heat of formation for the reference structure. It is demonstrated that for calculation the heat of formation of the annulenes (**1-10**) could use from a simple summation type function of the number of bonds in (**1-10**).<sup>26,29-35</sup> The Eq.-5 shows the  $\Delta H_f$  :

$$\Delta H_f = n_c (E_{C-C}) + [(n_c + 1)(E_{C-C})] + [(2n_c + 4)(E_{C-H})] \quad (\text{Eq.-5})$$

Where, " $n_c$ " is the number of carbon-carbon single bonds in compounds (**1-10**).<sup>25</sup> In this study, the molecular structure of the annulenes (**1-10**) have been considered with ab initio methods by using GAUSSIAN-98 computer program that is implemented on a Pentium-PC computer. Firstly, optimizations were performed at 6-31G basis set at the HF-level in the gas phase. To investigate further effect of electron correlation, the geometries were also optimized at the B3LYP/6-31G\* level. The results were reverberated in Table-1 and Table-2.<sup>25</sup>

For determining the DRE in annulenes (**1-10**) could compute the  $\Delta H_f^{\text{loc.}}$  by the use of Eq.-6 (in kcal mol<sup>-1</sup>)<sup>26</sup>:

$$\Delta H_f^{\text{loc.}} = 7.435 (n) - 0.605 (N_H) \quad (\text{Eq.-6})$$

In this equation, " $n$ " and " $N_H$ " are the number of carbon and hydrogen atoms in compounds (**1-10**), respectively. The related results of these calculations are shown in Table-1 and Table-2.

### GRAPHS:

For drawing the graphs of results, we used the Microsoft Office Excel-2003 program.

### DISCUSSION:

The values of the relative structural coefficients of the annulenes Randić index ( $\chi$ ) and  $\det(A)$  to

the Dewar resonance energy (DRE) of the compounds and their logarithmic data were shown in Table-1 and Table-2, respectively. The values shown in table-1 demonstrate that the Randić indices increases with molecular size of compounds (**1-10**). The table-1 reveals the three numerical progression apparent of the Randić indices. On this basis, the distance number of the Randić indices of  $\{C_4H_4, C_{10}H_{10}, C_{16}H_{16}, C_{22}H_{22}\}$ ,  $\{C_6H_6, C_{12}H_{12}, C_{18}H_{18}, C_{24}H_{24}\}$  and  $\{C_{14}H_{14}, C_{20}H_{20}\}$  is two (2) units of Randić index. The numbers shown in Fig.-2 (and extended in Table-1 and -2 for larger compounds **1-10**) have some mathematical structures. For example, in lieu of increase each C=C bond in the linear simple conjugated polyenes (**1**),  $\Delta H_f$ ,  $\Delta H_f^{loc}$  and DRE were increased. The distance between the values of  $\Delta H_f$ ,  $\Delta H_f^{loc}$  and DRE from  $\{C_4H_4(\mathbf{1})$  to  $C_6H_6(\mathbf{2})\}$  and  $\{C_{12}H_{12}(\mathbf{4})$  to  $C_{24}H_{24}(\mathbf{10})\}$  are 8.0, 13.66 and 5.6 kcal mol<sup>-1</sup>, respectively. But, [10]annulene ( $C_{10}H_{10}$ ) created rudeness in some of the diagrams (see Fig.-3 to Fig.-10). It seems that this rudeness concerns to the special property of **3**. [10]Annulene was produced in low temperatures. The compound **3** is very unstable because of its high angle strain.<sup>37,38</sup>

The DRE values increase with the Randić values of the **1-10**. The values of "log  $|A_d|$ ", were utilized for consideration of the relationship between the values of the relative structural coefficients of the annulenes **1-10**. According to the data of Table-2, the logarithmic values of Randić indices and det  $|A|$  increase by increasing the number of double bonds of **1-10**. The values of log(D<sub>RE</sub>) increase with increasing the above topological indices.

In Fig.-3 to Fig.-10 were shown two dimensional diagrams of the relationship between the main values of  $\chi$  and det  $|A_d|$  with  $\Delta H_f$ ,  $\Delta H_f^{loc}$ , DRE (see Table-1) and the logarithmic of topological indices (log( $\chi$ ) and log $|A_d|$ ) with the values of the log( $\Delta H_f$ ), log( $\Delta H_f^{loc}$ ) and log(D<sub>RE</sub>) (see Table-2). The Fig.-is the three dimensional diagram. The Fig.-11 shows the concerning of log( $\chi$ ), log( $A_d$ ) with log(D<sub>RE</sub>).

The Fig.-3 is a plot of the values of " $\chi$ " versus the " $\Delta H_f^{loc}$ " for compounds (**1-10**). The Fig.-3 shows a high linear correlation between

Randić indices and the localize energy ( $\Delta H_f^{loc}$ ). The  $\Delta H_f^{loc}$  was increased by increasing the double bonds in (**1-10**).

(See Table-1). Only,  $C_{10}H_{10}$  is not on the line of this correlation because of its unusual instability among these annulenes.

In Fig.-4 could distinguish a very good linear correlation between Randić indices and the calculated heats of formation ( $\Delta H_f$ ) by ab-initio method (HF/6-31G//B3LYP/6-31G) of **1-10** (see mathematical methods section).

In Fig.-5, was demonstrated the relationship between Randić indices and Dewar resonance energy (D<sub>RE</sub>). The DRE was increased by increasing the C=C double bonds in (**1-10**). Again, similar to Fig.-3, in Fig.-5 could see a rudeness in the diagram because of the property of **3**.

