

Topological Organic Chemistry. 6.¹ Graph Theory and Molecular Topological Indices of Cycloalkanes

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Adjacency (A), distance (D), and degree (v) matrices of representative cycloalkanes were used to generate molecular topological indices derived from the graphs of the cycloalkanes. Invariant indices (descriptors) were derived from the following matrix operations: the sum of the elements of the product of the degree vector and the distance matrix; the sum of the elements of the product of the degree vector and the sum of the adjacency and distance matrices; the determinant of the distance matrix and its principal eigenvalue; the determinant of the sum of the adjacency and distance matrices and its principal eigenvalue; the permanent of the distance matrix; the product of the row sums of the distance matrix; the short and long hafnians of the distance matrix; and the *N*-iteration value of the adjacency matrix, where *N* equaled the number of vertices in the graph. One variant index (code) was calculated—the sum of the elements obtained by multiplying the degree and decimalized adjacency vectors.

INTRODUCTION

Graph theory offers the means to numerically characterize chemical structures. Balaban,² Randić,³ Hansen and Jurs,⁴ and Rouvray⁵ are among investigators who have reviewed methods for calculating molecular topological indices. This paper reports the extension to cycloalkanes of the earlier studies of this series which examined the utility of structure-descriptive matrices as sources of single-sum numbers reflective of linear alkane structures.

Preliminary to determining the various kinds of topological indices of representative cycloalkanes, the intricacy (complexity) number of each carbon atom in those various molecules of the two series of C₃–C₁₀ matching, unsubstituted alkanes and cycloalkanes was calculated. This was done to arrive at a prior assessment of the influence of the all-identical secondary carbon atoms in the unsubstituted cycloalkanes, of the extra edges in the graphs of given cycloalkanes, and of the lower edge counts, about half, for the vertices of distance matrices of cycloalkanes—all, as contrasted with the corresponding acyclic, unsubstituted alkanes.

This paper, then, reports the results of experiments which use the structure-descriptive adjacency (A), distance (D), and degree (v) matrices for deriving various topological indices of cycloalkanes. In succeeding portions of this study each one of the above indices is evaluated with reference to the uniqueness, single-sum character, monotonicity, and invariance of the function. Also, an attempt, only partially successful, was made to evaluate the quantitative–structural potential of each kind of function, using the boiling points of the cycloalkanes as a guide for such comparisons.

COMPUTATIONS

Molecular graphs, hydrogen-suppressed and with the interatomic carbon–carbon atom edge counts set at unity, were derived from the representative C₃–C₁₀ compounds listed

in the accompanying tables. Both the canonical CIP and IUPAC systems⁸ were used in all calculations, although all but the last one of the surveyed matrix functions were invariant. Reference is made to past papers^{1,6–9} of this series for each specific mode of computation for the various functions discussed in the succeeding portions of this presentation.

INTRICACY NUMBERS

The intricacy, or complexity, numbers of the vertices of a graph were earlier defined⁶ as the elements of the matrix products of the degree vector and the sums of the adjacency and distance matrices, compactly summarized by Mihalić et al.,¹⁰ as

$$v(A + D) = e_1, e_2, \dots, e_N$$

where e_1, e_2, \dots, e_N are the elements of the product row ($1 \times N$) vector. The desired data for Table I were acquired for the cycloalkanes in the course of computing the values of the $v(A + D)$ molecular topological indices of Table II.^{6,10}

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

The data for the corresponding alkanes were accessed at the time of preparing the first paper of this series.⁶

The data of Table I, assessing as they do the combined influence of valence, adjacency, and distance for each comparable set of vertices of alkane and cycloalkane, show marked differences in the complexity values for all the secondary vertices of the propane/cyclopropane and butane/cyclobutane pairs (100 and 50%, respectively, on basis of the lower of the contrasting sets of values), remembering that the lower is the element number, the more intricate or complex is the vertex. As the size of the ring increases beyond four vertices, the intricacy numbers of all the identical secondary cyclic vertices of a given cycloalkane increasingly approach the value of the central secondary vertex of the corresponding acyclic alkane.

