

The Number of Spanning Trees in Buckminsterfullerene

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The theorem of Gutman et al. (1983) is applied to calculate the number of spanning trees in the carbon-carbon connectivity-network of the recently diagnosed C_{60} -cluster buckminsterfullerene. This "complexity" turns out to be approximately 3.75×10^{29} and it is found necessary to invoke the device of modulo arithmetic and the "Chinese Remainder Theorem" in order to evaluate it precisely on a small computer. The exact spanning-tree count for buckminsterfullerene is 375 291 866 372 898 816 000, or, $2^{25} \times 3^4 \times 5^3 \times 11^5 \times 19^3$. A "ring-current" calculation by the method of McWeeny may be based on any desired one of this vast number of spanning trees.

INTRODUCTION

In the short time since it was originally reported,¹ in 1985, the cluster of 60 carbon atoms that is variously becoming known as "icosahedral C_{60} ," "footballene," "soccerballene," and "buckminsterfullerene" (Fig. 1) has been the object of intense theoretical interest.²⁻²²

References 2-22 are merely a representative selection from the many investigations so far published, which range from assessments of the species' stability¹⁶ to the number of Kekulé structures that may be devised for it.^{3,4,21,22} Its predicted magnetic properties have been especially thoroughly studied.^{10,11,20} Underlying the latter is the graph-theoretical concept of the several *spanning trees*^{23,24} latent in the carbon-atom skeleton that features in the structural formula (Fig. 1) of the C_{60} system. The idea of a spanning tree is inherent in McWeeny's now-classic method²³⁻³¹ of calculating π -electron "ring-current" magnetic-properties of conjugated molecules. These developments have coincided with recently revised attention, in the *microscopic* context of molecules, to an old problem initiated, at the *macroscopic* level, by Kirchhoff, midway through the last century³²—namely, that of estimating the number of spanning trees in an electrical network. In 1983, Gutman, Essam and one of the present authors³³ proved a new theorem for counting the spanning trees of a molecular graph. This theorem, which is valid for any (graph-theoretically) planar graph, requires the development of a determinant only of the order of the number of *rings* in a given

conjugated molecule, rather than knowledge of the determinant or eigenvalues of a matrix approximately of the order of the number of *atoms* participating in its conjugation, as previous theorems for spanning-tree enumeration^{34,35} had done. Thus, in the case of naphthalene, for example, a mere 2×2 determinant has to be evaluated when the theorem of Gutman et al.³³ is applied, which is to be compared with the one of order 9×9 that has to be expanded when the so-called "matrix-tree" theorem^{34,23} is used. Furthermore, if the late D.A. Waller's elegant extension³⁵⁻³⁷ involving the eigenvalue spectra of "row-regularized" graphs were to be invoked in order to count the spanning trees in naphthalene, a 10×10 matrix would have to be diagonalized.^{33b} Now it is well known to mathematicians (e.g., reference 38) that any result proved for a planar graph is also valid when that graph is embedded on the surface of a sphere. Because of this, O'Leary and one of the present authors subsequently pointed out³⁹ to potential chemical users that the theorem of Gutman et al.,³³ announced in 1983, two years before icosahedral C_{60} was first reported, is in fact also applicable to that novel species. Accordingly, in the present article, we use this theorem³³ in order to obtain a precise count of the number of spanning trees in buckminsterfullerene. The recent remarkable synthesis⁴⁰ of C_{60} in macroscopic quantities, and the consequent availability of its ¹³C-NMR spectrum,⁴¹ make this especially timely.

