

## Papers

# On the use of iterated line graphs in quantitative structure-property studies

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For a molecular graph  $G$ , the iterated line graph sequence is  $L^i(G)$ ,  $i = 0, 1, 2, \dots$  where  $L^0(G) \equiv G$  and  $L^i(G)$  is the line graph of  $L^{i-1}(G)$ ,  $i = 1, 2, \dots$ . We determine some basic properties of this sequence and examine the possibility to use it in quantitative structure-property studies. In particular, we examine the dependency of certain physico-chemical properties of alkanes (boiling point, molar volume, molar refraction, heat of vapourization, critical temperature, critical pressure and surface tension) on the Bertz indices of  $L^i(G)$ .

For a graph  $G$  with  $n$  vertices and  $m$  edges (edges denoted as  $e_1, e_2, \dots, e_m$ ) the line graph  $L(G)$  is defined as a graph with  $m$  vertices, say  $u_1, u_2, \dots, u_m$ ; two vertices  $u_i$  and  $u_j$  of  $L(G)$  are adjacent if and only if the edges  $e_i$  and  $e_j$  of  $G$  are incident<sup>1</sup>.

An example of a hydrogen depleted molecular graph of 2, 3, 4-trimethylpentane and its corresponding line graph is shown in Fig. 1.

The  $i$ -th iterated line graph of  $G$  can be mentioned as  $L^i(G)$  ( $i = 0, 1, 2, \dots$ ) where  $L^0(G)$  denotes  $G$ ,  $L^1(G)$  denotes the line graph of  $G$ ,  $L^2(G)$  denotes the line graph of  $L^1(G)$ , and so on. It is both consistent and convenient to denote  $G$  and  $L(G)$  by  $L^0$

( $G$ ) and  $L^1(G)$ , respectively.

The series of graphs  $L^i(G)$ ,  $i = 0, 1, 2, \dots$ , is referred to as the iterated line graph sequence (ILGS) of the graph  $G$ . An example of ILGS is given in Fig. 2.

The use of line graphs in chemistry can be traced back to 1952, when Lennard-Jones and Hall published a work<sup>2</sup> on the ionization of paraffin molecules, in which they used C-C and C-H bonds as equivalent orbitals. In 1971, Herndon<sup>3</sup> extended this approach to the correlation of NMR chemical shifts, bond strengths, and photoelectron spectra. The method was further developed by Heilbronner *et al.*<sup>4,5</sup> and more recently by Gineityte.<sup>6</sup> Similar line graph based models of saturated molecules were elaborated by Sana and Leroy<sup>7</sup> and others<sup>8-10</sup>. Line graphs have found applications in other chemical theories as well, in particular in an algebraic formulation of Clar's aromatic sextet theory<sup>11-13</sup>.

An unrelated approach in which line graphs are encountered was put forward by Bertz<sup>14-17</sup>. He considered a topological index, equal to the number of edges of the line graph and eventually<sup>17</sup> proposed to examine the edge-counts of the higher members of

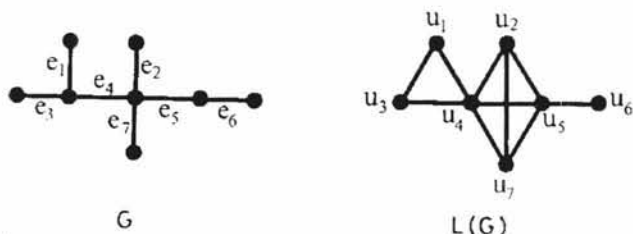


Fig. 1 – The molecular graph  $G$  of 2,3,3-trimethylpentane and its line graph  $L(G)$ : the edge  $e_i$  of  $G$  corresponds to the vertex  $u_i$  of  $L(G)$ ,  $i = 1, 2, \dots, 7$ .

