

Topological Organic Chemistry. 7.¹ Graph Theory and Molecular Topological Indices of Unsaturated and Aromatic Hydrocarbons

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Adjacency, distance, and degree matrices of representative unsaturated and aromatic hydrocarbons acquired from the appropriate graphs were used to generate molecular topological indices. Invariant indices were obtained from the following distance matrix calculations: the sum of the elements of the product of the degree vector and the distance matrix; the determinant and principal eigenvalue of the distance matrix; the permanent, the product of the row sums, and the short and long hafnians of the distance matrix. Descriptors were also derived from three adjacency-plus-distance matrix calculations: the sum of the elements of the product of the degree vector and the adjacency-plus-distance matrices; the determinant and principal eigenvalue of the sum of the two matrices.

INTRODUCTION

Balaban,² Randić,³ Hansen and Jurs,⁴ Rouvray,⁵ and Mihalić et al.^{6,7} are among many who have gathered references about, and reviewed methods for, calculating molecular topological indices of saturated hydrocarbons. Fewer, including Balaban,⁸ Barysz et al.,⁹ and Kvasnička and Pospíchal,¹⁰ have reviewed and presented techniques that lead to topological indices of unsaturated and/or aromatic hydrocarbons. This paper reports the extension to selected unsaturated and aromatic hydrocarbons of the earlier studies of this series which reported the utility of structure-descriptive matrices as sources of single-sum topological indices for linear and cyclic alkanes.

COMPUTATIONS

Molecular (multi)graphs, with hydrogens suppressed and with the interatomic carbon-carbon edge counts set at unity for tetrahedral, 1.5 for trigonal aromatic, 2 for trigonal aliphatic, and 3 for digonal hybridized carbon atoms, were derived from the representative unsaturated and aromatic hydrocarbons listed in Table I. The valence values reflected the corresponding edge counts cited above. Unsubstituted alkene and alkyne vertices were assigned valence values of 3 and 4, respectively, if internal bonds; one less if terminal, one more if an internal, substituted alkene. The aromatic carbon atoms, if internal and secondary as in most aromatic compounds, were assigned valences of 3; if internal and tertiary, as in the bridge of naphthalene, a valence of 4 was designated. Both the IUPAC and CIP numbering systems were used in all calculations; however, all of the matrix functions reported in this paper were invariant—descriptors. Particulars about specific substances utilize the IUPAC system of nomenclature. Reference is made to past papers^{1,11-15} of this series for each of the different modes of calculation of the various functions described in succeeding portions of this account. Table I lists

the results of experiments with representative C₂–C₁₀ unsaturated and aromatic hydrocarbons.

The adjacency (A) matrix was utilized with reluctance in some experiments, for the A matrix of any unsaturated or aromatic hydrocarbon was the same as that of its saturated congener, the corresponding linear or cyclic alkane, and was not, therefore, the source of new and unique information. The A matrix may be regarded as merely a limited (to 1) distance matrix; further, in the instance of these current studies, the A matrix did not convey complete information about the valences of the unsaturated or aromatic vertices of a graph, unlike the saturated hydrocarbon alkane A matrix which, in addition to its adjacency function, might be regarded as a stack of degree or valence (v) vectors. As Mihalić et al.^{6,7} have observed, the distance (D) matrix provides an abundance of graph information. In this paper distances and valences were defined so that the D matrix reflected the distances (edge counts) and valences (total edge counts about a vertex) of the vertices of these unsaturated and aromatic hydrocarbons, thus simultaneously weighting valences and edges of all these homonuclear graphs. In three sets of these studies the v·D (MTI') and the v(A + D) (MTI) matrix indices, as well as the determinant and principal eigenvalue indices of the D and (A + D) matrices, were contrasted. The conclusions drawn from such comparisons are recounted in subsequent sections and condensed in Table I.

