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Short communication

Quantitative structure-retention relationship studies for predicting the gas chromatography retention indices of polycyclic aromatic hydrocarbons

Quasi-length of carbon chain and pseudo-conjugated system surface

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Abstract

A new method of quantitative structure-retention relationship studies is reported for predicting capillary gas chromatography (GC) retention indices of polycyclic aromatic hydrocarbons (PAHs) by using two physicochemical parameters: pseudo-conjugated π -system surface (S_{π}) and quasi-length of carbon chain (N'), which represent the effect of the molecular π electronic conjugated surface and the molecular polarizability effect of PAHs on their corresponding gas chromatographic retention indices, respectively. Regression analysis is performed with regression coefficient being 0.9968 by using the above two parameters for capillary GC indices of 100 PAHs on SE-52 capillary columns. The results demonstrates a good linear relationship between the gas chromatographic retention index of PAHs and both their parameters N' and S_{π} . The method developed is successfully used for estimating and predicting the capillary GC retention index of PAHs. © 1998 Elsevier Science B.V.

Keywords: Quantitative structure–retention relationships; Quasi-length of carbon chain; Pseudo-conjugated system surface; Polynuclear aromatic hydrocarbons

1. Introduction

Polycyclic aromatic compounds (PACs) have been studied for well over a century, and the carcinogenic and mutagenic properties of numerous polycyclic compounds have been documented [1] and many others are presently under investigation. Because of the known hazards associated with the increasing emission of PACs into our environment, and the developing social environmental awareness there is a need for both further structural identification and more accurate quantitative measurement of these substances.

Gas chromatography (GC) employing either packed or capillary columns is a common analytical tool used for the separation and analysis of PACs. However, there has been a general lack of chromatographic data on isomeric PACs due to the un-

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availability of reference compounds. Thus methods that can predict chromatographic retention data of PACs from its structure are important. The earliest structure-retention relationship in GC is the correlation with retention volume and Wilmhust [3] discussed the relationship between GC retention data and the molecular mass of polycyclic aromatic hydrocarbons (PAHs), reporting that the retention data of PAHs increased almost linearly with their molecular mass. However, in his study substituted PAHs show some departure from the linear plot. Kaliszan and Lamparczyk [4] found a correlation between the GC retention data of PAHs and the connectivity index on a nonpolar GC phase.

Several workers have studied the influence of the molecular shape of PAHs on their chromatographic retention behavior on liquid crystal stationary phases [5–9] and various chemically bonded stationary phases [10,11]. Wise and co-workers [12–14] reported a relationship between the shape of PAHs and the reversed-phase LC retention on C_{18} bonded phases, and demonstrated the importance of unique selectivity of the C_{18} phase for PAHs and, particularly, for methyl-substituted PAHs.

In addition, some authors have reported the relation between the chromatographic retention and the physicochemical parameters of PAHs [15–21] and their nitro derivatives [22,23].

In this paper a relationship between the GC retention index on SE-52 capillary columns and two novel parameters from the molecular structure of PAHs, quasi-length of carbon chain [24] (N') and pseudo-conjugated system surface area (S_{π}), is reported.

2. Description of two main parameters

2.1. Pseudo-conjugated system surface area (S_{π})

As described earlier, a number of workers have studied the influence of the molecular structure, size and shape of PAHs on their chromatographic retention in both liquid–solid adsorption chromatography (LSC) and GC on liquid crystal stationary phases [5–7]. Radecki et al. [9] correlated the relative shape parameter, η , for PAHs with the relative GC retention on liquid crystal phases. The

shape parameter, η , was defined as the ratio of the longer side to the shorter side of a rectangle having a minimum area, which enclosed the molecule. Wise and co-workers [12-14] found a relationship between retention on polymeric C18 phase and the shape of the solute, defined as length-breadth ratio (L/B). The L/B value is determined by drawing the PAH molecule using the appropriate bond lengths and then constructing a rectangle around the structure which provides the maximum length to breadth ratio. In these works, the shape parameters of PAHs, specifically the length-to-breadth ratio is successfully used in predicting the retention behavior of PAHs with the same molecular mass on polymeric and monomeric C18 bonded phases, however, it does not adequately account for the retention behavior of PAHs with different molecular mass.

In this paper, the authors believe that the interaction between the molecular plane of PAHs and the stationary phase can be approximately regarded as a kind of frictional action and/or adsorptional action, which is related to the molecular surface. According to the interaction mechanism of PAH molecules in GC capillary columns, the greater the molecular plane of the PAH, the stronger the interaction and the longer the retention time. It is well known that the molecular structure of PAHs is nearly a planar, close ring and also, conjugated π -electron system. However, not all planes in the PAH molecule can influence the chromatographic retention data; in our opinion, only the main part which acts with the plane of the stationary phase can. So, in fact the effective area in the molecular plane of a PAH can be named pseudo-conjugated system surface (S_{π}) , and the sequence of the elution behavior of PAHs can be influenced by this pseudo-conjugated system surface.

The value of the pseudo-conjugated system surface (S_{π}) of PAHs can be calculated by the geometry arithmetic from the molecular structure formula. In order to simplify the calculation process all the bond lengths of a PAH take approximately the bond length of benzene, i.e., $1.39 \cdot 10^{-10}$ m. For example, the molecular structure formula of benzene is drawn as a regular hexagon and its length of edge is $1.39 \cdot 10^{-10}$ m, so its surface is $5.0197 \cdot 10^{-20}$ m², i.e. the pseudo-conjugated system surface area of benzene is $S_{\pi} = 5.0197 \cdot 10^{-20}$ m². The molecular surface area of naphthalene is about twice that of benzene, its

surface area is equal to $10.0394 \cdot 10^{-20} \text{ m}^2$. For PAHs with a branched ring such as 1-phenylnaphthalene, we study only its main ring and consider the surface of naphthalene. According to the above method, we can get conjugated system surface area (S_{π}) values for 100 PAHs (Table 1). In practice, the predicted results of such PAHs are in good agreement with the experimental values [25] (see Table 1 for details).

2.2. Quasi-length of carbon chain

As we know, there is a linear relationship between retention data and the number of carbons of a homologous series [2]. Here we define a parameter named quasi-length of carbon chain (N') in order to relate the retention index of PAHs directly. That is, for both the straight chain alkanes and PAHs having the same carbon atom number $N_{\rm C}$, if the inner molecule polarizability index value of the straight chain alkane is IMPI_{str} [24] and that of PAHs is equal to IMPI_{PAH} [24], then the quasi-length of carbon chain is expressed as Eq. (1):

$$N' = [IMPI_{str} / IMPI_{PAH}] N_{C}$$
(1)

Here, N' stands for the quasi-length of the carbon chain, rather than the not existing real length of the carbon chain, for PAHs under inner molecular polarizability sense.

3. Results and discussion

The experimental values of retention index data (I) of PAHs were taken from the literature [25]. The correlation of retention index data (I) with the corresponding molecular structure parameters N' and S_{π} was carried out for the 100 compounds containing unsubstituted and substituted PAHs in Table 1, and the multiple linear regression (MLR) analysis equation was obtained as follows:

$$I = -40.2643 + 23.1624N' + 6.2136S_{\pi}$$

$$F = 6197.01, \ S = 7.0965, \ R = 0.9961, \qquad (2)$$

$$n = 100$$

In Eq. (2), the two parameters N' and S_{π} represent the contribution of the molecular polarizability effect

and the molecular shape and size to the retention index, respectively.

Eq. (2) demonstrates that the molecular structure parameters N' and S_{π} are not only applicable for the unsubstituted PAHs but also for the substituted PAHs. In our study the quasi-length of carbon chain (N'), a molecular structure parameter based on the molecular polarizability theory [26], is employed in estimating the GC retention index for PAHs. We found that quasi-length of carbon chain (N') itself yielded a one-variable equation I = -78.58 +34.44N' with a correlation coefficient of R = 0.9651and standard deviation of S = 20.97 for 100 PAHs. This means that quasi-length of carbon chain (N') is an important descriptor for the influence of molecular structure on retention behavior for PAHs. We can also observe that the prediction model developed only by employing quasi-length of carbon chain (N')is not accurate enough for PAHs. As shown above in Eq. (2) and in Table 1, a novel descriptor, S_{π} , the pseudo-conjugated system surface area, is also introduced to reflect the molecular shape and size. The predicted results are in good agreement with the experimental values [25]. Another structural parameter, the number of rings in PAHs (S_c) simpler than S_{π} , may alternatively be considered together with the parameter N'. A similar relationship with the retention index of PAHs is obtained:

$$I = -31.1478 + 21.9534N' + 32.3837S_{c}$$

$$F = 2895.05, S = 10.3369, R = 0.9914,$$
 (3)

$$n = 100$$

where the parameter S_c represents the contribution of the number of rings in PAHs to the retention index.

