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Role of Solvent and Noncovalent Interactions in Alkaline Reactivity of Strained and Strain-Free Macrocyclic Disulfides

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Streszczenie

This study employs ab initio molecular dynamics simulations to investigate the impact of solvent and non-bonded interactions on the structure-reactivity relationship of both strain-free and strained macrocyclic disulfides. Our findings reveal that interactions with water as a solvent significantly influence the minimum energy geometry structures of both conformers of the studied macrocycle. In particular, our simulations identify short contacts, specifically S···π-aromatic interactions, which suppress reactivity for the strained isomer by obstructing the reaction cone at the minimum free energy. Surprisingly, the free energy barriers for the disulfide reaction with a simple nucleophile (OH- anion) remain very similar, despite one conformer having a markedly more strained disulfide bond than the other. Enhanced molecular dynamics simulations in explicit solution elucidate this apparent contradiction by revealing different solvent exposures of the two sulfur atoms in the macrocycles.

Słowa kluczowe

disulfide reduction, meta-dynamics, ab initio molecular dynamics, macrocycle, solvent exposure

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