

# Theory of the PCP effect and related phenomena

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**Abstract** Recent studies of cyclic conjugation in the five-membered ring of acenaphthylene and fluoranthene congeners revealed some peculiar regularities, of which the so-called PCP effect attracted the greatest attention. The PCP effect is a significant increase in the magnitude of cyclic conjugation in the five-membered ring caused by the six-membered rings separated from the five-membered ring by a single carbon–carbon bond. We now present the mathematical formalism of a general theory capable of treating cyclic–conjugation phenomena of this kind, of which the PCP effect is just a special case. Namely we calculate the influence of any cycle present in a polycyclic conjugated molecule on the energy effect of cyclic conjugation of any other cycle.

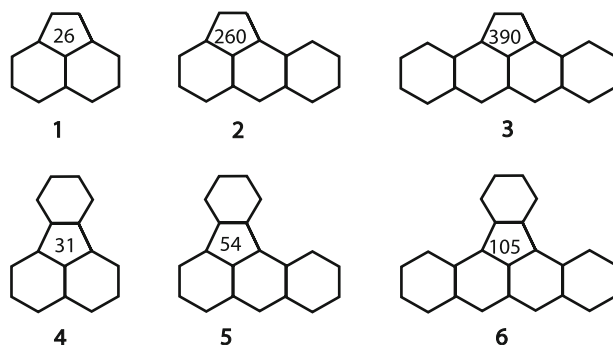
**Keywords** Cyclic conjugation · Energy effect (of cyclic conjugation) · Pairwise energy effect (of cyclic conjugation) · PCP effect · Graph theory · Spectral graph theory

## 1 Introduction

Within our studies of the  $\pi$ -electron properties of polycyclic conjugated molecules that are congeners of acenaphthylene and fluoranthene [1–4], we discovered several regularities for the structure–dependency of the intensity of cyclic conjugation in the five-membered ring. These findings are outlined in due detail in a number of recent papers [2–6], and will not be re-stated here. We only point out that these regularities were initially detected at the HMO level of theory, but were eventually corroborated by several other, more advanced, quantum chemical approaches [5–7].

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**Fig. 1** The energy-effect (in  $\beta$ -units times  $10^4$ ) of the five-membered ring in acenaphthylene (**1**), fluranthene (**4**), and its benzo- and dibenzo-derivatives. The benzene-rings attached to acenaphthylene and fluranthene are in PCP constellation (i.e., are connected to the five-membered ring by a single carbon-carbon bond). The energy-effect increases with the increasing number of six-membered rings in PCP constellation. Until now not a single exception of the PCP rule has been observed. For details see [2–6]

The most remarkable of these regularities is the so-called *PCP effect* (or *PCP rule*) which is illustrated by examples depicted in Fig. 1.

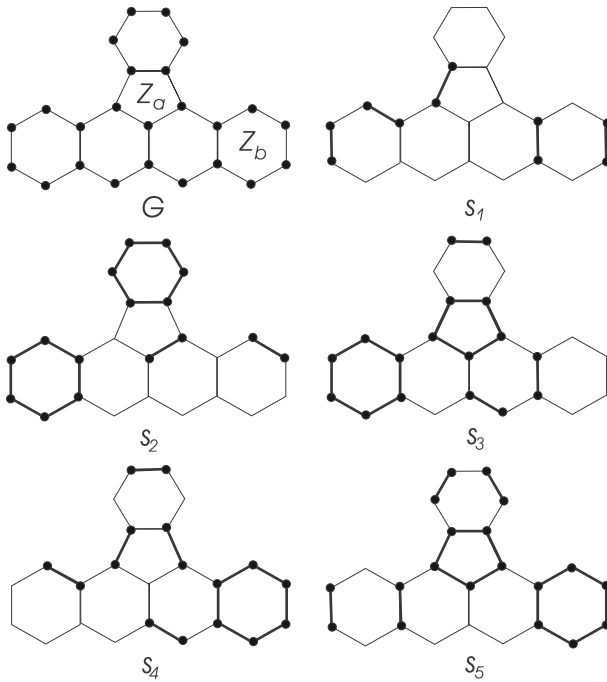
Chemists will without any hesitation accept the conclusion that the increase of the intensity of cyclic conjugation in the five-membered ring (measured by means of its energy-effect) is caused by the six-membered ring(s) attached to the acenaphthylene or fluranthene system. Although we do not intend to challenge this conclusion, we point out that the situation is far less “obvious” and “self-evident”. Namely, when we compare cyclic conjugation (or whichever property) in the five membered ring of acenaphthylene (**1**), benzoacenaphthylene (**2**) and dibenzoacenaphthylene (**3**), or fluranthene (**4**), benzofluranthene (**5**) and dibenzofluranthene (**6**), we must not overlook the fact that these molecules differ significantly: these have different numbers of carbon and hydrogen atoms, different number of  $\pi$ -electrons, different Kekulé structure counts, etc. Therefore, one cannot *a priori* exclude the possibility that the increase of the energy-effect is caused by some quite different structural factor, or by several mutually acting structural factors.

