QSPR for Physical Properties of *cata*-Condensed Benzenoids Using Two Simple Dualist-Based Descriptors

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Dualists of benzenoids are a special type of graphs that have as vertices the centers of hexagons and as edges the pairs of condensed rings. Catafusenes (*cata*-condensed benzenoids) have acyclic dualists. Codes of catafusenes with *h* benzenoid rings start from one end of a dualist and consist of digits 0 (indicating linear annelation, angle of 180° between two adjacent edges) and 1 or 2 for kinks (120° or 240° angles) with the convention of choosing the lowest number formed from these $h-2$ digits. A shape parameter (*n*) for the dualist consists of the number of adjacent zeros in the code plus 1. It is shown in the present communication that many molecular properties of catafusenes depend mainly on *n*, whereas most bulk properties depend mainly on *h*. Monoparametric or biparametric correlations in terms of the simple integer parameters *n* and/or *h* are presented for molecular properties (energy of the *p*-band in electronic absorption spectra, ionization potentials, electron affinities, hardness and softness) and bulk properties (normal boiling point, chromatographic retention index, the logarithm of the water solubility, and lipophilicity).

1. Introduction

Benzenoid polycyclic aromatic hydrocarbons (PAHs) are molecules that have a carbon skeleton which is a portion of a graphene sheet, with benzenoid rings that share carbon−carbon bonds. Thus, biphenyl and related molecules do not belong to this category. It has been known for more than 50 years that some PAHs are carcinogenic, and efforts have been made to reduce the amount of benzanthracene or benzopyrene and related carcinogens from exhaust gases. On the positive side, some PAHs have become the basis of large industries such as plastics, pharmaceuticals, or dyestuffs, and pentacene or its derivatives have recently demonstrated their usefulness in organic thin-film transistors or organic light-emitting diodes.[1−3] The high thermal resistance of PAHs is both a blessing for many uses (such as heat transfer fluids, or neutron moderators in nuclear reactors) and a curse (due to carcinogenic PAHs, and to the high persistence and high toxicity of polyhalo derivatives of biphenyl, dibenzofuran, and dibenzodioxin).

The inner duals (or dualists) of benzenoid polycyclic aromatic hydrocarbons (which will be called benzenoids for brevity) consist of vertices situated in the centers of benzenoid rings, and of edges connecting vertices corresponding to condensed rings, that is, rings sharing one C−C bond.[3,4] In dualists, bond lengths and angles do matter, unlike the situation in graphs. There is a one-to-one correspondence between structures of benzenoids and their dualists, which therefore characterize benzenoids uniquely.

Benzenoids are classified as *cata*-condensed (catafusenes), *peri*-condensed (perifusenes), and *corona*-condensed (coronoids). Catafusenes have no carbon atoms common to three benzenoid rings, and their dualists are acyclic; perifusenes have carbon atoms common to three benzenoid rings, and their dualists have three-membered rings (and possibly also acyclic branches); whereas coronoids have dualists with larger rings (and possibly also three-membered rings and/or acyclic branches).

The notation introduced for catafusenes, indicating the geometry of their condensation by means of digits 0, 1, and 2 for their dualists, contains essential information on many properties of these catafusenes. The digit 0 indicates linear annelation (angle of 180° between two edges in the dualist) giving rise to anthracenic portions, whereas digits 1 and 2 denote kinked annelation (angles of 120° or 240° starting from one extremity of the catafusene, keeping the right/left direction of annelation in correspondence with digits 1 and 2, respectively, and choosing among possible notations by the minimal number formed by digits 0, 1, and 2).[4−7] In particular, the number of zeros (i.e., of linearly condensed benzenoid rings) represents the number of anthracenoid subgraphs of the catafusene. The highest number of adjacent zeros (i.e., of linearly condensed benzenoid rings) plus 1 is an important parameter, denoted by *n*. The number of benzenoid rings in a longest acenic portion is $n + 1$. Branching of the dualist is denoted by brackets enclosing the notation for the dualist of the branch (when this branch is an isolated benzenoid ring as in triphenylene, it is denoted by a dot in the brackets).

The number *h* of benzenoid rings, which is also the number of vertices of the dualist, is linearly correlated with the molecular weight, MW (approximate integer values), as seen from eq 1.

$$\mathrm{MW} = 28 + 50h \qquad (1)$$

Among other applications and uses of dualists we cite only one, namely, weighted dualists.[7]

In a recent paper, it was shown that the half-wave reduction potentials of catafusenes are correlated satisfactorily with *n* (one plus the number of adjacent zeros in the code) and the total number *h* of benzenoid rings.[8] For naphthalene, we postulate that $n = 0$. In the present paper, a quantitative structure−property relationship (QSPR) study for other physical properties

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TABLE 1: Catafusenes with Their Names, CAS Registry Numbers, *h* and *n* Parameters, and Physical Properties

