

# Moments of Inertia of Spectra and Distribution Moments as Molecular Descriptors

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## Abstract

Frequencies and intensities of molecular spectra are used to construct a new kind of molecular descriptors. In this work two kinds of descriptors have been defined: one is a linear combination of squares of the frequencies and another one - a linear combination of squares of the intensities. If the frequencies and the intensities are interpreted as 'co-ordinates' of fictitious points forming one-dimensional rigid bodies and the coefficients of the combinations as their 'masses' then the descriptors may be interpreted as 'moments of inertia' of the spectrum. The new descriptors correctly represent the molecular structure. The results derived from the new descriptors are compared with the ones given by the spectral density distribution moments and the intensity distribution moments used as molecular descriptors. An analysis of the infrared spectra of chloronaphthalenes illustrates the theory. The descriptors not only allow to indicate the number of the chlorine atoms in a molecule but also to distinguish between different isomers.

## 1 Introduction

The aim of this work is developing methods used in the theory of molecular similarity [1–4]. The basic assumption of the quantitative structure-property relationships (QSPR) is that similar molecules have similar properties. In some sense, similarity is like beauty. It depends on the properties considered. It is not obvious how to represent the molecular structure and how to define the similarity measure. New approaches are still developing [5–11].

The basic quantities in the theory of molecular similarity are the molecular descriptors – properly defined numerical quantities which characterize the molecular properties [12].

A rich information about the molecular properties is contained in the molecular spectrum. In the present work we propose a nonconventional view on the spectrum. We treat it as a rigid body and calculate its moments of inertia. Then the moments of inertia are taken as the molecular descriptors. The results show that the new descriptors give an adequate representation of the molecular structure. Similar methodology (treating graphs as rigid bodies and calculating their moments of inertia) have already been successfully used in studies of the DNA sequences [13]. Another nonconventional view on the molecular spectrum is considering it as a statistical distribution. The basic quantities in such an approach are distribution moments. In the present work we consider two kinds of distribution moments: spectral density distribution moments and intensity distribution moments. The present studies are the continuation of our earlier investigations [14]. We have also applied spectral density distribution moments as novel descriptors for developing a QSPR model that predicts the logarithmic values of subcooled liquid vapor pressure [15] and intensity distribution moments as molecular descriptors [16–19].

Similar methodology, based on the distribution moments, we applied in other areas of science such as deterministic chaos [20,21], stellar spectra [22,23], and DNA sequences [24].

In the present work we construct the new descriptors, referred to as the *moments of inertia of spectra*, as well as the distribution moments, from the infrared spectra of chloronaphthalenes. We study the relations between the descriptors and the structure of the molecules. We show that the results derived from the intensity distribution moments can be treated for these molecules as corrections to the ones obtained from the spectral density distribution moments.

## 2 Theory

In the present work we introduce new ways of the description of the molecular spectra. The methodology is applied to the infrared spectra but it can be implemented to any other kind of spectra. Two non-standard ways of the analysis of spectra are compared: the first one is a *dynamic* description in which the spectra are treated as "rigid bodies", and the second one is a statistical description in which the spectra are considered as "statistical distributions".

The distribution of mass in a rigid body is characterized by its moment of inertia. In particular the moment of inertia of a rigid body composed of  $D$  material points with masses  $m_i$ ,  $i = 1, 2, \dots, D$ , with respect to an axis is defined as

$$T_x = \sum_{i=1}^D m_i x_i^2,$$

where  $x_i$  is the distance of the point  $m_i$  from the axis. In standard approach the moment of inertia of an object about a given axis is a measure how difficult is to induce an angular rotation of this object about this axis. It is easy to accelerate into spinning fast if the mass is concentrated close to the axis. The closer are the points to the axis, the smaller is the moment of inertia with respect to this axis.

In fact, one can use the notion of the moment of inertia to characterize the distribution of any kind of quantities - in particular, the molecular spectra. A molecular spectrum is composed of a series of lines which may be numbered in the same way as material points. If we assign to each line a 'mass' then we can define some analogs of the standard moment of inertia.

