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Computing the Permanent of the Adjacency Matrix for Fullerenes

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Computing the Permanent of the Adjacency Matrix for Fullerenes[#]

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Abstract

Motivation. Novel carbon allotropes, with finite molecular structure, including spherical fullerenes are nowadays currently produced and investigated. These compounds have beautiful architectures and show unusual properties that are very promising for the development of nanotechnologies. The Kekulé structure count and permanent of the adjacency matrix are computed for these molecules.

Method. A method for computation of the permanent of the adjacency matrix is herein optimized for fullerenes. The method finds exact values for permanents of adjacency matrices up to 60×60.

Results. The results provide linear and non–linear correlations between different structural parameters involving the presence of contiguous pentagons, $\ln[\mathrm{per}(\mathbf{A})]/\ln K$, $\ln K$ and $\ln[\mathrm{per}(\mathbf{A})]$.

Conclusions. A method for computing the permanent of the adjacency matrix is optimized for fullerenes. As $\ln[\mathrm{per}(\mathbf{A})]/\ln K$ can be related with thermodynamic stability, this aspect of chemistry could be useful for designing or predicting unknown fullerenes and their structure. The non–linear correlation for $\ln[\mathrm{per}(\mathbf{A})]/\ln K$ is improved. The variance decreases 49% and the risk of co–linearity diminishes.

Availability. The software programs are available on request from the author (Francisco.Torrens@uv.es) and are free for academics.

Keywords. Kekulé structure count; permanent of a matrix; adjacency matrix; graph theory; fullerene.

1 INTRODUCTION

Much chemical graph–theory work revolved around the adjacency matrices of the compounds under investigation. Many studies involving the determinants, characteristic polynomials and eigenvalues were published [1]. With the last few years dramatic improvements in computer power, the previously unapproachable matching polynomials have come under scrutiny [2]. Still relatively neglected because of their computational inaccessibility, however, are the permanents of these matrices [3]. The determinant of the 3×3 matrix [*a b c, d e f, g h i*] is *aei – ahf – dbi + dhc + gbf –*

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gec. This computation is far too cumbersome for larger matrices, and many shortcuts are available. The permanent of this matrix is the sum of the same six terms. Thus, computing the permanent of an $n \times n$ matrix involves adding $n!$ terms, each of which is the product of n matrix elements. Since $20! \approx 2.4 \cdot 10^{18}$, computing the permanent of any matrix of reasonable size by brute force is out of the question. There are some approximate methods, but computer time tends to increase with the quality of the approximation.

Cash published an algorithm that brings permanents of sparse matrices such as adjacency matrices within the reach of a desktop computer [4–6]. This algorithm takes advantage of the facts that zero times anything is zero, that the elements of an adjacency matrix are mostly zeroes, and that the non–zero elements are all ones. Acting on this basis, the algorithm counts the non–zero terms in the summation and provides an exact answer for the permanent. The time required for this computation is highly dependent on the number of non–zero elements in the matrix. Thus, of all polycyclic aromatic hydrocarbons (PAH), fullerenes take the longest because their adjacency matrices have $3n$ non–zero elements, the maximum number possible. For example, computing the permanent of a C_{44} fullerene took approximately 150 times as long as the computation for a $C_{44}H_{22}$ PAH on the same machine. There is, however, no straightforward relationship between matrix size, number of non–zero matrix elements and computation time. Computation times for distinct fullerenes of the same size can easily differ by a factor of two.

Cash computed the permanents of the adjacency matrices for representative smaller fullerenes and determined whether this parameter has any obvious use in quantitative structure–property relationships [7]. For all–polyhex hydrocarbons, the permanent is equal to the square of the Kekulé structure count, K, but this is not the case for fullerenes. In any instance, K for fullerenes is easily computed by the signed adjacency matrix method invented by Kasteleyn [8,9] and illustrated by Klein and Liu [10] and this method was used by Cash to determine K. He examined the relationships between structural parameters for 28 fullerenes and per(**A**). In particular, he related the examined structural parameters to the adjoining of pentagons [11–13]. Cash introduced a new parameter, r, which counts contiguous pentagon triplets that have no single vertex in common. The quantity well correlated with structure was not per(**A**) itself, but $\ln[\text{per}(\textbf{A})]/\ln K$. For all 28 fullerenes, $\ln[\text{per}(\textbf{A})]/\ln K > 2$, contrary to expectations.