Table 1 lists 100 PAHs that have been considered in our study. This table includes the measured [25] retention index values together with two calculated retention indices, one from the two parameters $N' S_{\pi}$ equation and another from Eq. (3). By comparing Eqs. (2) and (3), it is clear that, in the calculation accuracy, the developed parameter S_{π} is better than parameter S_c , especially for estimating retention index of PAHs which contain unconjugated ring and aromatic substituted groups, such as benzo[*ghi*]fluoranthene, triphenylene, 1-phenylnaphthalene and 9-phenylphenanthrene. Consequently, for solving the above problem, a predicting model for the capillary

Table 1 The retention index data and molecular structure parameters of 100 PAHs

No.	Compound	N'	<i>S</i>	Ι	I I		Ι	
	r r		π	observed ^a	Calculated ^b	difference	Calculated ^c	difference
1	Naphthalene	7.83	10.0395	200.00	203.44	-3.44	205.54	-5.54
2	2-Methylnaphthalene	8.69	10.0395	218.14	223.47	-5.33	224.50	-6.36
3	Azulene	7.81	11.3938	219.95	211.40	8.55	205.12	14.83
4	1-Methylnaphthalene	8.67	10.0395	221.04	222.82	-1.78	223.89	-2.85
5	2-Ethylnaphthalene	9.63	10.0395	236.08	245.19	-9.11	245.06	-8.98
6	1-Ethylnaphthalene	9.59	10.0395	236.56	244.24	-7.68	244.16	-7.60
7	2,6-Dimethylnaphthalene	9.56	10.0395	237.58	243.43	-5.85	243.39	-5.81
8	2,7-Dimethylnaphthalene	9.55	10.0395	237.71	243.39	-5.68	243.36	-5.65
9	1,3-Dimethylnaphthalene	9.52	10.0395	240.25	242.55	-2.30	242.56	-2.31
10	1,7-Dimethylnaphthalene	9.52	10.0395	240.66	242.68	-2.02	242.68	-2.02
11	1,6-Dimethylnaphthalene	9.53	10.0395	240.72	242.75	-2.03	242.74	-2.02
12	2,3-Dimethylnaphthalene	9.53	10.0395	243.55	242.87	0.68	242.87	0.68
13	1,4-Dimethylnaphthalene	9.50	10.0395	243.57	242.04	1.53	242.08	1.49
14	1,5-Dimethylnaphthalene	9.50	10.0395	244.98	242.04	2.94	242.08	2.90
15	1,2-Dimethylnaphthalene	9.50	10.0395	246.49	242.23	4.26	242.26	4.23
16	1,8-Dimethylnaphthalene	9.49	10.0395	249.52	241.91	7.61	241.96	7.56
17	2,3,6-Trimethylnaphthalene	10.39	10.0395	263.31	262.73	0.58	261.66	1.65
18	2,3,5-Trimethylnaphthalene	10.36	10.0395	265.90	261.98	3.92	260.95	4.95
19	Phenanthrene	10.64	15.0592	300.00	299.79	0.21	299.63	0.37
20	Anthracene	10.70	15.0592	301.69	301.11	0.58	300.88	0.81
21	3-Methylphenanthrene	11.48	15.0592	319.46	319.32	0.14	318.12	1.34
22	2-Methylphenanthrene	11.49	15.0592	320.17	319.46	0.71	318.25	1.92
23	2-Methylphenanthrene	11.55	15.0592	321.57	320.79	0.78	319.51	2.06
24	9-Methylphenanthrene	11.45	15.0592	323.06	318.48	4.58	317.32	5.74
25	4-Methylphenanthrene	11.45	15.0592	323.17	318.48	4.69	317.32	5.85
26	1-Methylphenanthrene	11.46	15.0592	323.90	318.74	5.16	317.57	6.33
27	1-Methylanthracene	11.52	15.0592	323.33	320.07	3.26	318.82	4.51
28	9-Methylanthracene	11.48	15.0592	329.13	319.19	9.94	318.00	11.13
29	9-Ethylphenanthrene	12.34	15.0592	337.05	339.26	-2.21	336.99	0.06
30	2-Ethylphenanthrene	12.41	15.0592	337.50	340.76	-3.26	338.41	-0.91
31	3,6-Dimethylphenanthrene	12.32	15.0592	337.83	338.80	-0.97	336.55	1.28
32	2,7-Dimethylphenanthrene	12.34	15.0592	339.23	339.11	0.12	336.85	2.38
33	9-Isopropylphenanthren	13.24	15.0592	345.78	360.08	-14.30	356.70	-10.92
34	1,8-Dimethylphenanthrene	12.27	15.0592	346.26	337.63	8.63	335.44	10.82
35	9-n-Propylphenanthrene	13.27	15.0592	350.30	360.64	-10.34	357.22	-6.92
36	9,10-Dimethylphenanthrene	12.25	15.0592	355.49	337.17	18.32	335.01	20.48
37	9-Methyl-10-ethylphenanthrene	13.88	15.0592	359.91	374.82	-14.91	370.65	-10.74
38	9,10-Dimethylphenanthrene	13.98	15.0592	367.97	377.30	-9.33	373.00	-5.03
39	1-Methyl-7-isopropylphenanthrene	14.07	15.0592	368.67	379.20	-10.53	374.79	-6.12
40	9,10-Dimethyl-3-ethylphenanthrene	13.97	15.0593	381.85	377.04	4.81	372.75	9.10
41	Benzo[ghi]fluoranthene	12.71	20.0790	389.60	378.94	10.66	409.82	-20.22
42	Benzo[c]phenanthrene	13.55	20.0790	391.39	398.30	-6.91	395.76	-4.37
43	Benzo[a]anthracene	13.51	20.0790	398.50	397.48	1.02	394.99	3.51
44	Chrysene	13.46	20.0790	400.00	396.21	3.79	393.78	6.22
45	Naphthacene	13.55	20.0790	408.30	398.50	9.80	395.95	12.35
46	11-Methylbenzo[a]anthracene	14.35	20.0790	412.72	416.99	-4.27	413.45	-0.73
47	2-Methylbenzo[a]anthracene	14.34	20.0790	413.78	416.78	-3.00	413.25	0.53
48	1-Methylbenzo[a]anthracene	14.30	20.0790	414.37	415.89	-1.52	412.42	1.95
49	9-Methylbenzo[a]anthracene	14.35	20.0790	416.50	416.96	-0.46	413.42	3.08
50	3-Methylbenzo[a]anthracene	14.35	20.0790	416.63	416.96	-0.33	413.42	3.21
51	8-Methylbenzo[a]anthracene	14.32	20.0790	417.56	416.22	1.34	412.72	4.84

