

Theoretical Studies of the Schizophrenic Effects of Geminal Fluorination on Organic Reactions: Explanations and Predictions

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Experiments by Dolbier and coworkers have found that geminal fluorination has a large effect on lowering the barrier to *cis*–*trans* isomerization of 1,2-dimethylcyclopropane and an even larger effect on lowering the barrier to racemization of optically active 1-ethyl-2-methylcyclopropane. In contrast, Dolbier has found that geminal fluorination has almost no effect on the barrier to rearrangement of methylenecyclopropane; and Lemal and coworkers have shown that geminal fluorination actually stabilizes [2.2.2]propellane toward ring opening and bicyclo[2.2.0]hex-1(4)-ene toward dimerization. In order to understand these very different effects of geminal fluorination, *ab initio* calculations have been performed and, from the results, explanations proposed and experimentally testable predictions made.