SCHEME OF CALCULATION

According to the theorem of Gutman et al.,³³ the number of spanning trees in a network—sometimes

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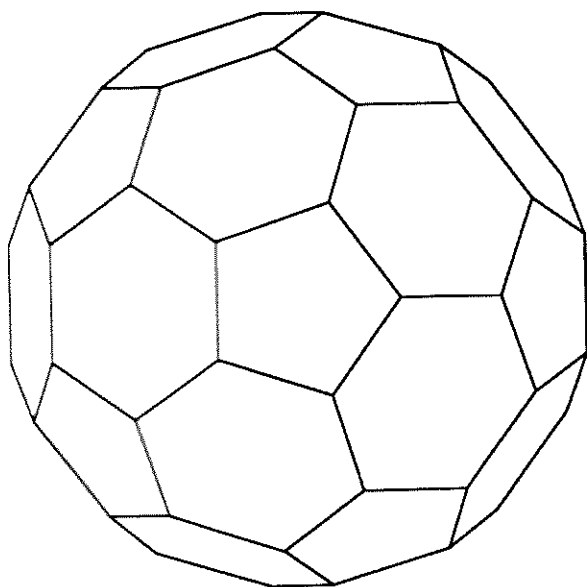


Figure 1. The carbon-carbon connectivity of icosahedral C_{60} (buckminsterfullerene).

called its “complexity”—is given by $|\mathbf{B}^* - \mathbf{A}^*|$, where the $(n^* \times n^*)$ matrix \mathbf{A}^* is an adjacency matrix of the *inner dual* of the network (graph) in question and \mathbf{B}^* is an entirely diagonal $(n^* \times n^*)$ matrix such that its (i, i) element ($i = 1, 2, \dots, n^*$) is equal to the number of edges possessed by that face of the original graph which is in 1 - 1 correspondence with vertex i of the inner dual—that inner dual having, in all, n^* vertices. (The reader is referred to references 33 and 39 for the definitions of “adjacency matrix” and “inner dual,” in this context). This process can be shown³³ to be equivalent to taking *any* cofactor of the analogously defined (equi-cofactorial) matrix $(\mathbf{B}^+ - \mathbf{A}^+)$, of dimension $(n^* + 1) \times (n^* + 1)$, pertaining to the *complete* (“geometric”) *dual* of the original network. \mathbf{B}^+ and \mathbf{A}^+ are here defined similarly as for \mathbf{B}^* and \mathbf{A}^* , but their orders are appropriate to the complete (“geometric”) dual, which comprises $(n^* + 1)$ vertices (including the so-called “infinite-face” vertex), rather than the inner dual (which has only n^* vertices, the “infinite-face” vertex—and all edges incident upon it—being, by definition, suppressed, in the inner dual.^{33,39})

The required matrix $(\mathbf{B}^+ - \mathbf{A}^+)$ for the complete dual of buckminsterfullerene was in practice obtained by the following procedure:

1. The 12 pentagons and 20 hexagons that feature in the structural formula of icosahedral C_{60} (Fig. 1) were first labeled 1 to 32 (inclusive). It was found to be a conceptual help actually to carry out this labeling process, physically, on a standard, European soccer-ball, but for illustrative purposes here, it is convenient to depict a Schlegel diagram of the three-dimensional system, similar to the one devised by Randić et al.¹⁵ The Schlegel diagram, and the numbering system we

used, is shown in Figure 2. It may be noted that, on *this* scheme, the “infinite face” is one of the pentagons, labeled “32.” For our purposes, any arbitrary labeling of the polygons on the buckminsterfullerene surface would in principle have been equally as satisfactory as any other. However, we felt disposed to effect the numbering process in such a way that diametrically opposite polygons were assigned numerical values that added to 33; (1 opposite 32, 2 opposite 31, 16 opposite 17, etc.) As will be seen, this choice had pleasant repercussions for the symmetry of the resulting (32×32) matrix $(\mathbf{B}^+ - \mathbf{A}^+)$.

2. The matrix $(\mathbf{B}^+ - \mathbf{A}^+)$ for the complete (“geometric”^{33,39}) dual of buckminsterfullerene could then immediately be written down, as follows:
 - a. if the face labeled i be a pentagon, the (i, i) element of $(\mathbf{B}^+ - \mathbf{A}^+)$ is 5;
 - b. if the face labeled i be a hexagon, the (i, i) element of $(\mathbf{B}^+ - \mathbf{A}^+)$ is 6;
 - c. if the face labeled i should have an edge in common with the face labeled j ($i \neq j$), the (i, j) and (j, i) elements of $(\mathbf{B}^+ - \mathbf{A}^+)$ are both -1 ; otherwise, all (i, j) elements of $(\mathbf{B}^+ - \mathbf{A}^+)$ ($i \neq j$) are zero.