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Table I. Intricacy (Complexity) Numbers^a of Vertices of Related C₃–C₁₀ Nonsubstituted Alkanes and Cycloalkanes

<i>N</i>	alkanes										cycloalkanes			
3					6		4		6					8
4				11		8		8		11				12
5			18		13		12		13		18			16
6			27		20		17		17		20		27	22
7		38		29		24		22		24		29		28
8		51		40		33		29		33		40		36
9		66		53		44		38		38		44		44
10	83		68		57		49		45		49		57	54

^a The lower the number, the more intricate or complex is the vertex.

By any system of indexing, therefore, one might expect greater deviations from any norm in those instances where the highly strained three- and four-membered rings are part of a series. Three- or four-unit straight chains attached to three- or four-vertex cycles might be expected to yield very anomalous index values.

CYCLOALKANE INDICES DERIVED FROM THE GRAPH-THEORETICAL DISTANCE MATRIX

Table II lists the limited sample of cycloalkane isomers studied in this paper. Quite especially, one short series of isomers, the five cyclopentane isomers, shows at a glance the relationships among the various index values. These stand in strong contrast to the various values for the 29 different cycloheptanes (omitting geometrical isomers from both series), so lengthy as to defy intuitive apprehension.

Many of the structures listed in Table II have apparently not yet been synthesized, for which, therefore, no boiling point data are listed. Boiling points for known geometrical isomers are recorded in the table, although the data are not germane to these described experiments because these adjacency and distance matrices convey only structural, not stereochemical, information.

v·D Index (Table II, Column 4). Mihalić et al.¹⁰ defined the index as

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

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

$$v \cdot D = e_1, e_2, \dots, e_N$$

That is, the value of the index is obtained by multiplying the valence vector by the distance matrix and summing the resulting vector elements.⁶ Müller et al.¹¹ have also described this MTI' index, as well as the succeeding MTI index, in detail.

Our results were disappointing, displaying 13 instances of replication and by inspection giving no evidence of monotonicity over the entire series. However, the values were invariant and single-sum. The unsubstituted cycloalkanes (1, 2, 4, 9, 10, 39–41) appeared to present a rational series of values, and when the cycloalkane boiling points were plotted against these MTI' index values, a straight line was obtained which was described by the equation

$$bp/^{\circ}C = -202.23 + 145.47[\log(v \cdot D)]$$

$$n = 8 \quad r^2 = 0.989 \quad s = 9.2 \quad F = 537$$

In addition to the above fit with unsubstituted cycloalkanes, both the unsubstituted and monosubstituted cycloalkanes for which boiling points were found were regressed against the

(v·D) indices. (The di- and trisubstituted cycloalkanes were not included because the consequent different diastereoisomers would be expected to possess different boiling points.) The combination of these two classes gave a slightly poorer fit than was obtained using only the unsubstituted cycloalkanes.

$$bp/^{\circ}C = -58.43 + 12.19(v \cdot D)^{1/2}$$

$$n = 16 \quad r^2 = 0.970 \quad s = 11.2 \quad F = 459$$

v(A + D) Index (Table II, Column 5). This index is closely related to the prior index and was derived by multiplying the valence vector by the sum of the adjacency and distance matrices and summing the resultant vector elements.⁶ The index has also been examined in detail by both Mihalić et al.¹⁰ and Müller et al.¹¹ for the linear alkanes themselves. Among the values obtained in this paper for the cycloalkanes there was no evidence of uniqueness (11 replications) or of monotonicity. But, values for the unsubstituted cycloalkanes appeared to present a monotonic series of values which, when plotted against the boiling points of the substances, gave a straight line described by the equation

$$bp/^{\circ}C = -277.50 + 173.07[\log(v(A + D))]$$

$$n = 8 \quad r^2 = 0.997 \quad s = 5.1 \quad F = 1789$$

det|D| Index and Its Principal Eigenvalue ($\lambda_1(D)$) Index (Table II, Columns 6 and 7). These indices, the determinant of the distance matrix and its principal eigenvalue, were both examined in earlier publications.^{7,10} The values, invariant and single-sum, but not at all unique, were surprising nonetheless. All the even-numbered, nonsubstituted cycloalkanes possessed determinants of 0, as did the few examples of monomethyl-substituted cycloalkanes listed in column 6. Moreover, Table II displays the identical determinants for all isomeric structures possessing the same cycle, regardless of substitution! Thus, the numerous isomers of cycloheptane exhibit among the 29 substances only 4 different determinant values: 0 (9×), 12 (1×), 44 (4×), and 128 (15×). Knop et al.¹² commented on an interesting parallelism observed in the determinants of the distance matrices of the acyclic alkanes. In spite of the total lack of uniqueness observed in the determinants of the limited samples of cycloalkanes listed, all the corresponding principal eigenvalues were different, although several only slightly so; all eigenvalues were single-sum and invariant. Of the two complete isomer series listed in columns 6 and 7 of Table II, neither that of the short series, cyclopentanes, nor of the long series, cycloheptanes, appeared to be monotonic.