Table 1. Continued

No. Compound N S. I Ifference Calculated ² difference 52 6-Methyberao(a/janhracene 14.30 20.0790 417.57 415.76 1.80 412.29 5.27 53 3-Methyberao(a/janhracene 14.30 20.0790 418.10 415.49 2.81 412.42 6.60 55 2-Methybherao(a/janhracene 14.32 20.0790 418.80 415.57 3.13 412.42 6.60 55 5-Methybherao(a/janhracene 14.32 20.0790 418.80 414.84 6.13 411.08 9.53 56 6-Methybherao(a/janhracene 14.32 20.0790 422.87 414.44 5.44 410.85 8.83 59 6-Methybherao(a/janhracene 15.05 20.0790 423.14 415.21 7.93 411.51 11.36 61 1.2-Methybherao(a/janhracene 15.05 20.0790 43.84 432.39 10.99 48.80.3 -4.04 64 7.12-Dimethyl(a/janhracene 15.05			N7/	G	7		7		7
Conserve Calculate Calculate <thcalculate< th=""> <thcalculate< th=""> <thca< th=""><th>NO.</th><th>Compound</th><th>N</th><th>\mathcal{S}_{π}</th><th><i>I</i></th><th>Calanda d^b</th><th>1 1:55</th><th>Calanda d^c</th><th>1</th></thca<></thcalculate<></thcalculate<>	NO.	Compound	N	\mathcal{S}_{π}	<i>I</i>	Calanda d ^b	1 1:55	Calanda d ^c	1
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56 12.Methylbenzojalpanthracene 14.26 20.0790 419.67 41.622 3.45 41.272 6.95 58 5.Methylchrysene 14.23 20.0790 419.68 41.622 3.45 41.272 6.95 58 5.Methylchrysene 14.23 20.0790 420.61 414.48 6.13 411.08 9.63 61 1.Methylchrysene 14.25 20.0790 422.87 414.94 7.93 411.77 11.37 63 1.12-Dimethyl[a]anthracene 15.05 20.0790 438.8 433.28 3.54 42.8.87 7.95 64 7.12-Dimethyl[a]anthracene 16.20 23.0986 495.01 491.45 3.56 486.82 8.19 65 Pentacene 16.40 25.0986 495.43 493.67 1.78 488.93 6.52 67 Dibenzoja/ajanthracene 15.20 20.090 404.24 7.55 487.77 12.23 70 Dibenzoja/ajanthracene 15.26 15.092 396.38 406.84 -10.46 433.34 -36.96 71 2-Phen	55	2-Methylchrysene	14.29	20.0790	418.80	415.67	3.13	412.20	6.60
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58 5-Methylchrysene 14.23 20.0790 419.68 414.24 5.44 410.08 8.83 60 4-Methylchrysene 14.25 20.0790 420.81 414.48 6.13 411.08 9.53 61 1-Methylchrysene 14.25 20.0790 422.87 414.94 7.93 411.17 11.37 63 1.12-Dimethyllc/anthracene 15.05 20.0790 433.84 432.39 10.99 428.03 15.35 64 7.12-Dimethyllc/anthracene 16.40 25.0986 495.61 491.45 3.56 486.82 8.19 65 Pentacene 16.41 25.0986 495.64 493.67 1.78 488.93 6.52 68 Benzols/a.hunthracene 16.31 25.0986 490.65 7.55 487.77 1.23 70 1-Phenylnaphithalene 12.61 10.0395 315.19 314.29 18.30 342.85 -102.6 73 9-Phenylnaphithalene 12.51 15.0592 306.34 406.84 0.06 433.34 -36.96 74 1-Phenylnaphit	57	4-Methylbenzo[a]anthracene	14.32	20.0790	419.67	416.22	3.45	412.72	6.95
59 6-Methylchrysene 14.24 20.0790 420.61 414.48 6.13 411.08 9.53 60 4-Methylchrysene 14.25 20.0790 422.87 414.91 6.22 411.20 9.63 61 1-Methylchrysene 14.26 20.0790 423.81 415.21 7.93 411.51 11.36 62 7-Methylbencolalnthracene 15.02 20.0790 433.84 432.39 10.99 428.03 15.35 64 Dibenzola.2 lanthracene 16.42 25.086 495.01 491.45 3.56 486.82 8.19 67 Dibenzola.2 lanthracene 16.23 25.0986 495.01 491.45 3.56 486.82 8.19 68 Benzola/lehynthene 12.51 10.0395 315.19 312.32 2.87 340.98 -25.79 71 2-Phenylnaphthalene 12.61 10.0395 312.52 2.87 340.82 -10.26 72 9-Henylnaphthalene 12.61 10.0395 312.52	58	5-Methylchrysene	14.23	20.0790	419.68	414.24	5.44	410.85	8.83
60 4-Methylchrysene 14,25 20,0790 422,83 414,64 6.22 411,20 9,63 61 1-Methylchrysene 14,26 20,0790 423,14 415,21 7,93 411,17 11,37 62 7.12-Dimethyl[a]anthracene 15,05 20,0790 443,38 3,54 428,87 7,95 63 1,12-Dimethyl[a]anthracene 15,02 20,0790 443,38 432,39 10,99 442,803 15,35 65 Pentacene 16,40 25,0986 495,61 491,45 3,56 488,893 6,52 66 Dibenzo[a,l]anthracene 16,31 25,0986 497,66 493,67 1,78 488,93 8,73 71 2-Phenylanphthalene 12,61 10,0395 315,19 312,32 2.87 340,98 -25.79 71 2-Phenylanphthalene 12,61 10,0395 332,59 314,29 13,30 342,85 -10,26 73 9-Phenylanthracene 15,26 15,0592 20,63 406,84 -10,46 433,34 -26,44 74 1-Pheny	59	6-Methylchrysene	14.24	20.0790	420.61	414.48	6.13	411.08	9.53
61 1-Methylchrysene 14.26 20.0790 422.87 414.94 7.93 411.51 11.36 62 7-Methylbenzo[a]anthracene 16.05 20.0790 423.82 433.28 3.54 428.87 7.95 64 7.12-Dimethyl[a]anthracene 15.02 20.0790 436.82 433.28 3.54 428.87 7.95 64 Dibenzo[a , $]$ anthracene 16.40 25.0966 495.61 491.45 3.56 486.82 8.19 66 Dibenzo[a , $]$ anthracene 16.31 25.0986 497.64 493.67 7.99 488.93 6.52 67 Picene 16.62 25.0986 497.64 493.67 7.99 488.93 6.52 71 2-Phenylnaphtalene 12.31 10.0395 332.59 314.29 18.30 342.85 -10.26 72 9-Phenylnaphtalene 15.26 15.0592 396.38 406.84 -10.46 433.34 -36.96 73 9-Phenylphenanthrene 15.26 15.0592 406.90 400.64 433.34 -26.44 74	60	4-Methylchrysene	14.25	20.0790	420.83	414.61	6.22	411.20	9.63
627-Methylenzolalanthracene14.2720.0790432.14415.217.93411.7711.37631.12-Dimethyllalanthracene15.0520.0790436.82433.283.54428.837.95647.12-Dimethyllalanthracene15.0220.0790443.33432.3910.99428.0315.3565Pentacene16.4025.0986495.01491.453.56486.828.1967Dibenzola.lanthracene16.3125.0986495.45493.671.78488.936.5268Benzolbchrysene16.3125.0986500.00492.457.55487.7712.23701-Phenyhaphthalene12.3310.0395315.19312.322.87340.98-25.79712-Phenyhaphthalene15.2615.0592396.38406.84-10.46433.34-36.96729-Phenyhphenanthracene15.2615.0592416.64475.7714.09434.03-12.37759-Methyl-10-phenyhphenanthrene15.0920.0790406.840.64433.34-26.44741-Phenyhphenanthrene15.0920.0790440.22433.213.1140.986.44759-Methyl-10-phenyhphenanthrene16.0015.0592411.64471.71-8.45463.79-2.07759-Methyl-10-phenyhphenanthrene15.4020.0790442.24433.18-0.66428.873.4576Triphenyhene15.422	61	1-Methylchrysene	14.26	20.0790	422.87	414.94	7.93	411.51	11.36
63 1,12-Dimethyl[a]anthracene 15.02 20.0790 436.82 433.28 3.54 428.87 7.95 64 7,12-Dimethyl[a]anthracene 15.02 20.0790 443.38 432.39 10.99 428.03 15.35 65 Pentacene 16.40 25.0986 495.01 491.45 3.56 486.82 8.19 66 Dibenzo[a,]anthracene 16.31 25.0986 495.67 1.78 488.93 8.73 68 Benzo[b]chrysene 16.31 25.0986 500.00 492.45 7.55 487.77 1.22.3 70 1-Phenylpaphthalene 12.51 10.0395 315.19 312.32 2.87 340.98 -25.79 71 2-Phenylpaphthalene 12.61 10.0395 332.59 314.29 18.30 342.85 -10.26 72 9-Phenylphenanthrene 15.26 15.0592 401.64 0.066 433.34 -26.44 74 1-Phenylphenanthrene 15.20 15.0592 471.64 441.31 -6.97 44.90 43.03 -12.37 75 9	62	7-Methylbenzo[a]anthracene	14.27	20.0790	423.14	415.21	7.93	411.77	11.37
64 7,12-Dimethyl[a]anthracene 15.02 20.0790 443.38 432.39 10.99 428.03 15.35 65 Pentacene 16.40 25.0986 486.81 495.71 8.90 490.85 4.04 66 Dibenzo[a,I]anthracene 16.31 25.0986 495.45 493.67 1.78 488.93 6.52 68 Benzo[b]chrysene 16.31 25.0986 497.66 493.67 3.59 488.93 8.73 69 Picene 16.26 25.0986 500.00 492.45 7.55 487.77 12.23 70 1-Phenylnaphthalene 12.51 10.0395 331.19 312.32 2.87 340.98 -25.79 71 2-Phenylphenanthrene 15.26 15.0592 314.64 40.06 433.34 -36.96 73 9-Phenylphenanthrene 15.29 15.0592 41.64 40.77 14.09 434.03 -12.37 75 9-Methyl-10-phenylphenanthrene 15.09 20.0790 461.32 431.31 -6.97 449.70 -32.54 76 Tripheny	63	1,12-Dimethyl[a]anthracene	15.05	20.0790	436.82	433.28	3.54	428.87	7.95
