ANALYTICAL CHALLENGE

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Goldberg Variations Challenge

We would like to invite you to participate in the Analytical Challenge, a series of puzzles to entertain and challenge our readers. The special ABC feature "Analytical Challenge" has established itself as a truly unique quiz series, with a new scientific puzzle published every second month. Readers can access the complete collection of published problems, with their solutions, on the ABC homepage at http://springer.com/journal/00216. Test your knowledge and tease your wits in diverse areas of analytical and bioanalytical chemistry by viewing this collection.

In this challenge fullerenes are the topic. And please note: there is a prize to be won (a Springer book from our catalogue up to a value of €75,-). Please read on...

Meet the Goldberg variations challenge

In approximately 1741 Johann Sebastian Bach wrote one of his enigmatic works for keyboard—the set of thirty variations on a theme nowadays known as the Goldberg Variations (BWV 988). In music, variation is the repetition of a theme with modification of rhythm, tune, harmony, or key; structural isomers of molecules on the other hand can be regarded as the chemical counterpart of this concept—variations on the theme "molecular connectivity". Two centuries later other Goldberg variations appeared, this time in a chemically related journal article. The latter variations were related to the structural isomers of carbon. Interestingly enough, as a consequence of these variations it seemed that the reasons for the non-existence of some molecular isomers were not chemical but rather mathematical. In this challenge readers are invited to trace a few fullerenes that do not exist because of such restrictions.

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Meet the challenge

Ever since the discovery of the spherical C_{60} molecule with 60 carbon atoms bonded into a soccer ball-shaped molecule [1], this carbon cluster has become an icon for chemistry, because of to its media-friendly appeal. This molecule has charisma that fascinates scientists, delights lay people, and infects children with new enthusiasm for science, as Sir Harald Kroto once expressed [2, 3]. A fullerene is a carbon-only molecule which can be seen as a simple mathematical polyhedron. Fullerene-type polyhedra occur not only in chemistry; they have been captured in architecture (the C_{60} dome of the Arctic institute (Buffin island) or the C_{20} fullerene as one of the Salvador Dali's houses) and are found in virus capsid structures (e.g. C_{20} in the gemini virus and C_{60} in the turnip yellow mosaic virus) [4].

Mathematically, fullerenes are trivalent pseudospherical polyhedra. Such polyhedra with v vertices (atoms), e edges (bonds), and f faces (double bonds+rings) obey Euler's theorem:

$$v + f = e + 2. \tag{1}$$

Because each carbon atom in fullerenes is bonded to three others (hence trivalent polyhedra), this forces the condition $2e=3v$. This expression is the first and the most obvious mathematical restriction to fullerene structure. It indicates the number of carbon atoms in a fullerene (v) must be an even number (for the number of edges, e, to be an integer). There are, however, more intricate restrictions on fullerene structures. In a structure made of pentagons (p_5) and hexagons (p_6), the total number of faces $f = p_5 + p_6$. From here, the Euler's formula can be re-written as:

$$v + p_5 + p_6 = 3v/2 + 2. \tag{2}$$

In a pseudo-spherical polygon consisting only of p_5 pentagons and p_6 hexagons the total number of vertices v
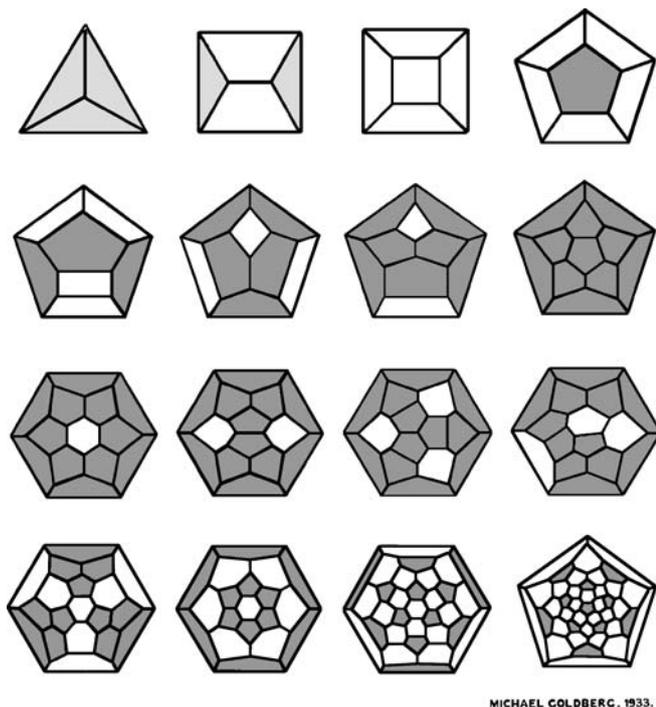
Fig. 1 Goldberg variations on several polyhedra (planar projections). Modified from Ref. [6]

(atoms) equals $(5 \cdot p_5 + 6 \cdot p_6)/3$. Combining this expression with Eq. (2) leads to a rather elegant solution, namely p_5=12. This is yet another mathematical restriction on fullerene structure postulating that any fullerene must have no more, or fewer, than twelve pentagons. This obviously means that the smallest possible fullerene is one with 12 pentagons and no hexagons at all (C_{20} fullerene) [5].

In the nineteen-thirties it was discovered that trihedral polyhedra with the same number of hexagons in addition to 12 regularly and symmetrically disposed pentagons can be topologically different. In other words, some of these polyhedra can have several isomers. From Fig. 1 (drawn in 1933!) one can see, for example, that the polyhedron with

12 pentagons and three hexagons (a C_{28} fullerene) can occur in two different topological forms (row 3, columns 3 and 4) meaning that a C_{28} fullerene has two isomers.

In the same year Michael Goldberg noted that one particular fullerene, a polyhedron made of only pentagons and hexagons, cannot exist, even though it conforms to all the previously outlined restrictions (more than 20 carbon atoms, even number of carbon atoms, twelve pentagons).

Can you name the forbidden fullerene and show why it cannot exist? Are there any other "forbidden" fullerenes?

We invite our readers to participate in the Analytical Challenge by solving the puzzle above. Please send the correct solution to abc-challenge@springer.com by June 15, 2006. Make sure you enter "Goldberg Variations Challenge" in the subject line of your e-mail. The winner will be notified by e-mail and his/her name will be published on the "Analytical and Bioanalytical Chemistry" website at http://springer.com/journal/00216 and in the Journal. Readers will find the solution and a short explanation on the "Analytical and Bioanalytical Chemistry" website after June 15, 2006, and in the Journal (Issue 386/1) .

The next Analytical Challenge will be published in Issue 385/5, July 2006. If you have enjoyed solving this Challenge you are invited to try the previous puzzles on the "Analytical and Bioanalytical Chemistry" website http://springer.com/journal/00216).

References

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