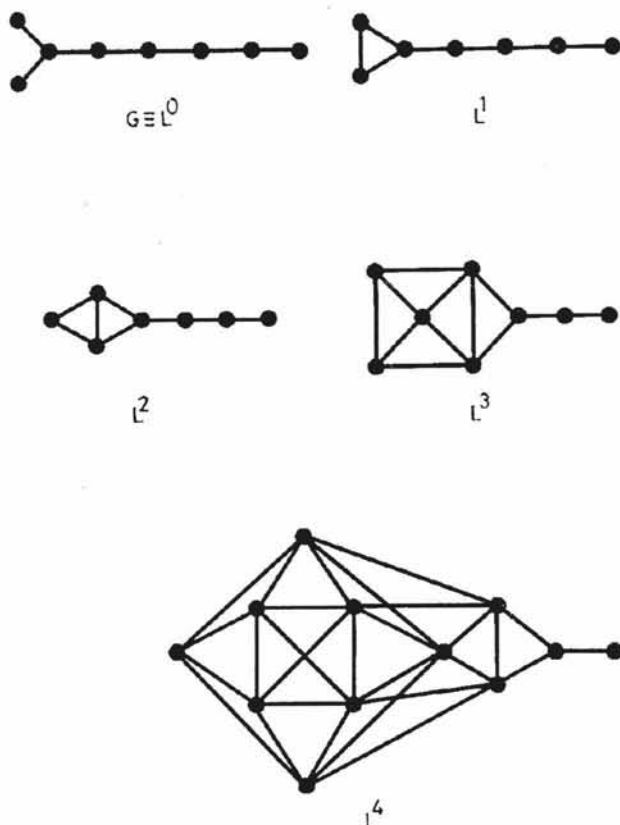


Fig. 2 – The first few members of the iterated line graph sequence (ILGS) of the molecular graph of 2-methyl pentane.

the ILGS. Iterated line-graphs also occur in the works by Diudea *et al.*<sup>18,19</sup>.

The first connections between topological indices of line graphs and physico-chemical properties of alkanes were communicated in 1995, independently by Diudea<sup>19</sup> and Estrada<sup>20</sup>. In the work of Diudea<sup>19</sup> critical pressures of octane isomers were correlated with the centrality and centrocomplexity indices and with the connectivity index, both of  $G$  and  $L(G)$ . In the work of Estrada<sup>20</sup> a correlation between molar volumes and the connectivity index of  $L(G)$  was reported. Eventually such considerations were extended to numerous other molecular-graph-based structure-descriptors and to other physico-chemical properties<sup>21-34</sup>. The ILGS has been employed only in a few studies<sup>31-34</sup>.

A more detailed bibliography on the chemical investigations involving line graphs can be found elsewhere<sup>32</sup>.

In this work we offer further results related to the properties of the ILGS of molecular graphs and to their applicability in quantitative structure-property (QSPR) studies.

### *Some properties of the iterated line graph sequence*

When dealing with iterated line graphs the first property that becomes evident is that with increasing  $i$ , the number of vertices of  $L^i(G)$  rapidly increases. This makes any computer manipulation with higher-order iterated line graphs very difficult.

It is known for sometime<sup>35,36</sup> that the only (connected) graphs whose iterated line graphs  $L^i$  remain finite as  $i \rightarrow \infty$  are the path-graphs  $P_n$  and the circuits  $C_n$ . [It is elementary to show that  $L(P_n) = P_{n-1}$  and  $L(C_n) = C_n$ ]. With the exception of these two classes of graphs, the vertex count of  $L^i(G)$  tends to infinity as  $i$  increases.

We now determine the approximate law of this increase. Denote by  $\delta_k$  the degree (= number of first neighbours) of this  $k$ -th vertex of the graph  $G$ . Then as is well-known<sup>1</sup>,

$$\sum_{k=1}^n \delta_k = 2m.$$

The number of edges of the line graph of  $G$  is equal to<sup>1,14</sup>

$$\sum_{k=1}^n \binom{\delta_k}{2} = \frac{1}{2} \sum_{k=1}^n \delta_k^2 - m.$$

Now,

$$\frac{1}{n} \sum_{k=1}^n \delta_k^2 - \left( \frac{1}{n} \sum_{k=1}^n \delta_k \right)^2 = \text{Var}(\delta|G)$$

is the variance of the vertex degrees in the graph  $G$ . In view of this, the number of edges of  $L(G)$  is given by

$$\frac{2m^2}{n} + \left[ m - \frac{n}{2} \text{Var}(\delta|G) \right] \quad \dots(1)$$