65Pentacene16.4025.0986495.71 -8.90 490.85 -4.04 66Dibenzola, janthracene16.2225.0986495.01491.453.56486.828.1967Dibenzola, janthracene16.3125.0986495.64493.671.78488.938.5268Benzol/b/thrysene16.3125.0986497.66493.673.99488.938.7369Picene16.2625.0986500.00492.457.55487.7712.23701-Phenylanphthalene12.5110.0395315.19312.322.87340.98 -25.79 712-Phenylanthracene15.2615.0592306.84406.64433.34 -36.96 739-Phenylanthracene15.2615.0592406.90406.840.06433.34 -26.44 741-Phenylphenanthrene15.0215.0592417.16424.13 -6.97 449.07 -32.54 759-Methyl-10-phenylphenanthrene15.0020.0790402.32433.18 -0.86 428.87 3.45 759-Methyl-10-phenylphennet16.0015.0592471.16424.13 -6.97 449.07 -32.54 76Triphenylene15.4020.0790452.32433.18 -0.86 428.87 3.45 791.6.11-Tirtimethyltriphenylene15.4220.0790445.2244.6325.24 -7.18 446.040.20801.3,6,11-Tirtimethyltriphenylene15.42 <td>64</td> <td>7,12-Dimethyl[a]anthracene</td> <td>15.02</td> <td>20.0790</td> <td>443.38</td> <td>432.39</td> <td>10.99</td> <td>428.03</td> <td>15.35</td>	64	7,12-Dimethyl[a]anthracene	15.02	20.0790	443.38	432.39	10.99	428.03	15.35
66Dibenzo[a, l]anthracene16.2225.0986495.01491.453.56486.828.1967Dibenzo[a, l]anthracene16.3125.0986495.45493.673.99488.936.5268Benzo[b]chrysnene16.3125.0986497.66493.673.99488.938.7369Picene16.6225.0986500.00492.457.55487.7712.23701-Phenylnaphthalene12.6310.0395315.19312.322.87340.98-25.79712-Phenylnaphthalene15.2615.0592396.38406.84-10.46433.34-36.96739-Phenylahenanthrene15.2615.0592406.90406.840.06433.34-26.44741-Phenylphenanthrene15.09241.66407.5714.09434.03-12.37759-Methyl-10-phenylphenanthrene15.09241.66407.5714.09434.03-12.3776Triphenylene13.4020.0790416.32413.213.11409.886.44781.3-Dimethyltriphenylene15.8220.0790426.24413.213.11409.886.44781.3-L1-Timethyltriphenylene15.8420.0790461.72470.17-8.45463.79-2.0781Accnaphthylene15.4220.0790451.22252.84-5.18466.400.2083Fluoranthene11.7219.2423344.01350.78-	65	Pentacene	16.40	25.0986	486.81	495.71	-8.90	490.85	-4.04
67Dibenzo[a/a]nathracene16.3125.0986495.45493.671.78488.936.5268Bernzo[b]chrysene16.2025.0986690.00492.457.55487.771.2.23701-Phenylnaphthalene12.5310.0395315.19312.322.87340.98 -25.79 712-Phenylnaphthalene12.6110.0395332.59314.2918.30342.85 -10.26 729-Phenylathracene15.2615.0592406.90406.84 -0.06 433.34 -26.44 741-Phenylphenanthrene15.2015.0592421.66407.5714.09434.03 -12.37 759-Phenylphenanthrene16.0015.0592417.16424.13 -6.97 449.70 -32.54 76Triphenylene14.1920.0790400.00394.945.06392.587.42771-Methyltriphenylene15.0520.0790446.24413.213.11409.886.44813.10inethyltriphenylene15.0520.0790446.24451.42 -5.18 446.040.20801.3.6.11-Tetramethyltriphenylene16.4220.0790446.24451.42 -5.18 446.040.20821-Methylacenaphthylene9.6614.2226265.24271.87 -6.63 278.12 -12.88 83Fluoranthene11.7219.2423344.01350.78 -6.77 323.3120.7084Pyrene11.63 <t< td=""><td>66</td><td>Dibenzo[<i>a</i>,<i>z</i>]anthracene</td><td>16.22</td><td>25.0986</td><td>495.01</td><td>491.45</td><td>3.56</td><td>486.82</td><td>8.19</td></t<>	66	Dibenzo[<i>a</i> , <i>z</i>]anthracene	16.22	25.0986	495.01	491.45	3.56	486.82	8.19
68Benzo[b]chrysene16.3125.0986497.66493.673.99488.938.7369Picene16.2625.0986500.00492.457.55487.7712.23712-Phenylanphthalene12.5110.395312.522.87340.98 -25.79 712-Phenylanphthalene12.6110.0395332.59314.2918.30342.85 -10.26 729-Phenylanthracene15.2615.0592496.840.06433.34 -26.44 741-Phenylphenanthrene15.2915.0592421.66407.5714.09434.03 -12.37 759-Methyl-10-phenylphenanthrene13.4020.0790406.22413.213.11409.886.44741-Methyltriphenylene13.4020.0790416.32413.213.11409.886.4476Triphenylenpine14.1920.0790446.24451.42 -5.18 446.00.00811.3-Dimethyltriphenylene15.0520.0790446.24451.42 -5.18 446.379 -2.07 81Acenaphthylene8.8414.2226244.63252.84 -8.21 260.10 -15.47 821-Methylacenaphthylene9.6614.2226252.4421.87 33.31 -2.52 854-Methylpyrene12.4320.0790351.22353.90 -2.68 353.74 -2.52 854-Methylpyrene12.4420.0790371.55373.05 -2.90 <td>67</td> <td>Dibenzo[a,h]anthracene</td> <td>16.31</td> <td>25.0986</td> <td>495.45</td> <td>493.67</td> <td>1.78</td> <td>488.93</td> <td>6.52</td>	67	Dibenzo[a,h]anthracene	16.31	25.0986	495.45	493.67	1.78	488.93	6.52
69Picene16.2625.0986500.00492.457.55487.7712.23701-PhenyInaphthalene12.5310.0395315.19312.322.87340.98 -25.79 712-PhenyInaphthalene12.6110.0395332.59314.2918.30342.85 -10.26 729-PhenyIanthracene15.2615.0592396.38406.84 -10.46 433.34 -36.96 739-PhenyIphenanthrene15.2015.0592416.6407.5714.09434.03 -12.37 759-Methyl-10-phenyIphenanthrene16.0015.0592417.16424.13 -6.97 449.70 -32.54 76TriphenyIene13.4020.0790416.32413.213.11499.886.44781.3-DimethyItriphenyIene15.0520.0790446.24451.42 -5.18 446.040.20801.3,6.11-TirmethyItriphenyIene15.6420.0790446.24451.42 -5.18 446.040.20801.3,6.11-TirmethyItriphenyIene16.6420.0790446.24451.42 -5.18 446.040.2081AccnaphthyIene9.6614.2226245.24271.87 -6.63 278.12 -12.88 83Fluoranthene11.7219.2423344.01350.78 -6.77 323.3120.7084Pyrene11.6320.0790370.15373.05 -2.90 371.86 -1.71 84Pyrene11.6320.07	68	Benzo[b]chrysene	16.31	25.0986	497.66	493.67	3.99	488.93	8.73
701-Phenylnaphthalene12.5310.0395315.19312.322.87340.98 -25.79 712-Phenylanthracene12.6110.0395332.59314.2918.30342.85 -10.26 739-Phenylanthracene15.2615.0592406.90406.84 -10.46 433.34 -26.44 741-Phenylphenanthrene15.2915.0592421.66407.5714.09434.03 -12.37 759-Methyl-10-phenylphenanthrene16.0015.0592417.16424.13 -6.97 449.70 -32.54 76Triphenylene13.4020.0790416.32413.213.11409.886.44781.3-Dimethyltriphenylene15.0520.0790432.32433.18 -0.86 428.873.45791.6.11-Timethyltriphenylene15.0420.0790461.72470.17 -8.45 463.79 -2.07 81Acenaphthylene8.8414.2226244.63252.84 -8.21 260.10 -15.47 821-Methylacenaphthylene9.6614.2226245.24271.87 -6.63 278.12 -12.88 83Fluoranthere11.7219.2423344.01350.78 -6.77 323.31 20.70 84Pyrene12.4620.0790351.22353.90 -2.68 353.74 -2.52 854.Methylpyrene12.4620.0790373.55372.551.00371.392.16881.Futhylpyrene12.44 </td <td>69</td> <td>Picene</td> <td>16.26</td> <td>25.0986</td> <td>500.00</td> <td>492.45</td> <td>7.55</td> <td>487.77</td> <td>12.23</td>	69	Picene	16.26	25.0986	500.00	492.45	7.55	487.77	12.23
712-Phenylmaphthalene12.6110.0395332.59314.2918.30342.85 -10.26 729-Phenylnthracene15.2615.0592396.38406.84 -10.46 433.34 -36.96 739-Phenylphenanthrene15.2615.0592421.66407.5714.09434.03 -12.37 759-Methyl-10-phenylphenanthrene16.0015.0592417.16424.13 -6.97 449.70 -32.54 76Triphenylene13.4020.0790400.00394.945.06392.58 7.42 711-Methyltriphenylene15.0520.0790432.32433.18 -0.86 428.87 3.45 791.6,11-Trimethyltriphenylene15.8420.0790446.24451.42 -5.18 446.040.20801.3,6,11-Tetramethyltriphenylene16.6420.0790461.72470.17 -8.45 463.79 -2.07 81Acenaphthylene8.8414.2226265.24271.87 -6.63 278.12 -12.88 83Fluoranthene11.7219.2423344.01350.78 -6.77 323.3120.07084Pyrene12.4320.0790373.55372.551.00371.392.16854-Methylpyrene12.4420.0790375.55373.05 -2.90 371.86 -1.71 862-Methylpyrene13.2820.0790385.35393.09 -7.74 390.83 -5.48 892,7-Dimethylprene	70	1-Phenylnaphthalene	12.53	10.0395	315.19	312.32	2.87	340.98	-25.79