In order to overcome these doubts, we developed a method which makes it possible to “extract” the influence of an individual cycle (e. g., of a six-membered ring) on the energy-effect of another cycle (e. g., of the five-membered ring) within one and the same molecule.

## 2 Preparations: Sachs graph formalism

The present considerations are based on the concept of Sachs graphs and uses the Sachs theorem; details on these matters are found in books [8–11] and surveys [12–17].

Let  $G$  be a (molecular) graph. Any subgraph of  $G$  consisting of disjoint cycles and/or connected two-vertex graphs  $K_2$  is said to be a *Sachs graph* contained in  $G$ ; for examples see Fig. 2. Also the empty graph (possessing no cycles and no  $K_2$ -graphs) is



**Fig. 2** The molecular graph  $G$  of dibenzofluoranthene and its rings  $Z_a$  and  $Z_b$ . By heavy lines are indicated five Sachs graphs of  $G$ . The Sachs graph  $s_1$  has five components,  $p(s_1) = 5$ , of which no one is cyclic,  $c(s_1) = 0$ , and 10 vertices,  $n(s_1) = 10$ . Analogously,  $p(s_2) = 4$ ,  $c(s_2) = 2$ ,  $n(s_2) = 16$ ,  $p(s_3) = 5$ ,  $c(s_3) = 2$ ,  $n(s_3) = 17$ ,  $p(s_4) = 6$ ,  $c(s_4) = 1$ ,  $n(s_4) = 16$ , and  $p(s_5) = 6$ ,  $c(s_5) = 2$ ,  $n(s_5) = 19$ . Further,  $s_1, s_2 \in \mathcal{S}_0(G)$ ,  $s_3, s_5 \in \mathcal{S}_a(G)$ ,  $s_4, s_5 \in \mathcal{S}_b(G)$ , and  $s_5 \in \mathcal{S}_{ab}(G)$

considered to be a Sachs graph of  $G$ . The set of all Sachs graphs of  $G$  will be denoted by  $\mathcal{S}(G)$ .

Let  $s$  be a Sachs graph of  $G$ , that is  $s \in \mathcal{S}(G)$ . By  $p(s)$ ,  $c(s)$ , and  $n(s)$  we denote the number of components, cyclic components, and vertices of  $s$ .

Let  $\phi(G, \lambda)$  be the characteristic polynomial of the graph  $G$  [9, 10]. If  $G$  has  $n$  vertices, then according to the famous *Sachs theorem*,

$$\phi(G, \lambda) = \sum_{s \in \mathcal{S}(G)} (-1)^{p(s)} 2^{c(s)} \lambda^{n-n(s)}. \tag{1}$$

In what follows, summations of the form occurring on the right-hand side of Eq. (1) will frequently be encountered. Therefore, for the sake of brevity we use the symbol  $Sum[\mathcal{X}]$  to denote the polynomial

$$\sum_{s \in \mathcal{X}} (-1)^{p(s)} 2^{c(s)} \lambda^{n-n(s)}$$

where  $\mathcal{X}$  is either the set  $\mathcal{S}(G)$  or some of its subsets. Thus, Eq. (1) will be written as

$$\text{Sum}[\mathcal{S}(G)] = \phi(G, \lambda).$$

From the definition of Sachs graphs and Eq. (1) we see that  $\text{Sum}[\mathcal{S}(G)]$  contains the effect of all cycles present in the (molecular) graph  $G$  on the value of the characteristic polynomial. Now, we will be interested in expressions in which the effect of some particular cycles are excluded.

Let  $Z_a$  and  $Z_b$  be two cycles contained in the graph  $G$ . [In the case of the molecular graphs of acenaphthylene and fluoranthene congeners,  $Z_a$  may be the five-membered ring, and  $Z_b$  a six-membered ring, cf. Fig. 2.]