Another way of analysis of spectra is to compose statistical distributions using the spectra. The frequencies and the intensities are not random values, however using the language of statistics one can reveal new properties of the systems. In this treatment we are not concentrated on the details of spectra but on their global characteristics. Frequencies and intensities are considered as statistical ensembles, analogously as in the statistics. Such an approach called *statistical spectroscopy* has been developed starting from several, rather diverse, motivations. During decades this approach was mainly applied in nuclear physics where not exactly known character of the interparticle interactions supplied the main motivation for using the language of statistics [25]. Later it was noticed that some useful information about properties of spectra may also be derived by applying methods of statistical spectroscopy to systems for which the Hamiltonian matrix is known exactly [26]. This lead to the development of the statistical theory of atomic and molecular spectra. The basic quantities in this approach are distribution moments.

The molecular descriptors considered in this work are derived from the dynamic and from the statistical description. They are directly correlated with the measured quantities which characterize the molecule: they are expressed in terms of intensities and of frequencies of the molecular spectra.

- Moments of inertia of a spectrum

Let us consider a molecular spectrum  $I(\nu)$  as a set of material points characterized by their masses and their coordinates. Let us project the spectrum to two orthogonal axes. As a consequence we obtain two sets of points:

1.  $(\nu_1, 0), (\nu_2, 0), \dots, (\nu_D, 0),$
2.  $(0, I_1), (0, I_2), \dots, (0, I_D),$

where  $\nu_i$  is the frequency and  $I_i$  the intensity of the  $i$ -th line, and  $D$  is the number of lines in the spectrum. Let us assign a mass  $m_i$  to each point and calculate the moments of inertia of two one-dimensional rigid bodies defined in this way. The moments of inertia of these bodies may be expressed as

$$T_1 = \sum_{i=1}^D m_i \tilde{\nu}_i^2, \quad (1)$$

$$T_2 = \sum_{i=1}^D m_i \tilde{I}_i^2, \quad (2)$$

where  $(\tilde{\nu}_i, 0)$  and  $(0, \tilde{I}_i)$  are the coordinates of the mass  $m_i$  in the Cartesian coordinate system for which the origin has been selected at the center of mass, i.e.

$$\tilde{\nu}_i = \nu_i - \nu_a, \quad (3)$$

$$\tilde{I}_i = I_i - I_a. \quad (4)$$

$(\nu_a, 0), (0, I_a)$  are the coordinates of the centers of mass of the two bodies, respectively, i.e.  $\nu_a, I_a$  are the appropriate averaged values:

$$\nu_a = \frac{1}{D} \sum_{i=1}^D \nu_i, \quad (5)$$

$$I_a = \frac{1}{D} \sum_{i=1}^D I_i. \quad (6)$$

We assume that  $m_i = 1$  for all the points. Then, the total mass of the spectrum is equal to the total number of points:

$$\sum_{i=1}^D m_i = D. \quad (7)$$

Since the masses are defined to be dimensionless,  $T_1$  is expressed in the units of the squares of the frequencies and  $T_2$  is expressed in the units of the squares of the intensities. The selection of the units is, however, irrelevant for the similarity relations. Of course, all quantities which characterize the set of systems compared have to be expressed in the same units.

- Spectral density distribution moments and intensity distribution moments

The molecular descriptors used in this paper are also moments of different kinds of statistical distributions. Let us consider a discrete finite set of values treated as a statistical ensemble:  $V_1, V_2, \dots, V_D$ . A common approach in statistical spectroscopy is introducing a distribution of the type:

$$\beta(V) = \mathcal{N} \sum_{i=1}^D w_i \delta(V - V_i), \quad (8)$$

where  $w_i$  is the weight of  $V_i$  and  $\delta(V - V_i)$  is the Dirac delta. The distribution is normalized

$$\int_{-\infty}^{\infty} \beta(V) dV = 1. \quad (9)$$

Statistical distributions may be characterized by their moments. The  $q$ -th moment of  $\beta(V)$  is defined as

