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Electronic structure of C_{40} possible structures

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Abstract

C_{40} is a fullerene with a conformation that has been proposed as T_d, D_{2d}, D_{4h} and D_{5d} symmetry groups. The correct structure has not been determined because it has not been possible to isolate the molecule, but there have been several studies of minor fullerenes that include it. In this work we present a theoretical study at the GAUSSIAN 94 HF/3-21G level that gives answers about the principal differences between the mentioned structures and the possible thermodynamic stability of each one. Furthermore, we include a similar study on the new D_{2h} structure that we propose. © 1998 Elsevier Science B.V.

Keywords: C_{40}; Fullerenes; Electronic structure; Symmetry

1. Introduction

Since the discovery of C_{60} [1] there have been numerous experimental and theoretical studies on the fullerenes, exploring the structures of these types of compounds (see for example [2]). It has been found that C_{60} and C_{70} are the stable ones; the structure of the C_{60} is very well know to be a truncated icosahedron with symmetry I_h [3]. Several studies have been done to determine the structure of other fullerenes, mainly directed towards bigger fullerenes since they can be detected experimentally (see for example [4]). Other studies have looked at small carbon-only compounds, C_n, but these have been limited to special experimental techniques as laser vaporization [5], mass spectroscopy [6,7] and photoelectron spectroscopy [8]. These studies have shown that for small n the structures are linear chains or cyclic forms, and that only when $n \geq 32$ are cages formed.

On the theoretical side, most of the work has concentrated on the C_{60}. The geometry has been optimised by several methods [9–13] and all of them predict an I_h symmetry and bond alternation. Raghavachari and Binkley [14] have done an accurate ab initio calculation for carbon clusters for $n = 2–10$; they find that for odd n, the geometries of the clusters are linear chains while for even n, cyclic structures are preferred. Bakowies and Thiel [15] did MNDO calculations with complete geometry optimisation for 30 polyhedral carbon clusters for $20 \leq n \leq 540$ and provided structures, heats of formation and orbital energies.

C_{40} is one of these cages and several symmetries have been proposed. Bakowies and Thiel [15] found that the optimised geometry has symmetry D_{5d}, Ying-Duo and Herndon [16] studied fullerenes that have two four-membered rings and found that symmetry D_{4h} is preferred and Adams et al. [17], using first-principle

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