729-Phenylanthracene15.2615.0592396.38406.84 -10.46 433.34 -36.96 739-Phenylphenanthrene15.2615.0592406.90406.840.06433.34 -26.44 741-Phenylphenanthrene15.2915.0592421.66407.5714.09434.03 -12.37 759-Methyl-10-phenylphenanthrene16.0015.0592411.61424.13 -6.97 449.70 -32.54 76Triphenylene13.4020.0790400.00394.945.06392.587.42771-Methyltriphenylene15.0520.0790416.22413.213.11409.886.44781.3-Dimethyltriphenylene15.0520.0790446.24451.42 -5.18 446.040.20801.3.6,11-Tetramethyltriphenylene16.6420.0790446.24451.42 -5.18 446.040.2081Acenaphthylene8.8414.2226244.63252.84 -8.21 260.10 -15.47 821-Methylacenaphthylene9.6614.2226255.24271.87 -6.63 278.12 -12.88 83Fluoranthene11.7219.2423344.01350.78 -6.77 323.3120.07084Pyrene11.6320.0790370.15373.05 -2.90 371.86 -1.71 854.Methylpyrene12.4620.0790373.55372.551.00371.392.16881-Ethylpyrene13.28 <td>71</td> <td>2-Phenylnaphthalene</td> <td>12.61</td> <td>10.0395</td> <td>332.59</td> <td>314.29</td> <td>18.30</td> <td>342.85</td> <td>-10.26</td>	71	2-Phenylnaphthalene	12.61	10.0395	332.59	314.29	18.30	342.85	-10.26
739-Phenylphenanthrene15.2615.0592406.90406.840.06433.34 -26.44 741-Phenylphenanthrene15.0592421.66407.5714.09434.03 -12.37 759-Methyl-10-phenylphenanthrene16.0015.0592417.16424.13 -6.97 449.70 -32.54 76Triphenylene13.4020.0790416.32413.213.11409.886.44771-Methyltriphenylene15.0520.0790432.32433.18 -0.86 428.873.45791.6.11-Trimethyltriphenylene15.8420.0790446.24451.42 -5.18 446.040.2081Acenaphthylene16.6420.0790461.72470.17 -8.45 463.79 -2.07 81Acenaphthylene8.8414.2226244.63252.84 -8.21 260.10 -15.47 821-Methylacenaphthylene9.6614.2226255.24271.87 -6.63 278.12 -12.88 83Fluoranthene11.7219.2423344.01350.78 -6.77 323.3120.7084Pyrene11.6320.0790370.15373.05 -2.90 371.86 -1.71 862-Methylpyrene12.4620.0790370.15373.05 -2.90 371.86 -1.71 871-Methylacenaphthylene13.2820.0790386.34392.18 -5.84 389.97 -3.63 90Cyclopental cal/pyrene13.282	72	9-Phenylanthracene	15.26	15.0592	396.38	406.84	-10.46	433.34	-36.96
741-Phenylphenanthrene15.2915.0592421.66407.5714.09434.03 -12.37 759-Methyl-10-phenylphenanthrene16.0015.0592417.16424.13 -6.97 449.70 -32.54 76Triphenylene13.4020.0790400.00394.945.06392.587.42761-Methyltriphenylene14.1920.0790416.32413.213.11409.886.44781,3-Dimethyltriphenylene15.0520.0790432.32433.18 -0.86 428.873.45791,6,11-Trimethyltriphenylene16.6420.0790461.2470.17 -8.45 463.79 -2.07 81Acenaphthylene8.8414.2226244.63252.84 -8.21 260.10 -15.47 821-Methylacenaphthylene9.6614.2226265.24271.87 -6.63 278.12 -12.88 83Fluoranthene11.7219.2423344.01305.90 -2.68 353.74 -2.52 854-Methylpyrene12.4320.0790351.22353.90 -2.68 353.74 -2.52 854-Methylpyrene13.3220.0790373.55373.05 -2.90 371.86 -1.71 862-Methylpyrene13.2320.0790385.35393.09 -7.74 390.83 -5.48 892,7-Dimethylpyrene13.2820.0790385.35393.09 -7.74 390.83 -5.48 892,7-Dimethylpyrene<	73	9-Phenylphenanthrene	15.26	15.0592	406.90	406.84	0.06	433.34	-26.44
759-Methyl-10-phenylphenanthrene16.00 15.0592 417.16 424.13 -6.97 449.70 -32.54 76Triphenylene13.40 20.0790 400.00 394.94 5.06 392.58 7.42 771-Methyltriphenylene14.19 20.0790 416.32 413.21 3.11 409.88 6.44 781.3-Dimethyltriphenylene15.05 20.0790 432.32 433.18 -0.86 422.87 3.45 791.6.11-Trimethyltriphenylene15.84 20.0790 446.24 451.42 -5.18 446.04 0.20 801.3.6.11-Tetramethyltriphenylene16.64 20.0790 446.24 451.42 -5.18 446.04 0.20 81Acenaphthylene 8.84 14.226 244.63 222.84 -8.21 260.10 -15.47 821-Methylacenaphthylene9.66 14.226 252.42 271.87 -6.63 278.12 -12.88 83Fluoranthene11.72 19.2423 344.01 350.78 -6.77 323.31 20.70 84Pyrene12.43 20.0790 373.55 372.35 1.00 371.39 2.16 862-Methylpyrene12.44 20.0790 373.55 372.55 1.00 371.39 2.16 881-Ethylpyrene13.28 20.0790 385.35 393.09 -7.74 390.83 -5.48 90Cyclopenta[cd]pyrene13.28 20.0790 385.35 </td <td>74</td> <td>1-Phenylphenanthrene</td> <td>15.29</td> <td>15.0592</td> <td>421.66</td> <td>407.57</td> <td>14.09</td> <td>434.03</td> <td>-12.37</td>	74	1-Phenylphenanthrene	15.29	15.0592	421.66	407.57	14.09	434.03	-12.37
76Triphenylene13.40 20.0790 400.00 394.94 5.06 392.58 7.42 771-Methyltriphenylene14.19 20.0790 416.32 413.21 3.11 409.88 6.44 781,3-Dimethyltriphenylene15.05 20.0790 432.32 433.18 -0.86 428.87 3.45 791,6,11-Trimethyltriphenylene15.84 20.0790 446.24 451.42 -5.18 446.04 0.20 81Acenaphthylene8.84 14.2226 244.63 252.84 -8.21 260.10 -15.47 821-Methylacenaphthylene9.66 14.2226 252.24 271.87 -6.63 278.12 -12.88 83Fluoranthene11.72 19.2423 344.01 350.78 -6.77 323.31 20.70 84Pyrene11.63 20.0790 351.25 373.05 -2.208 353.74 -2.52 854-Methylpyrene12.43 20.0790 370.15 373.05 -2.90 371.86 -1.71 871-Methylpyrene13.32 20.0790 385.35 372.55 1.00 371.39 2.16 881-Ethylpyrene13.32 20.0790 385.35 392.90 -7.74 390.83 -5.48 892,7-Dimethylpyrene13.32 20.0790 385.35 372.55 1.00 371.33 -16.51 90Cyclopenta(cd pyrene13.32 20.0790 385.34 392.18 -5.8	75	9-Methyl-10-phenylphenanthrene	16.00	15.0592	417.16	424.13	-6.97	449.70	-32.54
771-Methyltriphenylene14.1920.0790416.32413.213.11409.886.44781,3-Dimethyltriphenylene15.0520.0790432.32433.18 -0.86 428.873.45791,6,11-Trimethyltriphenylene15.8420.0790446.24451.42 -5.18 446.040.20801,3,6,11-Tetramethyltriphenylene16.6420.0790446.72470.17 -8.45 463.79 -2.07 81Acenaphthylene8.8414.226244.63252.84 -8.21 260.10 -15.47 821-Methylacenaphthylene9.6614.2226265.24271.87 -6.63 278.12 -12.88 83Fluoranthene11.7219.2423344.01350.78 -6.77 323.3120.7084Pyrene11.6320.0790351.22353.90 -2.68 353.74 -2.52 854-Methylpyrene12.4620.0790370.15373.05 -2.90 371.86 -1.71 871-Methylpyrene12.4620.0790385.35392.09 -7.74 390.83 -5.48 892,7-Dimethylpyrene13.2820.0790386.34392.18 -5.84 389.97 -3.63 90Cyclopenta[cd]pyrene12.6724.2621396.54403.87 -7.33 408.84 -12.30 911-n-Butylpyrene15.1720.0790414.87435.94 -21.07 431.38 -16.51 92Benzo[a]pyrene	76	Triphenylene	13.40	20.0790	400.00	394.94	5.06	392.58	7.42
781,3-Dimethyltriphenylene15.0520.0790432.32433.18 -0.86 428.873.45791,6,11-Trimethyltriphenylene15.8420.0790446.24451.42 -5.18 446.040.20801,3,6,11-Tetramethyltriphenylene16.6420.0790461.72470.17 -8.45 463.79 -2.07 81Accenaphthylene8.8414.2226244.63252.84 -8.21 260.10 -15.47 821-Methylacenaphthylene9.6614.2226265.24271.87 -6.63 278.12 -12.88 83Fluoranthene11.7219.2423344.01350.78 -6.77 323.3120.7084Pyrene11.6320.0790351.22353.90 -2.68 353.74 -2.52 854-Methylpyrene12.4420.0790370.15373.05 -2.90 371.86 -1.71 862-Methylpyrene12.4420.0790385.35393.09 -7.74 390.83 -5.48 892,7-Dimethylpyrene13.2220.0790386.34392.18 -5.84 389.97 -3.63 90Cyclopenta[cd]pyrene15.1720.0790346.34392.18 -5.84 389.97 -3.63 911- <i>n</i> -Butylpyrene15.1720.079044.87 435.94 -21.07 431.38 -16.51 92Benzo[c]pyrene14.3725.1168450.27443.2312.99441.0715.1593Benzo[c]pyrene	77	1-Methyltriphenylene	14.19	20.0790	416.32	413.21	3.11	409.88	6.44
791,6,11-Trimethyltriphenylene15.8420.0790446.24451.42 -5.18 446.040.20801,3,6,11-Tetramethyltriphenylene16.6420.0790461.72470.17 -8.45 463.79 -2.07 81Acenaphthylene8.8414.2226244.63252.84 -8.21 260.10 -15.47 821-Methylacenaphthylene9.6614.2226265.24271.87 -6.63 278.12 -12.88 83Fluoranthene11.7219.2423344.01350.78 -6.77 323.3120.7084Pyrene11.6320.0790351.22353.90 -2.68 353.74 -2.52 854-Methylpyrene12.4420.0790370.15373.05 -2.90 371.86 -1.71 862-Methylpyrene12.4420.0790373.55372.551.00371.392.16871-Methylpyrene13.3220.0790386.34392.18 -5.84 389.97 -3.63 90Cyclopenta[<i>cd</i>]pyrene13.2820.0790386.34392.18 -5.84 389.97 -3.63 911- <i>n</i> -Butylpyrene15.1720.0790414.87435.94 -21.07 431.38 -16.51 92Benzo[<i>a</i>]pyrene14.4325.1168450.73448.682.05446.234.5093Benzo[<i>a</i>]pyrene14.4325.1168450.22443.2312.99441.0715.1595Indeo[1,23- <i>cd</i>]pyrene15.42<	78	1,3-Dimethyltriphenylene	15.05	20.0790	432.32	433.18	-0.86	428.87	3.45