Diudea *et al*. devised a novel way in constructing toroidal fullerenes from square tiled tori [14]. Aihara and Hirama concluded that anti–aromatic species are scarcely formed in interstellar space [15]. Aihara studied the spherical aromaticity in charged fullerenes and the $2(N+1)^2$ rule [16]. Ivanciuc *et al*. presented a qualitative resonance–theoretic view for the description of a variety of conjugated π–network species identified with subgraphs of the graphite network [17].

In a previous paper, Cash's program for computing the permanent of adjacency matrices was applied to alternant hydrocarbons [18]. This paper uses our version of this program, which finds

exact values for permanents of sparse matrices, with examples of chemical adjacency matrices up to 60×60. Section 2 presents the computer algorithm. In Section 3, the calculation results for fullerenes are discussed. Section 4 summarizes the conclusions.

2 COMPUTER ALGORITHM

For an adjacency matrix, the permanent computation reduces to finding the number of different products of matrix elements A_{i1}, A_{j2}, A_{k3}… such that the elements are all equal to one and the first subscripts are all different, *i.e.*, no two elements are in the same row. For each such combination that exists, the permanent increases by 1.

Cash reported a computer algorithm that finds these combinations [4–6]. This algorithm first examines all A_{i1} until it finds an $A_{i1} = 1$. Then, after storing the active i, it examines all A_{j2} until it finds an $A_{j2} = 1$. Next, it checks to see that $i \neq j$. If $i = j$, it proceeds to the next $A_{j2} = 1$; if not, it begins searching for an $A_{k3} = 1$, keeping track of the active i and j so it can verify that $i \neq k$ and $j \neq k$. Whenever the tree thus grown reaches all the way to the last column in the matrix, the algorithm increments a counter. If the non–zero elements were other than one, it could compute a product and update a running total. The key to examining all possible combinations in a reasonable number of CPU cycles is timely pruning of the tree. Once the algorithm finds an $A_{i1} = 0$, it never examines another tree beginning with that A_{i1}. Similarly, if $A_{i1} = 1$ but $A_{j2} = 0$, it never examines another tree beginning with that A_{i1}, A_{j2}. Thus, the tree with n! potential branches is quickly pruned to a manageable size.

The only restriction in the method is that all the vertices should be divalent or trivalent. Thus, the method can be applied to tori. For instance, it has been applied to toroidal polyhex [5] and double–toroid, almost polyhex fulerenes [19]. Cash reported implementations of the algorithm in the C and Fortran 77 programming languages. In this work, a version of this algorithm has been optimised for Fortran 77. The program is available from the author (Francisco.Torrens@uv.es).

3 RESULTS AND DISCUSSION

One might intuitively assign the greater stability to the more symmetrical fullerene structures. However, neither $\ln K$ nor $\ln[\text{per}(\mathbf{A})]$ values support this idea, but, as discussed in some detail by Klein *et al*. $\ln K$ is not necessarily a reliable predictor of stability for fullerenes, as it is for all–polyhex systems [20]. In seeking possible quantitative structure–property relationship parameters, it became obvious that the ratio $\ln[\text{per}(\mathbf{A})]/\ln K$ for these fullerenes was almost constant, but not quite, ranging in value from 2.0199 for C_{20}, the unique smallest fullerene, to 2.2034 for a C_{30} structure with C_{2v} symmetry. The values for K, per($\mathbf{A}$) and $\ln[\text{per}(\mathbf{A})]/\ln K$, along with values for the structural parameters involving the presence of contiguous pentagons, are listed in Table 1. It was

stated that $per(A) = K^2$ (and thus $\ln[per(A)]/\ln K = 2$) generally for conjugated systems [21,22]. However, $per(A)$ was not equal to K^2 for any of the compounds studied in this paper. Indeed, $per(A)$ was generally not the square of any integer. At the present time, the general relationships among structure, $per(A)$ and K are unclear at best, at least for non–alternants.