The matrix that results from this process is illustrated in Figure 3. It will be seen that, in addition to the symmetry that it displays about its leading diagonal—which, from the definition of the matrix (just given), it must possess, whatever labeling scheme be adopted for the faces—it also manifests reflectional symmetry about the other (secondary) diagonal (the one running from the bottom left to

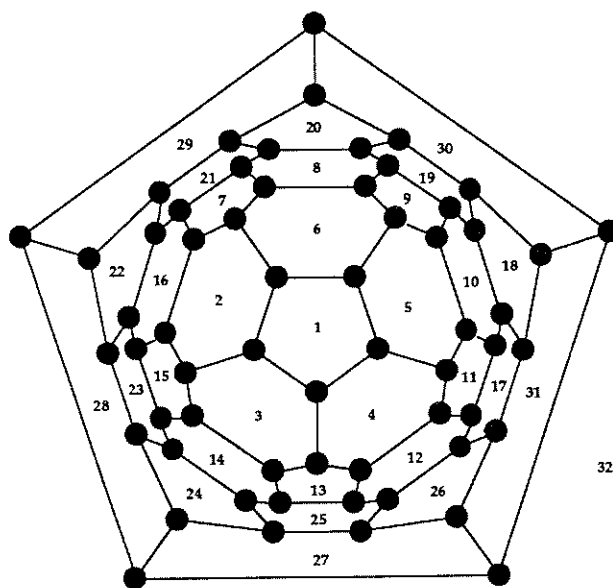


Figure 2. Schlegel diagram for buckminsterfullerene, with the numbering scheme adopted for the faces (and hence for the vertices of the inner dual and the complete (“geometric”) dual; note that, in the latter, the “infinite-face” vertex—in 1 - 1 correspondence with one of the pentagons—is here labeled 32.)

Table I. The (32, 32)-cofactor of the matrix ($\mathbf{B}^+ - \mathbf{A}^-$) (Fig. 3) for the complete ("geometric"^{33,39}) dual of buckminsterfullerene (Fig. 1), evaluated to each of the prime moduli from 31 to 89, inclusive.

| Modulus (n) | (32, 32)-Cofactor of ($\mathbf{B}^+ - \mathbf{A}^-$), modulo n |
|-------------------|---|
| 31 | 13 |
| 37 | 29 |
| 41 | 33 |
| 43 | 20 |
| 47 | 43 |
| 53 | 34 |
| 59 | 7 |
| 61 | 15 |
| 67 | 7 |
| 71 | 52 |
| 73 | 32 |
| 79 | 64 |
| (83) ^a | (42) ^a |
| (89) ^a | (63) ^a |

^aThese values are needed only later in the analysis—see Concluding Remarks.

of those two moduli.⁴² (The reader interested in the details of this is referred to our Mathematical Appendices 3 and 4). The (32, 32)-cofactor of ($\mathbf{B}^+ - \mathbf{A}^-$) (Fig. 3) was, accordingly, computed in 14 different coprime moduli—all the prime numbers from 31 to 89 (inclusive)—yielding the results that are given in Table I. By repeatedly combining all the modulo forms in steps (see Appendix 4), the cofactor was calculated to an ever-increasing modulus. As soon as the current working-modulus exceeded the approximately known value of the desired cofactor itself (and $31 \times 37 \times 41 \times \dots \times 79$ is already greater than 3.75×10^{30} , without the need for the results modulo the other two prime factors available from Table I), the answer arising from this process of continually combining the moduli represented the exact value of the cofactor we were seeking to evaluate. This value—and, hence, the required complexity of buckminsterfullerene—is

$$375\ 291\ 866\ 372\ 898\ 816\ 000$$

or, factorized into powers of prime numbers,⁴³

$$2^{25} \times 3^4 \times 5^3 \times 11^5 \times 19^3.$$

This result was checked by calculating several other cofactors of ($\mathbf{B}^+ - \mathbf{A}^-$) (Fig. 3), all of which agreed with the value just stated for the (32, 32)-cofactor.