$$M_{\beta,q} = \int_{-\infty}^{\infty} V^q \beta(V) dV. \quad (10)$$

Using the form of  $\beta(V)$  we get

$$M_{\beta,q} = \mathcal{N} \sum_{i=1}^D \int_{-\infty}^{\infty} V^q w_i \delta(V - V_i) dV = \mathcal{N} \sum_{i=1}^D w_i V_i^q, \quad (11)$$

where we used the well known property of the Dirac delta

$$\int_{-\infty}^{\infty} V^q w_i \delta(V - V_i) dV = V_i^q w_i. \quad (12)$$

The normalization condition (9) yields:

$$\mathcal{N} = \left( \sum_{i=1}^D w_i \right)^{-1}. \quad (13)$$

Very often properly scaled moments  $M'_{\beta,q}$  and  $M''_{\beta,q}$  are used. The centered moments for which  $M'_{\beta,1} = 0$  are defined as

$$M'_{\beta,q} = \mathcal{N} \sum_{i=1}^D w_i (V_i - M_{\beta,1})^q. \quad (14)$$

The moments for which  $M''_{\beta,1} = 0$  and  $M''_{\beta,2} = 1$  are

$$M''_{\beta,q} = \mathcal{N} \sum_{i=1}^D w_i \left[ \frac{(V_i - M_{\beta,1})}{\sqrt{M_{\beta,2} - (M_{\beta,1})^2}} \right]^q. \quad (15)$$

For the characterization of the distributions usually  $M_{\beta,1}$ ,  $M'_{\beta,2}$ , and  $M''_{\beta,q}$ , where  $q = 3, 4, 5, \dots$  are used.  $M_{\beta,1}$  is the mean of the distribution,  $M'_{\beta,2}$  characterizes the

width of the distribution,  $M''_{\beta,3}$  - the asymmetry of the distribution, and  $M''_{\beta,4}$  is the excess. Higher-order moments do not have a direct geometrical explanation.

In the present work we consider two kinds of distributions derived from the molecular spectrum.

1.  $V_1, V_2, \dots, V_D$  is a discrete frequency spectrum  $\nu_1, \nu_2, \dots, \nu_D$  and all the weights are the same. For simplicity we put  $w_i = 1, i = 1, 2, \dots, D$ . Then  $\beta$  represents the spectral density distribution  $\rho(\nu)$ :

$$\beta(V) \equiv \rho(\nu) = \mathcal{N} \sum_{i=1}^D \delta(\nu - \nu_i), \quad (16)$$

where

$$\mathcal{N} = D^{-1} \quad (17)$$

and  $\rho(\nu)$  describes the distribution of the frequencies (the density of the frequencies). The intensities of the lines are not taken into account, i.e. the weight of each frequency is the same. The moments of the distribution  $\rho(\nu)$  (spectral density distribution moments) are equal to

$$M_{\rho,q} = \frac{1}{D} \sum_{i=1}^D \nu_i^q. \quad (18)$$

2.  $V_1, V_2, \dots, V_D$  is a discrete frequency spectrum  $\nu_1, \nu_2, \dots, \nu_D$  and the corresponding weights are equal to the intensities,  $w_i = I_i, i = 1, 2, \dots, D$ . Then  $\beta$  represents the intensity distribution  $I(\nu)$ :

$$\beta(V) \equiv I(\nu) = \mathcal{N} \sum_{i=1}^D I_i \delta(\nu - \nu_i), \quad (19)$$

where

$$\mathcal{N} = \left( \sum_{i=1}^D I_i \right)^{-1}. \quad (20)$$

The moments of the distribution  $I(\nu)$  (intensity distribution moments) are equal to

$$M_{I,q} = \left( \sum_{i=1}^D I_i \right)^{-1} \sum_{i=1}^D I_i \nu_i^q. \quad (21)$$

Let us note that  $M''_{\beta,q}$  are dimensionless for both  $\beta \equiv \rho$  and  $\beta \equiv I$  while  $M_{\beta,q}$  and  $M'_{\beta,q}$  are expressed in the units of the q-th powers of frequencies for both  $\beta \equiv \rho$  and  $\beta \equiv I$ . Any change of units is here irrelevant for the molecular similarity relations since it results in a multiplicative factor, the same for all moments of a given kind.

