

The mechanism of ozonolysis on the surface of C₇₀ fullerene. The free energy surface theoretical study.

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Streszczenie

Density functional theory based metadynamics simulations of the room temperature ground state free energy surfaces (FES) of a,a-C₇₀O₃ /a,a-C₇₀O, c,c-C₇₀O₃ /c,c-C₇₀O, d,d-C₇₀O₃ /d,d-C₇₀O and e,e-C₇₀O₃ /e,e-C₇₀O systems have revealed several structures relevant for the thermal decomposition of the experimentally known c,c-C₇₀O₃ and hypothetical a,a-C₇₀O₃, d,d-C₇₀O₃ and e,e-C₇₀O₃ ozonides. Criegee intermediate, an open structure with carbonyl oxide and carbonyl groups, plays an important role in the possible mechanism of decomposition of all studied ozonides, while only for e,e-C₇₀O₃ /e,e-C₇₀O system it is related to the minimum on the underlying FES. The differences between the topography of FES and the previously reported related potential energy surface indicates the influence of a thermal factor on processes on C₇₀ surface. Only c,c-C₇₀O₃ should decompose thermally to form c,c-C₇₀O epoxide as the final product while for the other studied ozonides the preferred reaction channel seems to be the one leading to the structures with O₂ moiety entrapped over the C–C bonds adjacent to the C–O–C group. Hypothetical oxidoannulene form of c,c-C₇₀O is not related to a clear minimum on the free energy surface.

Słowa kluczowe

ozonide, epoxide, oxidoannulene, carbonyl oxide, DFT

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