80 $1,3,6,11$ -Tetramethyltriphenylene 16.64 20.0790 461.72 470.17 -8.45 463.79 -2.07 81Acenaphthylene 8.84 14.2226 244.63 252.84 -8.21 260.10 -15.47 82 1 -Methylacenaphthylene 9.66 14.2226 252.24 271.87 -6.63 278.12 -12.88 83Fluoranthene 11.72 19.2423 344.01 350.78 -6.77 323.31 20.70 84Pyrene 11.63 20.0790 351.22 353.90 -2.68 353.74 -2.52 85 4 -Methylpyrene 12.43 20.0790 370.15 373.05 -2.90 371.86 -1.71 86 2 -Methylpyrene 12.44 20.0790 373.55 372.55 1.00 371.39 2.16 88 1 -Ethylpyrene 13.32 20.0790 386.34 392.18 -5.84 389.97 -3.63 90Cyclopenta[cd]pyrene 12.67 24.2621 396.54 403.87 -7.33 408.84 -12.30 91 1 -n-Butylpyrene 15.17 20.0790 414.87 435.94 -21.07 431.38 -16.51 92Benzo[c]pyrene 14.43 25.1168 450.73 448.68 2.05 446.23 4.50 93Benzo[c]pyrene 14.43 25.1168 450.73 448.68 2.05 446.23 4.50 94Perylene 14.13 25.1168 450.73 <td< td=""><td>79</td><td>1,6,11-Trimethyltriphenylene</td><td>15.84</td><td>20.0790</td><td>446.24</td><td>451.42</td><td>-5.18</td><td>446.04</td><td>0.20</td></td<>	79	1,6,11-Trimethyltriphenylene	15.84	20.0790	446.24	451.42	-5.18	446.04	0.20
81Acenaphthylene8.8414.2226244.63252.84 -8.21 260.10 -15.47 821-Methylacenaphthylene9.6614.2226265.24271.87 -6.63 278.12 -12.88 83Fluoranthene11.7219.2423344.01350.78 -6.77 323.3120.7084Pyrene11.6320.0790351.22353.90 -2.68 353.74 -2.52 854-Methylpyrene12.4320.0790369.54372.32 -2.78 371.17 -1.63 862-Methylpyrene12.4620.0790370.15373.05 -2.90 371.86 -1.71 871-Methylpyrene13.3220.0790385.35393.09 -7.74 390.83 -5.48 892,7-Dimethylpyrene13.2220.0790386.34392.18 -5.84 389.97 -3.63 90Cyclopenta[<i>cd</i>]pyrene12.6724.2621396.54403.87 -7.33 408.84 -12.30 911- <i>n</i> -Butylpyrene15.1720.0790414.87435.94 -21.07 431.38 -16.51 92Benzo[<i>a</i>]pyrene14.3325.1168450.73448.682.05446.234.5093Benzo[<i>a</i>]pyrene15.4229.2819481.87499.00 -17.13 501.77 -19.90 94Perylene15.1330.1185503.89503.660.23501.272.6297Benzo[<i>d</i>] <i>h</i>]uoranthene15.1324.2621440	80	1,3,6,11-Tetramethyltriphenylene	16.64	20.0790	461.72	470.17	-8.45	463.79	-2.07
821-Methylacenaphthylene9.6614.2226265.24271.87 -6.63 278.12 -12.88 83Fluoranthene11.7219.2423344.01350.78 -6.77 323.3120.7084Pyrene11.6320.0790351.22353.90 -2.68 353.74 -2.52 854-Methylpyrene12.4320.0790369.54372.32 -2.78 371.17 -1.63 862-Methylpyrene12.4620.0790370.15373.05 -2.90 371.86 -1.71 871-Methylpyrene13.3220.0790385.35393.09 -7.74 390.83 -5.48 892,7-Dimethylpyrene13.2820.0790386.34392.18 -5.84 389.97 -3.63 90Cyclopenta[cd]pyrene12.6724.2621396.54403.87 -7.33 408.84 -12.30 911-n-Butylpyrene15.1720.0790414.87435.94 -21.07 431.38 -16.51 92Benzo[e]pyrene14.4325.1168450.73448.682.05446.234.5093Benzo[a]pyrene15.4229.2819481.87499.00 -17.13 501.77 -19.90 94Perylene15.1330.1185503.39503.660.23501.272.6297Benzo[dphiprene15.1330.1185501.32497.383.94495.335.9998Benzo[dphilovanthene14.5124.2621440.66 -5.7	81	Acenaphthylene	8.84	14.2226	244.63	252.84	-8.21	260.10	-15.47
83Fluoranthene 11.72 19.2423 344.01 350.78 -6.77 323.31 20.70 84Pyrene 11.63 20.0790 351.22 353.90 -2.68 353.74 -2.52 85 4 -Methylpyrene 12.43 20.0790 369.54 372.32 -2.78 371.17 -1.63 86 2 -Methylpyrene 12.46 20.0790 370.15 373.05 -2.90 371.86 -1.71 87 1 -Methylpyrene 12.44 20.0790 373.55 372.55 1.00 371.39 2.16 88 1 -Ethylpyrene 13.32 20.0790 385.35 393.09 -7.74 390.83 -5.48 89 $2,7$ -Dimethylpyrene 13.28 20.0790 386.34 392.18 -5.84 389.97 -3.63 90Cyclopenta[<i>cd</i>]pyrene 12.67 24.2621 396.54 403.87 -7.33 408.84 -12.30 91 1 -n-Butylpyrene 15.17 20.0790 414.87 435.94 -21.07 431.38 -16.51 92Benzo[<i>e</i>]pyrene 14.43 25.1168 450.73 448.68 2.05 446.23 45.09 93Benzo[<i>e</i>]pyrene 14.43 25.1168 456.22 443.23 12.99 441.07 15.15 94Perylene 14.13 25.1168 456.22 443.23 12.99 441.07 15.15 95Indeno[1,23- <i>cd</i>]pyrene 15.42 29.2819 481.87 49	82	1-Methylacenaphthylene	9.66	14.2226	265.24	271.87	-6.63	278.12	-12.88
84Pyrene11.6320.0790 351.22 353.90 -2.68 353.74 -2.52 854-Methylpyrene12.4320.0790 369.54 372.32 -2.78 371.17 -1.63 862-Methylpyrene12.4620.0790 370.15 373.05 -2.90 371.86 -1.71 871-Methylpyrene12.4420.0790 373.55 372.55 1.00 371.39 2.16 881-Ethylpyrene13.3220.0790 385.35 393.09 -7.74 390.83 -5.48 892,7-Dimethylpyrene13.2820.0790 386.34 392.18 -5.84 389.97 -3.63 90Cyclopenta[cd]pyrene12.67 24.2621 396.54 403.87 -7.33 408.84 -12.30 91 $1-n$ -Butylpyrene15.17 20.0790 414.87 435.94 -21.07 431.38 -16.51 92Benzo[e]pyrene14.43 25.1168 450.73 448.68 2.05 446.23 4.50 93Benzo[a]pyrene14.43 25.1168 456.22 443.23 12.99 441.07 15.15 94Perylene14.13 25.1168 456.22 443.23 12.99 441.07 15.15 95Indeno[1,23-cd]pyrene15.42 29.2819 481.87 499.00 -17.13 501.77 -19.90 95Indeno[1,23-cd]pyrene15.43 30.1185 503.89 503.66 0.23 501.27	83	Fluoranthene	11.72	19.2423	344.01	350.78	-6.77	323.31	20.70
854-Methylpyrene12.4320.0790 369.54 372.32 -2.78 371.17 -1.63 862-Methylpyrene12.4620.0790 370.15 373.05 -2.90 371.86 -1.71 871-Methylpyrene12.4420.0790 373.55 372.55 1.00 371.39 2.16 881-Ethylpyrene13.3220.0790 385.35 393.09 -7.74 390.83 -5.48 892,7-Dimethylpyrene13.2820.0790 386.34 392.18 -5.84 389.97 -3.63 90Cyclopenta[cd]pyrene12.67 24.2621 396.54 403.87 -7.33 408.84 -12.30 911-n-Butylpyrene15.1720.0790 414.87 435.94 -21.07 431.38 -16.51 92Benzo[e]pyrene14.3725.1168 450.73 448.68 2.05 446.23 4.50 93Benzo[a]pyrene14.4325.1168 453.44 450.07 3.37 447.55 5.89 94Perylene14.1325.1168 456.22 443.23 12.99 441.07 15.15 95Indeno[1,23-cd]pyrene15.4229.2819 481.87 499.00 -17.13 501.77 -19.90 96Dibenzo[def,mno]chrysene15.40 30.1185 503.89 503.66 0.23 501.27 2.62 97Benzo[jhi]perylene15.13 30.1185 501.32 497.38 3.94 495.33	84	Pyrene	11.63	20.0790	351.22	353.90	-2.68	353.74	-2.52
862-Methylpyrene12.4620.0790370.15373.05 -2.90 371.86 -1.71 87 1-Methylpyrene12.4420.0790373.55372.551.00371.392.16 88 1-Ethylpyrene13.3220.0790385.35393.09 -7.74 390.83 -5.48 89 2,7-Dimethylpyrene13.2820.0790386.34392.18 -5.84 389.97 -3.63 90 Cyclopenta[cd]pyrene12.6724.2621396.54403.87 -7.33 408.84 -12.30 91 1- n -Butylpyrene15.1720.0790414.87435.94 -21.07 431.38 -16.51 92 Benzo[e]pyrene14.3725.1168450.73448.682.05446.234.50 93 Benzo[a]pyrene14.4325.1168453.44450.073.37447.555.89 94 Perylene14.1325.1168456.22443.2312.99441.0715.15 95 Indeno[1,23- cd]pyrene15.4229.2819481.87499.00 -17.13 501.77 -19.90 96 Dibenzo[def,mno]chrysene15.4030.1185503.89503.660.23501.272.62 97 Benzo[ghi]perylene15.1330.1185501.32497.383.94495.335.99 98 Benzo[j]fluoranthene14.5124.2621440.92446.68 -5.76 449.36 -8.44 99 Benzo[b]fluoranthene	85	4-Methylpyrene	12.43	20.0790	369.54	372.32	-2.78	371.17	-1.63
871-Methylpyrene12.4420.0790373.55372.551.00371.392.16 88 1-Ethylpyrene13.3220.0790385.35393.09 -7.74 390.83 -5.48 89 2,7-Dimethylpyrene13.2820.0790386.34392.18 -5.84 389.97 -3.63 90 Cyclopenta[cd]pyrene12.6724.2621396.54403.87 -7.33 408.84 -12.30 91 1- n -Butylpyrene15.1720.0790414.87435.94 -21.07 431.38 -16.51 92 Benzo[e]pyrene14.3725.1168450.73448.682.05446.234.50 93 Benzo[a]pyrene14.4325.1168453.44450.073.37447.555.89 94 Perylene14.1325.1168456.22443.2312.99441.0715.15 95 Indeno[1,23- cd]pyrene15.4229.2819481.87499.00 -17.13 501.77 -19.90 96 Dibenzo[def,mno]chrysene15.4030.1185503.89503.660.23501.272.62 97 Benzo[ghi]perylene15.1330.1185501.32497.383.94495.335.99 98 Benzo[j]fluoranthene14.5124.2621440.92446.68 -5.76 449.36 -8.44 99 Benzo[b]fluoranthene14.5124.2621441.74446.60 -4.86 449.29 -7.55 100 Benzo[k]flu	86	2-Methylpyrene	12.46	20.0790	370.15	373.05	-2.90	371.86	-1.71