In both Fig.-6 and Fig.-7, were shown the curves of the adjacency matrixes  $|A_d|$  of **1-10** versus  $\Delta H_f^{loc}$  and  $\Delta H_f$ , respectively. In these figures could see a high curvature, specially after  $C_{18}H_{18}$  (**7**). It seems that the relationships of adjacency matrixes with  $\Delta H_f^{loc}$  and  $\Delta H_f$  are not suitable for prediction the related properties of annulenes.

The Fig.-8 shows a curve between logarithm values of  $|A_d|$  and D<sub>RE</sub> for (**1-10**). Similar to the results of two previous figures, there is no good situation for prediction of DRE in this family compounds. Also, the high curvature was started from [18]annulene.

In Fig.-9, was shown the relationship between logarithm values of Randić indices log( $\chi$ ) and log(D<sub>RE</sub>) of (**1-10**). Similar to Fig.-3 and Fig.-5 could distinguish the effect of the compound **3** ( $C_{10}H_{10}$ ) in this figure. Even though, [10]annulene created a rudeness in the diagram, there is a good correlation similar to Fig.-5.

Fig.-10 shows the relationship between logarithm values of Log $|A_d|$  and log(D<sub>RE</sub>) for annulenes **1-10**. The effect of the properties of **3** was appeared. However, the logarithm values of adjacency matrixes  $|A_d|$  show better correlation that the main values of det  $|A_d|$  with logarithm values of Dewar resonance energy (DRE).

Three dimensional figure-11 demonstrates comparative relations between log( $\chi$ ) and log  $|A_d|$  and log(D<sub>RE</sub>) in annulenes **1-10**. The

proportion of the  $\log(\chi)$  and  $\log(D_{RE})$  is more near than the  $\log|A_d|$  and  $\log(D_{RE})$  of these annulenes. On this basis, the correlations in Fig.-3 to Fig.-5, Fig.-9, Fig.-10 and Fig.-11 were better. By using and combining of Eq.-3 and Eq.-6, the Eq.-7 was achieved. This equation describes correlation of DRE and Randić index ( $\chi$ ) for the annulenes (**1-10**).

$$DRE = 22.305(\chi) - \Delta H_f - 0.605(N_H) \quad (\text{Eq.-7})$$

Where, "DRE" in  $\text{kcal mol}^{-1}$ , " $\chi$ ", " $\Delta H_f$ " and " $N_H$ " are Dewar resonance energy, Randić index, heat of formation for the reference structure and the number of hydrogen atoms in **1-10**, respectively.

## CONCLUSIONS

A characteristic polynomial is constructed for the reference structure with the graphs for the given molecule taken into account. TIs contain valuable structural information as evidenced by the success of their widespread applications in QSAR and QSPR. In this study, the structural relationship between Randić indices and the determinants of the adjacency matrixes with Dewar resonance energy of annulenes

(**1-10**) were presented and discussed. Computations of the DRE were based on the Dewar resonance energy definitions. In lieu of increase each C=C bond in the cyclic compounds (**1-10**),  $\Delta H_f$ ,  $\Delta H_f^{loc}$  and DRE were increased with a good discipline and show very good mathematical structures. The correlation of the Randić index values and  $\log(\chi)$  with Dewar resonance energy and  $\log(D_{RE})$  of **1-10** can show better results, in the comparison of using adjacency matrixes and logarithmic values of this index for prediction the same of the properties in annulenes **1-10**.

## ACKNOWLEDGMENT

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**Table1.** The values of the relative structural coefficients of annulenes **1-10**

No.	Compounds	n	A	Electronic System	Randić index ( $\chi$ )	Adjacency Det $ A_d $	$\Delta H_f^*$ ( $\text{kcal mol}^{-1}$ )	$\Delta H_f^{loc}$ ( $\text{kcal mol}^{-1}$ )	DRE ( $\text{kcal mol}^{-1}$ )
1	C <sub>4</sub> H <sub>4</sub>	4	2	4n	1.33	9	16.01	27.32	11.31
2	C <sub>6</sub> H <sub>6</sub>	6	3	4n+2	2.00	81	24.02	40.98	16.96
3	C <sub>10</sub> H <sub>10</sub>	10	5	4n+2	3.33	1221	40.06	54.64	14.58
4	C <sub>12</sub> H <sub>12</sub>	12	6	4n	4.00	3969	48.06	81.96	33.90
5	C <sub>14</sub> H <sub>14</sub>	14	7	4n+2	4.66	16383	56.07	95.62	39.55
6	C <sub>16</sub> H <sub>16</sub>	16	8	4n	5.33	64005	64.08	109.28	45.18
7	C <sub>18</sub> H <sub>18</sub>	18	9	4n+2	6.00	263169	72.10	122.94	50.84
8	C <sub>20</sub> H <sub>20</sub>	20	10	4n	6.66	1046529	80.10	136.60	56.50
9	C <sub>22</sub> H <sub>22</sub>	22	11	4n+2	7.33	4198401	88.10	150.26	62.16
10	C <sub>24</sub> H <sub>24</sub>	24	12	4n	8.00	16769025	96.09	163.92	67.82

\* The heats of formation ( $\Delta H_f$  in  $\text{kcal mol}^{-1}$ ) were calculated by the use of HF/6-31G//B3LYP/6-31G\* methods.

