Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Describing the chemical bonding in C_{70} and $C_{70}O_3$ - a quantum chemical topology study.

Autorzy

Andrzej Bil

Zdzisław Latajka

Jürg Hutter

Carole A. Morrison

Rok wydania

2014

Czasopismo

Chemical Physics

Numer woluminu

433

Strony

22-30

DOI

10.1016/j.chemphys.2014.02.003

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

C_c–C_c and C_a–C_b bonds in C_{70} have dominant characteristics of double bonds, whereas the remaining six other types of bonds are single bonds with contributions from π-electron density. ‘Single’ bonds can act as active sites in chemical reactions which would typically require a multiple bond, such as addition of an ozone molecule, due to the fact that all adjacent bonds can serve as an efficient source of π-electron density. Thus any alteration in the electron density distribution following functionalization has far-reaching impact. We note that formation of the most stable ozonide isomer causes the smallest total perturbation in the electron density of the parent fullerene and C–C bond evolution correlates well with the shape of the minimum energy path for the ozone ring opening reaction on the fullerene surface. Finally, we observe that the O–O bond in $C_{70}O_3$ is protocovalent, and as such resembles the O–O bond in H_2O_2.

Słowa kluczowe

Fullerene, Molozonides, AIM, ELI-D, Reaction mechanism

Adres publiczny

http://dx.doi.org/10.1016/j.chemphys.2014.02.003

Strona internetowa wydawcy

http://www.elsevier.com

Plik został wygenerowany dnia 2026-11-08 11:24:14

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/teXT5uo.