The synthesis of pyrrole from C4-olefinated isoxazole catalyzed by ruthenium: a DFT study

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Abstract

The mechanisms of ruthenium-catalyzed synthesis of pyrrole from C4-olefinated isoxazole were investigated by employing the density functional theory (DFT) calculations. Three main steps are included in this reaction: N-O cleavage, 1,5-cyclization, and H-transfer steps. The H-transfer is calculated to be the rate-determining step. The role of Cu(OAc)2 employed in this reaction is to supply HOAc molecule to facilitate the H-transfer step.

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