The determinants of the nonsubstituted cycloalkanes, when plotted against the corresponding boiling points, appeared to give a reasonable curve for the unsubstituted cycloalkanes with an odd number of carbon atoms. However, since the

Table II. Topological Indices Derived from the Distance and Adjacency Matrices of Representative C₃-C₁₀ Cycloalkanes

no.	compound	bp, °C (cis/trans)	vD	v(A + D)	del[D]	$\lambda_1(D)$	del[A + D]	$\lambda_1(A + D)$	per(D)	PRS(D)	shaf(D)	lhaf(D)	N - A ₂ iterations	vA _{in}
1	cyclopropane	-32.9	12	24	2	2	16	4	2	8	3	3	54	28
2	cyclobutane	13.1	32	48	0	4	-48	6	36	256	6	18	216	60
3	methylcyclopropane	0.7	30	48	-7	4.09965	-48	-48	25	240	5	9	260	73
4	cyclopentane	49.2	60	80	6	6	128	8	366	7 776	35	105	810	124
5	methylcyclobutane	37.2	61	83	0	6.53812	144	8.42443	432	10 080	38	126	984	151
6	ethylcyclopropane	36.2	64	86	20	7.00861	176	8.85835	516	13 230	42	156	1 044	166
7	1,1-dimethylcyclopropane	21	54	80	20	6.17644	128	8	268	7 056	32	78	1 322	180
8	1,2-dimethylcyclopropane	(37.2/28.2)	58	82	20	6.63752	144	8.42443	360	9 600	36	102	1 222	177
9	cyclohexane	80.7	108	132	0	9	-297	11	10 772	531 441	98	1286	2 916	252
10	cycloheptane	119	168	196	12	12	686	14	270 128	35 831 808	889	12803	10 206	508
11	methylcyclohexane	100.9	163	193	0	12.1704	756	14.0747	237 360	33 976 800	848	11520	12 576	519
12	ethylcyclopentane	103.5	164	194	44	12.6468	1408	14.4909	224 812	37 544 364	842	9768	13 643	682
13	1,1-dimethylcyclopentane	87.9	146	180	44	11.3866	1024	13.2111	122 236	19 468 800	644	5394	17 370	732
14	1,2-dimethylcyclopentane	(99.6/91.9)	150	182	44	11.7171	1120	13.5217	144 180	23 051 952	690	6288	15 724	721
15	1,3-dimethylcyclopentane	(90.8/91.6)	154	186	44	12.0465	1152	13.8580	170 428	27 225 000	742	7620	15 308	645
16	propylcyclobutane	183	213	0	14.1904	1924	16.0286	14.7469	459 648	79 119 040	1160	20680	13 906	688
17	isopropylcyclobutane	91	165	197	0	12.9508	1536	14.7469	264 032	43 740 000	908	11 944	16 192	753
18	1-ethyl-1-methylcyclobutane	(-/90.1)	155	189	0	12.4160	1392	14.1816	176 320	31 006 976	764	7 512	19 254	802
19	1-ethyl-2-methylcyclobutane	(91.0/88.0)	163	195	0	13.0163	1536	14.7778	249 184	42 962 400	884	10 856	17 160	784
20	1-ethyl-3-methylcyclobutane		171	203	0	13.6775	1524	15.4533	332 400	57 760 560	1004	15 040	15 819	712
21	1,1,2-trimethylcyclobutane		145	181	0	11.7666	1104	13.5020	135 168	22 486 464	676	5 976	21 892	835
22	1,1,3-trimethylcyclobutane		153	189	0	12.4397	1104	14.1876	185 152	31 046 400	776	8 544	20 996	739
23	1,2,3-trimethylcyclobutane		153	187	0	12.4227	1176	14.1497	186 576	31 185 000	776	8 384	19 792	805
24	1-cyclopropylbutane	99.5	196	226	128	15.0565	2372	16.9205	737 080	121 651 200	1422	33 910	14 085	688
25	2-cyclopropylbutane	91	168	200	128	13.2932	1872	15.0731	296 072	50 379 840	954	12 814	17 272	784
26	1-cyclopropyl-2-methylpropane		178	210	128	13.8216	1920	15.6472	438 256	69 696 000	1130	20 454	15 758	709
27	2-cyclopropyl-2-methylpropane		150	186	128	12.0449	1344	13.8023	161 440	26 733 096	732	7 080	21 282	788
28	1-methyl-1-propylcyclopropane		166	200	128	13.3272	1728	15.0970	279 456	49 827 960	938	12 390	20 200	806
29	1-isopropyl-1-methylcyclopropane	82.1	148	184	128	12.0830	1344	13.8023	155 016	26 417 664	722	6 866	23 323	973
30	2-methyl-1-propylcyclopropane	(96.6/88.9)	178	210	128	14.2596	1924	16.0286	436 328	77 597 520	1140	19 960	18 030	796
31	1-isopropyl-2-methylcyclopropane		160	194	128	13.0259	1536	14.7469	249 744	42 768 000	890	11 458	20 574	861
32	1,1-diethylcyclopropane	88.7	156	190	128	12.7798	1680	14.4942	192 600	35 684 352	798	7 974	21 718	866
33	1,2-diethylcyclopropane	(93.5/86.5)	172	204	128	14.0230	1900	15.7528	351 248	65 707 200	1038	15 150	19 040	722
34	1-ethyl-1,2-dimethylcyclopropane		150	186	128	12.4928	1392	14.1816	163 432	30 201 600	744	6 960	24 954	912
35	1-ethyl-2,2-dimethylcyclopropane		154	190	128	12.7902	1408	14.4909	193 136	35 625 744	800	8 364	24 374	874
36	1-ethyl-2,3-dimethylcyclopropane		158	192	128	13.1335	1584	14.8176	219 592	41 310 000	846	9 198	22 742	798
37	1,1,2,2-tetramethylcyclopropane		136	176	128	11.5453	1024	13.2111	102 872	18 279 040	606	4 434	30 744	956
38	1,1,2,3-tetramethylcyclopropane	75.9	140	178	128	11.8954	1152	13.544	117 016	21 464 352	642	4 878	30 078	953
39	cyclooctane	(-/77.6)	150	256	0	16.000	0	18.000	12 979 264	4294 967 296	3192	264 250	34 992	1020
		171	360	396	20	20.000	88	22.000	587 828 900	512 × 10 ⁹			118 098	2044
40	cyclodecane	201	500	540	0	25.000	-29236	27.000	42 795 063 000	95 367 × 10 ⁹			393 660	4092