no.	name	CAS -RN	*h*	*n*	code	IP	EA	*E*-ga p	η	ΔE_p	NBP	RI	log *S*	log K_{ow}	ΔH_f
1	naphthalene	91-2 0-3	2	0	.	8.57	0.332	8.24	0.618	4.38	217.9	2.00	1.49	3.33	150.6
2	phenanthrene	85-0 1-8	3	1	1	8.48	0.481	7.997	0.605	4.23	340	3.00	0.061	4.55	209.1
3	anthracene	120-12-7	3	2	0	8.05	0.842	7.21	0.414	3.38	339.9	3.20	−1.36	4.54	218.3
4	chrysene	218-01-9	4	1	12	8.26	0.718	7.54	0.52	3.87	431	4.10	−2.46	5.84	267.7
5	triphenylene	217-59-4	4	1	1(.)	8.5	0.557	7.95	0.684		425	3.70	−1.39	5.45	258.5
6	benzo[*c*]phenanthrene	195-19-7	4	1	11	8.28	0.692	7.59	0.568	3.84		3.64	−2.46	5.84	280.5
7	benz[*a*]anthracene	56-5 5-3	4	2	01	8.11	0.83	7.28	0.452	3.53	437.6	4.00	−2.03	5.91	276.9
8	tetracene	92-2 4-0	4	3	00	7.72	1.185	6.54	0.295	2.71	440	4.51	−2.82	5.96	286.1
9	picene	213-46-7	5	1	121	8.24	0.751	7.49	0.502	3.8	519	5.18	−2.37	7.11	326.3
10	benzo[*c*]chrysene	194-69-4	5	1	112	8.27	0.747	7.52	0.55		519	4.45		7.11	335.5
11	dibenzo[*c*,*g*]phenanthrene	188-52-3	5	1	111	8.22	0.822	7.35	0.535		519	4.07		7.11	333
12	benzo[*g*]chrysene	196-78-1	5	1	1(.)1	8.157	0.815	7.341				4.27			329.8
13	benzo[*b*]chrysene	214-17-5	5	2	012	7.972	0.995	6.997	0.405	3.27	524	5.00		7.11	339
14	dibenz[*a*,*h*]anthracene	53-7 0-3	5	2	102	8.15	0.829	7.32	0.473	3.57	524	4.73	−2.60	6.75	335.5
15	dibenz[*a*,*j*]anthracene	224-41-9	5	2	101	8.17	0.829	7.32	0.492	3.6	524	4.56	−2.99	6.54	335.5
16	dibenz[*a*,*c*]anthracene	215-58-7	5	2	01(.)	8.17	0.823	7.35	0.499		524	4.40		7.19	326.3
17	dibenzo[*b*,*g*]phenanthrene	195-06-2	5	2	011	7.972	0.967	7.005				4.33			348.3
18	pentaphene	222-93-5	5	2	010	8.11	0.844	7.27	0.437	3.55		4.67		6.81	344.7
19	benzo[*a*]tetracene	226-88-0	5	3	001	7.797	1.145	6.65	0.327	2.83		4.99		6.81	
20	pentacene	135-48-8	5	4	000	7.499	1.43	6.07	0.22	2.23	529			7.19	353.9
21	dibenzo[*g*,*p*]chrysene	191-68-4	6	1	1(.)1(.)	8.01	0.9199	7.09	0.512					8.39	
22	benzo[*c*]picene	217-37-8	6	1	1212	8.15	0.867	7.28	0.471	3.66					403.2
23	dibenzo[*c*,*l*]chrysene	4285 0-69 -1	6	1	1122	8.14	0.872	7.27	0.539						
24	hexahelicene	187-83-7	6	1	1111				0.546						
25	dibenzo[*a*,*n*]triphenylene	196-64-5	6	2	0(.)11	7.99	0.962	7.03	0.447						
26	benzo[*c*]pentaphene	222-54-8	6	2	0101					3.42					406.8
27	benzo[*b*]picene	217-42-5	6	2	0121					3.34					
28	naphtho[1,2-*b*]chrysene	220-77-9	6	2	1012					3.39					
29	dibenzo[*b*,*k*]chrysene	217-54-9	6	2	0120	7.82	1.16	6.66	0.348	3.02					
30	benzo[*h*]pentaphene	214-91-5	6	2	0(.)10	8.19	0.835	7.35	0.506						408.8
31	dibenzo[*a*,*j*]tetracene	227-04-3	6	3	1002	7.87	1.11	6.76	0.358	2.95					
32	dibenzo[*a*,*l*]tetracene	226-86-8	6	3	1001	7.87	1.11	6.77	0.361	2.95					
33	dibenzo[*a*,*c*]tetracene	216-00-2	6	3	001(.)	7.85	1.13	6.72	0.356						
34	hexaphene	222-78-6	6	3	0010				0.336	2.94					
35	naphtho[2,1-*a*]tetracene	220-82-6	6	3	0011					2.72					
36	benzo[*a*]pentacene	239-98-5	6	4	0001	7.566	1.39	6.176	0.244	2.37					384.8
37	hexacene	258-31-1	6	5	0000	7.34	1.61	5.74	0.169	1.9					
38	dinaphtho[2,3-*c*:2,3-*g*]phenanthrene	188-51-2	7	2	01110				0.394						
39	naphtho[2,3-*c*]pentaphene	222-58-2	7	2	01020					3.28					
40	benzo[*b*]naphtho[1,2-*k*]chrysene	214-15-3	7	2	01201					3.1					
41	dibenzo[*b*,*n*]picene	213-44-5	7	2	01210					3.37					
42	dibenzo[*c*,*m*]pentaphene	222-51-5	7	2	10201					3.43					
43	heptaphene	222-75-3	7	3	00100					2.97					
44	benzo[*b*]naphtho[2,3-*k*]chrysene	214-16-4	7	3	00120					2.65					
45	dibenzo[*a*,*l*]pentacene	227-09-8	7	4	10002				0.269	2.47					
46	naphtho[2,3-*a*]pentacene	222-81-1	7	4	00010					2.39					
47	benzo[*a*]hexacene	240-04-0	7	5	00001					2					
48	heptacene	258-38-8	7	6	00000	7.23	1.74	5.49							
49	benzo[*b*]naphtho[2,3-*m*]picene	5204 5-15 -5	8	2	012120					3.09					
50	dinaphtho[1,2-*b*: 1,2-*k*]chrysene	214-13-1	8	2	102101					3.18					
51	benzo[*b*]naphtho[2,3-*n*]picene	7444 3-32 -6	8	3	001210					2.75					
52	octacene	258-33-3	8	7	000000	7.15	1.85	5.31							

of catafusenes is presented. Numerical data for these properties were obtained from the literature, as will be indicated for each property.

