match no. 20 pp. 283-287 1986

RESEARCH NOTE: ON THE MATCHING AND THE CHARACTERISTIC POLYNOMIAL OF THE GRAPH OF TRUNCATED OCTAHEDRON

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(Received: March 1986)

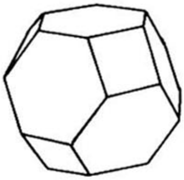
In recent experiments graphite has been evaporated by laser irradiation, producing a remarkably stable cluster consisting of 60 carbon atoms [1] . It has been suggested that this cluster has the structure of a truncated icosahedron and as it resambles a football the cluster has been named the footballene.

However, there are other Archimedean solids which may be realized in molecular form from carbon atoms only [2] . Archimedean solids are facially regular, i.e. each face is a regular polygon, but the faces are not all of the same kind. However, the vertices are all congruent.

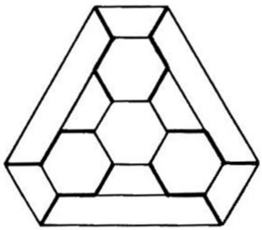
One of the simplest of these solids is a truncated octahedron(1) which is depicted below. It is composed of 24 vertices arranged in 6 four-membered and 8 six-membered rings. Each four-membered ring is surrounded by 4 six-membered rings.

In the present note we show how one could easily compute the mathching and the characteristic polynomial of the graph of the truncated octahedron but the similar approach could be applied to other Archimedean solids as well.

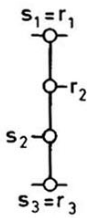
Let us represent the truncated octahedron by a planar graph G as it is shown below. This graph could be understood as a rotagraph [3] composed from some number of repeating monographs [5] . If a monograph indicated in G by heavy lines is chosen, G appears composed from 6 such monographs. This monograph is denoted by A and it is together with its linking edges shown below too.



(1)



(G)



(A)

By following the method of Refs. [4-7] the square matrix T(A) of the order 8 has to be formed. Its matrix elements are given by:

$T_{11} = \alpha(A;x)$

$T_{12} = -\alpha(A-r_1;x)$

$T_{13} = -\alpha(A-r_2;x)$

$T_{14} = -\alpha(A-r_3;x)$

$T_{15} = \alpha(A-r_1-r_2;x)$

$T_{16} = \alpha(A-r_1-r_3;x)$

$T_{17} = \alpha(A-r_2-r_3;x)$

$T_{18} = -\alpha(A-r_1-r_2-r_3;x)$

$T_{21} = \alpha(A-s_1;x)$

$T_{23} = -\alpha(A-s_1-r_2;x)$

$T_{24} = -\alpha(A-s_1-r_3;x)$

$T_{27} = \alpha(A-s_1-r_2-r_3;x)$

$T_{31} = \alpha(A-s_2;x)$

$T_{32} = -\alpha(A-s_2-r_1;x)$

$T_{34} = -\alpha(A-s_2-r_3;x)$

$T_{36} = \alpha(A-s_2-r_1-r_3;x)$

$T_{41} = \alpha(A-s_3;x)$

$T_{42} = -\alpha(A-s_3-r_1;x)$

$T_{43} = -\alpha(A-s_3-r_2;x)$

$T_{45} = \alpha(A-s_3-r_1-r_2;x)$

$T_{51} = \alpha(A-s_1-s_2;x)$

$T_{54} = -\alpha(A-s_1-s_2-r_3;x)$

$T_{61} = \alpha(A-s_1-s_3;x)$

$T_{63} = -\alpha(A-s_1-s_3-r_2;x)$

$T_{71} = \alpha(A-s_2-s_3;x)$

$T_{72} = -\alpha(A-s_2-s_3-r_1;x)$

$T_{81} = \alpha(A-s_1-s_2-s_3;x)$

while the remaining matrix elements of T equal zero. Non-zero matrix elements of T are easily calculated by using the basic recursion for the matching polynomial $\alpha(H;x)$ of graph H:

$$\alpha(H;x) = \alpha(H-e;x) - \alpha(H-u-v;x)$$

where e is an arbitrary edge of H with end-points u and v. Indeed, the method of Refs. [4-7] is based on asystematic application of the above recursion.

The matching polynomial of G equals the trace of T^6 [4-7] and after some algebra one obtains:

$$\mathcal{A}(G) = \mathrm{tr}\ T^6 = x^{24} - 36\ x^{22} + 558\ x^{20} - 4884\ x^{18} + 26619\ x^{16} - 94008\ x^{14} + 217172\ x^{12} - 323976\ x^{10} + 301203\ x^8 - 163444\ x^6 + 46182\ x^4 - 5508\ x^2 + 169$$

The last coefficient equals the number of perfect matchings, **K**, of G: K = 169.

By using the cyclic symmetry of G [3] one could factorize and compute the characteristic polynomial $\Phi(G;x)$ of G. After some algebra one derives:

$$\Phi(G;x) = (x^4 - 10\ x^2 + 9\ )\ (x^4 - 6x^2 + 1)^3\ (x^4 - 4x^2 + 3)^2 = x^{24} - 36\ x^{22} + 546\ x^{20} - 4564\ x^{18} + 23103\ x^{16} - 73416\ x^{14} + 147484\ x^{12} - 185160\ x^{10} + 141519\ x^8 - 62740\ x^6 + 14946\ x^4 - 1764\ x^2 + 81$$

The last coefficient of $\Phi(G;x)$ equals the square of the Algebraic Structure Count, ASC, of G; therefore: ASC = 9.

Although $\mathcal{A}(G;x)$, $\Phi(G;x)$, K and ASC have found applications in chemistry we will not derive any chemical conclusions here because the carbon cluster of the truncated octahedron is probably a candidate for alkane and not for alkene **as** well as because the strain in this cluster could be relatively large [2] .

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