Denote by  $n_i$  the number of vertices of the  $i$ -th iterated line graph  $L^i(G)$ , and recall that  $n_0 = n$ ,  $n_1 = m$  and that the line graph of  $G$  has  $n_2$  vertices. Then Eq. (1) becomes

$$n_2 = \frac{2n_1^2}{n_0} + \left[ n_1 - \frac{n_0}{2} \text{Var}(\delta | L^0(G)) \right]$$

which is readily generalized for  $i = 0, 1, 2, \dots$  as

$$n_{i+2} = \frac{2n_{i+1}^2}{n_i} + q_i(G)$$

where

$$q_i(G) = \left[ n_{i+1} - \frac{n_i}{2} \text{Var}(\delta | L^i(G)) \right].$$

With increasing  $i$ , in the case of molecular graphs (and probably in the case of all graphs) the term  $q_i$  becomes negligibly small compared to  $2n_{i+1}^2/n_i$ . For instance, for 2,6-dimethyl heptane and for  $i = 6$ ,  $q_i = 17475.3$  whereas  $2n_{i+1}^2/n_i = 666878.7$ ; for 2, 3, 5-trimethyl hexane and  $i = 5$ ,  $q_i = 1239.1$  whereas  $2n_{i+1}^2/n_i = 1060752.9$ .

Consequently, in the above expression for  $n_{i+2}$ ,  $q_i$  may safely be neglected, resulting in an approximate recurrence relation

$$n_{i+1} \approx \frac{2n_i^2}{n_{i-1}}$$

i.e.,

$$\frac{n_{i+2}}{n_{i+1}} \approx 2 \frac{n_{i+1}}{n_i}$$

The latter relation implies

$$\frac{n_{i+1}}{n_i} \approx C 2^i \quad \dots(2)$$

where  $C$  is some constant,  $C \approx n_1/n_0 = 2m/n$ . From (2) we further obtain

$$n_i \approx C_0 C^i 2^{1+2+\dots+i} = C_0 C_i 2^{i(i+1)/2}$$

where  $C_0$  is another constant,  $C_0 \approx n_0 = n$ .

We thus arrive at the law of the increase of the number of vertices of the members of an ILGS

$$n_i \approx C_0 (C_i)^{(\sqrt{2})}$$

or, in logarithmic form

$$\ln n_i \approx \frac{\ln 2}{2} i^2 + \alpha i + \beta.$$

We see that  $\ln n_i$  increases as a quadratic polynomial of  $i$ , whose leading coefficient is independent of molecular structure (and is equal to  $\ln 2/2 = 0.34657\dots$ ), whereas the other two coefficients ( $\alpha$  and  $\beta$ ) are structure-dependent.

Anyway,  $n_i$  increases enormously rapidly, much faster than exponentially.

Because of this rapid increase in the size of the members of an ILGS until now only the first few such members could have been examined<sup>31-34</sup>. We have now prepared a special computer program in FORTRAN-90, by which we could go a step further.

In Table 1 the calculated  $n_i$ -values for the isomeric octanes are given. (Analogous data for other alkanes, up to nonanes, are available from the authors upon request.) If  $h$  is the maximal value of  $i$  for which  $n_i$  could be evaluated, then the  $n_{h-2} \times n_{h-2}$  adjacency matrix of the line graph  $L^{h-2}(G)$  was constructed (in the computer), whereas  $n_{h-1}$  and  $n_h$  were calculated by using the relations

$$n_{h-1} = m(L^{h-2}(G)); \quad n_h = \sum_k \binom{\delta_k(L^{h-2}(G))}{2}.$$

### The Bertz topological index and a QSPR model based on it

As already mentioned, Bertz<sup>14</sup> proposed the number of edges of the line graph of a molecular graph as a chemically useful structure-descriptor. Therefore, it is justified to call this quantity the *Bertz topological index*. Each member of an ILGS has its Bertz index, and then we speak of the *higher-order*