### 3 Results and discussion

The theory is illustrated by the calculations for the infrared spectra of 76 molecules listed in Table 1 and also considered in [14, 15].

Fig. 1 panel (a) shows moment of inertia  $T_1$  for all the molecules labeled by  $r$  displayed in the horizontal axis (see Table 1).  $T_1$  clearly represents the molecular structure: these descriptors indicate the number of chlorine atoms in the molecules. Similar properties of the molecules are described by the spectral density distribution moments shown in Fig. 2 panel (a) ( $q = 1$ ), and Fig. 2 panel (b) ( $q = 3$ ).

The information contained in  $T_1$  is similar to the one contained in  $M'_{\rho,2}$ . The second-order ( $q = 2$ ) distribution moments are measures of the width of the distributions. Therefore the values of both  $T_1$  (the measure of the concentration of the mass around the axis) and  $M'_{\rho,2}$  describe the dispersion of the oscillation frequencies. The values of these descriptors increase if the dispersion increases. Comparing the appropriate equations we get  $M'_{\rho,2} = T_1/D$ . In particular, if  $D$  is the same for all the molecules, then the similarity relations are identical using  $T_1$  or  $M'_{\rho,2}$  ( $D$  is only a multiplicative factor which does not change the similarity relations). For all the considered molecules the number of lines is the same ( $D = 48$ ). Generally, standard values used in dynamics:  $T_1$  and  $T_2$  should be normalized by dividing them by the total mass  $D$ . As a consequence, in the case of  $T_1$  the dynamic and the statistical descriptions are equivalent. New information is contained in  $T_2$ .

A detailed description of the spectral density distribution moments has been given in our previous work [14]. The information contained in  $T_1$  and in spectral density distribution moments supply the main information about the structure of chloronaphthalenes. In order to obtain more specific information and to distinguish between different isomers, intensity distribution moments or  $T_2$  can be considered. The behavior of  $T_2$  is shown in Fig. 1 panel (b). The intensity distribution moments are shown in Fig. 1 panel (c) for  $q = 2$ , Fig. 2 panel (c) for  $q = 1$ , and Fig. 2 panel (d) for  $q = 3$ . Though the behavior of these moments is not very regular when the number of the chlorine atoms increases, we can see some clear trends: an increase of  $T_2$  and a decrease of  $M'_{I,2}$  [Fig. 1 panels (b), (c)].