Hückel system:  $4n+2$ , Mübuis system:  $4n$ .

A= The number of conjugated double bonds.

n = The number of conjugated carbon atoms.

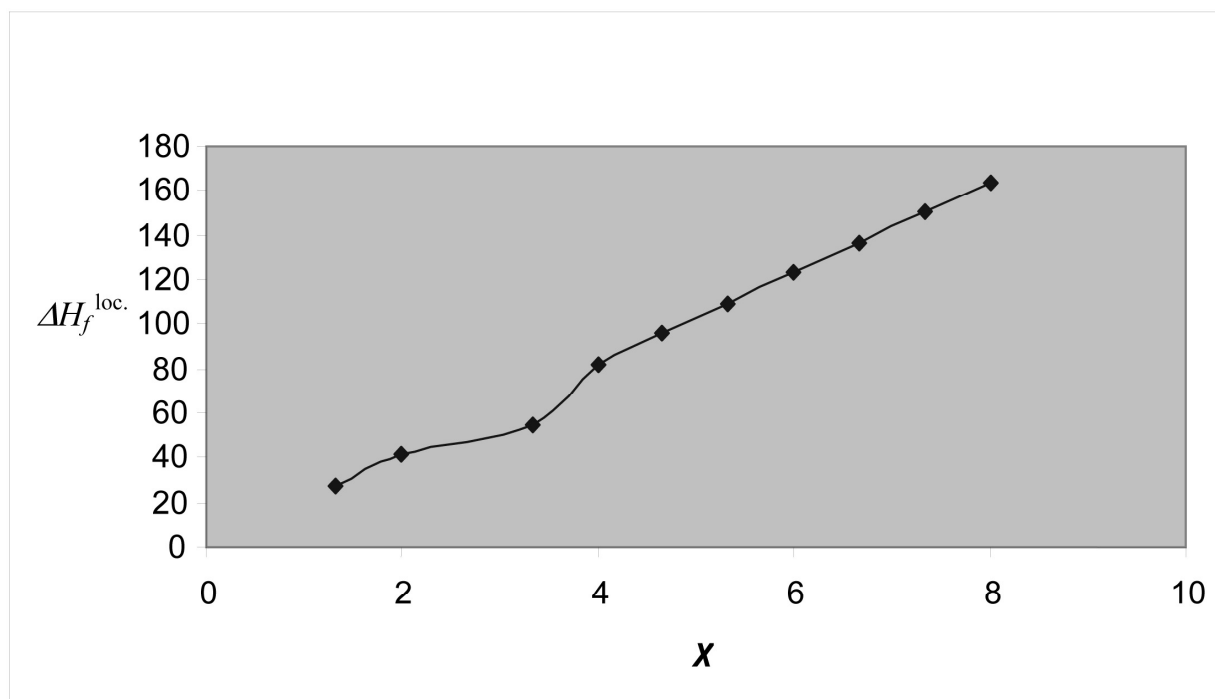
**Table2.** The logarithmic values of the relative structural coefficients of annulenes 1-10

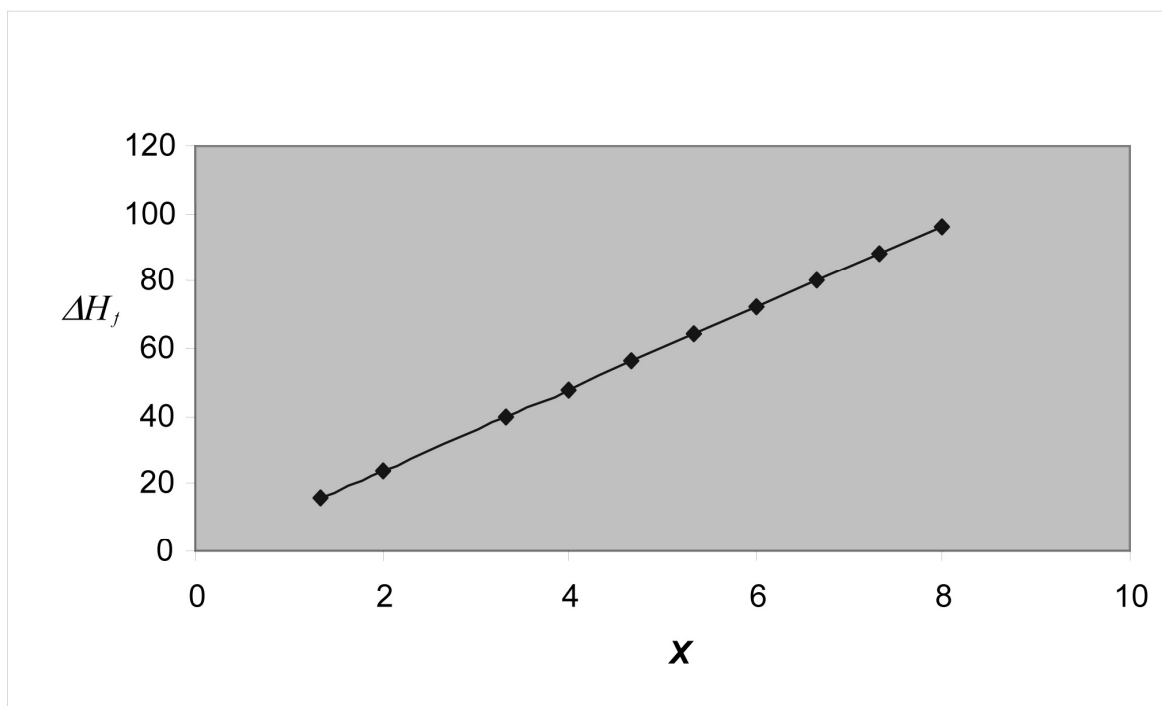
No	Compounds	n	A	Electronic System	Log ( $\chi$ )	Log A <sub>d</sub>	Log( $\Delta H_f$ )	Log( $\Delta H_f^{\text{loc.}}$ )	Log( $D_{RE}$ )
1	C <sub>4</sub> H <sub>4</sub>	4	2	4n	0.1238	0.9540	1.2044	1.4365	1.0535
2	C <sub>6</sub> H <sub>6</sub>	6	3	4n+2	0.3010	1.9085	1.3806	1.6126	1.2294
3	C <sub>10</sub> H <sub>10</sub>	10	5	4n+2	0.5224	3.0867	1.6027	1.7375	1.1638
4	C <sub>12</sub> H <sub>12</sub>	12	6	4n	0.6021	3.5986	1.6818	1.9136	1.5302
5	C <sub>14</sub> H <sub>14</sub>	14	7	4n+2	0.6684	4.2144	1.7487	1.9805	1.5971
6	C <sub>16</sub> H <sub>16</sub>	16	8	4n	0.7267	4.8062	1.8067	2.0385	1.6550.
7	C <sub>18</sub> H <sub>18</sub>	18	9	4n+2	0.7781	5.4202	1.8579	2.0897	1.7062
8	C <sub>20</sub> H <sub>20</sub>	20	10	4n	0.8235	6.0190	1.9036	2.1355	1.7520
9	C <sub>22</sub> H <sub>22</sub>	22	11	4n+2	0.8651	6.6231	1.9450	2.1768	1.7935
10	C <sub>24</sub> H <sub>24</sub>	24	12	4n	0.9031	7.2245	1.9827	2.2146	1.8313