Table 1 – The vertex counts ( $n_i$ ) of the members of the ILGS of isomeric octanes;  $n_0$  and  $n_1$  are not recorded, since for alkanes  $n_1 = n_0 - 1$  whereas for octanes  $n_0 = 8$ ; note that  $n_{i+j}$  is the  $i$ -th Bertz index; for details see text.

| Isomer    | i= 2 | i= 3 | i= 4 | i= 5 | i= 6  | i= 7    | i= 8    | i= 9   |
|-----------|------|------|------|------|-------|---------|---------|--------|
| 8         | 6    | 5    | 4    | 3    | 2     | 1       | 0       | 0      |
| 2M7       | 7    | 8    | 12   | 28   | 114   | 850     | 12068   | 335183 |
| 3M7       | 7    | 9    | 17   | 54   | 307   | 3277    | 67938   | -      |
| 4M7       | 7    | 9    | 18   | 60   | 356   | 3973    | 86272   | -      |
| 3E6       | 7    | 10   | 23   | 90   | 638   | 8614    | 228149  | -      |
| 22MM6     | 9    | 17   | 55   | 324  | 3573  | 76089   | -       | -      |
| 23MM6     | 8    | 13   | 35   | 167  | 1488  | 25674   | 875810  | -      |
| 24MM6     | 8    | 12   | 26   | 92   | 586   | 7132    | 171142  | -      |
| 25MM6     | 8    | 11   | 20   | 54   | 242   | 1956    | 30036   | 901930 |
| 33MM6     | 9    | 19   | 70   | 464  | 5795  | 140798  | -       | -      |
| 34MM6     | 8    | 14   | 40   | 203  | 1936  | 35931   | 1322806 | -      |
| 23ME5     | 8    | 14   | 41   | 213  | 2078  | 39449   | 1485676 | -      |
| 33ME5     | 9    | 21   | 84   | 606  | 8286  | 221310  | -       | -      |
| 223MMM5   | 10   | 23   | 92   | 681  | 9700  | 272214  | -       | -      |
| 224MMM5   | 10   | 20   | 65   | 381  | 4252  | 92799   | -       | -      |
| 233MMM5   | 10   | 24   | 101  | 783  | 11664 | 342427  | -       | -      |
| 234MMM5   | 9    | 17   | 53   | 297  | 3173  | 66793   | -       | -      |
| 2233MMMM4 | 12   | 33   | 162  | 1512 | 27702 | 1011474 | -       | -      |

Bertz indices. The  $i$ -th order Bertz index, pertaining to the molecular graph  $G$ , will be denoted by<sup>31,34</sup>  $\theta_i(G)$ . Hence,  $\theta_i(G)$  is the number of edges of  $L^i(G)$ . Evidently,

$$\theta_i(G) = n_{i+1}.$$

In previous multiple- regression studies<sup>31,33,34</sup> involving the Bertz indices of the ILGS, attempts were made to calculate various physico-chemical properties of alkanes by means of the model

$$M(0,1,2, \dots k) = a_0\theta_0 + a_1\theta_1 + a_2\theta_2 + \dots + a_k\theta_k + b \quad \dots(3)$$

with  $a_0, a_1, a_2, \dots, a_k$  and  $b$  being determined by least squares fitting, using some pertinently chosen data base. We now use a more flexible QSPR approach, namely

$$M(i_0, i_1, i_2, \dots, i_k) = a_0\theta_{i_0} + a_1\theta_{i_1} + a_2\theta_{i_2} + \dots + a_k\theta_{i_k} + b \quad \dots(4)$$

where  $\{i_0, i_1, i_2, \dots, i_k\}$  is a  $(k+1)$ -element subset of the set  $\{0, 1, 2, \dots, p\}$ . In our case  $p = 6$  (see below). We determine an approximation of the form (4), which is optimal within all possible choices of  $k+1$  distinct higher-order Bertz indices.