TOPOLOGICAL INDICES DERIVED FROM THE GRAPH-THEORETICAL DISTANCE MATRIX

Table I lists the limited examples of various alkenes, alkynes, and aromatics studied and experimented with for this paper. In most compounds the functional groups of primary interest were the trigonal hybridized carbon atoms of the alkene and aromatic groups. In a few instances (3, 6, 7, 27, 31, 40, 42) multiple unsaturated, mostly conjugated, groups were inserted into the molecules; three alkynes (16, 17, 18) and one mythical cyclic triene (32) were also examined. Compounds 40 and 42, precursors of the charged aromatic compounds 41 and 43, were also included in Table I. The rather broad spectrum of structural qualities represented by the compounds of Table

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Table I. Topological Indices Derived from the Distance and Adjacency Matrices of Representative C₇-C₁₀ Unsaturated and Aromatic Hydrocarbons

no.	compound	bp, °C (cis/trans)	v(D)	det[D]	λ_1 (D)	per(D)	PRS(D)	shaf(D)	lhaf(D)	v(A + D)	det[A + D]	λ_1 (A + D)
1	ethene	-102	8	-4	2	4	4	2	4	12	-9	3
2	propene	-48	23	12	4	12	60	6	14	32	36	5.589
3	propadiene	-34.5	40	32	5.46410	32	144	8	24	52	72	6.69042
4	1-butene	-6	50	-32	6.80262	144	1 575	12	56	63	-128	8.13231
5	2-butene	(3.7/0.9)	52	-32	7.12311	324	2 304	18	146	66	-143	8.52494
6	1,3-butadiene	-4.4	76	-80	8.38517	324	3 600	18	122	92	-260	9.68466
7	1-butene-3-yne	5.1	110	-144	10.0194	576	7 007	24	216	129	-432	11.3011
8	1-pentene	30	93	80	10.1171	2 304	68 992	78	550	110	464	11.5138
9	2-pentene	(36.9/36.3)	97	80	10.6712	4 608	112 320	102	1 030	115	508	12.1395
10	2-methyl-1-butene	31.2	81	80	9.21411	1 568	45 360	66	358	101	380	10.5667
11	3-methyl-1-butene	20	83	80	9.28632	1 392	44 226	64	336	102	368	10.6398
12	2-methyl-2-butene	38.6	87	80	9.83132	3 072	75 600	86	686	108	428	11.2668
13	1-hexene	63.3	156	-192	14.0799	61 504	4 608 000	232	5 280	177	-1 636	15.5367
14	2-hexene	(68.8/68)	162	-192	14.8283	112 996	7 621 185	314	9 942	184	-1 801	16.3463
15	3-hexene	(66.4/67.1)	164	-192	15.0331	17 440	9 144 576	400	19 616	186	-1 785	16.5662
16	1-hexyne	71.3	214	-336	16.1373	96 388	8 690 825	290	8 070	238	-2 665	17.5597
17	2-hexyne	84	226	-336	17.5807	280 900	21 048 105	494	24 486	252	-3 049	19.1104
18	3-hexyne	81.5	230	-336	17.9789	629 764	28 676 025	770	80 582	256	-3 009	19.5334
19	2-methyl-1-pentene	60.7	138	-192	12.9272	41 412	2 953 665	190	3 318	162	-1 337	14.3392
20	3-methyl-1-pentene	51.1	136	-192	12.6954	30 016	2 419 200	160	2 048	159	-1 316	14.0849
21	4-methyl-1-pentene	53.9	142	-192	13.0452	36 388	2 861 001	178	2 870	165	-1 344	14.4604
22	2-methyl-2-pentene	67.3	152	-192	13.9839	113 572	6 016 725	322	12 278	175	-1 520	15.4835
23	3-methyl-2-pentene	(67.6/70.4)	142	-192	13.4249	62 020	4 266 405	230	4 566	167	-1 505	14.8864
24	4-methyl-2-pentene	(56.3/58.5)	148	-192	13.7803	70 432	4 939 200	248	5 728	172	-1 460	15.2631
25	2,3-dimethyl-1-butene	55.7	124	-192	11.8800	23 968	1 769 472	144	1 760	150	-1 088	13.2433
26	2,3-dimethyl-2-butene	73.2	136	-192	12.9282	72 224	3 841 600	256	7 504	164	-1 280	14.3899
27	2,3-dimethyl-1,3-butadiene	68-78	166	-448	13.6838	51 268	3 956 121	210	3 590	196	-2 240	15.0164
28	1-heptene	93.6	243	448	18.7051	2 225 400	437 404 968	2 316	86 520	268	5 538	20.2145
29	1-octene	121.3	358	-1024	24.0020	109 340 000	56 017 891 615	9 200	1 525 104	387	-18 167	25.5566
30	cyclohexene	83	142	-17	10.0492	18 293	980 100	127	1 829	170	-585	12.0459
31	1,3-cyclohexadiene	80.5	188	0	11.7185	46 244	2 474 329	202	4 886	220	-873	13.7139
32	1,3,5-cyclohexatriene	80.1	234	-52	13.0000	93 784	4 826 809	286	9 456	270	-1 620	15.0000
33	benzene	80.1	243	0	13.5	122 700	6 053 445.14	330.75	14 648.3438	279	-1 356	15.5
34	<i>o</i> -xylene	144	440	0	21.0204	85 331 000	32 349 619 600	8 079.75	1 185 908.3440	490	-8 344	22.8959
35	<i>m</i> -xylene	139	446	0	21.3659	104 320 000	35 771 369 681.2	8 991	1 660 464.5616	496	-8 175	23.2448
36	<i>p</i> -xylene	138	452	0	21.7898	120 680 000	43 645 000 000	9 720	2 077 703.1566	502	-7 975	23.6710
37	phenylbenzene	136.2	462	0	22.0149	111 390 000	44 000 551 362.5	9 213.75	1 459 420.0302	509	-11 840	23.9065
38	phenylethene	145.2	545	0	24.1322	181 330 000	77 519 441 698.5	11 738.25	2 277 282.0930	598	-22 815	25.9639
39	phenylethyne	142.4	644	0	26.3881	268 020 000	128 632 601 234	14 262.75	3 306 979.4052	697	-36 140	28.1679
40	1,3-cyclopentadiene	40	118	22	8.4183	1 926	41 472	69	435	146	368	10.4162
41	cyclopentadienyl anion	-	135	45.562	9.0000	2 779.3	59 049	78.75	531.5625	165	578.187	11.0000
42	1,3,5-cycloheptatriene	117	344	0	17.1615	3 274 600	432 972 864	2 596	115 040	384	2 100	19.1601
43	cycloheptatrienyl cation	-	378	205.03	18.0000	4 615 400	612 220 032	3 000.375	145 834.1710	420	5 040.31	20.0000
44	naphthalene	218	1032	0	33.2385	461 730 000 000	12 660 300 000 000 000			1104	69 984	35.3533