Hückel system:  $4n+2$ , Möbius system:  $4n$ .

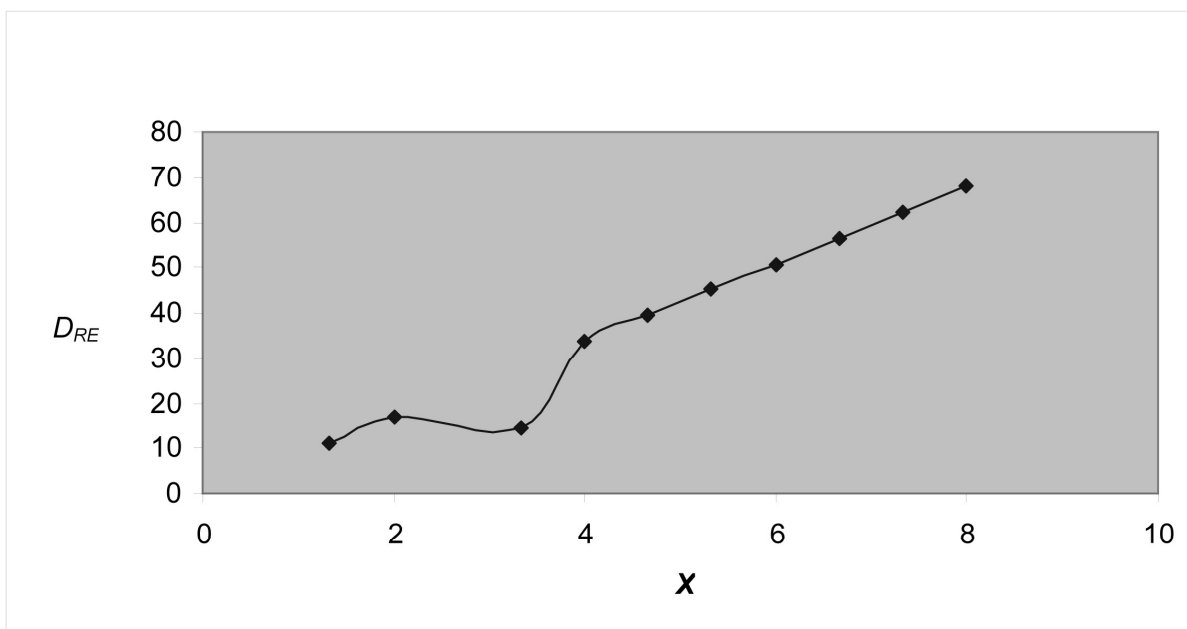
n = The number of conjugated carbon atoms.

A= The number of conjugated double bonds.