cata-Condensed benzenoid hydrocarbons have some physical properties that depend in large measure on the presence of linearly condensed benzenoid rings, that is, parameter *n* (e.g., half-wave reduction potentials, energies of the *p*-band (^1L_a-band) in electronic absorption spectra, ionization potentials, electron affinities, HOMO−LUMO gap), and bulk properties that reflect in a large measure the weak intermolecular forces. The former properties are *molecular (intrinsic) properties* that are almost independent of the aggregation state, whereas the latter are *bulk properties* that are manifest in condensed phase (usually liquid phase). In crystalline phase, packing forces add further complications.

It should also be mentioned that some chemical properties, such as the reactivity toward dienophiles in Diels−Alder reactions, depend on *n* to a large extent.[9] Also, one should be aware that catafusenes that differ only by permuting some digits 1 and 2 (e.g., **9**−**11**, or **22**−**24**, or **31** and **32**) are isoarithmic (having the same number of Kekulé structures,[10,11] or even isoresonant[12,13]), and they are similar in many other properties. In the *L*-transform of their 3-digit code, one replaces digits 1 and 2 by letter *l* (which looks like the digit 1), and such catafusenes then have the same *L*-transformed code.[14] An equivalent idea had been proposed by Gutman as the LA sequence.[15]

In Table 1 we show the catafusenes that are discussed in the present paper with their names and *Chemical Abstracts Service* reference numbers (CAS RN), the code of their dualists, parameters *h* and *n*, four molecular properties that depend mainly on *n*: energies of the *p*-band (Platt's ^1L_a-band) in electronic absorption spectra, ionization potentials, electron affinities, and HOMO−LUMO gap, as well as four bulk properties that depend

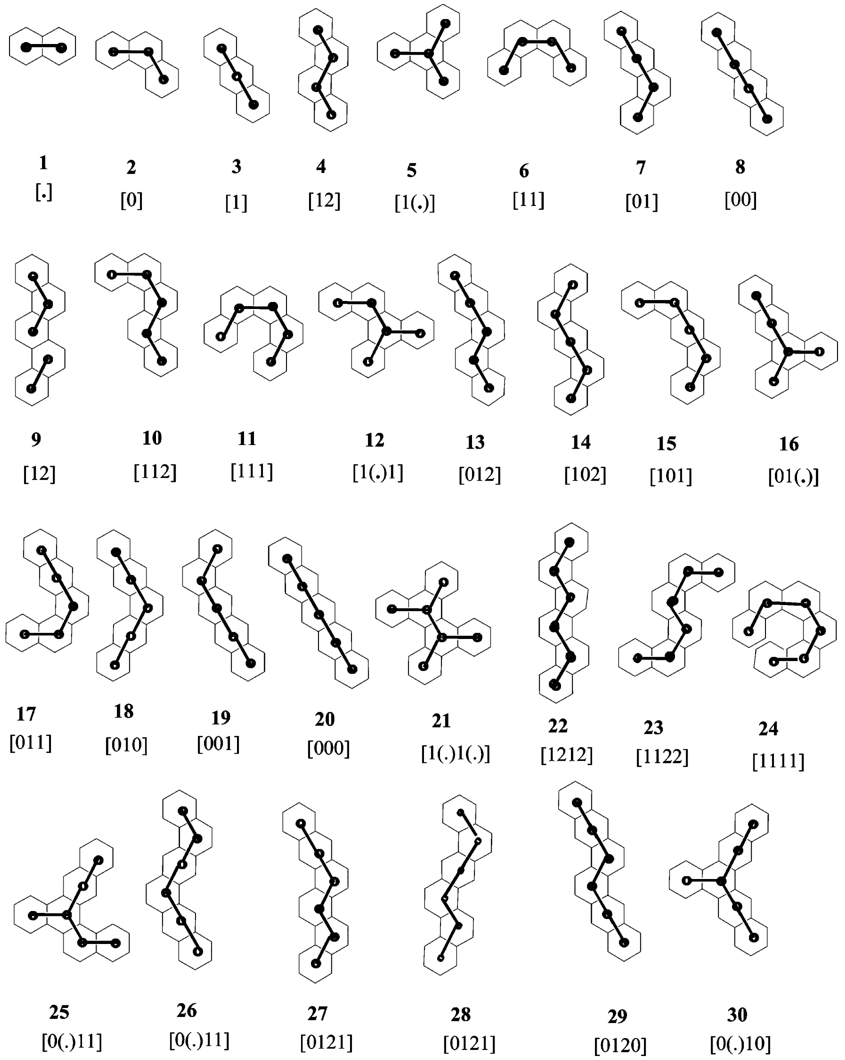

Figure 1. Structures and codes of benzenoids **1**−**30**.

mainly on *h*: normal boiling point (NBP, in °C), chromatographic retention index (RI), the logarithm of the water solubility (log *S*), and the logarithm of the lipophilicity measured by the octanol−water partition coefficient (log K_{ow}). For naming benzenoids the IUPAC nomenclature is usually followed, even when a trivial name is available (e.g., fulminene or zigzag-[6]fibonacene is called benzo[*c*]picene, **22**); however, for brevity we use occasionally shorter names such as hexahelicene, **24**. Tetracene (**8**) is preferred to naphthacene (also when condensed with benzo rings as in **19**, **31**−**35**). Compound **34** may also be called benzo[*b*]pentaphene, and **16** may also be called benzo-[*b*]triphenylene.

