



Density functional theory based molecular dynamics simulations of C₇₀O₃ doped with light molecules.

Autorzy

Andrzej Bil

Zdzisław Latajka

Carole A. Morrison

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Streszczenie

We demonstrate that light molecules such as H₂, N₂, H₂O, NH₃, BH₃, CH₄, and HCl can move freely inside C₇₀ in the space roughly defined between planes of d-type carbon atoms. Contrary to that, two H₂ molecules, when inserted into C₇₀, do not cross the equatorial plane of the fullerene. The enthalpy of the ozone ring opening in C₇₀O₃ monoozonide doped with light molecules depends little on the identity of the guest. Surprisingly, two H₂ molecules inside the cage modify the relative stability of the C₇₀O₃ isomer series by some 3.5 kcal mol⁻¹.

Słowa kluczowe

Fullerene, endohedral guest, ozonide, reaction mechanism

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