**Fig3.** A plot of the Randić index versus the  $\Delta H_f^{\text{loc.}}$  for annulenes 1-10.



**Fig.4.** The linear relationship between the values of *Randić* indices and  $\Delta H_f$  of **1-10**.



**Fig.5.** A plot of the *Randić* index versus the  $D_{RE}$  for compounds **1-10**.



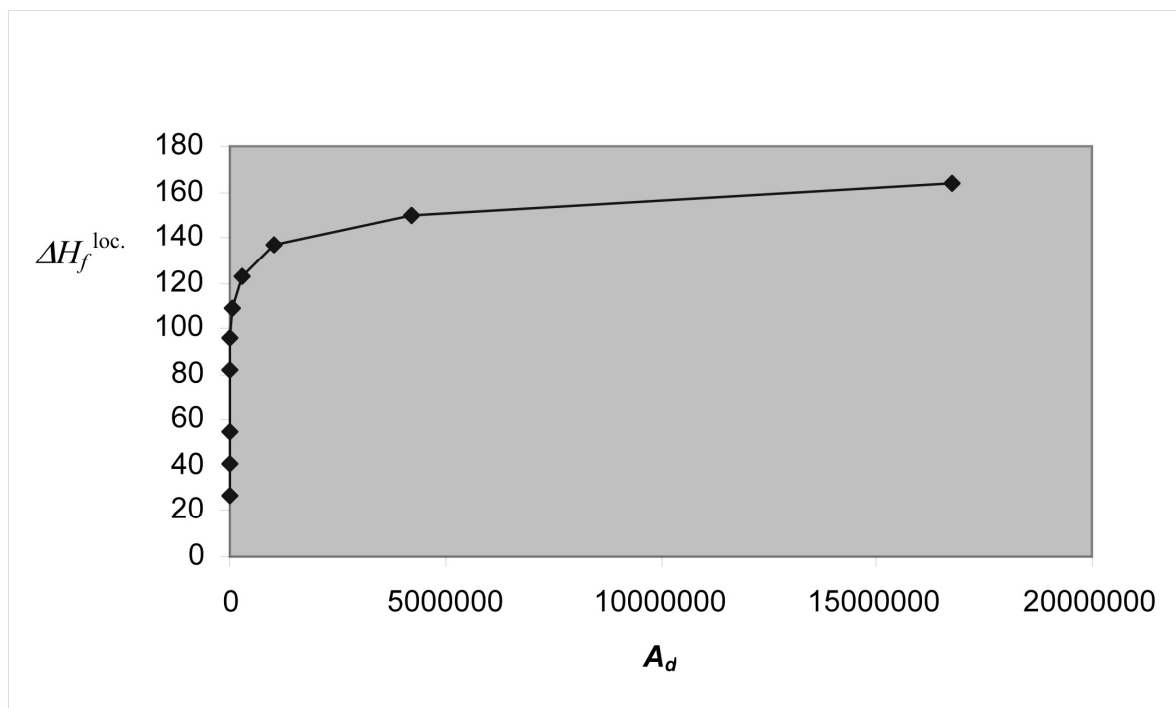


Fig. 6. The curve of the *adjacency* matrixes of 1-10 and  $\Delta H_f^{loc.}$ .

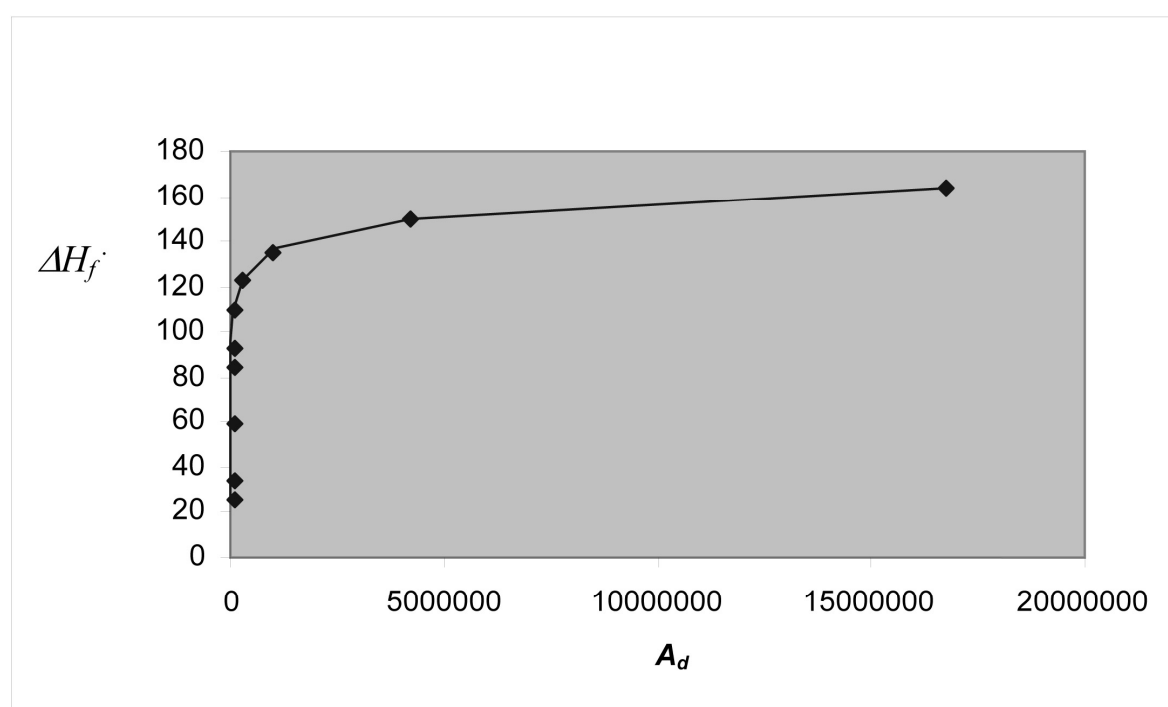


Fig.7. The curve of the *adjacency* matrixes of 1-10 and  $\Delta H_f$ .