FINAL COMMENTS ON "RING-CURRENT" CALCULATIONS

We conclude by drawing attention to the fact that the method of McWeeny²³⁻³¹ requires *just one* spanning tree on which to base a calculation of the π -electron "ring-current" intensity in a given conjugated system (usually expressed²⁵⁻²⁷ as a ratio to the

corresponding "ring-current" intensity calculated, by the same method, for benzene). The present investigation has confirmed that, in the case of icosahedral C_{60} (Fig. 1), this sole, required spanning-tree may be chosen from a truly vast number—ca. 3.75×10^{20} . If the McWeeny unitary transformation^{23a,25,27} is used in the calculation, it must be based on a spanning tree that is "unbranched" (i.e., one that represents a Hamiltonian²³ path through the molecular-graph in question). If the Gayoso-Boucekkine unitary transformation,^{23a,24,27} is invoked, however, *any* spanning tree, including a branched one,^{23a,27} may be used. The "ring-current" intensities that result from a computation based on any of these numerous spanning-trees will, however, be entirely independent of which particular spanning-tree is favored for selection.^{23-27,31} Now it has already been pointed out by several authors^{23-27,31} that precisely because a "ring-current" calculation by the McWeeny method^{23-31,10} may be based on *any* spanning tree extant within the network under study, and yet the "ring-current" intensities eventually calculated must finally be invariant to such a choice, it follows that there must be many more relations^{25,31} among the imaginary bond-bond polarizabilities (and the Coulson bond-orders) that arise in a McWeeny "ring-current" calculation^{23-27,31} than there are among the bond orders and the *real* bond-bond polarizabilities, originally defined by Coulson and Longuet-Higgins.⁴⁴ This is true, as was pointed out by McWeeny in his pioneering paper,²⁵ even for a very small unsaturated system like naphthalene with only two rings and 10 carbon atoms participating in its conjugation. In the case of buckminsterfullerene (Fig. 1), it can, therefore, be concluded with confidence that only a tiny proportion of its ($^{90}C_2 + 90$) = 4095 mutual- and self-bond-bond polarizabilities, and its 90 bond orders, will in fact actually be *distinct*.

CONCLUDING REMARKS

We might observe in passing that the original ("brute-force") computer-determination of the complexity, carried out in Porto in order to gain an order-of-magnitude estimate, could have been obviated by the following reasoning: The Schlegel diagram for the buckminsterfullerene structure (Fig. 2) comprises 90 bonds and 31 rings; now, the number of "rings" in a molecule (in the chemical sense of that term) is the same as the number of "fundamental circuits" in its molecular graph.^{23,45} Furthermore, it is well known^{23,33-36} that if a graph has N fundamental circuits, precisely N edges (bonds) have to be removed from the parent graph in order to obtain a spanning tree. In the case of C_{60} , therefore, 31 bonds have to be removed, from among the 90 available, to form a spanning tree⁴⁶; hence, $^{90}C_{31} \approx 1.30 \times 10^{24}$ is an *upper bound* for the number of spanning trees (since, of course, removal of an arbitrary combina-

tion of 31 bonds does not necessarily give rise to a spanning tree). The modulus to which we previously knew the complexity (the product of all the prime factors in Table I up to and including the 83) was ca. 4.13×10^{22} . Since $89 \times 4.13 \times 10^{22} \approx 3.68 \times 10^{24}$, it can be seen that doing just one more calculation of the required cofactor (to a modulus of the next highest prime number, 89—see Table I) would have been sufficient to obtain the cofactor to a composite modulus exceeding the upper bound just stated (${}^{90}C_{31}$), and hence to yield the true value of the complexity, without the need for the initial approximate computer-determination of this quantity.

