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RECEIVED for review April 23, 1984. Accepted August 13, 1984.
This work was supported by the National Foundation for Scientific Research (NFWO-FNRS), Belgium.

Relationship between Gas Chromatographic Retention Indices and Molecular Connectivities of Nitrated Polycyclic Aromatic Hydrocarbons

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Gas chromatographic retention indices of nitrated polycyclic aromatic hydrocarbons (nitro-PAH) on SE-52, a methylphenylsilicone stationary phase, are linearly related to molecular connectivities. The data set of mononitrated and dinitrated PAH on the same stationary phase allows the correlation of retention indices with different topological parameters. On the basis of these findings, chromatographic retention behavior is predicted.

Recent interest has focused on development of analytical methods for the determination of nitrated polycyclic aromatic hydrocarbons (nitro-PAH) in environmentally significant samples. This interest has been generated because of the remarkably facile nitration of some polycyclic aromatic hydrocarbons (PAH) (1-3) in the presence of nitrating agents and because some nitro-PAH are potent bacterial mutagens. Nitro-PAH have caused increasing health-related concerns due to their direct-acting mutagenic responses in salmonella tests (4-6), positive mutagenic responses in mammalian cells (7), and carcinogenic activity in animal experiments (8). Schuetzle et al. (9) have estimated that approximately 30% of the direct-acting mutagenicity of the solvent-extractable portion of diesel engine exhaust is due to the presence of one compound, 1-nitropyrene. Nitro-PAH are found in diesel exhaust gases and particulates (10-12), in carbon black (13), and in other environmentally significant materials. Numerous analytical methods have been used to determine nitro-PAH. These include direct-probe high-resolution mass spectrometry (HRMS), MS-MS, thin-layer chromatography (TLC) with fluorescence detection, high-performance liquid chromatography (HPLC) with electrochemical, MS, and fluorescence detection, and gas chromatography employing mass spectrometric, nitrogen-selective, electron capture, and flame ionization detection.

High-resolution capillary gas chromatography utilizing a thermionic ionization detector in a nitrogen environment has previously been used for the analysis of nitro-PAH (14). This detector responded linearly with respect to nitro-PAH, detected as little as 3 pg of some nitro-PAH, and responded selectively toward nitro-PAH spiked into an aromatic fraction of a Homestead, KY, coal extract. On the other hand, the detector did not respond uniformly toward all nitro-PAH. The gas chromatographic retention characteristics (relative retentions determined isothermally and linear temperature-programmed retention indices) of 56 nitro-PAH on fused-silica columns coated with SE-52 were discussed in another publication (15).

This paper reports the linear relationship between relative retention (i.e., retention index) and topology (molecular connectivity) of nitro-PAH. The linear relationships obtained were used to predict the gas chromatographic retention indices of nitro-PAH. Although the correlations between retention index and molecular connectivity provided only an approximation of the gas chromatographic retention characteristics of nitro-PAH, nevertheless, the ability to predict retention indices is extremely important since few analytical reference standards are commercially available, and moreover, over 1000 different isomeric nitro-PAH having between two and five condensed rings and one and four nitro substitutions can be envisioned.

EXPERIMENTAL SECTION

Molecular Connectivity Calculations. Molecular connectivity, χ , as described by Kier and Hall (16) is a topological description of molecular structure based on a count of skeletal atom groupings, weighted by the degree of skeletal branching. Molecular connectivities have been correlated with solubility parameters, boiling points, densities, partition coefficients, and retention data (16-21). An example of a $^m\chi_v$ calculation is illustrated below for 1-nitronaphthalene (m denotes order and v , valence). The molecule is shown in its skeletal form (see Figure

