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

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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

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