I was devised to test the practicality of the matrix representations and operations utilized in this paper.

Several alkenes listed in Table I exhibit geometrical isomerism; hence, each is encountered as a pair of diastereoisomers—5, 9, 14, 15, 23, 24. For these substances the representative matrices reflected only the structure and not the stereochemistry of the graph, and although the boiling points of the geometrical isomers are listed in column 3 of Table I, none of the data were used in the quantitative-structural relationship studies which are a part of this report.

All of the topological indices presented in Table I and described in the following sections were single-sum and invariant, circumstances that will not usually be referred to again. In the entire listing of data in Table I very few replications were observed, except for the **D** determinant indices which are described and analyzed at length in the appropriate section. Additionally, column 4, Table I, the MTI' index, showed replicate values for a triad (21/23/30) and a dyad (28/33) of substances; columns 7 and 9, Table I, the permanent and short hafnian indices, displayed one pair (5/6) of duplicates in common.

Some generalizations about all of the topological indices listed in Table I are usefully summarized at this point.

Unsaturates. All the data, except the **D** matrix determinants, disclosed that as the unsaturated group moved from the terminus to the center of a linear molecule, the index value increased. The more compact alkenes of the same carbon atom content were, the lower the index value usually was. Likewise, the index value decreased from linear to cyclic alkene of the same vertex count. Expectedly, if the unsaturation in a molecule was increased, either by introducing more double bonds or by substituting an alkene group with an alkyne function, the topological index increased.