Let  $\mathcal{S}_0(G)$  be the set of Sachs graphs of  $G$  which contain (as components) neither  $Z_a$  nor  $Z_b$ . Let  $\mathcal{S}_a(G)$  be the set of Sachs graphs of  $G$  which contain (as component)  $Z_a$ . Let  $\mathcal{S}_b(G)$  be the set of Sachs graphs of  $G$  which contain (as component)  $Z_b$ . Let  $\mathcal{S}_{ab}(G)$  be the set of Sachs graphs of  $G$  which contain (as components) both  $Z_a$  and  $Z_b$ . For examples see Fig. 2.

Of course,

$$\mathcal{S}_0(G) \cup \mathcal{S}_a(G) \cup \mathcal{S}_b(G) = \mathcal{S}(G)$$

and

$$\mathcal{S}_a(G) \cap \mathcal{S}_b(G) = \mathcal{S}_{ab}(G).$$

Consider an element  $s$  of  $\mathcal{S}_a(G)$ . By definition, one component of  $s$  is the cycle  $Z_a$ . If this cycle is deleted from the Sachs graphs  $s$ , what remains is a Sachs graph of the subgraph  $G - Z_a$ . It is easy to see that there is a one-to-one correspondence between the elements of  $\mathcal{S}_a(G)$  and  $\mathcal{S}(G - Z_a)$ , cf. Fig. 3.

If  $s' \in \mathcal{S}(G - Z_a)$  corresponds to  $s \in \mathcal{S}_a(G)$ , then  $p(s') = p(s) - 1$ ,  $c(s') = c(s) - 1$  and  $n(s') = n(s) - |Z_a|$ , where  $|Z_a|$  is the number of vertices (= size) of the cycle  $Z_a$ . Since, in addition,  $n(G - Z_a) = n(G) - |Z_a|$ , we obtain

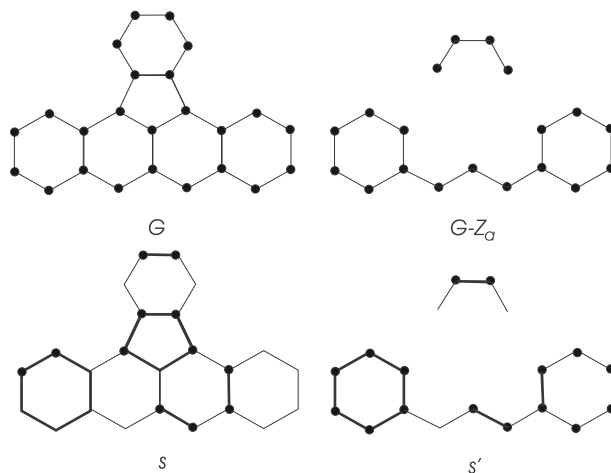
$$\text{Sum}[\mathcal{S}_a(G)] = -2 \text{Sum}[\mathcal{S}(G - Z_a)] = -2 \phi(G - Z_a, \lambda). \quad (2)$$

In a fully analogous manner we have

$$\text{Sum}[\mathcal{S}_b(G)] = -2 \text{Sum}[\mathcal{S}(G - Z_b)] = -2 \phi(G - Z_b, \lambda). \quad (3)$$

If  $s \in \mathcal{S}_{ab}(G)$ , then  $s$  contains as components both  $Z_a$  and  $Z_b$ . If these cycles are deleted from  $s$ , what remains is a Sachs graph of the subgraph  $G - Z_a - Z_b$ . Again, there is a one-to-one correspondence between the elements of  $\mathcal{S}_{ab}(G)$  and  $\mathcal{S}(G - Z_a - Z_b)$ . If  $s' \in \mathcal{S}(G - Z_a - Z_b)$  corresponds to  $s \in \mathcal{S}_{ab}(G)$ , then  $p(s') = p(s) - 2$ ,  $c(s') = c(s) - 2$  and  $n(s') = n(s) - |Z_a| - |Z_b|$ . In addition,  $n(G - Z_a - Z_b) = n(G) - |Z_a| - |Z_b|$ , which implies

$$\text{Sum}[\mathcal{S}_{ab}(G)] = (-1)^2 (2)^2 \text{Sum}[\mathcal{S}(G - Z_a - Z_b)] = 4 \phi(G - Z_a - Z_b, \lambda). \quad (4)$$



**Fig. 3** The molecular graph  $G$  and its cycle-deleted subgraph  $G - Z_a$ . The Sachs graphs  $s$  of  $G$  corresponds to the Sachs graph  $s'$  of  $G - Z_a$ ; for details see text