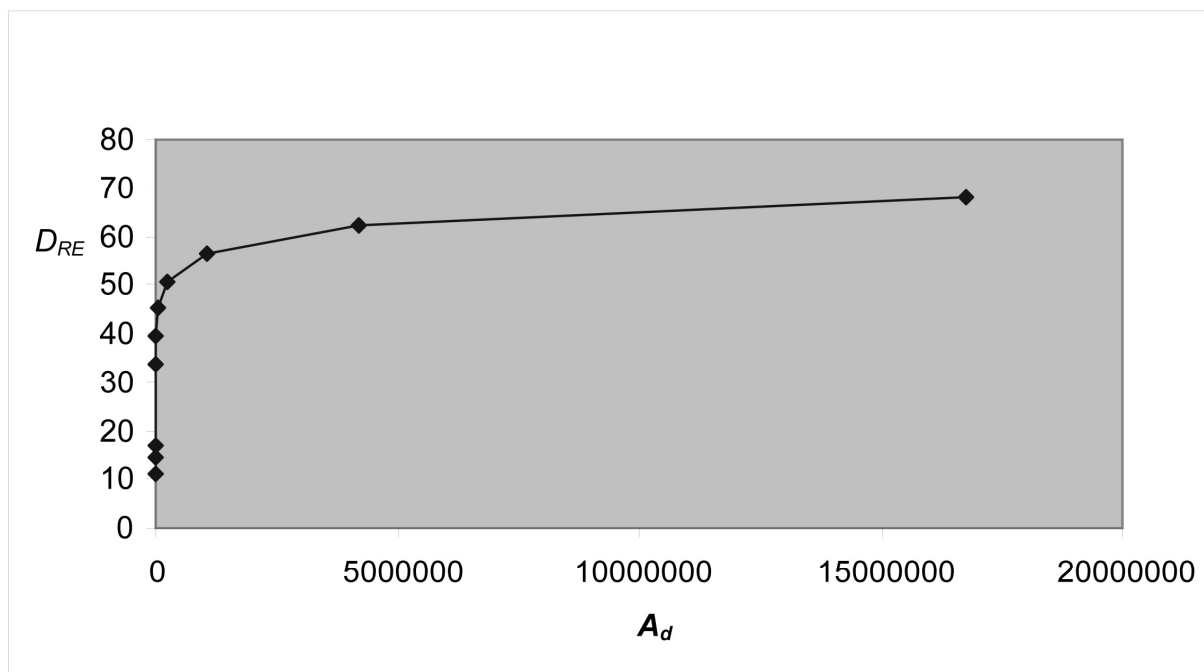


Fig.8. A curve between logarithm values of  $|A_d|$  and  $D_{RE}$  for (1-10).

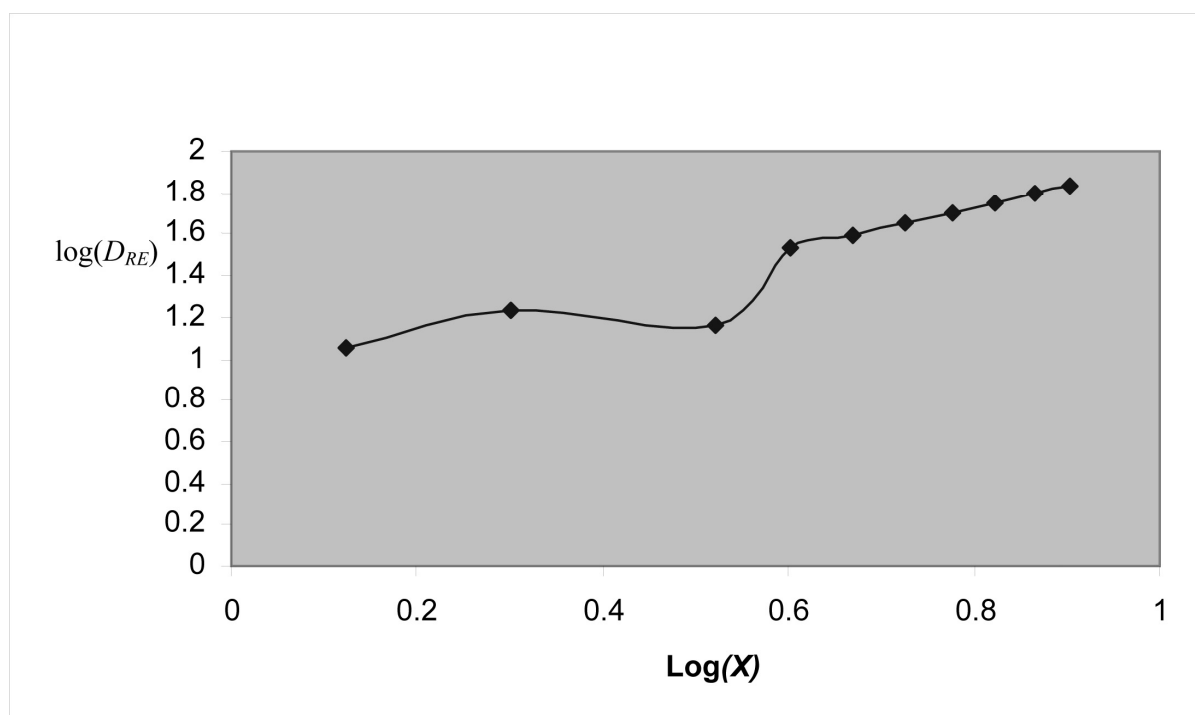


Fig.9. The relationship between logarithm values of *Randić* indices and  $\log(D_{RE})$  of (1-10).