881-Ethylpyrene13.3220.0790 385.35 393.09 -7.74 390.83 -5.48 892,7-Dimethylpyrene13.2820.0790 386.34 392.18 -5.84 389.97 -3.63 90Cyclopenta[cd]pyrene12.67 24.2621 396.54 403.87 -7.33 408.84 -12.30 911-n-Butylpyrene15.1720.0790 414.87 435.94 -21.07 431.38 -16.51 92Benzo[e]pyrene14.37 25.1168 450.73 448.68 2.05 446.23 4.50 93Benzo[a]pyrene14.43 25.1168 453.44 450.07 3.37 447.55 5.89 94Perylene14.13 25.1168 456.22 443.23 12.99 441.07 15.15 95Indeno[1,23-cd]pyrene15.42 29.2819 481.87 499.00 -17.13 501.77 -19.90 96Dibenzo[def,mno]chrysene15.40 30.1185 503.89 503.66 0.23 501.27 2.62 97Benzo[ghi]perylene15.13 30.1185 501.32 497.38 3.94 495.33 5.99 98Benzo[j]fluoranthene14.51 24.2621 440.92 446.68 -5.76 449.36 -8.44 99Benzo[b]fluoranthene14.51 24.2621 442.56 447.87 -5.31 450.48 -7.92	87	1-Methylpyrene	12.44	20.0790	373.55	372.55	1.00	371.39	2.16
892,7-Dimethylpyrene13.2820.0790386.34392.18 -5.84 389.97 -3.63 90Cyclopenta[cd]pyrene12.6724.2621396.54403.87 -7.33 408.84 -12.30 911-n-Butylpyrene15.1720.0790414.87435.94 -21.07 431.38 -16.51 92Benzo[e]pyrene14.3725.1168450.73448.682.05446.234.5093Benzo[a]pyrene14.4325.1168453.44450.073.37447.555.8994Perylene14.1325.1168456.22443.2312.99441.0715.1595Indeno[1,23-cd]pyrene15.4229.2819481.87499.00 -17.13 501.77 -19.90 96Dibenzo[def,mno]chrysene15.4030.1185503.89503.660.23501.272.6297Benzo[ghi]perylene15.1330.1185501.32497.383.94495.335.9998Benzo[jfluoranthene14.5124.2621440.92446.68 -5.76 449.36 -8.44 99Benzo[b]fluoranthene14.5124.2621441.74446.60 -4.86 449.29 -7.55 100Benzo[k]fluoranthene14.5624.2621442.56447.87 -5.31 450.48 -7.92	88	1-Ethylpyrene	13.32	20.0790	385.35	393.09	-7.74	390.83	-5.48
90Cyclopenta[cd]pyrene12.6724.2621396.54403.87 -7.33 408.84 -12.30 911- n -Butylpyrene15.1720.0790414.87435.94 -21.07 431.38 -16.51 92Benzo[e]pyrene14.3725.1168450.73448.682.05446.234.5093Benzo[a]pyrene14.4325.1168453.44450.073.37447.555.8994Perylene14.1325.1168456.22443.2312.99441.0715.1595Indeno[1,23- cd]pyrene15.4229.2819481.87499.00 -17.13 501.77 -19.90 96Dibenzo[def,mno]chrysene15.4030.1185503.89503.660.23501.272.6297Benzo[ghi]perylene15.1330.1185501.32497.383.94495.335.9998Benzo[j]fluoranthene14.5124.2621440.92446.68 -5.76 449.36 -8.44 99Benzo[b]fluoranthene14.5124.2621441.74446.60 -4.86 449.29 -7.55 100Benzo[k]fluoranthene14.5624.2621442.56447.87 -5.31 450.48 -7.92	89	2,7-Dimethylpyrene	13.28	20.0790	386.34	392.18	-5.84	389.97	-3.63
911-n-Butylpyrene15.1720.0790414.87435.94 -21.07 431.38 -16.51 92Benzo[e]pyrene14.3725.1168450.73448.682.05446.234.5093Benzo[a]pyrene14.4325.1168453.44450.073.37447.555.8994Perylene14.1325.1168456.22443.2312.99441.0715.1595Indeno[1,23-cd]pyrene15.4229.2819481.87499.00 -17.13 501.77 -19.90 96Dibenzo[def,mno]chrysene15.4030.1185503.89503.660.23501.272.6297Benzo[ghi]perylene15.1330.1185501.32497.383.94495.335.9998Benzo[j]fluoranthene14.5124.2621440.92446.68 -5.76 449.36 -8.44 99Benzo[b]fluoranthene14.5124.2621441.74446.60 -4.86 449.29 -7.55 100Benzo[k]fluoranthene14.5624.2621442.56447.87 -5.31 450.48 -7.92	90	Cyclopenta[cd]pyrene	12.67	24.2621	396.54	403.87	-7.33	408.84	-12.30
92Benzo[e]pyrene 14.37 25.1168 450.73 448.68 2.05 446.23 4.50 93Benzo[a]pyrene 14.43 25.1168 453.44 450.07 3.37 447.55 5.89 94Perylene 14.13 25.1168 456.22 443.23 12.99 441.07 15.15 95Indeno[1,23-cd]pyrene 15.42 29.2819 481.87 499.00 -17.13 501.77 -19.90 96Dibenzo[def,mno]chrysene 15.40 30.1185 503.89 503.66 0.23 501.27 2.62 97Benzo[ghi]perylene 15.13 30.1185 501.32 497.38 3.94 495.33 5.99 98Benzo[j]fluoranthene 14.51 24.2621 440.92 446.68 -5.76 449.36 -8.44 99Benzo[b]fluoranthene 14.51 24.2621 441.74 446.60 -4.86 449.29 -7.55 100Benzo[k]fluoranthene 14.56 24.2621 442.56 447.87 -5.31 450.48 -7.92	91	1-n-Butylpyrene	15.17	20.0790	414.87	435.94	-21.07	431.38	-16.51
93 Benzo[a]pyrene 14.43 25.1168 453.44 450.07 3.37 447.55 5.89 94 Perylene 14.13 25.1168 456.22 443.23 12.99 441.07 15.15 95 Indeno[1,23-cd]pyrene 15.42 29.2819 481.87 499.00 -17.13 501.77 -19.90 96 Dibenzo[def,mno]chrysene 15.40 30.1185 503.89 503.66 0.23 501.27 2.62 97 Benzo[ghi]perylene 15.13 30.1185 501.32 497.38 3.94 495.33 5.99 98 Benzo[j]fluoranthene 14.51 24.2621 440.92 446.68 -5.76 449.36 -8.44 99 Benzo[b]fluoranthene 14.51 24.2621 441.74 446.60 -4.86 449.29 -7.55 100 Benzo[k]fluoranthene 14.56 24.2621 442.56 447.87 -5.31 450.48 -7.92	92	Benzo[e]pyrene	14.37	25.1168	450.73	448.68	2.05	446.23	4.50
94Perylene 14.13 25.1168 456.22 443.23 12.99 441.07 15.15 95Indeno[1,23-cd]pyrene 15.42 29.2819 481.87 499.00 -17.13 501.77 -19.90 96Dibenzo[def,mno]chrysene 15.40 30.1185 503.89 503.66 0.23 501.27 2.62 97Benzo[ghi]perylene 15.13 30.1185 501.32 497.38 3.94 495.33 5.99 98Benzo[j]fluoranthene 14.51 24.2621 440.92 446.68 -5.76 449.36 -8.44 99Benzo[b]fluoranthene 14.51 24.2621 441.74 446.60 -4.86 449.29 -7.55 100Benzo[k]fluoranthene 14.56 24.2621 442.56 447.87 -5.31 450.48 -7.92	93	Benzo[a]pyrene	14.43	25.1168	453.44	450.07	3.37	447.55	5.89
95 Indeno[1,23-cd]pyrene 15.42 29.2819 481.87 499.00 -17.13 501.77 -19.90 96 Dibenzo[def,mno]chrysene 15.40 30.1185 503.89 503.66 0.23 501.27 2.62 97 Benzo[ghi]perylene 15.13 30.1185 501.32 497.38 3.94 495.33 5.99 98 Benzo[j]fluoranthene 14.51 24.2621 440.92 446.68 -5.76 449.36 -8.44 99 Benzo[b]fluoranthene 14.51 24.2621 441.74 446.60 -4.86 449.29 -7.55 100 Benzo[k]fluoranthene 14.56 24.2621 442.56 447.87 -5.31 450.48 -7.92	94	Perylene	14.13	25.1168	456.22	443.23	12.99	441.07	15.15
96 Dibenzo[def,mno]chrysene 15.40 30.1185 503.89 503.66 0.23 501.27 2.62 97 Benzo[ghi]perylene 15.13 30.1185 501.32 497.38 3.94 495.33 5.99 98 Benzo[j]fluoranthene 14.51 24.2621 440.92 446.68 -5.76 449.36 -8.44 99 Benzo[b]fluoranthene 14.51 24.2621 441.74 446.60 -4.86 449.29 -7.55 100 Benzo[k]fluoranthene 14.56 24.2621 442.56 447.87 -5.31 450.48 -7.92	95	Indeno[1,23-cd]pyrene	15.42	29.2819	481.87	499.00	-17.13	501.77	-19.90
97 Benzo[ghi]perylene 15.13 30.1185 501.32 497.38 3.94 495.33 5.99 98 Benzo[j]fluoranthene 14.51 24.2621 440.92 446.68 -5.76 449.36 -8.44 99 Benzo[k]fluoranthene 14.51 24.2621 441.74 446.60 -4.86 449.29 -7.55 100 Benzo[k]fluoranthene 14.56 24.2621 442.56 447.87 -5.31 450.48 -7.92	96	Dibenzo[def,mno]chrysene	15.40	30.1185	503.89	503.66	0.23	501.27	2.62
98 Benzo[<i>j</i>]fluoranthene 14.51 24.2621 440.92 446.68 -5.76 449.36 -8.44 99 Benzo[<i>b</i>]fluoranthene 14.51 24.2621 441.74 446.60 -4.86 449.29 -7.55 100 Benzo[<i>k</i>]fluoranthene 14.56 24.2621 442.56 447.87 -5.31 450.48 -7.92	97	Benzo[ghi]perylene	15.13	30.1185	501.32	497.38	3.94	495.33	5.99
99 Benzo[b]fluoranthene 14.51 24.2621 441.74 446.60 -4.86 449.29 -7.55 100 Benzo[k]fluoranthene 14.56 24.2621 442.56 447.87 -5.31 450.48 -7.92	98	Benzo[<i>j</i>]fluoranthene	14.51	24.2621	440.92	446.68	-5.76	449.36	-8.44
100 Benzo[k]fluoranthene 14.56 24.2621 442.56 447.87 -5.31 450.48 -7.92	99	Benzo[b]fluoranthene	14.51	24.2621	441.74	446.60	-4.86	449.29	-7.55
	100	Benzo[k]fluoranthene	14.56	24.2621	442.56	447.87	-5.31	450.48	-7.92