In what follows the QSPR (4) will be referred to as a  $(k)$ -model.

The value of  $k$  in (4) was determined by the requirement that a  $(k)$ -model is significantly more accurate than the best  $(k-1)$ -model, and that no  $(k+1)$ -model is significantly more accurate than the best  $(k)$ -model. What is (statistically) "significant" was established by means of an  $F$ -test<sup>37</sup> at a 90% confidence level.

Although we evaluated  $\theta_i$  of some alkanes up to  $i = 8$  (see Table 1), the  $\theta_i$ -values of all alkanes with nine or less carbon atoms could be calculated only

Table 2 – Correlation coefficients  $\rho_{ij} = \rho_{ji}$  of the Bertz indices  $\theta_i$  and  $\theta_j$  of the 74 alkanes from the Needham data base<sup>38</sup>

|       | j = 1 | j = 2 | j = 3 | j = 4 | j = 5 | j = 6 |
|-------|-------|-------|-------|-------|-------|-------|
| i = 0 | 0.86  | 0.62  | 0.47  | 0.38  | 0.32  | 0.27  |
| i = 1 |       | 0.92  | 0.81  | 0.73  | 0.65  | 0.59  |
| i = 2 |       |       | 0.97  | 0.92  | 0.85  | 0.79  |
| i = 3 |       |       |       | 0.98  | 0.94  | 0.89  |
| i = 4 |       |       |       |       | 0.99  | 0.95  |
| i = 5 |       |       |       |       |       | 0.99  |

until  $i = 6$ . This makes possible to choose  $p = 6$  in formula (4). (Note that in previous studies<sup>31,33,34</sup> only the indices  $\theta_i$ ,  $i \leq 4$ , were employed.)

Table 3 – The best QSPR models, Eq. (4) for the following physico-chemical properties of alkanes: boiling points (BP) at normal pressure [K], molar volumes (MV) at 293 K [ $\text{cm}^3/\text{mol}$ ], molar refractions (MR) at 293 K [ $\text{cm}^3/\text{mol}$ ], heats of vapourization at 298 K [ $\text{kJ}/\text{mol}$ ], critical temperatures (CT) [K], critical pressures (CP) [ $10^3 \text{ kPa}$ ] and surface tensions (ST) [ $10^{-3} \text{ N/m}$ ]; experimental values taken from ref 38.

| Property | Optimal model                                 | k       | Correlation coeff. | Average rel.error(%) |
|----------|-----------------------------------------------|---------|--------------------|----------------------|
| BP       | $a_0\theta_0 + a_1\theta_1 + a_2\theta_4 + b$ | 2       | 0.992              | 1.26                 |
| MV       | $a_0\theta_0 + a_1\theta_1 + a_2\theta_2 + b$ | 2       | 0.997              | 0.65                 |
| MR       | $a_0\theta_0 + a_1\theta_1 + a_2\theta_2 + b$ | 2       | 0.9998             | 0.22                 |
| HV       | $a_0\theta_0 + a_1\theta_1 + a_2\theta_3 + b$ | 2       | 0.9985             | 0.62                 |
| CT       | $a_0\theta_0 + a_1\theta_1 + a_2\theta_2 + b$ | 2       | 0.983              | 1.53                 |
| CP       | $a_0\theta_0 + a_1\theta_1 + a_2\theta_2 + b$ | 2       | 0.966              | 2.79                 |
| ST       | $a_0\theta_0 + a_1\theta_1 + a_2\theta_2 + b$ | 2       | 0.974              | 1.72                 |
| Property | $a_0$                                         | $a_1$   | $a_2$              | $b$                  |
| BP       | 37.830                                        | -7.305  | 0.019              | 174.314              |
| MV       | 10.714                                        | 6.333   | -1.519             | 56.141               |
| MR       | 4.265                                         | 0.454   | -0.109             | 7.033                |
| HV       | 6.831                                         | -2.010  | 0.040              | 5.383                |
| CT       | 51.515                                        | -20.073 | 4.099              | 304.677              |
| CP       | -0.961                                        | -2.490  | 0.638              | 44.483               |
| ST       | 3.518                                         | -2.498  | 0.506              | 9.288                |

