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Dynamic intramolecular rearrangements with proton transfer in methanimine oxide

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Abstract

The structures of possible intermediates and transition states on the potential energy surface for the isomerization of methanimine oxide into formamide were determined by UHF/6-311G(3d) quantum-chemical calculations. Two possible reaction channels were revealed. The same processes were studied by the direct molecular mechanics method which also revealed two reaction channels. The time range of the examined dynamic processes was estimated at 90-300 fs.

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