Structures of catafusenes from Table 1 are shown in Figures 1 and 2. Benzene is not included in Table 1 because it is not a condensed benzenoid. Even naphthalene is an outlier in some of the regressions, and it will be occasionally omitted. Monoparametric intercorrelation coefficients (r^2) between the values of physical properties from Table 1 and the two integer parameters *h* and *n* are presented in Table 2, highlighting in boldface characters the major r^2 value.

We present in Table 2 the monoparametric r^2 values for the physical properties that are discussed in the present communication. It can be seen that molecular properties have higher r^2 values for *n* than for *h*, whereas the converse is true for bulk parameters. In the following sections we discuss separately each physical property, and then we present the selected monoparametric or biparametric regressions.

2. Experimental Methods

2.1. Data and Sources for Molecular Properties. *First ionization potentials* (IP) indicate energies (in eV) needed for removing one electron from the benzenoid in the gaseous state. They depend on the energies of the highest occupied molecular orbital (HOMO).[16]

Electron affinities (EA) are the energies (in eV) associated with the benzenoid in the gaseous state becoming an anion by acquiring an electron. This electron will then reside in the lowest unoccupied molecular orbital (LUMO).[16]

The HOMO−LUMO *gap* of the benzenoid (*E*-gap, in β-units) can be obtained from quantum-chemical calculations at various levels, e.g., Hückel-MO, PPP-MO, and so forth.[16]

The absolute hardness (η, in eV)[16] was defined by Parr, Pearson, and Zhou[17−19] as half of the difference between IP and EA. The inverse of absolute hardness is the chemical softness.[20]

The *p*-band in the electronic absorption spectrum (ΔE_p, in eV)[16,20] was identified by Clar as being due to an electronic transition from the HOMO to the LUMO.[21,22]

2.2. Data and Sources for Bulk Properties. Boiling points at normal pressure (NBP, in °C) were taken from refs 16, 23, and 24.

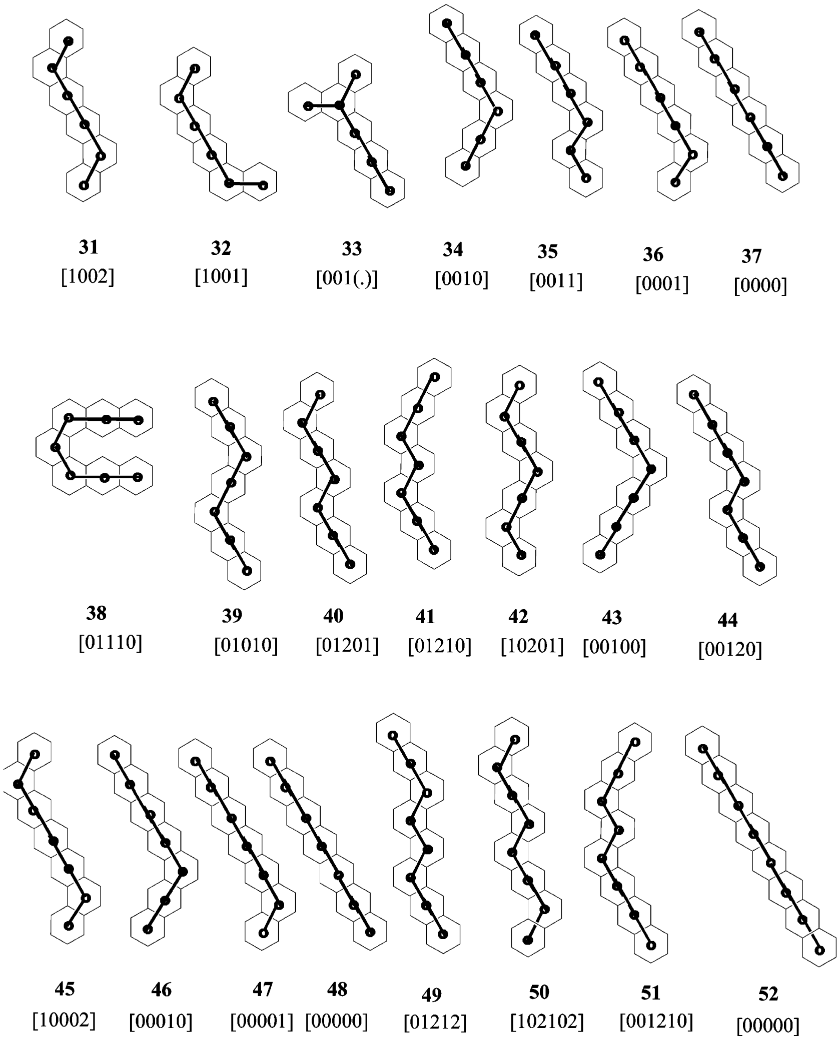

Figure 2. Structures and codes of benzenoids **31**−**52**.

TABLE 2: Monoparametric Correlation Coefficients r^2 for Physical Properties[a]

	molecular property					bulk property				
parameter	IP	EA	E-gap	η	ΔE_p	NBP	RI	log K_{ow}	log S	ΔH_f
h	0.467	0.548	0.510	0.217	0.287	**0.994**	**0.827**	**0.974**	**0.765**	**0.982**
n	**0.888**	**0.895**	**0.893**	**0.830**	**0.929**	0.208	0.340	0.119	0.443	0.198

[a] Major r^2 values are highlighted in boldface type.

The chromatographic retention index (RI) was determined by retention time (log I) for reversed-phase liquid chromatography on polymer.[16,25]

The solubility in water (log S) is as reported in refs 16 and 26.

Lipophilicity or n-octanol−water partition coefficient (log K_{ow}) is as reported in refs 16,26.

