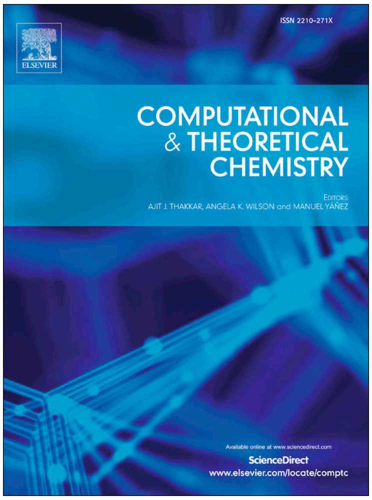

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Ab initio and DFT investigations on the ring opening of aziridines using singlet unsaturated carbenes

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Abstract

cis-2,3-dimethylaziridine undergoes ring cleavage with unsaturated carbenes to yield corresponding olefins. Ab initio and density functional investigations of this ring opening reaction show that this reaction takes place in a single step. Initially the reactants form a pre-reactive complex, followed by a transition state which gives alkene with the same stereochemistry. Computations suggest that the asynchronous concerted cleavage of C-N bonds leads to retention of stereochemistry. Intrinsic reaction coordinate analysis and Wiberg bond order analysis reveal the asynchronous nature of the transition state very well and fix the reaction mechanism. Substitution of groups at R_3 and R_4 of carbene carbon predict the same trend. The higher exothermicity observed in the reaction indicates the release of ring strain.

Keywords: *cis*-2,3- dimethylaziridine, ab initio and DFT, methylidenecarbene, ring opening, stereochemistry, deamination

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