Now,  $Sum[\mathcal{S}(G) \setminus \mathcal{S}_a(G)]$  is the polynomial resembling the characteristic polynomial, from which the effect of the cycle  $Z_a$  has been excluded. Bearing in mind Eqs. (2)–(4), by direct calculation we get

$$Sum[\mathcal{S}(G) \setminus (\mathcal{S}_a(G))] = Sum[\mathcal{S}(G)] - Sum[\mathcal{S}_a(G)]$$

resulting in

$$Sum[\mathcal{S}(G) \setminus (\mathcal{S}_a(G))] = \phi(G, \lambda) + 2\phi(G - Z_a, \lambda). \tag{5}$$

Analogously, the polynomial from which the effect of the cycle  $Z_b$  has been excluded is

$$Sum[\mathcal{S}(G) \setminus (\mathcal{S}_b(G))] = \phi(G, \lambda) + 2\phi(G - Z_b, \lambda). \tag{6}$$

If the want to exclude from the characteristic polynomial the effect of both cycles  $Z_a$  and  $Z_b$ , then we have:

$$Sum[\mathcal{S}(G) \setminus (\mathcal{S}_a(G) \cup \mathcal{S}_b(G))] = Sum[\mathcal{S}(G)] - Sum[\mathcal{S}_a(G)] - Sum[\mathcal{S}_b(G)] + Sum[\mathcal{S}_{ab}(G)] \tag{7}$$

which yields

$$Sum[\mathcal{S}(G) \setminus (\mathcal{S}_a(G) \cup \mathcal{S}_b(G))] = \phi(G, \lambda) + 2\phi(G - Z_a, \lambda) + 2\phi(G - Z_b, \lambda) + 4\phi(G - Z_a - Z_b, \lambda). \tag{8}$$

Note that the last term on the right-hand side of the formulas (7) and (8) had to be added because any Sachs graph  $s \in \mathcal{S}_{ab}(G)$  is contained in both  $\mathcal{S}_a(G)$  and  $\mathcal{S}_b(G)$ .

### 3 The main result

Within the HMO approximation, the total  $\pi$ -electron energy  $E_\pi$  of a conjugated molecule can be calculated from the characteristic polynomial of the underlying molecular graph. Details of this calculation are not important for the present considerations and can be found in appropriate textbooks [9–11]. Thus we may write

$$E_\pi = F[\phi(G, \lambda)]$$

with  $F$  indicating the procedure by means of which  $E_\pi$  is calculated from  $\phi(G, \lambda)$ .

As explained in the preceding section,  $\phi(G, \lambda)$  contains the contributions of all cycles present in the molecular graph. Therefore, also the actual value of  $E_\pi$  depends on all cycles present in the molecular graph, and thus present in the corresponding conjugated molecule.

In view of Eq. (5),

$$F[\phi(G, \lambda) + 2\phi(G - Z_a, \lambda)]$$

is a total- $\pi$ -electron-energy-like quantity, containing the same structural contributions as  $E_\pi$ , except the contributions coming from the cycle  $Z_a$ . Analogously, by Eq. (6),

$$F[\phi(G, \lambda) + 2\phi(G - Z_b, \lambda)]$$

differs from the total  $\pi$ -electron energy, by lacking the contributions coming from the cycle  $Z_b$ . Further, by Eq. (8),

$$F[\phi(G, \lambda) + 2\phi(G - Z_a, \lambda) + 2\phi(G - Z_b, \lambda) + 4\phi(G - Z_a - Z_b, \lambda)]$$

is the energy-like quantity, in which the effects of both cycles  $Z_a$  and  $Z_b$  are neglected, but all other structural effects are same as in the case of the ordinary total  $\pi$ -electron energy.

The difference

$$ef(G; Z_a) = F[\phi(G, \lambda)] - F[\phi(G, \lambda) + 2\phi(G - Z_a, \lambda)] \quad (9)$$

is thus the effect of the cycle  $Z_a$  on total  $\pi$ -electron energy. This quantity, first introduced in 1977 [18–21], has been much studied; for review see [22] and for some most recent applications see [23–25]

Applying the Coulson–Jacobs integral formula [26] we get

$$ef(G; Z_a) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \frac{\phi(G, ix)}{\phi(G, ix) + 2\phi(G - Z_a, ix)} dx \quad (10)$$

where  $i = \sqrt{-1}$ . This result is known for a long time [19,20]. For more details on Coulson–type integral formulas see [10,27–29].