Table I. Retention Indices and χ Values of Mononitrated PAH

no.	compounds	$^0\chi_v$	$^1\chi_v$	$^2\chi_{vp}$	$^3\chi_{vp}$	$^4\chi_{vp}$	$^5\chi_{vp}$	$^6\chi_{vp}$	$^3\chi_{vc}$	$^4\chi_{vpc}$
1	5-nitroindan	6.617	4.034	3.064	2.293	1.672	0.959	0.545	0.316	0.701
2	1-nitronaphthalene	6.805	3.910	2.755	1.963	1.367	0.900	0.399	0.257	0.585
3	1-nitro-2-methylnaphthalene	7.728	4.327	3.188	2.366	1.613	0.997	0.506	0.382	0.908
4	2-nitronaphthalene	6.805	3.904	2.789	1.944	1.290	0.888	0.425	0.278	0.562
5	2-nitrobiphenyl	7.960	4.577	3.140	2.186	1.495	0.979	0.414	0.257	0.585
6	3-nitrobiphenyl	7.960	4.571	3.173	2.164	1.430	0.953	0.422	0.278	0.562
7	4-nitrobiphenyl	7.960	4.571	3.170	2.185	1.406	0.922	0.433	0.278	0.575
8	7-nitro-1-tetralone	7.525	4.488	3.375	2.455	1.730	1.240	0.645	0.358	0.763
9	4-nitrophenyl phenyl ether	8.368	4.729	3.166	2.026	1.261	0.809	0.321	0.248	0.415
10	3-nitrofluorene	8.512	5.111	3.932	2.993	2.225	1.589	0.931	0.460	1.043
11	3-nitrodibenzofuran	8.213	4.812	3.536	2.571	1.828	1.272	0.694	0.374	0.814
12	5-nitroacenaphthene	8.065	4.951	3.841	3.051	2.391	1.634	0.999	0.441	1.082
13	2-nitrofluorene	8.512	5.111	3.932	2.988	2.245	1.573	0.917	0.460	1.046
14	3-nitro-9-fluorenone	8.713	5.108	3.862	2.920	2.128	1.492	0.851	0.452	1.053
15	9-nitroanthracene	8.960	5.320	3.925	2.925	2.186	1.581	0.849	0.404	0.949
16	2-nitro-9-fluorenone	8.713	5.108	3.862	2.920	2.130	1.490	0.841	0.452	1.053
17	2-nitroanthracene	8.960	5.310	3.988	2.900	2.041	1.515	0.851	0.445	0.922
18	9-methyl-10-nitroanthracene	9.883	5.743	4.321	3.555	2.520	1.787	1.000	0.057	1.034
19	1-methyl-9-nitrophenanthrene	9.883	5.737	4.368	3.295	2.414	1.752	1.023	0.535	1.248
20	1-nitroanthraquinone	9.622	5.568	4.161	3.127	2.279	1.598	0.870	0.483	1.148
21	1-nitrofluoranthene	9.960	6.071	4.666	3.707	2.953	2.238	1.400	0.257	1.350
22	7-nitrofluoranthene	9.960	6.071	4.666	3.703	2.974	2.220	1.369	0.527	1.349
23	2-nitrofluoranthene	9.960	6.065	4.700	3.680	2.907	2.202	1.381	0.546	1.330
24	3-nitrofluoranthene	9.960	6.071	4.663	3.722	2.952	2.199	1.366	0.525	1.367
25	1-nitropyrene	9.960	6.065	4.698	3.702	2.879	2.201	1.377	0.548	1.334
26	4-nitro- <i>p</i> -terphenyl	11.269	6.642	4.747	3.403	2.261	1.531	0.807	0.445	0.960

1), with each atom assigned a δ value corresponding to the difference between the number of valence electrons and the number of hydrogen atoms attached to that atom. For the zero-order valence term $^0\chi_v$

$$^0\chi_v = \sum_{i=1}^K (\delta_i)^{-1/2} \quad (1)$$

The first-order valence (v) term is calculated after assigning a δ value to adjacent atoms i and j . An example calculation of $^1\chi_v$ is presented in Figure 1, where

$$^1\chi_v = \sum_{q=1}^L (\delta_i \delta_j)_q^{-1/2} \quad (2)$$

and L is the number of bonds in the molecule. The second-order valence path term is described mathematically as