compounds with even-numbered carbon atoms possessed a value of 0, no equation was calculated.

But, the same exercise utilizing the principal eigenvalues,⁷ which were unique, gave a reasonable fit with the equation

$$\text{bp}/^{\circ}\text{C} = -115.81 + 65.02[\lambda_1(\text{D})]^{1/2}$$

$$n = 8 \quad r^2 = 0.993 \quad s = 7.4 \quad F = 837$$

det|A + D| Index and Its Principal Eigenvalue ($\lambda_1(\text{A} + \text{D})$) (Table II, Columns 8 and 9). These values, allied to the above topic, also extended earlier studies^{7,10} of this subject. The determinants of the adjacency-plus-distance matrices replicate repeatedly, as is seen for the five cyclopentane isomers, for which are recorded only three different figures: 128 (2×), 144 (2×), and 176 (1×). Again, these values appear to lack monotonicity within the series, as is also observed with the principal eigenvalues. The more extended series, the 29 cycloheptane isomer values, likewise lacks uniqueness, as do the corresponding principal eigenvalues, the latter to not quite the same extent, however. For example, although compounds **12** and **35** have the same determinants (1408) and the same principal eigenvalues (14.4909), comparison shows there are fewer instances of such replications (8) in the list of eigenvalues than in the corresponding determinants (17 replications). Although both series appear to be single-sum and invariant, both series lack monotonic character. A plot of the determinants versus the boiling points for the unsubstituted cycloalkanes gave a poor fit due in part to disparate values for compounds **39** and **40**. However, a similar comparison for the principal eigenvalues gave a good fit to the equation

