The mechanism of the ozonolysis on the surface of C70 fullerene : the electron localizability indicator study.

Autorzy

Andrzej Bil

Krzysztof Mierzwicki

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Streszczenie

The formation of $C_{70}O$ from $C_{70}O_3$ monomolozonide is a three-step process with the isomer dependent last step leading either to c,c-$C_{70}O$ epoxide or d,d-$C_{70}O$ oxidoannulene. The process involves the open intermediate (first O–O then C_c–C_c/C_d–C_d bonds broken), oxidoannulene-like structure intermediate (new C_c–O/C_d–O bond formed) and finally the oxide product. On the formation of c,c-$C_{70}O$ isomer, the final release of O_2 is followed by the restoration of C_c–C_c bond, which stabilizes the product. Neither C_d–C_d bond is restored nor the total energy essentially lowered upon d,d-$C_{70}O$ formation. At all steps of the studied process, the four CC bonds adjacent to C_c–C_c or C_d–C_d bond, respectively, play a crucial role donating or withdrawing the necessary electron density. $C_{70}(O)O_2$ products, with O_2 bridging one of the bonds adjacent to the parent C_c–C_c/C_d–C_d one, may compete with the oxide products. The OO bond in such structures is weak as suggested by its low electron population. For both c,c-$C_{70}O_3$ and d,d-$C_{70}O_3$, the shape of the potential energy surfaces (0 K) and the related, reported earlier, room temperature–free energy surfaces differ.

Słowa kluczowe

Molozonide, Epoxide, Oxidoannulene, ELI-D, Quantum chemical topology

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