Bearing in mind the previous discussion, we see that the right–hand sides of both (9) and (10) contain contributions coming from the cycle  $Z_b$ . Therefore,

$$\begin{aligned}
 pef(G; Z_a, Z_b) = & \{F[\phi(G, \lambda)] - F[\phi(G, \lambda) + 2\phi(G - Z_a, \lambda)]\} \\
 & - \{F[\phi(G, \lambda) + 2\phi(G - Z_b, \lambda)] - F[\phi(G, \lambda) \\
 & + 2\phi(G - Z_a, \lambda) \\
 & + 2\phi(G - Z_b, \lambda) + 4\phi(G - Z_a - Z_b, \lambda)]\} \quad (11)
 \end{aligned}$$

and its Coulson–type integral formulation

$$pef(G; Z_a, Z_b) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \Gamma(G; Z_a, Z_b, x) dx \quad (12)$$

where

$$\begin{aligned}
 & \Gamma(G; Z_a, Z_b, x) \\
 = & \frac{\phi(G, ix)[\phi(G, ix) + 2\phi(G - Z_a, ix) + 2\phi(G - Z_b, ix) + 4\phi(G - Z_a - Z_b, ix)]}{[\phi(G, ix) + 2\phi(G - Z_a, ix)][\phi(G, ix) + 2\phi(G - Z_b, ix)]} \quad (13)
 \end{aligned}$$

can be viewed as the effect of the cycle  $Z_b$  on the energy–effect of the cycle  $Z_a$ . Since, evidently,

$$pef(G; Z_a, Z_b) = pef(G; Z_b, Z_a)$$

formulas (11) and (12) express also the effect of the cycle  $Z_a$  on the energy–effect of the cycle  $Z_b$ . Therefore we speak of a *pairwise energy effect* and denote it by *pef*.

In the general case the integrand  $\ln \Gamma(G; Z_a, Z_b, x)$  is complex–valued. Bearing in mind that any complex number  $z$  can be written in the form  $z = |z|e^{i\varphi}$  i. e.,  $\ln z = \ln |z| + i\varphi$ , and since the integral in (12) is necessarily real–valued, we get

$$pef(G; Z_a, Z_b) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln |\Gamma(G; Z_a, Z_b, x)| dx. \quad (14)$$

At this point it should be mentioned that recently another approach for calculating the pairwise energy effects of two cycles was put forward [30]. This method was also aimed at explaining the PCP effect. However, it is based on a number of approximations and certain *ad hoc* assumptions. Therefore it cannot be considered as complete and satisfactory [31]. We maintain that the present formulas (11) and (12) provide the true and rigorous solution of the problem of pairwise energy effects of cyclic conjugation.

#### 4 Application to acenaphthylene and fluoranthene congeners

In this section we consider the special case of formula (12) when  $G$  is the molecular graph of an acenaphthylene or fluoranthene congener,  $Z_a$  is its (unique) five-membered ring, and  $Z_b$  is one of its six-membered rings. We assume that the molecule is Kekuléan, which implies that the number  $n$  of vertices of  $G$  is even. Then the polynomials occurring in Eq. (13) can be written as:

$$\phi(G, ix) = i^n [P(x) + i Q(x)]$$

$$\phi(G - Z_a, ix) = i^{n-5} P_a(x) \quad (15)$$

$$\phi(G - Z_b, ix) = i^{n-6} [P_b(x) + i Q_b(x)]$$

$$\phi(G - Z_a - Z_b, ix) = i^{n-11} P_{ab}(x). \quad (16)$$

Whereas the graphs  $G$  and  $G - Z_b$  are non-bipartite, the graphs  $G - Z_a$  and  $G - Z_a - Z_b$  are bipartite. Therefore  $\phi(G - Z_a, ix)$  and  $\phi(G - Z_a - Z_b, ix)$  are pure imaginary. The degrees of the polynomials  $P(x)$ ,  $Q(x)$ ,  $P_a(x)$ ,  $P_b(x)$ ,  $Q_b(x)$ , and  $P_{ab}(x)$  are equal to  $n$ ,  $n-5$ ,  $n-5$ ,  $n-6$ ,  $n-11$ , and  $n-11$ , respectively. Therefore  $Q(x) \ll P(x)$  and  $Q_b(x) \ll P_b(x)$ , and in what follows we adopt the approximations

