CALIFORNIA STATE SCIENCE FAIR
2010 PROJECT SUMMARY

Name(s)
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Project Number
S0506

Project Title
The Structures and Energetics of Non-Classical Fullerenes

Abstract

Objectives/Goals
To 1) provide computational (theoretical) data on 7 non-classical fullerene derivatives (all of which have no previously published characteristic values), 2) compare the calculated cage structures of the test fullerenes with the control X-ray structure, and 3) examine and explore the mechanism for C(62) synthesis and its applications.

Methods/Materials
The procedure consisted of a dry lab experiment; I obtained the computational data by running Gaussian 03 software for many weeks. (The calculations per molecule are very time-consuming.) All calculations were performed on a hybrid density functional level (B3LYP), based upon Becke's 3-parameter formulation, coupled with a 6-31G* (also called 6-31G(d)) basis set. I first tested these settings on the control molecule (C(62)tolyl(2)), to ensure that the results would match the X-ray structure for proper comparison, and then applied it to the 7 test molecules. Results included that for bond lengths, bond angles, pyramidalization angles, and band gap of the 4-membered carbon ring.

Results
The structural data for the seven C(62) derivatives very strongly supports my conclusion. The band gap for each derivative is higher than that of C(60). (The numbers are not included to conserve space.) Some categories varied more than others, most likely due to the sterics of the substituents attached to the fullerene cage. An analysis of the proposed mechanism reveals several slow steps with extremely high activation energies. A step was taken toward the possibility of more :CC: insertions; the structure and mechanism of C(64) was also explored, with similar structural and energetic results.

Conclusions/Discussion
The data strongly supports a cyclobutene structure for the 4-membered ring in C(62), answering the question of whether the ring structure is that of [4]radialene or cyclobutene. The molecule is overall energetically unstable and highly reactive (due to the high band gap, aka HOMO/LUMO energy gap). This could be useful in a commercial setting, with regards to photovoltaic efficiency (solar cells). The molecule's structure may also be of use in the field of immunology.

Summary Statement
The computational study carried out here of C62, which provided both structural and energetic data, is the first step toward extensive reactive and innovative research regarding this molecule and other non-classical fullerenes.

Help Received
Graduate student helped provide access to online publications and the Gaussian software (not available to high school students)