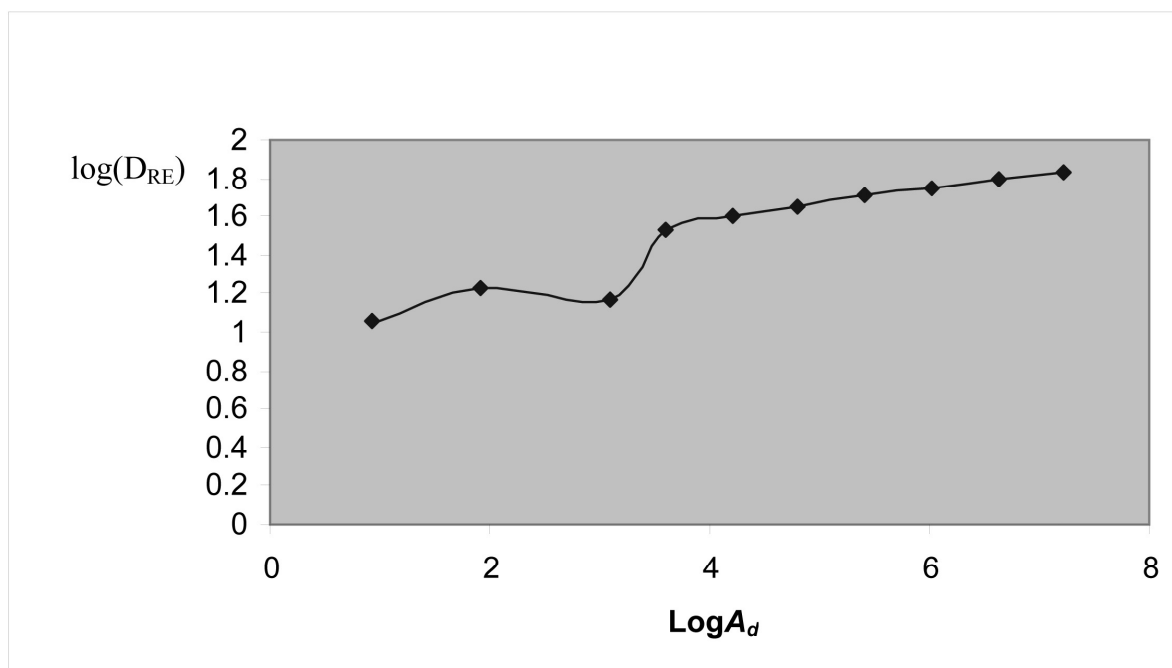


Fig.10. The relationship between logarithm values of  $\text{Log}|A_d|$  and  $\log(D_{RE})$  for annulenes 1-10.

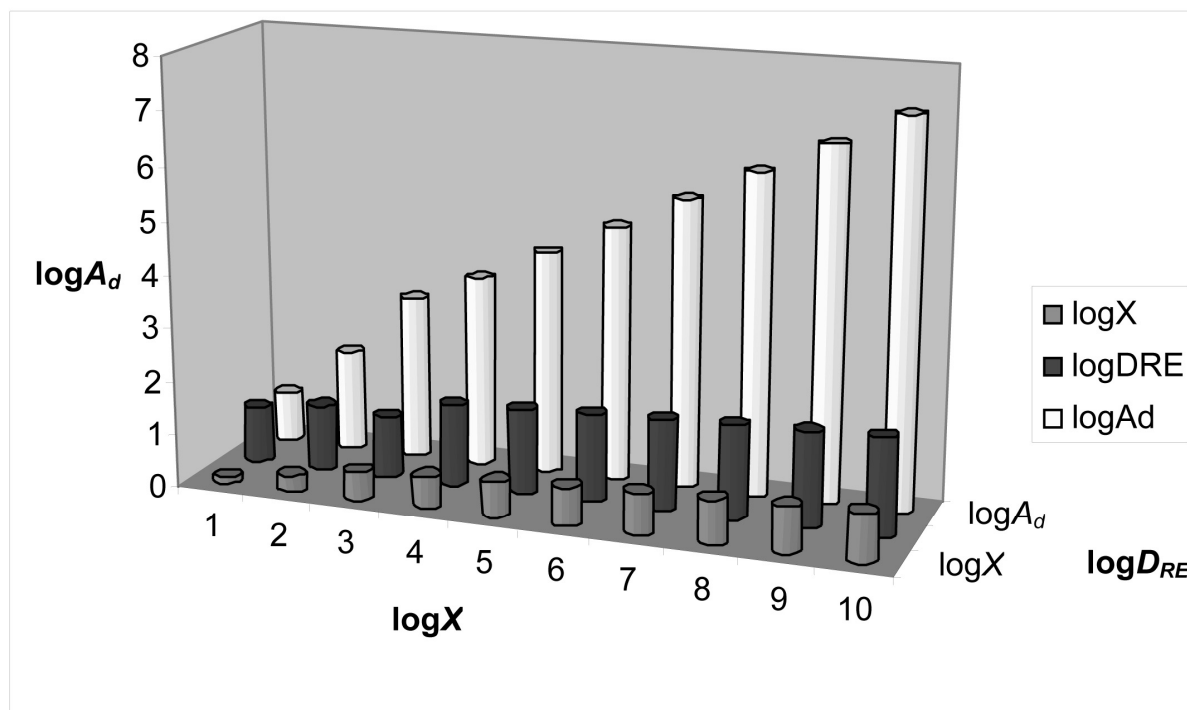


Fig.11. The three dimensional relationship between the  $\log(\chi)$ ,  $\log|A_d|$  and the  $\log(D_{RE})$  for annulenes 1-10 .