Visual inspection of all indices of all unsaturates listed in Table I reflected a lack of monotonicity in each separate series of data. Quantitative-structural comparisons of the boiling points and topological indices of the various unsaturates were experimentally regressed, with disappointing results. However, the related series of 16 alkenes listed in Table I—1, 2, 4, 8, 10, 11, 12, 13, 19, 20, 21, 22, 25, 26, 28, 29—when subjected to boiling point-topological index regression studies, did yield evidence of reasonable relationships, as described in subsequent paragraphs of this paper. Omitting the three nonterminal alkenes—12, 22, 26—from the regressions only slightly improved the results of the studies of the remaining 13 terminal alkenes. Unsaturated compounds excluded from the above comparisons were all alkynes, alkenes that exhibited geometric isomerism, and alkadienes, including compound 27, also excluded because of its broad-range boiling point.

Aromatics. Except for the **D** matrix determinants, every set of index data distinguished between *ortho*, *meta*, and *para* dialkyl substituted benzenes and further discriminated between the extent of unsaturation in a two-carbon side chain on a benzene ring, displaying markedly different topological indices for its ethyl, ethenyl, and ethynyl derivatives. Regressions that compared boiling points and aromatic topological index data were disappointingly negative. Quantitative-structural comparisons of these aromatic compounds are not further referred to in succeeding descriptions of these experiments.

v·D Index (Table I, Column 4). Mihalić et al.⁶ defined the index as

$$\text{MTI}' = \sum_{i=1}^N e_i$$

where e_i ($i = 1, 2, \dots, N$) are elements of the row ($1 \times N$)

vector, and

$$\mathbf{v} \cdot \mathbf{D} = e_1, e_2, \dots, e_N$$

The $\mathbf{v} \cdot \mathbf{D}$ index is the consequence of summing the vector elements obtained by multiplying the valence vector by the distance matrix. Müller et al.¹⁶ have also described this MTI' index.

When the MTI' index values of all 16 linear monoalkenes listed in Table I were compared with the respective boiling points, a straight line was obtained which was described by the equation

$$\text{bp}/^\circ\text{C} = -230.53 + 135.55(\log \text{MTI}')$$

$$n = 16 \quad r^2 = 0.985 \quad s = 6.723 \quad F = 946$$

The same exercise, but restricted to only the linear monoalkenes with the unsaturated group in the terminal position, gave modest statistical improvement.

$$\text{bp}/^\circ\text{C} = -229.71 + 134.23(\log \text{MTI}')$$

$$n = 13 \quad r^2 = 0.992 \quad s = 5.514 \quad F = 1135$$

det|D| Index and Its Principal Eigenvalue ($\lambda_1(\mathbf{D})$) Index (Table I, Columns 5 and 6). As in prior studies,^{1,12} the determinant index was the most interesting and within the purview of this paper the least useful of all the invariant indices, with alkenes of the same carbon content possessing the same **D** determinant index. Observe, however, the atypical indices for compounds 3–6, and the influence of the triple bond (16–18) versus that of the double bond (13–15); comparison of these alkene data with earlier published determinant data¹² for alkanes showed fascinating contrasts. For example, although the alkenes and alkadienes of the same carbon atom content did not possess the same **D** determinants, all had the same **D** determinant indices as did the alkane isomers containing one and two more carbon atoms, respectively. By contrast, the alkynes displayed no obviously parallel relationships to the alkanes. The expression cited by Knop et al.¹⁷ for the determinant of any saturated tree graph

$$\det|\mathbf{D}| = -(-2)^{N-2}N - 1$$

wherein N was the number of vertices in the alkane graph, was partially adapted to the alkenes, but with N representing the total number of edges, plus one, in the alkene graph; plus two in the alkadiene graph. Unfortunately, the equation yielded only the absolute value of the determinant, with not necessarily the correct sign. Observe in Table I the different signs for the same absolute $\det|\mathbf{D}|$ values for compounds 6 and 8–12, for example. This circumstance was corrected with the insertion of a numbers-of-vertices recognition factor (-1^{N-1}) into a modified algorithm that then gave the determinant **D** index for all acyclic alkenes and alkadienes in Table I,

