

Unclicking the click : metal-assisted mechanochemical cycloreversion of triazoles is possible.

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The mechanochemical cycloreversion of 1,2,3-triazole compounds, which serve as unusually stable building blocks in materials and biomolecular chemistry as a result of mild "click chemistry", remains puzzling. We show that the hitherto discussed straight-forward retro-click mechanism of the 1,4-disubstituted isomer, even if Cu^I catalyzed, can be ruled out in view of more favorable activation free energies of destructive pathways. In stark contrast, the 1,5-regioisomer can undergo cycloreversion under rather mild mechanochemical conditions owing to its favorable response to the external force in conjunction with standard Ru^{II} catalysis.

Słowa kluczowe

click chemistry, computational chemistry, mechanochemistry, reaction mechanisms, triazole

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