^a Taken from Ref. [25]. ^b Calculated from Eq. (2). ^c Calculated from Eq. (3).



Fig. 1. Plot of predicted retention index vs. measured retention index for 100 PAHs.

GC retention index of PAHs is developed by the combination of the quasi-length of carbon chain (N')with pseudo-conjugated system surface (S_{π}) . Good results by MLR (in Eq. (2)) illustrate this predicting model is applicable to the estimation and prediction of GC retention indices for both unsubstituted and substituted PAHs (shown in Fig. 1). Also, the authors examined the cross-correlation between the two paired parameters and obtained the unexpected correlation coefficients of R = 0.7885 (N' = 6.8705 + $0.3427S_{\pi}$) and $0.8377 (N' = 6.3923 + 1.8203S_c)$ for the $N' \sim S_{\pi}$ and $N' \sim S_{c}$ pairs, respectively. This demonstrates that N' cross-correlates less with S_{π} than with S_c and I relates better with N' and S_{π} than with N' and S_c . The results shown in Table 1 suggest that S_c should be an appropriate descriptor and S_{π} may be a better descriptor for expressing molecular structures of PAHs, to estimate and predict the capillary GC retention index.

4. Conclusions

In this work, a new model developed in our laboratories for predicting capillary GC retention index by utilizing two parameters calculated directly from the molecular structure of PAHs is reported. Furthermore this study illustrates the influence of the molecular polarizability effect and the structural shape on the relative retention behavior quantitatively by using quasi-length of carbon chain (N') and pseudo-conjugated system surface area (S_{π}). Further work is in progress.

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