$$\det|\mathbf{D}| = (-1^{N-1})2^{E-1}E$$

where E and N are the numbers of edges and vertices in the linear alkene or diene. None of the other topological indices reported in this paper exhibited a relationship similar to the determinant link observed to exist between the alkenes and the alkanes. As also recorded earlier,^{1,12} these determinant values alternated from negative for graphs of even-numbered vertices to positive for graphs of odd-numbered vertices. As expected, all aromatic compounds, except the two charged aromatics (41, 43), had determinants of zero. No quantitative-structural comparisons were attempted with the determinant

indices of compounds listed in Table I. However, every principal eigenvalue listed in column 6 of Table I was unique, and regression experiments with indices versus boiling points of the unsaturates were, therefore, executed. All the linear monoalkenes gave the equation

$$\text{bp}/^{\circ}\text{C} = -172.67 + 208.57 \log(\lambda_1(\mathbf{D}))$$

$$n = 16 \quad r^2 = 0.986 \quad s = 6.699 \quad F = 953$$

and the linear, terminal alkenes under like circumstances gave virtually the same equation

$$\text{bp}/^{\circ}\text{C} = -172.22 + 206.63 \log(\lambda_1(\mathbf{D}))$$

$$n = 13 \quad r^2 = 0.991 \quad s = 5.879 \quad F = 1173$$

per(D) Index (Table I, Column 7). The data for column 7 were calculated as outlined in a prior article.¹⁴ Excluding compounds 5 and 6, all the permanent values were unique. A plot of the boiling points of the linear monoalkenes versus the corresponding permanent indices gave the equation

$$\text{bp}/^{\circ}\text{C} = -163.40 + 103.70[\log(\text{per}(\mathbf{D}))]^{1/2}$$

$$n = 16 \quad r^2 = 0.981 \quad s = 7.729 \quad F = 712$$

A similar plot for the linear, terminal monoalkenes showed no improvement in the equation

$$\text{bp}/^{\circ}\text{C} = -163.83 + 103.36[\log(\text{per}(\mathbf{D}))]^{1/2}$$

$$n = 13 \quad r^2 = 0.983 \quad s = 7.869 \quad F = 650$$

PRS(D) Index (Table I, Column 8). The product of the row sums (PRS) index is related to the permanent index of the distance matrix; both are described in a prior publication.¹⁴ When the boiling points were plotted against the PRS index values for the linear monoalkenes listed in Table I, the following equation resulted

$$\text{bp}/^{\circ}\text{C} = -167.01 + 89.27[\log(\text{PRS}(\mathbf{D}))]^{1/2}$$

$$n = 16 \quad r^2 = 0.991 \quad s = 5.296 \quad F = 1533$$

The linear, terminal monoalkenes gave almost the same equation

$$\text{bp}/^{\circ}\text{C} = -167.05 + 88.55[\log(\text{PRS}(\mathbf{D}))]^{1/2}$$

$$n = 13 \quad r^2 = 0.996 \quad s = 3.761 \quad F = 2882$$

shaf(D) and lhaf(D) Indices (Table I, Columns 9 and 10). The derivations and applications of the short and long hafnians were described in a prior work¹⁵ of this series; as earlier observed, the complicated character of the hafnian calculations limited this study to compounds possessing no more than eight carbon atoms. Except for compounds 5 and 6, the short hafnians were unique; the same pair of degenerate values, for compounds 5 and 6, was exhibited by the permanent indices listed in column 7. It was interesting to observe that the squares of the short hafnians of compounds 1 and 4–7 were equal to the permanent index values for the same substances. An earlier paper¹⁵ describing hafnian indices has also commented on this curious happenstance.

A study of the relationship of the boiling points and short hafnian indices for the linear monoalkenes gave the equation

$$\text{bp}/^{\circ}\text{C} = -178.90 + 154.81[\log(\text{shaf}(\mathbf{D}))]^{1/2}$$

$$n = 16 \quad r^2 = 0.982 \quad s = 7.512 \quad F = 755$$

and when extended to the linear, terminal monoalkenes, no statistical improvement was observed

$$\text{bp}/^{\circ}\text{C} = -178.16 + 153.43[\log(\text{shaf}(\mathbf{D}))]^{1/2}$$

$$n = 13 \quad r^2 = 0.985 \quad s = 7.54 \quad F = 712$$

All of the long hafnian values displayed in column 10 were unique, and the linear monoalkene indices, when plotted against their boiling points, gave the equation