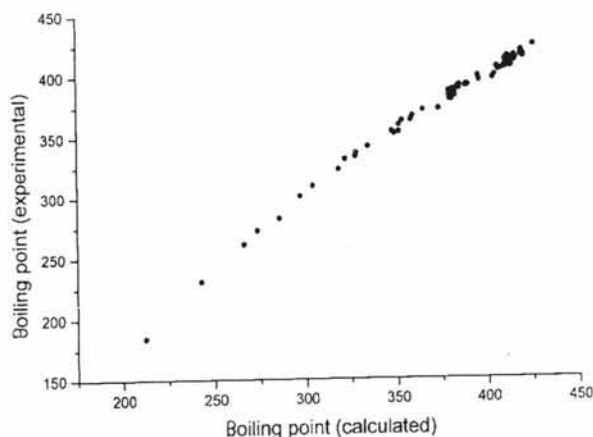


Fig. 3 – Experimental vs. calculated boiling points of 74 alkanes; for details see Table 3 and the text.

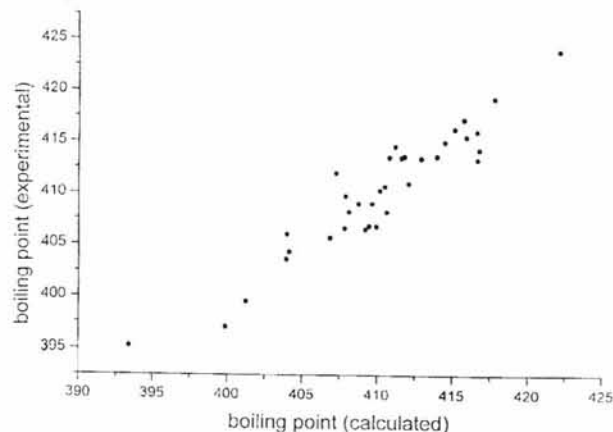


Fig. 4 — Experimental vs. calculated boiling points of isomeric nonanes; for details see Table 4 and the text.

## Numerical work

The first data base examined was that of Needham *et al.*<sup>38</sup> in which are collected experimentally determined boiling points (BP), critical temperatures (CT) and critical pressures (CP) for 74 alkanes, molar volumes (MV), molar refractions (MR) and heats of vapourization (HV) for 69 alkanes, and surface tensions (ST) for 68 alkanes. This data base embraces a total of 74 alkanes with 9 or less carbon atoms. The respective correlation coefficients between the  $i$ -th and  $j$ -th order Bertz indices,  $0 \leq i, j \leq 6$ , are recorded in Table 2. These data indicate that the various Bertz indices of alkanes are only weakly correlated.

In all cases studied, the (1)-model  $a_0\theta_0 + b$  was found to be far better than any other (1)-model. For instance, for the boiling point the correlation coefficient for  $a_0\theta_0 + b$  is 0.986, whereas for  $a_0\theta_i + b$ ,  $i = 1, 2, \dots, 6$ , the correlation coefficients are 0.804, 0.554, 0.411, 0.334, 0.284 and 0.245, respectively. Therefore, in Eq. (4) we always have  $i_0 = 0$ .

The optimization was continued by setting  $k = 1, k = 2$ , etc. For any given  $k$  all possible ( $k$ )-models were tested and the best model was selected. The search was ended when no ( $k+1$ )-model was found to be significantly better (as determined by  $F$ -test at 90% confidence level<sup>37</sup>), than the best ( $k$ )-model.

The optimal QSPR models found as well as the statistical data indicating their precision are given in Table 3. A characteristic (optimal) correlation is depicted in Fig. 3.