Table 1. Values of Kekulé Structure Count for Fullerenes

| Fullerene	K	$per(A)$	$\ln[per(A)]/\ln K$	p	q	r
C_{20} (I_h)	36	1392	2.0199	30	20	30
C_{24} (D_{6d})	54	4692	2.1192	24	12	36
C_{26} (D_{3h})	63	8553	2.1853	21	8	30
C_{28} (T_d)	75	15705	2.2378	18	4	24
C_{28} (D_2)	90	16196	2.1540	20	8	24
C_{30} (C_{2v})	107	29621	2.2034	17	4	20
C_{30} (C_{2v})	117	30053	2.1651	18	6	20
C_{30} (D_{5h})	151	31945	2.0672	20	10	20
C_{32} (D_3)	144	55140	2.1968	15	2	18
C_{32} (C_2)	151	55705	2.1780	16	4	16
C_{32} (C_2)	168	57092	2.1375	17	6	16
C_{32} (D_2)	184	58384	2.1045	18	8	15
C_{34} (C_{3v})	195	103665	2.1902	15	3	15
C_{34} (C_s)	196	104484	2.1896	15	3	16
C_{34} (C_2)	204	103544	2.1714	14	2	14
C_{34} (C_2)	212	107720	2.1632	17	6	16
C_{36} (D_{6h})	272	192528	2.1706	12	0	12
C_{36} (D_{2d})	288	192720	2.1489	12	0	12
C_{36} (C_{2v})	312	197340	2.1231	13	2	10
C_{36} (D_{3h})	364	207924	2.0764	15	6	6
C_{38} (C_{2v})	360	366820	2.1768	14	2	14
C_{38} (C_{3v})	378	363300	2.1572	12	1	9
C_{38} (D_{3h})	456	411768	2.1116	18	8	18
C_{40} (D_{5d})	562	515781	2.0775	10	0	10
C_{40} (T_d)	576	704640	2.1185	12	4	0
C_{40} (D_{5d})	701	803177	2.0750	20	10	20
C_{44} (T)	864	2478744	2.1775	12	4	0
C_{44} (D_{3h})	960	2436480	2.1416	9	2	0
C_{60} (I_h)	12500	395974320	2.0986	0	0	0

| p | q | r |
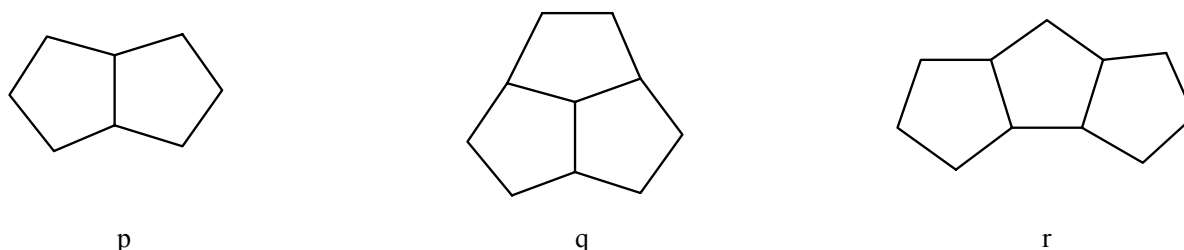
Figure 1. Substructures that contribute to the *p*, *q* and *r* counts.

The structural features involving adjacent pentagons are encoded by the *p*, *q* and *r* parameters as illustrated in Figure 1. The *p* and *q* parameters were introduced by Liu *et al*. for classifying fullerenes [23]. These enumerate, respectively, the number of edges common to two pentagons and the number of vertices common to three pentagons. The *r* parameter was introduced by Cash [7]. This parameter enumerates the number of pairs of non–adjacent pentagon edges shared with two

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other pentagons, *i.e.*, the number of ways of choosing from the structure three contiguous pentagons that do not share a common vertex. Thus, q and r complement each other by counting both possible arrangements of three contiguous pentagons.