$$^2\chi_{vp} = \sum_{q=1}^M (\delta_i \delta_j \delta_k)_q^{-1/2}$$

where $\delta_{i,j,k}$ are the δ values of the atoms of two adjacent bonds and M is the number of adjacent bonds in the molecule. Computation of third-, fourth-, fifth-, and sixth-order valence path terms is done in a similar fashion. In condensed rings and other highly branched molecules, a cluster grouping of atoms is possible in addition to the path subgraph, e.g., $^3\chi_{vp}$ and $^3\chi_{vc}$ (valence path and valence cluster, respectively). This is depicted in Figure 1b and described mathematically as

$$^3\chi_{vp,vc} = \sum_{q=1}^N (\delta_i \delta_j \delta_k \delta_l)_q^{-1/2} \quad (3)$$

In eq 3, N is the number of three adjacent bonds and $\delta_{i,j,k,l}$ values denote atoms of three adjacent bonds forming a path $^3\chi_{vp}$. On the other hand, $\delta_{i,j,k,l}$ values for atoms of three adjacent bonds forming a cluster (tripod-like structure) are defined as $^3\chi_{vc}$. Additional information for condensed rings may be obtained by computing the path/cluster four subgraph, $^4\chi_{vpc}$ (shown in Figure 1b). This index occurs at branch points of ring vertices and at nitro-substitution branches of the ring. The $^4\chi_{vpc}$ encodes information on the orientation of the condensed rings and their substituents.

Retention data for all nitro-PAH used in this study were published in an earlier paper (15) and were calculated from the relationship of Van Den Dool and Kratz (22). The molecular connectivity terms were calculated on a Digital Equipment Corp. Series 10 (DEC-10) computer at Tufts University. Multiple

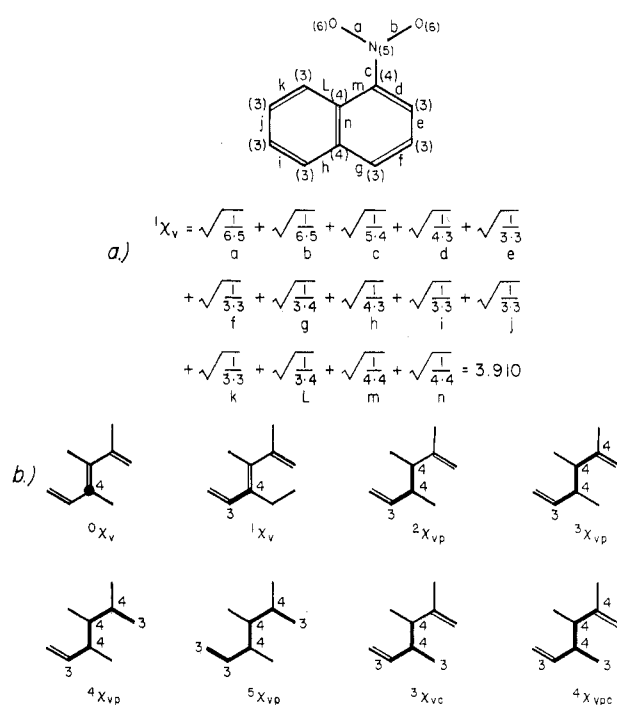


Figure 1. (a) Example calculation of the first-order valence molecular connectivity of 1-nitronaphthalene. Numbers in parentheses are the assigned δ values of the individual atoms. Bonds around the molecule are lettered to facilitate the calculations. (b) Subgraphs of 1-nitronaphthalene illustrating topological parameters, $^m\chi_v$.

regression analysis and correlations were computed by using programs supplied by Lowell Hall (Eastern Nazarene College, Quincy, MA) that were made compatible with the DEC-10 computer system.