Heat (enthalpy) of formation (ΔH_f, in kJ/mol) is as reported in ref 16.

3. Results and Discussion

Table 3 contains monoparametric or biparametric equations for predicting the various physical properties of catafusenes discussed in the present communication. For each equation, in addition to its number enclosed in brackets, one sees the number N of benzenoids for which the numerical value of the property is available, the correlation coefficient r^2, the standard error SE, the Fisher criterion F, the cross-validated correlation coefficient q^2 using the leave-one-out procedure, and the root-mean-square cross-validated standard error $\mathrm{RMS_{cv}}$. In the next section the discussion of the results will be based on q^2 and SE.

3.1. Molecular Properties: Ionization Potential, Electron Affinity, HOMO−LUMO Gap, Energy of the *p*-Band (^1L_a-band) in Electronic Spectra. The ionization potential (IP) is modeled satisfactorily with a single parameter n, and the addition of h as a second parameter adds only small or no improvements to r^2, SE, and q^2 values. Figure 3 presents the resulting monoparametric plot. It can be observed that because n takes only a few small integer values, the linear plot has only a few discrete values on the vertical axis.

However, for the electron affinity (EA) the biparametric correlation does improve somewhat the r^2, SE, and q^2 values. Figure 4 presents the resulting biparametric plot.

The HOMO−LUMO gap (E-gap) is modeled a little better with both parameters n and h. Figure 5 presents the resulting biparametric plot.

TABLE 3: Monoparametric and Biparametric Correlations with the Corresponding Statistical Parameters

eq no.	property	equation	N	r^2	SE	F	q^2	$\mathrm{RMS}_{\mathrm{CV}}$
1	IP	$\mathrm{IP} = -0.209n + 8.465$	33	0.888	0.117	244	0.870	0.122
2	IP	$\mathrm{IP} = -0.0430h - 0.187n + 8.638$	33	0.901	0.111	137	0.874	0.120
3	EA	$\mathrm{EA} = 0.206n + 0.514$	33	0.895	0.110	265	0.881	0.114
4	EA	$\mathrm{EA} = 0.0673h + 0.173n + 0.243$	33	0.930	0.092	198	0.910	0.099
5	E-gap	$E\text{-gap} = -0.413n + 7.946$	33	0.893	0.224	258	0.877	0.233
6	E-gap	$E\text{-gap} = -0.112h - 0.358n + 8.397$	33	0.916	0.201	164	0.893	0.218
7	η	$\eta = -0.0988n + 0.642$	33	0.867	0.0450	202	0.852	0.0460
8	η	$\eta = -0.00691h - 0.0957n + 0.671$	33	0.870	0.0452	101	0.844	0.0472
9	ΔE_{p}	$\Delta E_{\mathrm{p}} = -0.494n + 4.34$	37	0.929	0.155	457	0.922	0.158
10	ΔE_{p}	$\Delta E_{p} = -0.0500h - 0.465n + 4.56$	37	0.941	0.143	274	0.941	0.141
11	NBP	$\mathrm{BP} = 96.8h + 41.1$	15	0.994	7.69	2051	0.987	10.33
12	NBP	$\mathrm{BP} = 94.37h + 5.87n + 41.63$	15	0.997	5.66	1899	0.991	8.65
13	NBP no naph..	$\mathrm{BP} = 91.31h + 66.58$	14	0.996	4.50	3061	0.995	4.70
14	NBP no naph.	$\mathrm{BP} = 90.59h + 4.19n + 62.31$	14	0.999	2.42	5283	0.998	3.06
15	RI	$\mathrm{RI} = 0.792h + 0.689$	19	0.827	0.334	81	0.784	0.35
16	RI	$\mathrm{RI} = 0.701h + 0.263n + 0.667$	19	0.883	0.282	61	0.841	0.303
17	$\log K_{\mathrm{ow}}$	$\log K_{\mathrm{ow}} = 1.23h + 0.86$	19	0.974	0.197	646	0.970	0.202
18	$\log K_{\mathrm{ow}}$	$\log K_{\mathrm{ow}} = 1.23h + 0.00363n + 0.861$	19	0.974	0.203	304	0.966	0.215
19	$\log S$	$\log S = -1.275h + 3.26$	11	0.765	0.704	29	0.596	0.840
20	$\log S$	$\log S = -1.051h - 0.577n + 3.23$	11	0.859	0.577	24	0.761	0.644
21	ΔH_{f}	$\Delta H_{\mathrm{f}} = 62.55h + 24.63$	23	0.982	8.93	1139	0.979	9.21
22	ΔH_{f}	$\Delta H_{\mathrm{f}} = 61.31h + 3.226n + 24.78$	23	0.984	8.65	608	0.976	9.97

The absolute hardness (η) is modeled satisfactorily with a single parameter n, and the addition of h as a second parameter adds only small or no improvements to r^2, SE, and q^2 values. The resulting plot for the monoparametric correlation is shown in Figure 6.

For the energy of the p-band in the electronic absorption spectrum (ΔE_{p}) the monoparametric and biparametric regressions are both shown in Figures 7 and 8. The statistical parameters show a small increase on adding h as a second parameter, although n explains most of the variance.

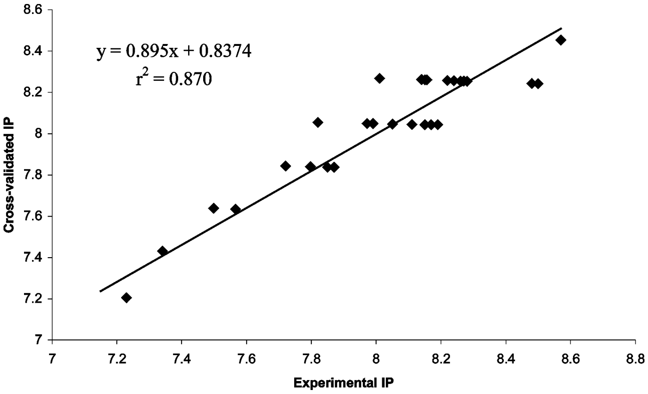

Figure 3. Plot of calculated versus tabulated ionization potentials according to eq 2.

