A Theoretical Study of Substituted Stepwise Fluorinated Cyclopropanone Keto-Enol System

Abdullah El-Alali, Ali A. Marashdeh, and Salim M. Khalil

Chemistry Department, College of Science, Mutah university, Karak, Jordan

Reprint requests to Prof. S. M. K.; e-mail: qukhalil@mutah.edu.jo

Z. Naturforsch. **58a,** 749 – 755 (2003); received September 24, 2003

MINDO-Forces calculations have been performed with complete optimization of the geometries on stepwise fluorinated cyclopropanones and their enols. Increase in the number of fluorine atoms causes destabilization of cyclopropanone. Perfluorinated enol was found to be present in substantial concentration, as was mentioned in previous work. This is supported by calculations of Gibbs free energies and isodesmic reactions. Geometrical parameters, heats of formation, electron densities, dipole moments and orbital energies (HOMO-LUMO) are reported.

Key words: Fluorinated Cyclopropanone; Keto-enol.