RESULTS AND DISCUSSION

The calculated molecular connectivities of some mononitrated PAH are listed in Table I while those of some dinitrated PAH are presented in Table II. The corresponding retention indices of the nitro-PAH cited in Tables I and II were obtained from White et al. (15). Table III lists the retention indices of some PAH obtained from Lee and co-

Table II. Retention Indices and χ Values of Dinitrated PAH

no.	compounds	$^0\chi_v$	$^1\chi_v$	$^2\chi_{vp}$	$^3\chi_{vp}$	$^4\chi_{vp}$	$^5\chi_{vp}$	$^6\chi_{vp}$	$^3\chi_{vc}$	$^4\chi_{vpc}$
1	1,4-dinitronaphthalene	7.992	4.416	3.164	2.271	1.586	1.050	0.526	0.348	0.786
2	1,5-dinitronaphthalene	7.992	4.416	3.164	2.269	1.595	1.047	0.504	0.348	0.786
3	1,3-dinitronaphthalene	7.992	4.410	3.200	2.232	1.531	1.062	0.528	0.369	0.752
4	2,2'-dinitrobiphenyl	9.146	5.082	3.549	2.492	1.721	1.131	0.522	0.348	0.786
5	1,8-dinitronaphthalene	7.992	4.416	3.167	2.254	1.606	1.073	0.505	0.349	0.769
6	2,4-dinitro-2'-methylphenyl phenyl ether	10.477	5.651	4.034	2.664	1.638	1.068	0.499	0.476	0.879
7	2,6-dinitro-9-fluorenone	9.900	5.608	4.303	3.207	2.280	1.616	0.980	0.563	1.231
8	2,7-dinitrofluorene	9.699	5.611	4.374	3.270	2.411	1.697	1.047	0.572	1.217
9	2,5-dinitrofluorene	9.699	5.617	4.344	3.275	2.486	1.756	1.050	0.552	1.221
10	2,7-dinitro-9-fluorenone	9.900	5.608	4.303	3.207	2.282	1.613	0.970	0.563	1.231
11	1,3-dinitropyrene	11.146	6.570	5.110	3.995	3.097	2.380	1.529	0.640	1.528
12	1,6-dinitropyrene	11.146	6.570	5.106	4.012	3.089	2.351	1.521	0.640	1.538
13	1,8-dinitropyrene	11.146	6.570	5.106	4.012	3.089	2.351	1.519	0.640	1.538

Table III. Retention Indices and $^1\chi_v$ Values of Some Polycyclic Aromatic Hydrocarbons

no.	PAH	I^a	$^1\chi_v$
1	naphthalene	200.00	3.405
2	azulene	219.95	3.405
3	acenaphthylene	244.63	4.149
4	acenaphthene	251.29	4.445
5	phenanthrene	300.00	4.809
6	anthracene	301.69	4.815
7	4H-cyclopenta[def]phenanthrene	322.08	5.356
8	fluoranthene	344.01	5.565
9	pyrene	351.22	5.559
10	benzo[a]fluorene	366.74	6.022
11	benzo[b]fluorene	369.39	6.016
12	benzo[ghi]fluoranthene	389.60	6.309
13	benzo[c]phenanthrene	391.39	6.226
14	cyclopenta[cd]pyrene	396.54	6.303
15	benz[a]anthracene	398.50	6.220
16	chrysene	400.00	6.226
17	triphenylene	400.00	6.232
18	benzo[j]fluoranthene	440.92	6.976
19	benzo[b]fluoranthene	441.74	6.976
20	benzo[k]fluoranthene	442.56	6.970
21	benzo[a]pyrene	453.44	6.970
22	perylene	456.22	6.976
23	indeno[1,2,3-cd]pyrene	481.87	7.720
24	pentacene	486.81	7.619
25	dibenz[a,c]anthracene	495.01	7.637
26	dibenz[a,h]anthracene	495.45	7.631
27	benzo[b]chrysene	497.66	7.631
28	picene	500.00	7.637
29	benzo[ghi]perylene	501.32	7.720
30	dibenzo[def,mno]chrysene	503.89	7.714

^a Retention indices were taken from ref 23.Table IV. Correlation Coefficient Relationships of χ Values of Mononitrated PAH Shown in Table I