The second sample studied consists of data for all (35) isomeric nonanes. This in fact is a subset of the Needham data base<sup>38</sup>. By means of this sample we intend to exclude the molecular size effects, which are known to cause artificially high correlation coefficients<sup>39</sup>.

For isomers the parameter  $\theta_0$  is constant (in our case  $\theta_0 = 8$ ) and, therefore, instead of (4) we have to employed the model

$$M(i_1, i_2 \dots i_k) = a_1\theta_{i_1} + a_2\theta_{i_2} + \dots + a_k\theta_{i_k} + b \quad \dots(5)$$

where  $\{i_1, i_2 \dots i_k\}$  is now a  $k$ -element subset of the set  $\{1, 2, \dots, 6\}$ . As anticipated, in the case of isomers the quality of the Bertz-index-based model (5) is markedly weaker than what we have observed with the Needham sample and the model (4). The respective QSPR formulae and the data indicating their precision are given in Table 4. A characteristic (optimal) correlation is shown in Fig. 4.

## Discussion and concluding remarks

For both the data sets and for all the seven physico-chemical properties examined the optimal QSPR formula has  $k = 2$ , which means that only two distinct Bertz indices need to be used (plus  $\theta_0$  in case of non-isomers). In all cases one of these two indices is  $\theta_1$  – the original Bertz topological index<sup>14</sup>. The second structure-descriptor occurring in our formulae is either  $\theta_2$  (for MV, MR, CT (first sample), CP and ST) or  $\theta_3$  (for HV and CT (second sample)) or  $\theta_4$  (for

Table 4 — Same data as in Table 3, corresponding to the set of isomeric nonanes

| Property | Optimal model                   | k      | Correlation coeff. | Average rel.error(%) |
|----------|---------------------------------|--------|--------------------|----------------------|
| BP       | $a_1\theta_1 + a_2\theta_2 + b$ | 2      | 0.945              | 0.38                 |
| MV       | $a_1\theta_1 + a_2\theta_4 + b$ | 2      | 0.912              | 0.58                 |
| MR       | $a_1\theta_1 + a_2\theta_2 + b$ | 2      | 0.890              | 0.21                 |
| HV       | $a_1\theta_1 + a_2\theta_3 + b$ | 2      | 0.984              | 0.54                 |
| CT       | $a_1\theta_1 + a_2\theta_3 + b$ | 2      | 0.865              | 0.68                 |
| CP       | $a_1\theta_1 + a_2\theta_2 + b$ | 2      | 0.867              | 2.20                 |
| ST       | $a_1\theta_1 + a_2\theta_2 + b$ | 2      | 0.917              | 1.39                 |
| Property | $a_1$                           | $a_2$  | $b$                |                      |
| BP       | -7.624                          | 0.023  | 475.475            |                      |
| MV       | 5.992                           | -1.478 | 144.562            |                      |
| MR       | 0.465                           | -0.112 | 41.097             |                      |
| HV       | -2.019                          | 0.040  | 60.126             |                      |
| CT       | -14.134                         | 0.577  | 693.859            |                      |
| CP       | -1.902                          | 0.516  | 33.605             |                      |
| ST       | -2.459                          | 0.508  | 36.940             |                      |

BP). In not a single case was the inclusion of the fifth- and/or sixth order Bertz index found to be necessary. It is almost certain that the Bertz indices of order greater than 6 would play hardly any role in QSPR studies.

It is also remarkable that the optimal models deduced for the two samples are practically identical, except in the case of CT. Not only are the required Bertz indices the same, but also the coefficients  $a_1$  and  $a_2$  have nearly equal values. In the case of critical temperature the two samples lead to different QSPR models: the formula for the calculation of CT in the isomer-sample should not be considered as significant, because its precision is quite weak.

With the exception of HV and, perhaps, BP, in the case of sets of isomers, the predictive power of the QSPR formulae based on Bertz indices is not as satisfactory as one would have expected (especially in the view of the analogous results obtained for the

samples containing non-isomers). This finding should certainly be taken into account in future QSPR applications of the Bertz indices and of other topological indices of iterated line graphs.

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