$$\text{bp}/^{\circ}\text{C} = -205.68 + 281.95[\log(\lambda_1(\text{A} + \text{D}))]$$

$$n = 8 \quad r^2 = 0.998 \quad s = 3.7 \quad F = 3424$$

per(D) Index (Table II, Column 10). The data for the permanent of the distance matrices were calculated as described in a previous paper⁹ of this series. All of the permanents were unique, invariant, and single-sum, but inspection of the five values listed for the isomers of cyclopentane indicated that the series lacked monotonicity, a circumstance that appeared to extend to the numerous cycloheptane isomers also. But again, as in the prior instances described above, the parent cycloalkanes themselves present a rational series of values when permanents are plotted against boiling points, giving the equation

$$\text{bp}/^{\circ}\text{C} = -89.90 + 88.44[\log(\text{per}(\text{D}))]^{1/2}$$

$$n = 8 \quad r^2 = 0.995 \quad s = 5.9 \quad F = 1294$$

All compounds of non- and monosubstituted cycloalkanes were also regressed. Again, as with the ($\nu\text{-D}$) index values, this combined regression gave a slightly inferior fit as compared to the fit when only unsubstituted cycloalkanes were used, as pictured in the equation

$$\text{bp}/^{\circ}\text{C} = -22.27 + 22.34[\log(\text{per}(\text{D}))]$$

$$n = 16 \quad r^2 = 0.969 \quad s = 11.4 \quad F = 445$$

PRS(D) Index (Table II, Column 11). This function, related to the permanents, is the product of the row sums of the distance matrix and is also described in the above citation.⁹ Like the permanents, these products of the row sums were found to be

invariant, unique within the limited sample shown in Table II, and single-sum but lacking in monotonicity through the two complete series of values for the cyclopentane and cycloheptane isomers. The PRS values of the unsubstituted parent cycloalkanes gave a straight line when plotted against the boiling points, fulfilling the equation

$$\text{bp}/^{\circ}\text{C} = -116.57 + 84.69[\log(\text{PRS}(\text{D}))]^{1/2}$$

$$n = 8 \quad r^2 = 0.998 \quad s = 3.4 \quad F = 3865$$

shaf(D) and lhaf(D) Indices (Table II, Columns 12 and 13). The modes of derivation for the short and long hafnians of the distance matrix were outlined in an earlier paper¹ of this series; the involved nature of the calculations limited this study to cyclic graphs of no larger than eight vertices. Both functions were found to be invariant, single-sum, and unique, except for the short hafnians (776) of compounds **22** and **23**, but the two series were not monotonic. A plot of the boiling points versus the short hafnians of the distance matrices of the unsubstituted cycloalkanes, C₃–C₈, gave a fairly straight line conforming to the equation

$$\text{bp}/^{\circ}\text{C} = -41.86 + 56.06[\log(\text{shaf}(\text{D}))]$$

$$n = 6 \quad r^2 = 0.973 \quad s = 12.5 \quad F = 142$$

Similarly the long hafnians gave the equation

$$\text{bp}/^{\circ}\text{C} = -35.81 + 36.24[\log(\text{lhaf}(\text{D}))]$$

$$n = 6 \quad r^2 = 0.977 \quad s = 11.4 \quad F = 172$$

Combination of the non- and monosubstituted cycloalkane long hafnians versus boiling points gave a plot conforming to the equation

$$\text{bp}/^{\circ}\text{C} = -32.59 + 32.90[\log(\text{lhaf}(\text{D}))]$$

$$n = 14 \quad r^2 = 0.956 \quad s = 11.4 \quad F = 172$$

CYCLOALKANE INDICES DERIVED FROM THE GRAPH-THEORETICAL ADJACENCY MATRIX

N – A₂ Iterations Index (Table II, Column 14). This invariant technique for deriving a molecular index is described in the third paper⁸ of this series. As the data demonstrate, the *N*-iteration values of the adjacency matrix (where *N* is the number of vertices in the graph) are not only invariant but also unique and single-sum and appear to constitute a monotonic series of values, the only such values to do so in this study of cycloalkane molecular topological indices. The cyclopentane isomer series indicates that the parent isomer has the lowest iteration figure (810), with values increasing (by this mode of measurement) to the most intricate isomer, 1,1-dimethylcyclopropane, with an *N*-iteration value of 1322. The order of increasing complexity—**4**, **5**, **6**, **8**, and **7**—is intuitively reasonable. And of the cycloheptane isomers, cycloheptane (**10**, 10 206), as the least complex isomer, and 1,1,2,2-tetramethylcyclopropane (**37**, 30 744), as the most intricate isomer, define the limits of what is also an intuitively acceptable series.