	$^0\chi_v$	$^1\chi_v$	$^2\chi_{vp}$	$^3\chi_{vp}$	$^4\chi_{vp}$	$^5\chi_{vp}$	$^6\chi_{vp}$	$^3\chi_{vc}$
$^1\chi_v$	0.98							
$^2\chi_{vp}$	0.37	0.36						
$^3\chi_{vp}$	0.43	0.45	0.99					
$^4\chi_{vp}$	0.50	0.52	0.96	0.99				
$^5\chi_{vp}$	0.57	0.60	0.94	0.97	0.99			
$^6\chi_{vp}$	0.61	0.65	0.88	0.94	0.97	0.99		
$^3\chi_{vc}$	0.47	0.48	0.96	0.98	0.97	0.96	0.93	
$^4\chi_{vpc}$	0.54	0.55	0.92	0.96	0.98	0.97	0.95	0.98

workers (23) and their corresponding $^1\chi_v$ values. Tables IV and V illustrate the relationship between the various χ values calculated for mononitrated and dinitrated PAH, respectively. The information in Tables IV and V reveals that the topological parameters are highly intercorrelated for each set of nitro-PAH studied. Multivariate regressions analysis does not give significantly better correlations than single-variant analysis. Figure 2 illustrates the best fit of retention index

Table V. Correlation Coefficient Relationships between χ Values of Dinitrated PAH Shown in Table II

	$^0\chi_v$	$^1\chi_v$	$^2\chi_{vp}$	$^3\chi_{vp}$	$^4\chi_{vp}$	$^5\chi_{vp}$	$^6\chi_{vp}$	$^3\chi_{vc}$
$^1\chi_v$	0.99							
$^2\chi_{vp}$	0.96	0.99						
$^3\chi_{vp}$	0.92	0.97	0.99					
$^4\chi_{vp}$	0.86	0.93	0.96	0.99				
$^5\chi_{vp}$	0.85	0.92	0.95	0.98	1.00			
$^6\chi_{vp}$	0.84	0.91	0.95	0.98	1.00	1.00		
$^3\chi_{vc}$	0.91	0.94	0.98	0.97	0.94	0.93	0.93	
$^4\chi_{vpc}$	0.88	0.94	0.97	0.99	0.99	0.98	0.99	0.97

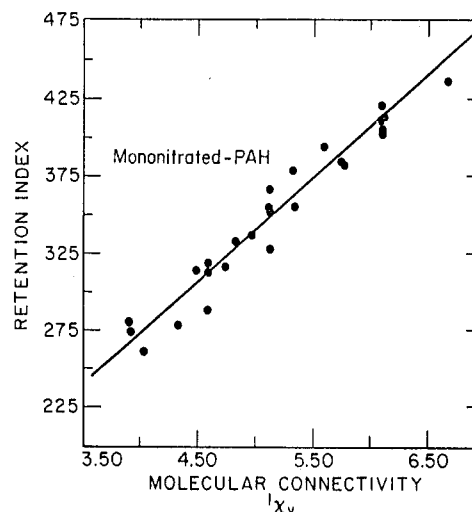


Figure 2. Plot of I vs. $^1\chi_v$ for mononitrated PAH; correlation coefficient = 0.975, slope = 67, intercept = 7.3, standard error = 11.6, and number of points = 26.

vs. the topological parameters listed in Table I for mononitrated PAH. The corresponding regression equation

$$I = 67^1\chi_v + 7.3 \quad (4)$$

was the only one whose correlation coefficient was greater than 0.970.

In the case of dinitrated PAH, only two topological parameters describe plots of similar statistical significance. Figures 3 and 4 illustrate plots of I vs. $^4\chi_{vpc}$ and $^3\chi_{vp}$, respectively. For dinitrated PAH, substitution seems to play a more important role in the relationship between chromatographic retention on SE-52 and the topology of the solute than in the case of mononitrated PAH. Each nitro group forms a cluster subgraph, and, thus, the $^4\chi_{vpc}$ encodes this cluster substituent one bond into the ring from the point of attachment. Similarly, the $^3\chi_{vp}$ term incorporated the NO segment of the nitro group one bond into the ring from the point of attachment (see Figure 1b). Regression analysis of

