Understanding the molecular mechanism of the chlorine atom transfer between ammonia and hypochlorous acid with electron localisation function (ELF).

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Streszczenie

The nature of the chlorine atom transferred between ammonia and hypochlorous acid was investigated using the bonding evolution theory (BET). The application of topological analysis of electron localisation function (ELF) and Thom's catastrophe theory enabled a detailed description of the evolution of chemical bonds and non-bonding electron density. The BET analysis was performed at the DFT(MN15)/def2-TZVPPD computational level. The Hausdorff distance was used as a qualitative view on the evolution of the ELF field. The molecular mechanism of the chlorination reaction consisted of 11 structural stability domains (SSDs) and 10 ELF catastrophes. Four SSDs were observed before the transition state (TS). The TS was found in SSD V, and six SSDs were distinguished after the TS. The energy barriers were analysed with six different DFT functionals (B3LYP, CAM-B3LYP, LC-ωPBE, M11, MN15, ωB97XD) and def2-TZVPPD basis set. The energy barrier between transition state and reagents was smaller than transition state and products, thus the chlorination of ammonia is thermodynamically favourable. Alongside BET analysis, NPA (natural population analysis), AIM (atoms in molecules) and APT (atomic polar tensor) charge analysis was also applied to the transferred chlorine atom.

Słowa kluczowe

BET, ELF, ammonia, hypochlorous acid, Hausdorff distance

Adres publiczny

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