An attempt to establish linearity between the known boiling points and the iteration numbers of the cyclopentane and cycloheptane series of isomers failed. However, a study of the relationship of boiling points and iteration numbers for

the nonsubstituted cycloalkanes gave a straight line represented by the equation

$$\text{bp}/^{\circ}\text{C} = -128.62 + 60.12[\log(N - A_2)]$$

$$n = 8 \quad r^2 = 0.995 \quad s = 6.2 \quad F = 1200$$

$v \cdot A_{10}$ Index (Table II, Column 15). This variant, single-sum index, the sum of the elements of the product of the valency vector and the decimalized adjacency matrix, also treated in the third paper⁸ of this series, was included in this study because of the fixed ratio of change observed between values for the nonsubstituted parent cycloalkanes, a ratio wherein each subsequent $v \cdot A_{10}$ index value was $2n + 4$ units greater than the immediately preceding value for a nonsubstituted cycloalkane, when the vertices of the cyclic graph were numbered according to the canonical CIP system.⁸ This circumstance presented the capacity to quantify the degree of intricacy, or complexity, of the substances reported in this paper. It is interesting to note that the $v \cdot A_{10}$ indices of all the nonsubstituted cycloalkanes were, in fact, invariant, a circumstance not true of the substituted cycloalkanes, except for a few simple substances for which the vertex numbers were the same for both the CIP and IUPAC systems of numbering: 1, 3, 5-7, 28-33, and 35-37.

The series appeared to be monotonic, with two sets of duplicate index values (688 for compounds 16 and 24; 784 for compounds 19 and 25), implying that, of the two pairs of compounds propylcyclopropane/1-cyclopropylbutane and 1-ethyl-2-methylcyclobutane/2-cyclopropylbutane, each set of pairs has the same complexity.

Comparisons were made between compounds of different carbon atom content. For example, the ratio of cyclopentane (4, 124) to 1,1-dimethylcyclopropane (7, 180), $124/180 = 0.689$, is about the same as the ratio of cycloheptane (10, 508) to 1,1-dimethylcyclopentane (13, 732), $508/732 = 0.693$, and to 1,1,3-trimethylcyclobutane (22, 739), $508/739 = 0.687$. On the basis of this premise, the conclusion is justified that compounds 7, 13, and 22 are of about the same complexity.

The data appear to be monotonic through the series, for by these standards the increasing order of complexity of the cyclopentane isomers is 4, 5, 6, 8, and 7, the same order as was observed when the N -iteration values of the binary adjacency matrices were used to the same end. And among the 29 cycloheptane isomers, cycloheptane (10, 508) is the least intricate, with 1-isopropyl-1-methylcyclopropane (29, 973) the most complex isomer, followed closely by compounds 37 and 38: again, an intuitively reasonable order of intricacy.

As with the other sets of experiments, boiling point correlations were only positive in the instances of the parent cycloalkane isomers. A straight line relationship with the equation

$$\text{bp}/^{\circ}\text{C} = -178.65 + 107.10[\log(v \cdot A_{10})]$$

$$n = 8 \quad r^2 = 0.994 \quad s = 6.9 \quad F = 966$$

resulted when boiling points and $v \cdot A_{10}$ indices were contrasted.

CONCLUSIONS

Earlier studies of this series which examined the utility of structure-descriptive matrices as sources of single-sum numbers reflective of alkane structures were extended with indifferent results to cycloalkane compounds. Using the distance matrices, only the permanent, product of row sums, and long hafnian functions were found to be invariant, unique, and single-sum. None of the above matrix functions reflected monotonic character within the totality of the various series, however.

And when the adjacency matrix was used as a source of topological indices, only the N -iterations function was observed to offer all four qualities of invariancy, uniqueness, monotonicity, and single-sum character.

Results of quantitative-structural physical property relationship studies were likewise disappointing, for in all instances that were examined only the nonsubstituted parent cycloalkanes were amenable to the establishment of boiling point-topological index correlations.

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