Table VI. Comparison of Experimental and Predicted Retention Indices

mononitrated PAH	exptl	predicted	% difference		
4-nitrobiphenyl	313.20	312.1	+0.4		
4-nitrophenyl phenyl ether	316.80	322.4	-1.7		
2-nitrofluorene	352.17	347.2	+1.4		
1-nitroanthraquinone	394.88	376.9	+4.7		
3-nitrofluoranthene	413.84	409.6	+0.9		
1-nitropyrene	421.08	409.2	+2.9		
$Y = 65^1x_v + 15 \quad R = 0.974 \quad S = 12.3 \quad N = 20$					
dinitrated PAH	exptl	predicted	% difference	predicted	% difference
1,3-dinitronaphthalene	332.75	332.0	-0.2	340.4	+2.2
2,7-dinitrofluorene	427.47	430.7	+0.7	433.4	+1.4
1,6-dinitropyrene	478.51	501.1	+4.5	497.6	+3.8
$Y = 95^3x_{vp} + 120$		$Y = 200^4x_{vpc} + 190$			
$R = 0.970$		$R = 0.965$			
$S = 11.9$		$S = 12.8$			
$N = 10$		$N = 10$			

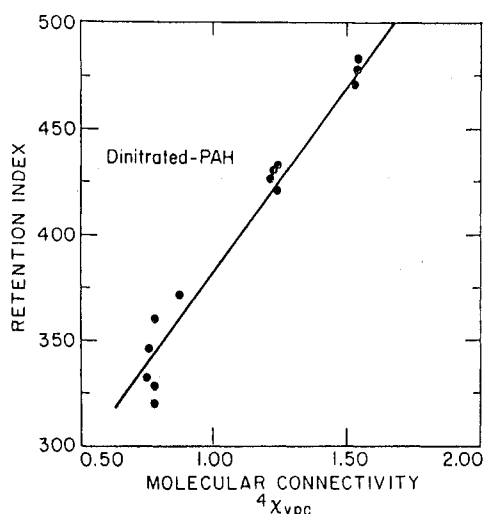


Figure 3. Plot of I vs. $^4\chi_{vpc}$ for dinitrated PAH; correlation coefficient = 0.982, slope = 180, intercept = 200, standard error = 11.6, and number of points = 13.

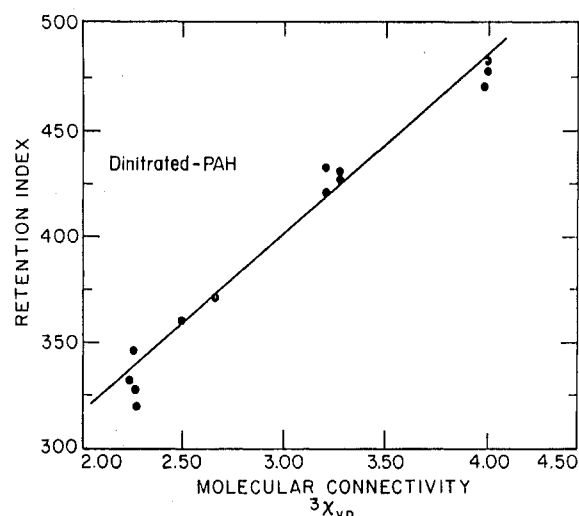


Figure 4. Plot of I vs. $^3\chi_{vp}$ for dinitrated PAH; correlation coefficient = 0.981, slope = 84, intercept = 150, standard error = 12.0, and number of points = 13.

other single-variable topological parameters yielded correlation coefficients less than 0.975.

A plot of retention index vs. $^1\chi_v$ for the 13 dinitrated PAH is shown in Figure 5. Interestingly, two sets of data points are observed. The slope of line A for the first set (compounds 4 and 7-13 in Table II) is within experimental error of the mononitrated PAH slope, while line B for the second set (compounds 1-4 and 6 in Table II) has a slope of one-half the mononitrated PAH slope. Moreover, a plot of retention index vs. $^1\chi_v$ for the 30 PAH shown in Table III yielded

$$I = 69^1\chi_v - 37 \quad (5)$$

with $R = 0.996$, $S = 8.8$, and $N = 30$. Thus, plots of retention index vs. $^1\chi_v$ for PAH, mononitrated PAH, and dinitrated PAH (line A) resulted in approximately parallel lines.