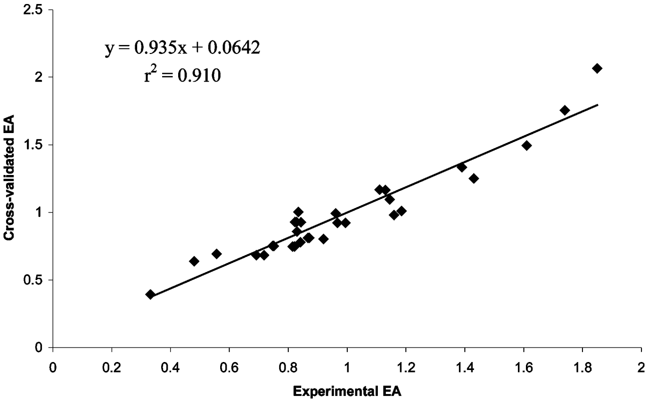

Figure 4. Plot of calculated versus tabulated electron affinity according to eq 5.

3.2. Bulk Properties: Normal Boiling Point, Chromatographic Retention Index, Solubility in Water, Lipophilicity, and Heat of Formation. For the normal boiling point (NBP), which is clustered according to h, two equations are presented including naphthalene, and two without it. The r^2 and q^2 values increase from eqs 11 to 12 and from eqs 13 to 14 only at the second or third decimal, but the standard error has a substantial steady decrease, most markedly between the last two equations. Therefore we present in Figures 9 and 10 the biparametric regressions according to eqs 12 and 14.

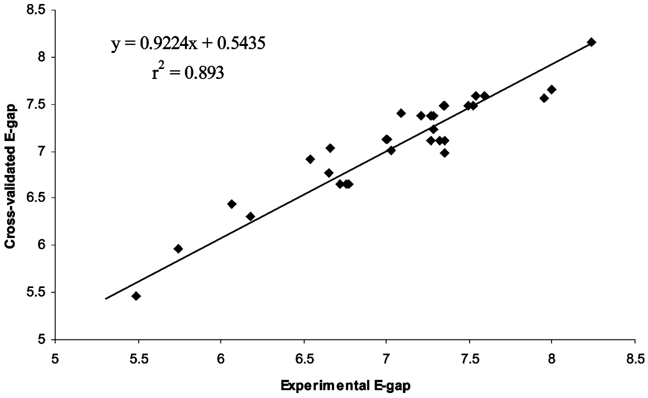

Figure 5. Plot of calculated versus tabulated HOMO−LUMO gap according to eq 7.

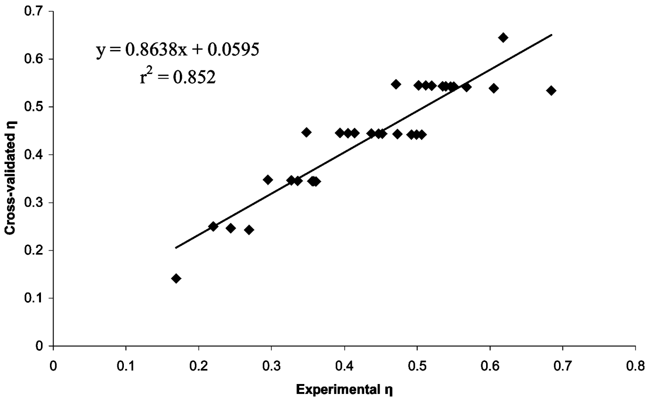

Figure 6. Plot of calculated versus tabulated hardness (η) according to eq 8.

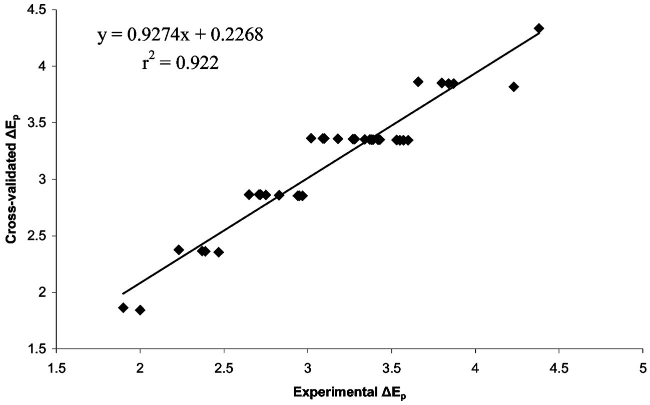

Figure 7. Plot of calculated versus tabulated energy of the electronic absorption *p*-band according to eq 10.

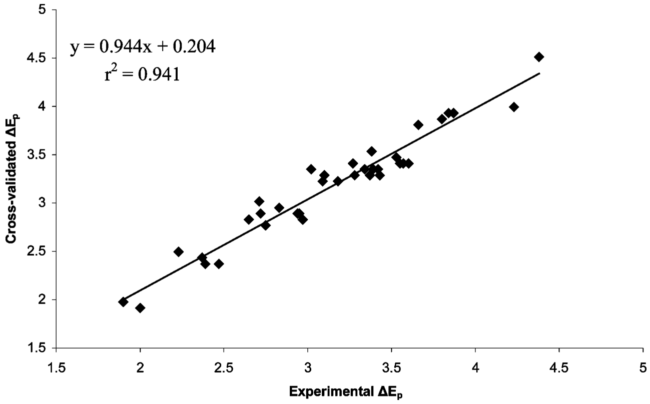

Figure 8. Plot of calculated versus tabulated energy of the electronic absorption *p*-band according to eq 11.