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APPENDIX 1: STORAGE AND PROCESSING OF NUMBERS AS ARRAYS

As explained in the text, the numbers generated in the calculations described soon exceeded the computer's limit of accuracy (eight significant figures). This problem was solved by storing numbers not as integer variables, but as arrays. Thus

$$a = 1234567890$$

would become

$$a(3) = 0012, a(2) = 3456, a(1) = 7890.$$

The arrays could have stored one digit in each element, but that would have been wasteful of the available eight-digit accuracy. Storing as four-digit blocks is equivalent to writing the numbers in base 10,000. All normal arithmetic now becomes an "element-wise" operation, such as would be carried out on paper. Routines were written to perform long multiplication, addition, and subtraction in this way. Within the capacity of the machine, the suite of programs could now operate with complete accuracy in numbers up to 160 elements—that is, 640 digits; (the actual problem, however, eventually required only 21 digits—or, on the system just described, six elements.)

An Example of Multiplication

$$a \times b, \text{ with } a = 12345678 \text{ and } b = 87654321$$

First

$$a(2) = 1234, a(1) = 5678,$$

$$b(2) = 8765, b(1) = 4321$$

Then

| | | | |
|------|------|------|------|
| | | 8765 | 4321 |
| | | 1234 | 5678 |
| | | 2453 | 4638 |
| | 4976 | 7670 | 0000 |
| | 533 | 2114 | 0000 |
| 1081 | 6010 | 0000 | 0000 |
| 1082 | 1520 | 2237 | 4638 |

ans(4) = 1082, ans(3) = 1520, ans(2) = 2237, ans(1) = 4638. Hence, final answer = 1082152022374638.

As described in the text, by looping through the above algorithm enough times to combine all the moduli in this way, we were finally able to obtain the reported 21-digit complexity of buckminsterfullerene.

APPENDIX 2: SCHEME FOR EVALUATION OF THE INTEGRAL DETERMINANT

To use only a small computer to evaluate precisely an integral determinant, Δ , of large order, such as the one described in the text, it is convenient to reduce a known, integral multiple of it, by row operations (as in the "pivotal condensation" method,⁴⁷ but *avoiding division*), to a "triangular" determinant—that is, one with only zeros above (or below) its principal diagonal—and thus to obtain an equation of the form

$$a\Delta = b.$$

Here, the integer b is the product of the elements along the leading diagonal of the resulting triangular determinant, and the integer a is the product of the scaling factors that have been used in the row operations that reduced the original determinant to its corresponding triangular-form. Then, if working is carried out to a modulus, m , the multiplicative inverse of a (that is, c , say, such that $a \times c \equiv 1 \pmod{m}$) is found by systematic trial-and-error and so, to modulus m ,

$$\Delta \equiv c \times b$$

APPENDIX 3: "THE CHINESE REMAINDER THEOREM"

In all that follows, all letters stand for integers; Greek letters represent integers of which the values need not be known.

Given $x \equiv a \pmod{p}$ and $x \equiv b \pmod{q}$, then if, and only if, p and q are coprime (i.e., $(p, q) = 1$), we can find λ and μ such that

$$\lambda p + \mu q = 1$$

and so, from

$$\begin{aligned}x &= a + \theta p \\x &= b + \phi q\end{aligned}$$

deduce that

$$\mu qx + \lambda px = \mu qa + \lambda pb + \psi pq$$

and hence that

$$x \equiv \mu qa - \lambda pb \pmod{pq}$$

Conversely, from this congruence, it follows that

$$x = a - \lambda pa + \lambda pb + \omega pq$$

and so

$$x \equiv a \pmod{p}$$

and, similarly,

$$x \equiv b \pmod{q}$$

i.e., the two initial congruences ($x \equiv a \pmod{p}$) and ($x \equiv b \pmod{q}$) $\Leftrightarrow x \equiv \mu qa - \lambda pb \pmod{pq}$.

APPENDIX 4: AN APPLICABLE ALGORITHM

Of p, q such that $(p, q) = 1$, let (for computational speed) p be the greater. Form in succession $a, (a + p), (a + 2p), \dots, (a + (q - 1)p)$, each modulo q (in the range $q > (a + ip) \geq 0$). One of these, and only one, is equal to b (as they are all different and form a complete set of residues, mod q), it being assumed that $q > b \geq 0$. Suppose it is $(a + kp)$. Clearly, this is congruent to $a \pmod{p}$. It is also congruent to $b \pmod{q}$ by its specification. Therefore, it is the " $\mu qa + \lambda pb \pmod{pq}$ " of Appendix 3.