An attempt was made to predict retention indices of six mononitrated PAH and three dinitrated PAH randomly selected from Tables I and II. Their experimental retention index values and respective $^1\chi_v$, $^3\chi_{vp}$, and $^4\chi_{vpc}$ values were omitted from the points used to generate the linear least-squares regression lines employed to predict their retention indices. The results are illustrated in Table VI and indicate good agreement between experimental and predicted retention indices for the relatively small sample population of nitro-PAH. Often the calculated molecular connectivities of isomeric nitro-PAH that differ only in the position of nitration are identical. This is evident from Figures 3-5, which reveal a

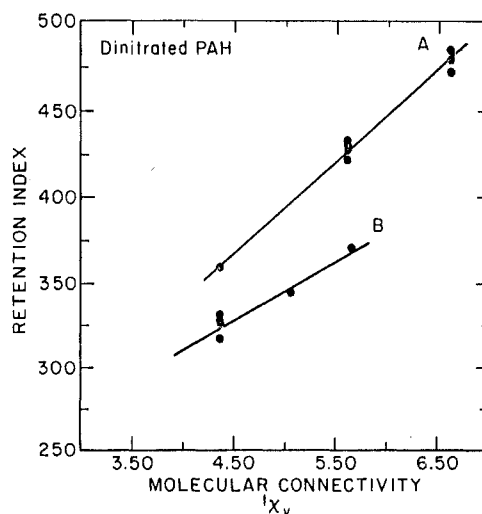


Figure 5. Plot of I vs. $^1\chi_v$ for dinitrated PAH. Line A: correlation coefficient = 0.993, slope = 54, intercept = 120, standard error = 6.0, and number of points = 8. Line B: correlation coefficient = 0.971, slope = 34, intercept = 180, standard error = 5.4, and number of points = 5.

clustering of the data points relative to isomeric nitro-PAH, limiting the accuracy of the correlation between retention index and molecular connectivity to predict retention char-

acteristics. Thus, the limited data set of 26 and 13 mono- and dinitro-PAH corresponds to only about 15 and 5 degrees of freedom for the correlations illustrated in Figure 2 and Figures 3-5, respectively. Because of this, only approximate retention indices of isomeric nitro-PAH can be predicted, each isomer having nearly the same predicted retention index. In the case of mononitrated PAH, the order of elution of these isomers can be further predicted, as described earlier, based on their predicted dipole moments and boiling points (15). It must be emphasized, however, that even though the correlation coefficients of the linear least-squares regression lines of retention indices vs. molecular connectivities are high, the accuracy of the predictions is not high enough to make the technique of practical use for identification purposes. For example, some of the predicted retention indices in Table VI are 10 or more index units away from the actual value. It does, however, provide for a good first approximation as to the possible identity of the compound which can then be confirmed by GC-MS or spiking experiments. In a forthcoming paper, correlations of the retention indices of nitro-PAH with molecular topological parameters, boiling point, polarizability, and dipole moment will be discussed.

The relationship between retention indices obtained by using SE-52, OV-101, and OV-17 and molecular connectivity has recently been evaluated with respect to planar PAH (24-28). Retention of an individual PAH on these phases is related to the logarithm of its vapor pressure and, consequently, to its boiling point and relative molecular mass. The same relationships have been observed by us concerning the retention of nitro-PAH (15). The relationship between molecular connectivity and retention is only approximate. Furthermore, the physicochemical explanations for the correlation between gas chromatographic retention and molecular connectivity are unclear. Although the relationship between retention indices and molecular connectivity is only approximate, it is nevertheless useful because it allows the approximate prediction of gas chromatographic retention characteristics of nitro-PAH. This is particularly important, since very few nitro-PAH reference standards are available for experimental determinations.

ACKNOWLEDGMENT

We thank Lowell Hall and Milton Lee for many helpful discussions.