Cash selected a group of 27 fullerenes (included in Table 1) to correlate $\ln[\text{per}(\mathbf{A})]/\ln K$, $\ln K$ and $\ln[\text{per}(\mathbf{A})]$ with the structural parameters p, q and r. After removing the outliers, he obtained the following fits with 25 points (Equation 1) or 27 points (Equations 2 and 3).

$$\ln[\text{per}(\mathbf{A})]/\ln K = 1.6895 + (0.0430\pm0.0039)p - (0.0402\pm0.0028)q - (0.0028\pm0.0008)r$$
$$n = 25 \qquad R = 0.962 \qquad s = 0.015 \tag{1}$$

$$\ln K = 9.3422 - (0.2946\pm0.0773)p + (0.2224\pm0.0511)q - (0.0210\pm0.0178)r$$
$$n = 27 \qquad R = 0.904 \qquad s = 0.368 \tag{2}$$

$$\ln[\text{per}(\mathbf{A})] = 18.8884 - (0.5183\pm0.1572)p + (0.3482\pm0.1039)q - (0.0482\pm0.0361)r$$
$$n = 27 \qquad R = 0.909 \qquad s = 0.748 \tag{3}$$

Despite the good results obtained by Cash, three important remarks should be made. First, the parameters p, q and r include some redundant information. There is a close relationship between each pair p–q and p–r. For instance, the minimum structure with $q = 1$ (Figure 1, q) needs $p = 3$, and the minimum structure with $r = 1$ (Figure 1, r) requires $p = 2$. Second, the error of some parameters is large, *e.g.*, the relative error of r is 85% in Equation (2) and 75% in Equation (3). Third, non–linear effects of p, q and r could affect $\ln[\text{per}(\mathbf{A})]/\ln K$, $\ln K$ or $\ln[\text{per}(\mathbf{A})]$.

Therefore, a different strategy has been assayed in this paper: (*a*) smaller superpositions of the p–q and p–r pairs are sought, (*b*) not all the three structural parameters are necessarily retained in the fits, and (*c*) non–linear correlations are allowed.

The best linear correlation of $\ln[\text{per}(\mathbf{A})]/\ln K$ with the structural parameters is:

$$\ln[\text{per}(\mathbf{A})]/\ln K = 2.14 - 0.0108q + 0.00364r$$
$$n = 29 \qquad R = 0.721 \qquad s = 0.036 \qquad F = 14.1 \tag{4}$$

The mean absolute percentage error (MAPE) is 1.21% and the approximation error variance (AEV) is 0.4803. All other models with greater MAPE and AEV have been discarded. Notice that there are several fullerenes with the same set of p, q and r parameters. If the different repetitions of $\ln[\text{per}(\mathbf{A})]/\ln K$ are substituted by their mean, a maximum correlation coefficient of 0.757 is obtained. Therefore, Equation (4) with $R = 0.721$ explains 95% of the correlation coefficient of the means. On the other hand, the best non–linear correlation of $\ln[\text{per}(\mathbf{A})]/\ln K$ with the structural parameters results:

$$\ln[\text{per}(\mathbf{A})]/\ln K = 2.13 + 0.0515z_{41}$$
$$z_{41} = 0.225z_{31} + 1.20z_{32}$$
$$z_{31} = -1.16 + 0.232q$$
$$z_{32} = 1.05z_{22} - 0.875z_{21}z_{22}$$
$$z_{21} = 1.22 - 0.0983r + 0.00277qr$$
$$z_{22} = -0.726z_{11} - 0.921z_{12} \tag{5}$$

$$z_{11} = -1.16 + 0.232q$$
$$z_{12} = 1.22 - 0.0983r + 0.00277qr$$
$$\text{MAPE} = 0.87\% \qquad \text{AEV} = 0.2432$$

and AEV decreases 49%. Due to the complexity of Equation (5), a Fortran program has been written to calculate $\ln[\text{per}(\mathbf{A})]/\ln K$.