$$\text{bp}/^{\circ}\text{C} = -183.11 + 127.65[\log(\text{lhaf}(\mathbf{D}))]^{1/2}$$

$$n = 16 \quad r^2 = 0.978 \quad s = 8.241 \quad F = 625$$

Under the same circumstances, the linear, terminal monoalkenes again gave approximately the same equation

$$\text{bp}/^{\circ}\text{C} = -184.26 + 128.15[\log(\text{lhaf}(\mathbf{D}))]^{1/2}$$

$$n = 13 \quad r^2 = 0.980 \quad s = 8.629 \quad F = 539$$

TOPOLOGICAL INDICES DERIVED FROM THE GRAPH-THEORETICAL ADJACENCY-PLUS-DISTANCE MATRICES

v(A + D) Index (Table I, Column 11). This earlier described¹¹ index is closely related to the v-D or MTI' index and was derived by multiplying the valence vector by the adjacency-plus-distance matrices and summing the consequent vector elements. This v(A + D) or MTI index has also been examined in detail by both Mihalić et al.⁶ and Müller et al.¹⁶ The MTI index series was entirely unique and possessed a numbers progression that implied a possible monotonic series of values, in effect paralleling the MTI' indices of column 4. Regression analysis for the boiling points versus these MTI values for the linear monoalkenes gave the equation

$$\text{bp}/^{\circ}\text{C} = -269.43 + 148.91(\log \text{MTI})$$

$$n = 16 \quad r^2 = 0.988 \quad s = 6.146 \quad F = 1135$$

and for the linear, terminal monoalkenes gave the slightly different equation

$$\text{bp}/^{\circ}\text{C} = -268.00 + 147.47(\log \text{MTI})$$

$$n = 13 \quad r^2 = 0.993 \quad s = 5.189 \quad F = 1509$$

det|A + D| Index and Its Principal Eigenvalue ($\lambda_1(\mathbf{A} + \mathbf{D})$) Index (Table I, Columns 12 and 13). All of these values were unique, in contrast to the above-described D determinant indices. As was true of the D determinant indices of column 5, the signs of the (A + D) determinant indices also varied from minus for substances containing an even number of carbon atoms to plus for graphs with an odd number of vertices. Unlike the D determinant indices described above, these (A + D) determinant indices were unique and displayed no obvious relationship to earlier published values for alkanes¹² and cycloalkanes.¹ Regression studies involving the linear alkenes' boiling points and the absolute values of the det|A + D| indices gave the equation

$$\text{bp}/^{\circ}\text{C} = -303.58 + 205.91[\log(\det|A + D|)]^{1/2}$$

$$n = 16 \quad r^2 = 0.989 \quad s = 5.789 \quad F = 1280$$

and the principal eigenvalues gave the equation

$$\text{bp}/^{\circ}\text{C} = -221.88 + 242.63[\log(\lambda_1(A + D))]$$

$$n = 16 \quad r^2 = 0.988 \quad s = 5.984 \quad F = 1197$$

CONCLUSIONS

Utilizing only the distance matrix, satisfactory representations of linear and cyclic unsaturated and aromatic hydrocarbons were attained. The edge counts of 2 or 3 for the various unsaturates adequately reflected the presence of double and triple bonds; valences were derived from the appropriate edge counts. The bonds of the aromatic hydrocarbons were assigned edge counts of 1.5; vertices, valences of 3. No problems were encountered in deriving the distance matrices of substances with the above edge and valence information, nor in operating upon the consequent matrices to obtain the desired invariant functions.

The addition of the adjacency matrix to the distance matrix was experimented with for three matrix functions—MTI, $\det|A + D|$, and $\lambda_1(A + D)$ indices. No obvious advantage seemed to accrue to the formulation of topological indices as a consequence of using the adjacency matrix as a hoped-for added source of graph information; the summing of the A and D matrices for the purpose of calculating any kind of a topological index was probably an operation of dubious utility.

None of the topological indices reported in this paper exhibited monotonicity within the totality of each of the series, but when quantitative-structural comparisons were restricted to similar sets of unsaturated hydrocarbons, reasonably acceptable regression results were obtained.

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