Table 1: Molecules

r		r	
0	Naphthalene	38	1,2,5,8-tetrachloronaphthalene
1	1-chloronaphthalene	39	1,2,6,7-tetrachloronaphthalene
2	2-chloronaphthalene	40	1,2,6,8-tetrachloronaphthalene
3	1,2-dichloronaphthalene	41	1,2,7,8-tetrachloronaphthalene
4	1,3-dichloronaphthalene	42	1,3,5,7-tetrachloronaphthalene
5	1,4-dichloronaphthalene	43	1,3,5,8-tetrachloronaphthalene
6	1,5-dichloronaphthalene	44	1,3,6,7-tetrachloronaphthalene
7	1,6-dichloronaphthalene	45	1,3,6,8-tetrachloronaphthalene
8	1,7-dichloronaphthalene	46	1,4,5,8-tetrachloronaphthalene
9	1,8-dichloronaphthalene	47	1,4,6,7-tetrachloronaphthalene
10	2,3-dichloronaphthalene	48	2,3,6,7-tetrachloronaphthalene
11	2,6-dichloronaphthalene	49	1,2,3,4,5-pentachloronaphthalene
12	2,7-dichloronaphthalene	50	1,2,3,4,6-pentachloronaphthalene
13	1,2,3-trichloronaphthalene	51	1,2,3,5,6-pentachloronaphthalene
14	1,2,4-trichloronaphthalene	52	1,2,3,5,7-pentachloronaphthalene
15	1,2,5-trichloronaphthalene	53	1,2,3,5,8-pentachloronaphthalene
16	1,2,6-trichloronaphthalene	54	1,2,3,6,7-pentachloronaphthalene
17	1,2,7-trichloronaphthalene	55	1,2,3,6,8-pentachloronaphthalene
18	1,2,8-trichloronaphthalene	56	1,2,3,7,8-pentachloronaphthalene
19	1,3,5-trichloronaphthalene	57	1,2,4,5,6-pentachloronaphthalene
20	1,3,6-trichloronaphthalene	58	1,2,4,5,7-pentachloronaphthalene
21	1,3,7-trichloronaphthalene	59	1,2,4,5,8-pentachloronaphthalene
22	1,3,8-trichloronaphthalene	60	1,2,4,6,7-pentachloronaphthalene
23	1,4,5-trichloronaphthalene	61	1,2,4,6,8-pentachloronaphthalene
24	1,4,6-trichloronaphthalene	62	1,2,4,7,8-pentachloronaphthalene
25	1,6,7-trichloronaphthalene	63	1,2,3,4,5,6-hexachloronaphthalene
26	2,3,6-trichloronaphthalene	64	1,2,3,4,5,7-hexachloronaphthalene
27	1,2,3,4-tetrachloronaphthalene	65	1,2,3,4,5,8-hexachloronaphthalene
28	1,2,3,5-tetrachloronaphthalene	66	1,2,3,4,6,7-hexachloronaphthalene
29	1,2,3,6-tetrachloronaphthalene	67	1,2,3,5,6,7-hexachloronaphthalene
30	1,2,3,7-tetrachloronaphthalene	68	1,2,3,5,6,8-hexachloronaphthalene
31	1,2,3,8-tetrachloronaphthalene	69	1,2,3,5,7,8-hexachloronaphthalene
32	1,2,4,5-tetrachloronaphthalene	70	1,2,3,6,7,8-hexachloronaphthalene
33	1,2,4,6-tetrachloronaphthalene	71	1,2,4,5,6,8-hexachloronaphthalene
34	1,2,4,7-tetrachloronaphthalene	72	1,2,4,5,7,8-hexachloronaphthalene
35	1,2,4,8-tetrachloronaphthalene	73	1,2,3,4,5,6,7-heptachloronaphthalene
36	1,2,5,6-tetrachloronaphthalene	74	1,2,3,4,5,6,8-heptachloronaphthalene
37	1,2,5,7-tetrachloronaphthalene	75	Octachloronaphthalene



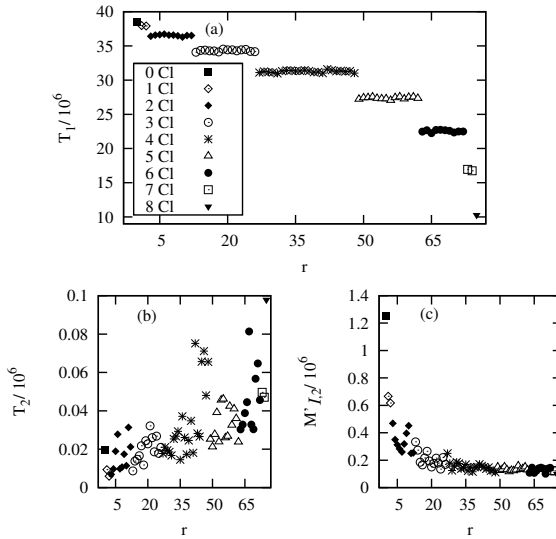


Figure 1: Moments of inertia of spectra [panels (a), (b)] and second-order intensity distribution moments [panel (c)].

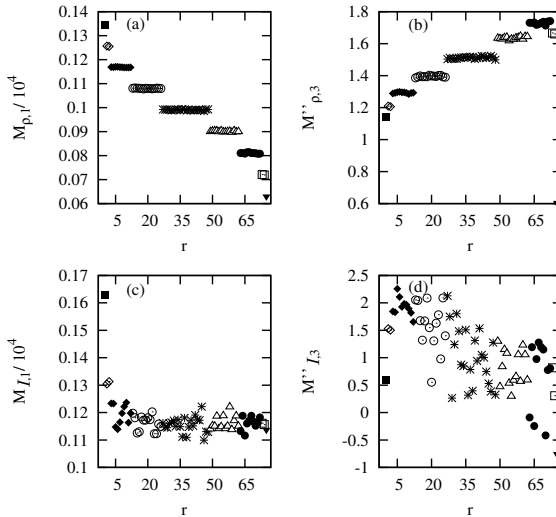


Figure 2: First-order distribution moments [panels (a), (c)] and third-order distribution moments [panels (b), (d)]. The symbols are the same as in Fig. 1.