For $\ln K$ alone, the best linear correlation for these parameters is

$$\ln K = 9.68 - 0.337p + 0.220q$$

n = 29 $R = 0.949$ $\qquad s = 0.366 \qquad F = 117.5 \qquad$ MAPE = 3.87% $\qquad$ AEV = 0.0996 $\qquad$ (6)

Equation (6) explains 97% of the correlation coefficient of the means (0.976). On the other hand, the best non–linear correlation results are obtained with:

$$\ln K = 9.57 - 0.339p + 0.324q - 0.00379pq$$
$$\text{MAPE} = 4.00\% \qquad \text{AEV} = 0.0896$$

(7)

and AEV decreases 10% with respect to the linear fit.

For $\ln[\text{per}(\mathbf{A})]$ alone, the best linear correlation is

$$\ln[\text{per}(\mathbf{A})] = 20.2 - 0.660p + 0.383q$$

$n = 29$ $R = 0.949$ $\qquad s = 0.757 \qquad F = 118.5 \qquad$ MAPE = 4.05% $\qquad$ AEV = 0.0988 $\qquad$ (8)

Equation (8) explains 97% of the correlation coefficient of the means (0.977). On the other hand, the best non–linear correlation results are obtained with:

$$\ln[\text{per}(\mathbf{A})] = 20.0 - 0.666p + 0.616q - 0.00850pq$$
$$\text{MAPE} = 3.91\% \qquad \text{AEV} = 0.0871$$

(9)

and AEV decreases 12% with respect to the linear fit.

The signs and magnitudes of the coefficients in Equations (1)–(9) are of some interest. One would intuitively expect that, for some property determined in part by the presence of abutting pentagons (Figure 1, *p)*, an arrangement such as Figure 1, *q* would make less of a contribution than would three isolated *p*–type pairs of pentagons. If this is true, then the sign of the *q* coefficient would be opposite that of the *p* coefficient, as is the case in Equations (1)–(3) and (6)–(9). By the same type of argument, one would expect the sign of the *r* coefficient to be opposite that of *p*, as is the case in Equation (1). One also would expect the magnitude of the *r* coefficient to be smaller than that of the *q* coefficient on the assumption that an *r*–type cluster is intermediate in properties between a *q*–type cluster and two isolated *p*–type pairs, as is the case in Equations (1)–(5). Indeed, Kroto proposed a similar ordering [13].

When comparing Equations (4)–(9) with (1)–(3), smaller superpositions of the *p–q* and *p–r* pairs are observed in Equations (4)–(9). This diminishes the risk of co–linearity [24] in the fits given the close relationship between each pair *p–q* and *p–r*.

The estimation of properties has been carried out from the fits for two fullerenes out of the

calibration domain. Isolated–pentagon fullerenes *(p = q = r = 0)* have been selected because of the following reasons: (1) Maximal thermodynamic stability is expected for these isomers [25]. (2) Isolated–pentagon isomers were computed as the most stable forms for C_{60}, C_{70} [11] and C_{82} [26]. (3) Isolated–pentagon C_{60} and C_{82} were used as models of endohedral fullerenes [27–30]. The calculation of the Kekulé structure count $\ln K$ from Equations (6)–(7) is given in Table 2. In particular, for $C_{70}(D_{5h})$ both linear and non–linear fitting results are inside the range of the reference results (9.3–10.9). The relative errors for the linear (–11%) and non–linear (–12%) fits are smaller than that obtained from Equation (2) taken as reference 1 (–14%). However, the results of the non–linear fit should be taken with care. The correction from the linear to the non–linear fit goes in the wrong direction. On the other hand, the correction in $\ln[per(\mathbf{A})]$ from the linear to the non–linear fit goes in the correct direction for both fullerenes with respect to Equation (3) taken as reference 1. The correction in $\ln[per(\mathbf{A})]/\ln K$ from the linear to the non–linear fit goes in the correct direction for both fullerenes with respect to Equation (1) taken as reference 1 and to references 2 to 4. Notice that MAPE and AEV do not refer to the consideration of examples inside or outside the calibration domain, but to the variance of the original data and that introduced by the fit. For examples inside the calibration domain, the expected value for the relative error should be equal to MAPE. However, for examples outside the calibration domain, the expected value for the relative error may be greater than MAPE. On the other hand, for a structure with $p, q, r \neq 0$, K is expected to be lower, according to Equations (6)–(7). For instance, for $p = 20$ and $q = 10$, $\ln K = 5.14$ in Equation (6) or 5.272 in Equation (7). Of course, this is what was expected from thermodynamic arguments because p, q and r tend to destabilize the fullerene structures, while K and $\ln K$ are likely inclined to increase the stability [18,31]. Consequently, $\ln[per(\mathbf{A})]/\ln K$ tends to decrease the stability.