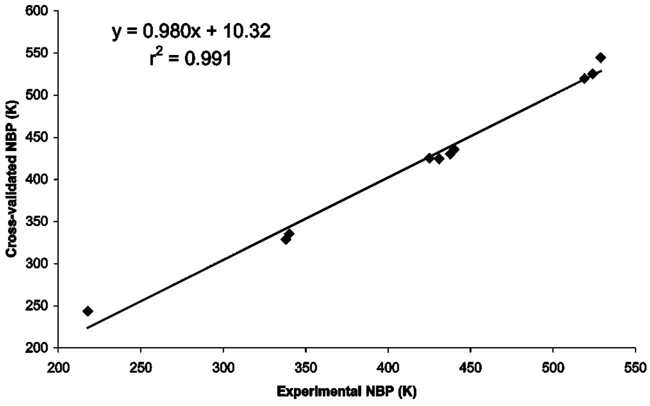

Figure 9. Plot of calculated versus tabulated normal boiling points for all catafusenes **1**−**52** according to eq 13.

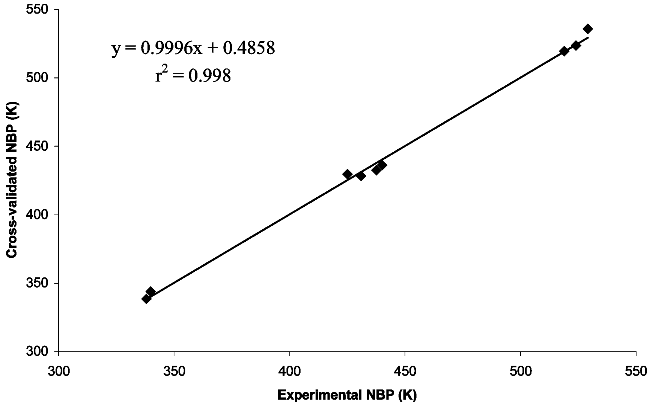

Figure 10. Plot of calculated versus tabulated normal boiling points for catafusenes **2**−**52** (without naphthalene) according to eq 15.

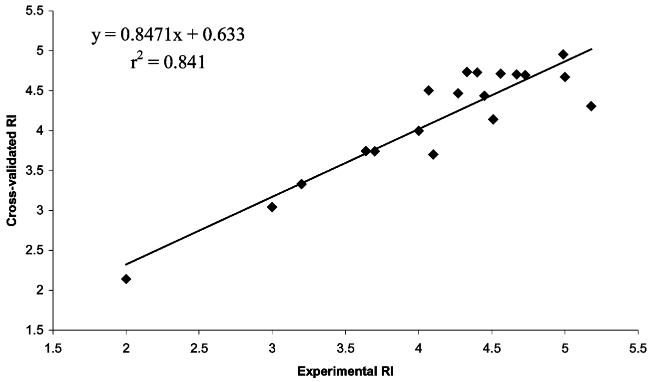

Figure 11. Plot of calculated versus tabulated retention index according to eq 17.

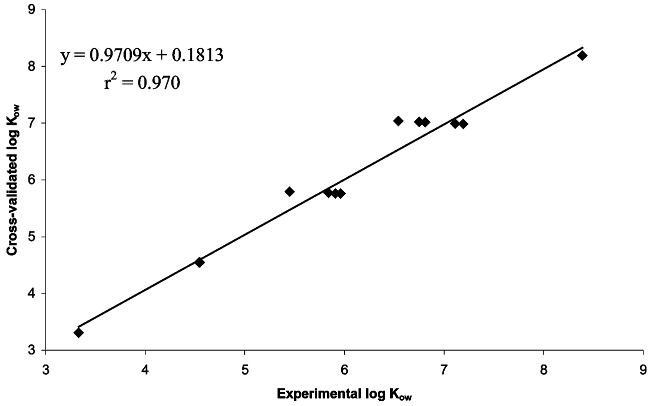

Figure 12. Plot of calculated versus tabulated hydrophobicity according to eq 18.

The correlation coefficients r^2 and q^2 for the retention index (RI) improve on adding n as a second parameter but reach only the value $q^2 = 0.841$, and the agreement between tabulated and calculated values shown in Figure 11 is poorer than in Figures 9 and 10.

By contrast, the hydrophobicity (log K_{ow}) shows no improvement on adding n, and therefore Figure 12 presents a monoparametric correlation in terms of h with fair agreement between tabulated and calculated values.

For the aqueous solubility of catafusenes (log S), the few available data allow only a moderate agreement between tabulated and calculated values, as seen in Figure 13 for the biparametric correlation, with the lowest value $q^2 = 0.761$ among all properties discussed in the present communication. Thus, this property would need additional parameters (possibly topological indices).

The heat of formation (ΔH_f) presents little improvement on adding n, and therefore Figure 14 presents a monoparametric correlation in terms of h with fair agreement between tabulated and calculated values.

A behavior similar to that of bulk properties is expected for the heat of vaporization, heat of sublimation, and heat of melting, which also depend on intermolecular forces, but at present few such data are available. By means of Trouton's Rule, one can approximate the heat of vaporization from the normal boiling point expressed in kelvins.