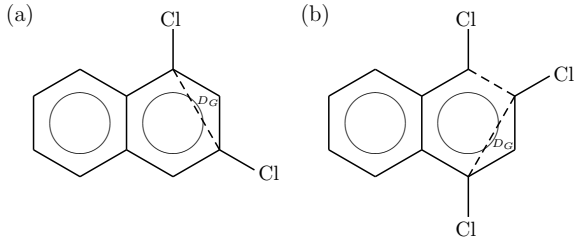


Figure 3:  $D_G$  (dashed lines) for 1,3-dichloronaphthalene [panel (a)], and for 1,2,4-trichloronaphthalene [panel (b)].

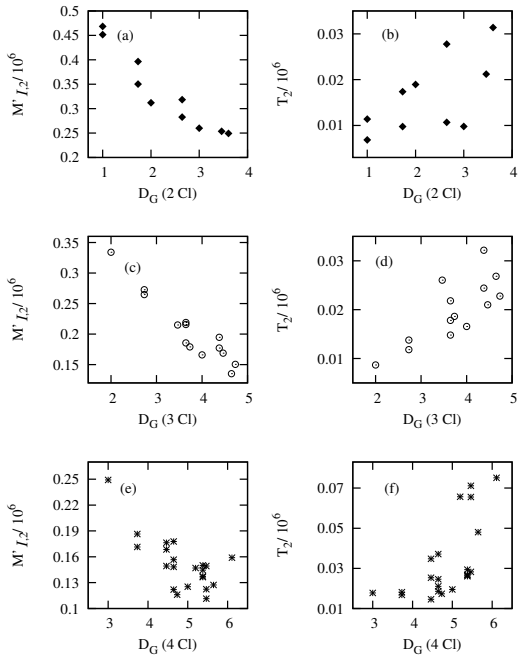


Figure 4: Correlation diagrams:  $M'_{I,2}$  versus  $D_G$  [panels (a), (c), (e)], and  $T_2$  versus  $D_G$  [panels (b), (d), (f)].

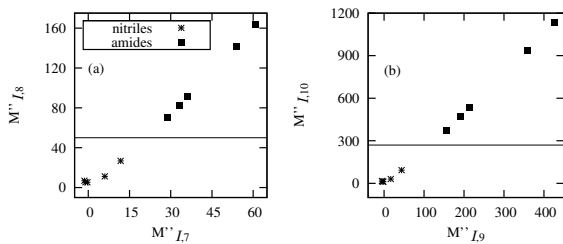


Figure 5: Classification diagrams: intensity-intensity distribution moments for nitriles and amides.

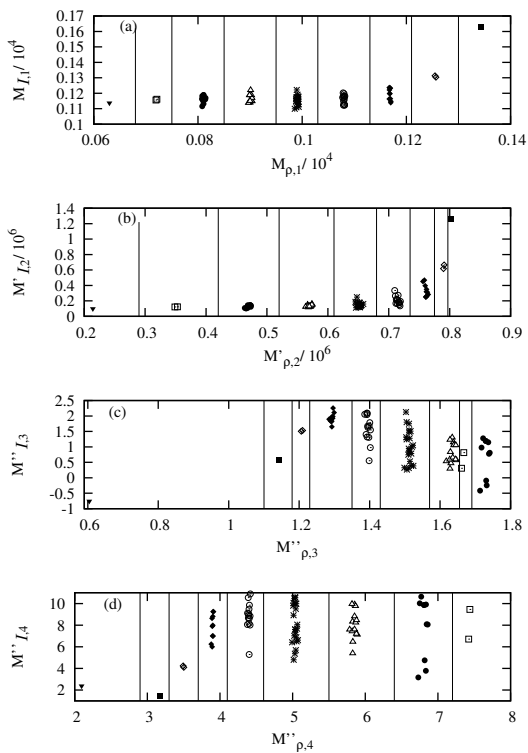


Figure 6: Classification diagrams: spectral density-intensity distribution moments [panel (a):  $q = 1$ ; panel (b):  $q = 2$ ; panel (c):  $q = 3$ ; panel (d):  $q = 4$ ]. The symbols are the same as in Fig. 1.