$$\phi(G, ix) \approx i^n P(x) \quad (17)$$

$$\phi(G - Z_b, ix) \approx i^{n-6} P_b(x). \quad (18)$$

Using the fact that acenaphthylenes and fluoranthenes contain just a single odd-membered ring, it can be shown that all polynomials  $P(x)$ ,  $P_a(x)$ ,  $P_b(x)$ , and  $P_{ab}(x)$  are of the form

$$c_0 x^h + c_1 x^{h-2} + c_2 x^{h-4} + c_3 x^{h-6} + \dots$$

where  $c_0, c_1, c_2, c_3, \dots$  are non-negative numbers and where  $h = n, n-5, n-6$ , and  $n-11$ , respectively. These polynomials are monic, i. e., their leading coefficients  $c_0$  are equal to unity. For what follows it is important that the second coefficient ( $c_1$ ) is equal to the number of edges of the underlying graph.

Combining Eqs. (15)–(18) with (13) we arrive at

$$\begin{aligned} & \ln |\Gamma(G; Z_a, Z_b, x)| \\ &= \frac{1}{2} \ln \left[ 1 + 4 \frac{[2P(x)P_a(x) + 4P_a(x)P_b(x)][P(x)P_{ab}(x) - P_a(x)P_b(x)]}{[P(x)^2 + 2P_a(x)^2]^2 + [2P(x)P_a(x) + 4P_a(x)P_b(x)]^2} \right]. \end{aligned} \quad (19)$$

It can be shown that

$$\ln |\Gamma(G; Z_a, Z_b, x)| = \ln |\Gamma(G; Z_a, Z_b, -x)|$$



and therefore we need to examine this integrand only for  $x > 0$ . For  $x > 0$ , all terms occurring on the right-hand side of formula (19) are positive-valued, except

$$P(x)P_{ab}(x) - P_a(x)P_b(x)$$

whose sign is not *a priori* evident.

Denote the number of edges of the graph  $G$  by  $m$ . Let the number of edges of the subgraphs  $G - Z_a$ ,  $G - Z_b$ , and  $G - Z_a - Z_b$  be  $m - m_a$ ,  $m - m_b$ , and  $m - m_{ab}$ , respectively.

Now, if the rings  $Z_a$  and  $Z_b$  are in a PCP-constellation, namely if a single edge of  $G$  is incident to both  $Z_a$  and  $Z_b$ , then  $m_{ab} = m_a + m_b - 1$  i. e.,  $m_a + m_b - m_{ab} = 1$ . Therefore

$$\begin{aligned} P(x)P_{ab}(x) - P_a(x)P_b(x) &= [x^n + m x^{n-2} + \dots][x^{n-11} + (m - m_{ab})x^{n-13} + \dots] \\ &\quad - [x^{n-5} + (m - m_a)x^{n-7} + \dots](x^{n-6} + (m - m_b)x^{n-7} + \dots) \\ &= [x^{2n-11} + (2m - m_{ab})x^{2n-13} + \dots] \\ &\quad - [x^{2n-11} + (2m - m_a - m_b)x^{2n-13} + \dots] \\ &= (m_a + m_b - m_{ab})x^{2n-13} + \dots \end{aligned}$$

Thus,  $P(x)P_{ab}(x) - P_a(x)P_b(x)$  is a polynomial of degree  $2n - 13$  with leading coefficient equal to  $+1$ . Consequently,  $P(x)P_{ab}(x) - P_a(x)P_b(x) > 0$  and therefore the expression in (19) under the logarithm is greater than unity, implying that the integrand in (14) is greater than zero for all values of  $x$ , implying that the pairwise energy effect of rings  $Z_a$  and  $Z_b$  in PCP-constellation is positive, i. e., stabilizing.

By analogous reasoning several other, previously observed [3,4], general regularities for cyclic conjugation in fluoranthene and acenaphthylene derivatives can also be rationalized.

For instance, we say that the five-membered ring  $Z_a$  and a six-membered ring  $Z_b$  are in linear constellation if they are separated by a single hexagon, but are not in PCP-constellation [3,4]. It can be shown that in this case,  $P(x)P_{ab}(x) - P_a(x)P_b(x)$  is a polynomial of degree  $2n - 15$  with negative leading coefficient. This implies  $pef < 0$ , in agreement with earlier observations [3,4].

## 5 Concluding remarks

In this paper the mathematical theory of the pairwise energy effect  $pef$  has been outlined in due detail. Numerical studies of  $pef$  are under way and will be communicated at a later moment. Some of our first numerical results, pertaining to benzo-annelated perylenes, have already been completed [32].

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