A repetition of this process leads to a sufficiently large modulus $pqr \dots$. The strategy adopted in the computation was thus to combine the first two moduli, 31 and 37 (see Table I), and then to combine this modulus, 1147, with the next one, 41, and so on until the required determinant was obtained modulo $(31 \times 37 \times 41 \times \dots \times 79)$, which was safely greater than its approximately known value.

References

- H.W. Kroto, J.R. Heath, S.C. O'Brien, R.F. Curl, and R.E. Smalley, *Nature*, **318**, 162 (1985).
- A.D.J. Haymet, a. *Chem. Phys. Letters*, **122**, 421 (1985). b. *J. Am. Chem. Soc.*, **108**, 319 (1986).
- D.J. Klein, T.G. Schmalz, G.E. Hite, and W.A. Seitz, *J. Am. Chem. Soc.*, **108**, 1301 (1986).
- H. Hosoya, *Computer Math. Appl.*, **12B**, 271 (1986).
- R.C. Haddon, L.E. Brus, and K. Raghavachari, a. *Chem. Phys. Letters*, **125**, 459 (1986); b. *Chem. Phys. Letters*, **131**, 165 (1986).
- R.L. Disch and J.M. Schulman, *Chem. Phys. Letters*, **125**, 465 (1986).
- T.G. Schmalz, W.A. Seitz, D.J. Klein, and G.E. Hite, *Chem. Phys. Letters*, **130**, 203 (1986).
- P.W. Fowler and J. Woolrich, *Chem. Phys. Letters*, **127**, 78 (1986).
- P.W. Fowler, *Chem. Phys. Letters*, **131**, 444 (1986).
- V. Elser and R.C. Haddon, a. *Nature*, **325**, 792 (1987). b. *Phys. Rev.*, **36**, 4579 (1987).
- R.B. Mallion, *Nature*, **325**, 760 (1987).
- H.W. Kroto, *Nature*, **329**, 529 (1987).
- S.H. Yang, C.L. Pettiette, J. Conceicao, O. Cheshnovsky, and R.E. Smalley, *Chem. Phys. Letters*, **139**, 233 (1987).
- K. Kavacević, A. Graovac, and D. Babić, *Int. J. Quant. Chem.*, **21**, 589 (1987).
- M. Randić, S. Nikolić, and N. Trinajstić, *Croatica Chem. Acta*, **60**, 595 (1987).
- P.W. Fowler and J.I. Steer, *J. Chem. Soc. Chem. Commun.*, 1403 (1987).
- T.G. Schmalz, W.A. Seitz, D.J. Klein, and G.E. Hite, *J. Am. Chem. Soc.*, **110**, 1113 (1988).
- J. Aihara and H. Hosoya, *Bull. Chem. Soc. Japan*, **61**, 2657 (1988).
- a. K. Balasubramanian and X. Liu, *J. Comp. Chem.*, **9**, 406 (1988). b. J. R. Dias, *J. Chem Education*, **66**, 1012 (1989).