## REFERENCES

- 1 P. J. Hansen and P. Jurs, *J. Chem. Edu.*, 1988, 65, 574-580. (and the literature cited therein).
- 2 H. Hosoya, *Bull. Chem. Soc. Jpn.*, 1971, 44, 2332-2339.
- 3 M. Randić, *Acta Chim. Slov.*, 1998, 45, 239-252.
- 4 G. Rücker and C. Rücker, *J. Chem. Inf. Comput. Sci.*, 1999, 39, 788-802.
- 5 H. Wiener, *J. Am. Chem. Soc.*, 1947, 17-20.
- 6 Y. P. Du, Y. Z. Liang, B. Y. Li and C. J. Xu, *J. Chem. Inf. Comput. Sci.*, 2002, 42, 1128-1138.
- 7 M. Randić, *J. Am. Chem. Soc.*, 1975, 97, 6609-6615.
- 8 A. Sabljic and N. Trinajstić, *Acta Pharm. Ugosl.*, 1981, 31, 189-214.
- 9 P. G. Sybold, M. May and U. A. Bagal, *J. Chem. Edu.*, 1987, 64, 575-582.
- 10 L. B. Kier and L. H. Hall, "Molecular Connectivity in Chemistry and Drug Research", Academic Press, New York, 1976.
- 11 M. Randić, *J. Math. Chem.*, 1991, 7, 155-168.
- 12 M. Randić and D. Mills and S. C. Basak, *Int. J. Quantum Chem.*, 2000, 80, 1199-1209.
- 13 M. Randić, D. Plavšić and N. Lerš, *J. Chem. Inf. Comput. Sci.*, 2001, 41, 657-662.
- 14 M. Randić and S. C. Basak, *J. Chem. Inf. Comput. Sci.*, 2001, 41, 614-618.
- 15 M. Randić and M. Pompe, *J. Chem. Inf. Comput. Sci.*, 2001, 41, 575-581.
- 16 J. Galvez, *J. Mol. Struct. (Theochem)*, 1998, 429, 255-264.
- 17 E. Estrada, *Chem. Phys. Lett.*, 2000, 336, 248-252.
- 18 D. Bonchev and N. Trinajstić, *J. Chem. Phys.*, 1977, 67, 4517-4533.
- 19 S. Bertz, *Discrete Applied Math.*, 1988, 19, 65-83.
- 20 R. B. King, "Chemical Applications of Topology and Graph Theory", Elsevier, Amsterdam, Netherland, 1983.
- 21 F. A. Carey, "Organic Chemistry", McGraw-Hill, Higher Education, 5<sup>th</sup> Ed. (International Edition), 2003.
- 22 S. Shaik, A. Shurki, D. Danovich and P. C. Hiberty, *Chem. Rev.*, 2001, 101 (5), 1501-1540. (and the literature cited therein).
- 23 H. C. Longuet-Higgins, L. Salem, *Proc. R. Soc. London*, 1959, A251, 172.
- 24 C. H. Choi, M. Kertesz, *J. Chem. Phys.* 1998, 108, 6681.
- 25 J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. B. Foresman, J. Cioslowski, J. V. Ortiz, B. B. Stefanov, G. Liu, A. Liashenko, C. Gonzalez, M. Challacombe, P. M. W. Gill, B. G. Johnson, W. C. M. Head-Gordon, E. S. Replogle, J. A. Pople, *Gaussian 98 (Revision A.7)*, Gaussian, Inc., Pittsburgh, PA, 2001.
- 26 J. M. Harris and C. C. Wamser, "Fundamentals of Organic Reaction Mechanisms", John Wiley & Sons, New York, USA, 1976.
- 27 G. W. Wheland, "Resonance in Organic Chemistry", Wiley, New York, USA, 1955.
- 28 A. Streitwieser, Jr., "Molecular Orbital Theory for Organic Chemists", Wiley, New York, USA, 1962.
- 29 M. J. S. Dewar, "The Molecular Orbital Theory of Organic Chemistry", McGraw-Hill, New York, USA, 1969.
- 30 M. J. S. Dewar, "Localization and Delocalization", Eds. J. F. Liberman and A. Greenberg, Ch. 1, VCH, New York, USA, 1988.
- 31 IUPAC Physical Organic Chemistry Glossary, IUPAC, *Pure Appl. Chem.*, 1999, 71(10), 1919-1981.
- 32 N. C. Baird, *J. Chem. Edu.*, 1971, 48, 509.
- 33 L. J. Schaad & B. A. Hess, Jr., *J. Chem. Edu.*, 1974, 51, 640.
- 34 B. A. Hess, Jr., and L. J. Schaad, *J. Am. Chem. Soc.*, 1971, 93, 305.
- 35 L. B. Kier and L. H. Hall, *J. Chem. Inf. Comput. Sci.*, 2000, 40, 729-795.
- 36 E. Estrada, *Internet Electron. J. Mol. Des.*, 2002, 1, 360-366. (and the literature cited therein).
- 37 E. E. van Tamelen, T. L. Burkoth and R. H. Greeley, *J. Am. Chem. Soc.*, 1971, 93, 6120.
- 38 S. Masamune and N. Darby, *Acc. Chem. Res.*, 1972, 5, 272.