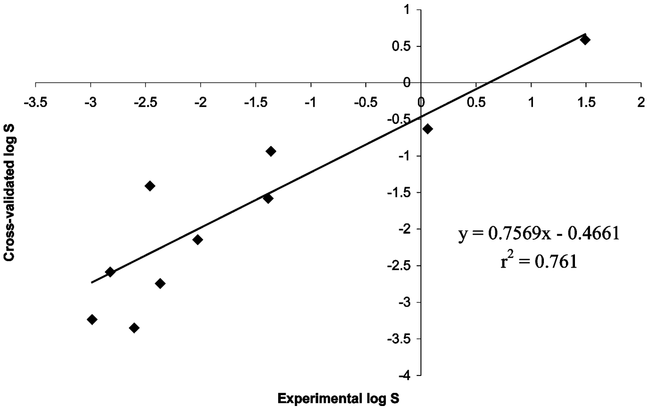

Figure 13. Plot of calculated versus tabulated water solubility according to eq 21.

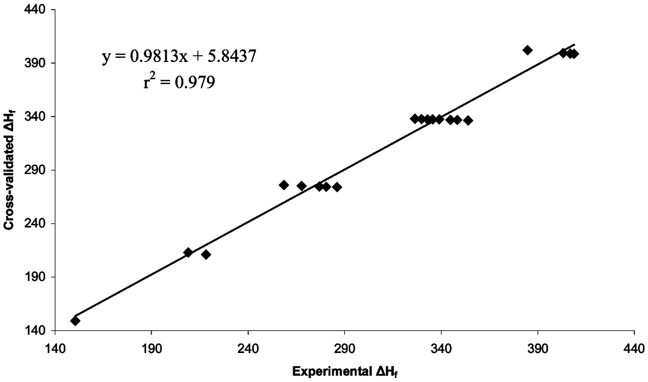

Figure 14. Plot of calculated versus tabulated enthalpy of formation according to eq 22.

4. Conclusions

We have shown that two very simple integer parameters characterizing the dualist of *cata*-condensed benzenoids contain sufficient information for satisfactory regressions and predictions of physical properties. For many molecular (intrinsic) properties, most of the variance is explained by parameter *n* characterizing the longest acenic portion of the benzenoid, whereas for many bulk properties (thermodynamic data, including phase transitions) the number of benzenoid rings explains most of the variance.

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References and Notes

(1) Weidkamp, K. P.; Afzali, A.; Tromp, R. M.; Hamers, R. J. *J. Am. Chem. Soc.* **2004**, *126*, 12740.

(2) Anthony, J. E. *Chem. Rev.* **2006**, *106*, 5028, and references therein.

(3) Wolak, M. A.; Jang, B.; Palilis, L. C.; Kafafi, Z. H. *J. Phys. Chem. B* **2004**, *108*, 5492, and references therein.

(4) Balaban, A. T.; Harary, F. *Tetrahedron* **1968**, *24*, 2505.

(5) Balaban, A. T. *Tetrahedron* **1969**, *25*, 2949.

(6) Balaban, A. T. *Pure Appl. Chem.* **1982**, *54*, 1075.

(7) Nikolić, S; Trinajstić, N.; Knop, J. V.; Müller, W. R.; Szymanski, K. *J. Math. Chem.* **1990**, *4*, 357.

(8) Singh, J; Singh, S.; Meer, S.; Agrawal, V. K.; Khadikar, P. V.; Balaban, A. T. *Arkivoc* **2006** (xv), 104.

(9) Balaban, A. T.; Biermann, D.; Schmidt, W. *Nouv. J. Chim.* **1985**, *9*, 443.

(10) Balaban, A. T.; Tomescu, I. *Commun. Math. Comput. Chem. (MATCH)* **1983**, *14*, 155.

(11) Balaban, A. T. *Commun. Math. Comput. Chem. (MATCH)* **1989**, *24*, 29.

(12) Živković, T. P.; Klein, D. J.; Schmalz, T. G. *Polycyclic Aromat. Compd.* **2000**, *13*, 457.

(13) Živković, T. P.; Schmalz, T. G.; Klein, D. J. *Polycyclic Arom. Comp.* **2000**, *18*, 13.

(14) Balaban, A. T. *Rev. Roum. Chim.* **1977**, *22*, 45.

(15) Gutman, I. *Theor. Chim. Acta* **1977**, *45*, 309.

(16) Ferreira, M. M. C. *Chemosphere* **2001**, *44*, 125.

(17) Parr, R. G.; Pearson, R. G. *J. Am. Chem. Soc.* **1983**, *105*, 7512.

(18) Pearson, R. G. *Proc. Natl. Acad. Sci. U.S.A.* **1986**, *83*, 8440.

(19) Zhou, Z.; Parr, R. G. *J. Am. Chem. Soc.* **1989**, *111*, 7371.

(20) Hiruta, K.; Tokita, S.; Nishimoto, K. *J. Chem. Soc., Perkin Trans. 2* **1995**, 1443.

(21) Clar, E. *Polycyclic Hydrocarbons*; AcademicPress: London, 1964.

(22) Clar, E. *The Aromatic Sextet*; Wiley: London, 1972.

(23) Alvas de Lima Ribeiro, F.; Ferreira, M. M. C. *J. Mol. Struct. (Theochem)* **2003**, *663*, 109.

(24) Karcher, W. *Spectral Atlas of Polycyclic Aromatic Compounds*; Kluwer Academic Publications: Dordrecht, 1988; Vol. 2, p 16.

(25) Sander, L. C.; Wise, S. A. *Adv. Chromatogr.* **1986**, *25*, 139.

(26) Mackay, D.; Callcot, D. In *The Handbook of Environmental Chemistry*, Vol. 3, *Part J, PAHs and Related Compounds*; Neilson, A. H., Ed.; Springer: Berlin, 1998; pp 325−346.