A DFT Study on the Stepwise Fluorinated Methylenecyclopropane ⇌ 1-Methylcyclopropene System

Salim M. Khalil

Chemistry Department, School of Basic Science, Academy of Graduate Studies,
P. O. Box 79031, Tripoli, Libya

Reprint requests to S. M. K.; E-mail: salimkhalil2002@yahoo.com

Z. Naturforsch. **63a,** 42 – 48 (2008); received July 5, 2007

Density functional theory (DFT) calculations have been performed to calculate the optimized geometries of stepwise fluorinated methylenecyclopropanes and 1-methylcyclopropenes. Increasing the number of fluorine atoms caused a destabilization of methylenecycopropane. Perfluorinated 1-methylcyclopropene was found to be present in substantial concentration. This is supported by calculations of the Gibbs free energy, isodesmic reactions and orbital energies (HOMO-LUMO). These results are compared with the fluorinated cyclopropanes keto-enol system. Enthalpies, entropies and dipole moments are reported.

Key words: Cyclic Alkene; Tautomerism; Fluorinated Cyclic Alkene; DFT.