- R.B. Mallion, *Math./Chem./Comp.*, 1988, in *Proceedings of an International Course and Conference on the Interfaces between Mathematics, Chemistry and Computer Science, Dubrovnik, Yugoslavia*, 20–25 June, 1988, A. Graovac, Ed., *Studies in Physical and Theoretical Chemistry*, **63**, pp. 505–510; Elsevier Science Publishers, B.V., Amsterdam, The Netherlands, 1989.
- E. Brendsdal and S.J. Cyvin, *J. Mol. Struct. (Theochem.)*, **188**, 55 (1989).
- a. W.R. Müller, K. Szymanski, J.V. Knop, and N. Trinajstić. Unpublished work, 1986, using 22b, the method described in reference 22c. b. N. Trinajstić, Personal communication to R.B.M., January 29, 1990. c. J.V. Knop, K. Szymanski, N. Trinajstić, and P. Krivka, *Computer Math. Appls.*, **10**, 369 (1984).
- R.B. Mallion, a. *Proc. Royal Soc. (London)*, Ser. A., **341**, 429 (1975). b. *Chem. Phys. Letters*, **36**, 170 (1975).
- J. Gayoso, and A. Boucekkine, *Comptes Rend. Acad. Sci. (Paris)*, Sér C, **272**, 184 (1971).
- R. McWeeny, *Mol. Phys.*, **1**, 311 (1958).
- R.B. Mallion, *Mol. Phys.*, **25**, 1415 (1973).
- C.W. Haigh and R.B. Mallion, *Prog. N.M.R. Spectrosc.*, **13**, 303 (1979).
- a. J. Aihara, *J. Am. Chem. Soc.*, **101**, 5913 (1979). b. J. Aihara, *Bull. Chem. Soc. Japan*, **54**, 1245 (1981). c. J. Aihara and T. Horikawa, *Bull. Chem. Soc. Japan*, **56**, 1853 (1983). d. J. Aihara, *Bull. Chem. Soc. Japan*, **58**, 1045 (1985). e. J. Aihara, *Bull. Chem. Soc. Japan*, **59**, 3781 (1986).
- A. Baba Ahmed and J. Gayoso, *Int. J. Quant. Chem.*, **23**, 71 (1983).
- B. O'Leary and R.B. Mallion, *J. Math. Chem.*, **3**, 323 (1989).
- a. R.B. Mallion, D. Phil. Thesis, University of Oxford (Christ Church), United Kingdom, 1979, Chapter VII, pp. 191–225. b. N. Mizoguchi, *Bull. Chem. Soc. Japan*, **60**, 2005 (1987). c. C.W. Haigh and R.B. Mallion, *Croatica Chem. Acta*, **62**, 1 (1989).
- a. G.R. Kirchhoff, *Annal. Phys. Chem.*, **72**, 497 (1847). b. English translation: J.B. O'Toole, *I.R.E. Trans. Circuit Theory*, **CT5**, 4 (1958). c. Another English translation: in N.L. Biggs, E.K. Lloyd, and R.J. Wilson, *Graph Theory 1736–1936*, Oxford University Press, Oxford, United Kingdom, 1976, pp. 133–135.
- I. Gutman, R.B. Mallion, and J.W. Essam, *Mol. Phys.*, **50**, 859 (1983).