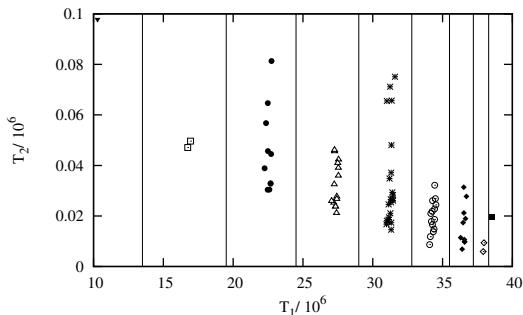


Figure 7: Classification diagram based on moments of inertia of spectra. The symbols are the same as in Fig. 1.

The changes of these descriptors for the molecules with a given number of chlorine atoms can add some new information about the molecules. In order to study the relations of the two descriptors with the geometry of the molecules, let us consider a simple descriptor: the geometrical distance  $D_G$  which is the shortest distance between the carbon atoms to which the chlorine atoms are bound. For our approximate relations we assume that all bond lengths between the carbon atoms are the same. As a unit of length we take the bond length carbon-carbon and  $D_G$  is expressed in these units. Two examples of  $D_G$  are shown in Fig. 3:  $D_G = \sqrt{3}$  in panel (a) and  $D_G = 1 + \sqrt{3}$  in panel (b). The relations of  $M'_{1,2}$  and of  $T_2$  with  $D_G$  are shown in Fig. 4. Approximately,  $T_2$  increase with  $D_G$ , and  $M'_{1,2}$  decrease. Panels (a), (b) correspond to the molecules with two chlorine atoms ( $r = 3, 4, \dots, 12$  - see Table 1), panels (c), (d) correspond to the molecules with three chlorine atoms ( $r = 13, 14, \dots, 26$ ), and panels (e), (f) correspond to the molecules with four chlorine atoms ( $r = 27, 28, \dots, 48$ ). For the molecules with larger number of chlorine atoms,  $D_G$  becomes similar for different isomers and such a simple descriptor ( $D_G$ ) does not correlate with the moments considered in this paper.

In our previous studies we have shown that intensity distribution moments can distinguish between different groups of molecules: nitriles and amides [19]. Two examples of classification diagrams based on the intensity distribution moments (both axes are represented by the intensity distribution moments) for nitriles and amides are shown in Fig. 5. The patterns are similar in the two diagrams and that suggests some correlations between the moments [compare panels (a) and (b)]. Usually, higher-order moments are correlated

with the lower ones [18]. They contain similar information and it is sufficient to consider several lowest moments.

For chloronaphthalenes intensity distribution moments do not contain sufficient information to compose intensity-intensity distribution moment classification diagrams. Here the intensity distribution moments play a different role: they are corrections to the spectral density distribution moments. The classification diagrams for these molecules are mainly based on spectral density distribution moments. For chloronaphthalenes we can only consider, either spectral density-spectral density distribution moments diagrams as in our previous work [14] or spectral density-intensity distribution moments diagrams (Fig. 6). We can also consider diagrams based on the moments of inertia of the spectra. The diagram  $T_1 - T_2$  is shown in Fig. 7 and it is similar to spectral density-intensity distribution moments diagrams. Different symbols denote molecules with different number of chlorine atoms. As one can see, different symbols are located in different parts of the diagrams and they are separated by lines.

Summarizing, moments of inertia of molecular spectra, spectral density distribution moments, and intensity distribution moments can be used as molecular descriptors for QSAR/QSPR. Their role depends on the systems and properties considered. In particular, for chloronaphthalenes intensity distribution moments and  $T_2$  which allow to distinguish between different isomers can be considered as corrections to the frequency distribution moments and to  $T_1$ .

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