Table 2. Estimation values of Kekulé structure count from fits for fullerenes

Fullerene[a]	$\ln K$				$\ln[per(\mathbf{A})]$		
	Linear fit	Non–lin. fit	Exact	Ref. 1.[b]	Linear fit	Non–lin. fit	Ref. 1.[b]
C_{70} (D_{5h})	9.6800	9.5700	10.8622[f]	9.3422	20.2000	20.0000	18.8884
C_{82} (C_s)	9.6800	9.5700	–	9.3422	20.2000	20.0000	18.8884

Fullerene[a]	$\ln[per(\mathbf{A})]/\ln K$					
	Linear fit	Non–linear fit	Ref. 1[b]	Ref. 2[c]	Ref. 3[d]	Ref. 4[e]
C_{70} (D_{5h})	2.1400	2.1169	1.6895	2.0218	2.0868	2.0899
C_{82} (C_s)	2.1400	2.1169	1.6895	2.0218	2.0868	2.0899

[a] Structural parameters $p = q = r = 0$.
[b] Reference 1: estimation carried out with Equations (1)–(3) taken from Cash
[c] Reference 2: estimation carried out with quotient $\ln[per(A)]/\ln K$ from Equations (2) and (3) taken from Cash
[d] Reference 3: estimation carried out with quotient from independent linear fits from Equations (6) and (8)
[e] Reference 4: estimation carried out with quotient from independent non–linear fits from Equations (7) and (9)
[f] The exact value of K for $C_{70}(D_{5h})$ is 52 168.

4 CONCLUSIONS

A method for determining the permanent of the adjacency matrix of fullerenes is optimised. The results are given for a series of structures up to C_{60}. The algorithm allows rapid computation of

per(**A**) for adjacency matrices of molecules large enough to be theoretically interesting. Within the limits imposed by available computer time, this method should be applicable to any fullerene. The algorithm should be readily adaptable to other types of sparse matrices, including those with elements other than zero and one, thus permitting wider exploration of the significance and uses of permanents. This is also true for the signed–adjacency–matrix method. With the permanent now open to computation, a great deal of work remains to be done to characterize the relationship of the permanent to chemical structure and properties. Much future work remains to be done in elucidating the extent to which the permanent encodes structural features in a quantitative way as well as in exploring the relationship of the permanent to structure in fullerenes.

The reproduction of $\ln[\text{per}(\mathbf{A})]/\ln K$, $\ln K$ and $\ln[\text{per}(\mathbf{A})]$ for fullerenes with structural parameters $p = q = r = 0$ as $C_{60}(I_h)$, $C_{70}(D_{5h})$ and $C_{82}(C_s)$ is far from trivial with linear fitting methods, as can be seen from Equations (1)–(3).

Linear and non–linear correlation models have been obtained for $\ln[\text{per}(\mathbf{A})]/\ln K$, $\ln K$ and $\ln[\text{per}(\mathbf{A})]$ of fullerenes as functions of structural parameters involving the presence of contiguous pentagons. The multivariable non–linear regression equation for $\ln[\text{per}(\mathbf{A})]/\ln K$ has been improved. The variance of the fit has decreased 49%. It has also diminished the risk of co–linearity in the fit.

Even with the greater number of fitted parameters, the predictions of this model are far from trivial with both linear and non–linear fitting methods from Equations (4)–(9) for fullerenes with $p = q = r = 0$.

Acknowledgment

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Biographies

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