34. a. C.W. Borchardt, *J. Reine Angewandte Math.*, **57**, 111 (1860). b. R.L. Brooks, C.A.B. Smith, A.H. Stone, and W.T. Tutte, *Duke Math. J.*, **7**, 312 (1940). c. W.T. Tutte, *Proc. Cambridge Phil. Soc.*, **44**, 463 (1948). d. J. Lantieri, *Ann. Telecommun.*, **5**, 204 (1950). e. H.M. Trent, *Proc. Nat. Acad. Sci. U.S.A.*, **40**, 1004 (1954). f. H. Hutschenreuter, *Wissenschaft. Z. Tech. Hochsch. Ilmenau*, **13**, 403 (1967). g. F. Harary, *Graph Theory*, Addison-Wesley, Reading, Massachusetts, 1969. h. J.W. Moon, *Counting Labelled Trees*, Canadian Mathematical Congress Monographs, No. 1: Canadian Mathematical Congress, Montreal, Quebec, Canada, 1970, pp. 41, 42. i. P. John, *Wissenschaft. Z. Tech. Hochsch. Ilmenau*, **35**, 41 (1989). j. P. John and H. Sachs, *J. Chem. Soc. Faraday Trans.*, **86**, 1033 (1990). k. P. John and H. Sachs, *Topics Curr. Chem.*, **153**, 147 (1990).
35. D.A. Waller, a. *Atti dei Convegni Lincei*, **17**, Proceedings of the *Colloquio Internazionale sulle Teori Combinatorie*, Rome, Italy, 1973 (in English), *Accademia Nazionale dei Lincei*, **I**, 313 (1976). b. in *Combinatorics*, T.P. McDonough and V.C. Mavron, Eds., London Mathematical Society Lecture-Notes Series, **13**, Cambridge University Press, London, United Kingdom, 1974, pp. 177-183. c. *I.E.E.E. Circuits Systems*, **23**, 467 (1976).
36. R.J. Wilson, in *Combinatorics*, D.J.A. Welsh and D.R. Woodall, Eds., Institute of Mathematics and its Applications, Southend-on-Sea, United Kingdom, 1973, pp. 295-321.
37. M.J. Rigby, R.B. Mallion, and D.A. Waller, *Chem. Phys. Letters*, **59**, 316 (1978).
38. R.J. Wilson, *Introduction to Graph Theory*, 3rd. ed., Longman, Harlow, Essex, United Kingdom, 1985, p. 65.
39. B. O'Leary and R.B. Mallion, in *Graph Theory and Topology in Chemistry*. A Collection of Papers Presented at an International Conference Held at the University of Georgia, Athens, Georgia, United States of America, 16-20 March, 1987, R.B. King and D.H. Rouvray, Eds., Studies in Physical and Theoretical Chemistry, **51**, pp. 544-551, Elsevier Science Publishers, B.V., Amsterdam, The Netherlands, 1987.
40. W. Krättschmer, L.D. Lamb, K. Fostiropoulos, and D.R. Huffman, *Nature*, **347**, 354 (1990).
41. R.D. Johnson, G. Meijer, and D.S. Bethune, *J. Am. Chem. Soc.*, **112**, 8983 (1990).
42. a. L.E. Dickson, *Introduction to the Theory of Numbers*, University of Chicago Press, Chicago, 1929, pp. 11-12. b. H. Midonick, *The Treasury of Mathematics*, Penguin, London, United Kingdom, 1965, Part I, p. 217.
- c. Reference 42b gives the context of the problem solved by Sun-Tsu (third century A.D.), who really gave a "rule of thumb" for solving $x \equiv a \pmod{3}$, $x \equiv b \pmod{5}$, $x \equiv c \pmod{7}$. The Indian Brahmagupta (seventh century A.D.) and then Ibn al-Haitam (ca. 1000 A.D.) posed more complicated problems.^{42a} The simple proof given by Dickson in reference 42a needs an algorithm to solve $ya \equiv 1 \pmod{m}$ where y is an unknown, and a and m are known and coprime (i.e., the greatest common divisor of $(a, m) = 1$); this can be done by continued fractions or the Euclidean Algorithm.^{42b,42c} d. R.B.M. is grateful to his colleague the Revd. Canon P.F. Johnson for very helpful discussion on this point. e. P.F. Johnson, Personal correspondence to R.B.M., April 14, 1990.
43. We noted with some amusement (though we do not claim it to have any particular significance!) that when the complexity of icosahedral C_{60} is expressed in the form
- $$2^{25} \times 3^4 \times 5^3 \times 11^5 \times 19^3,$$
- the sum of the bases, $(2 + 3 + 5 + 11 + 19)$, is equal to the sum of the powers, $(25 + 4 + 3 + 5 + 3)$, both being 40.
44. C.A. Coulson and H.C. Longuet-Higgins. *Proc. Royal Soc. (London)*, *Ser. A*, **191**, 39 (1947).
45. N. Mizoguchi, *Bull. Chem. Soc. Japan*, **63**, 765 (1990).
46. This could also be looked at in the following way, which may be intuitively rather more obvious: If F , V , and E be the number of faces, vertices, and edges, respectively, Euler's relation is
- $$F + V = E + 2,$$
- and so,
- $$E - (F - 1) = V - 1.$$
- It is evident that any spanning tree (which contains all V vertices of the network, but no circuits) must comprise $V - 1$ edges; an upper bound to the number of spanning trees is, therefore, ${}^E C_{V-1}$ which, by the above, amounts to ${}^E C_{E-(F-1)} = {}^E C_{F-1}$. Thus, for icosahedral C_{60} , with $E = 90$ and $F = 32$, this is ${}^{90}C_{31}$, as asserted in the text.
47. a. A.C. Aitken, *Determinants and Matrices*, 2nd ed., Oliver and Boyd, Edinburgh, Scotland, United Kingdom, 1942, pp. 46-48. b. P.M. Cohn, *Linear Equations*, Library of Mathematics Series, W. Ledermann, Ed., Routledge and Kegan Paul, London, United Kingdom, 1958, p. 64.