Registry No. 5-Nitroindan, 7436-07-9; 1-nitronaphthalene, 86-57-7; 1-nitro-2-methylnaphthalene, 881-03-8; 2-nitronaphthalene, 581-89-5; 2-nitrobiphenyl, 86-00-0; 3-nitrobiphenyl, 2113-58-8; 4-nitrobiphenyl, 92-93-3; 7-nitro-1-tetralone, 40353-34-2; 4-nitrophenyl phenyl ether, 620-88-2; 3-nitrofluorene, 5397-37-5; 3-nitrodibenzofuran, 5410-97-9; 5-nitroacenaphthene, 602-87-9; 2-nitrofluorene, 607-57-8; 3-nitro-9-fluorenone, 42135-22-8; 9-nitroanthracene, 602-60-8; 2-nitro-9-fluorenone, 3096-52-4; 2-nitroanthracene, 3586-69-4; 9-methyl-10-nitroanthracene, 84457-22-7; 1-methyl-9-nitrophenanthrene, 87517-97-3; 1-nitroanthraquinone, 82-34-8; 1-nitrofluoranthene, 13177-28-1; 7-nitrofluoranthene, 13177-31-6; 2-nitrofluoranthene, 13177-29-2; 3-nitrofluoranthene, 892-21-7; 1-nitropyrene, 5522-43-0; 4-nitro-*p*-terphenyl, 10355-53-0; 1,4-dinitronaphthalene, 6921-26-2; 1,5-dinitronaphthalene, 605-71-0; 1,3-dinitronaphthalene, 606-37-1; 2,2'-dinitrobiphenyl, 2436-96-6; 1,8-dinitronaphthalene, 602-38-0; 2,4-dinitro-2'-methylphenyl phenyl ether, 2363-26-0; 2,6-dinitro-9-fluorenone, 58160-30-8; 2,7-dinitrofluorene, 5405-53-8; 2,5-dinitrofluorene, 15110-74-4; 2,7-dinitro-9-fluorenone, 31551-45-8; 1,3-dinitropyrene, 75321-20-9; 1,6-dinitropyrene, 42397-64-8; 1,8-dinitropyrene, 42397-65-9; naphthalene, 91-20-3; azulene, 275-51-4; acenaphthylene, 208-96-8; acenaphthene, 83-32-9; phenanthrene, 85-01-8; anthracene, 120-12-7; 4*H*-cyclopenta[*def*]phenanthrene, 203-64-5; fluoranthene, 206-44-0; pyrene, 129-00-0; benzo[*a*]fluorene, 30777-18-5; benzo[*b*]fluorene,

30777-19-6; benzo[*ghi*]fluoranthene, 203-12-3; benzo[*c*]phenanthrene, 195-19-7; cyclopenta[*cd*]pyrene, 27208-37-3; benz[*a*]anthracene, 56-55-3; chrysene, 218-01-9; triphenylene, 217-59-4; benzo[*j*]fluoranthene, 205-82-3; benzo[*b*]fluoranthene, 205-99-2; benzo[*k*]fluoranthene, 207-08-9; benzo[*a*]pyrene, 50-32-8; perylene, 198-55-0; indeno[1,2,3-*cd*]pyrene, 193-39-5; pentacene, 135-48-8; dibenz[*a,c*]anthracene, 215-58-7; dibenz[*a,b*]anthracene, 53-70-3; benzo[*b*]chrysene, 214-17-5; picene, 213-46-7; benzo[*ghi*]perylene, 191-24-2; dibenzo[*def,mno*]chrysene, 191-26-4.

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RECEIVED for review April 19, 1984. Accepted July 10, 1984. Part of this investigation was accomplished at the Pittsburgh Energy Technology Center during the summer of 1982 when A. Robert, Jr., and R. M. Hoes were under appointments to the Faculty Research Participation program and the Laboratory Graduate Participation program, respectively. Both programs are administered by Oak Ridge Associated Universities for the United States Department of Energy. The donors of the Petroleum Research Fund, administered by the American Chemical Society partially supported the research by A. Robbat, Jr. Based in part on a master's thesis by Philip J. Doherty. Presented in part at the Pittsburgh Conference and exposition on Analytical Chemistry and Applied Spectroscopy, Atlantic City, NJ, March 1983.