Iranian Journal of Organic Chemistry IranJOC Vol.1, No.1, 2009 **Contents Graphical Abstracts** AIM analysis for the ylide rotamers from the reaction between pp 5-8 triphenylphosphine and dialkyl acetylenedicarboxylates in the presence of 2-pyrrolecarbaldehyde Sayyad Mostafa Habibi Khorassani,^{*} Ali Ebrahimi, Malek Taher Maghsoodlou, Pouya Karimi, Mohammad Amin Kazemian Department of Chemistry, University of Sistan and Balouchestan, P.O. Box 98135-674, Zahedan, Iran PPh₃ + ROOC — COOR + N-H -COOR PPh. R= Me. t-Bu H i RO RO (OR Ph.F (E)-4a(Z)-4aThe synthesis and conformational studies of 9-monosubstituted-10-chloro-9Hpp 9-12 cyclohepta[def]phenanthrene Saeed Taghvaei-Ganjali,^{a*} Reza Zadmard,^b Barsam Mirfattah,^a Shamimeh Seifi^b ^aDepartment of Chemistry, Islamic Azad University, North Tehran Branch, P.O.Box: 15875-5981, Tehran. Iran ^bChemistry and Chemical Engineering Research Center of Iran, P.O.Box: 14335-186, Tehran, Iran NH2CH2COOH Trichloromelamine and Triphenylphosphine as a versatile and efficient system pp 13-17 for oxidation of alcohols under solvent-free condition Bi Bi Fatemeh Mirjalili,^{a*} Abdolhamid Bamoniri,^b Mohammad Ali Amrollahi,^a Ebrahim Dastan^a ^aDepartment of Chemistry, College of Science, Yazd University, P.O. Box 89195-741, Yazd. Iran ^bDepartment of Chemistry, College of Science, University of Kashan, Kashan, Iran. CHOH $\xrightarrow{\text{TCM}}_{\text{PPh}_3, \text{Base}} \xrightarrow{\kappa_1}_{\text{Ph}} C=O$ R₁=Ar, R, H

Theoretical investigation of the interaction between glycine amino acid and fullerenes pp 19-23

K. Zare,^a M. D. Ganji^{b*}

^aDepartment of chemistry, University of Shahid Beheshti, Tehran, Iran ^bDepartment of Chemistry, Islamic Azad University of Ghaemshahr, Mazandaran, Iran

In this paper, the possibility of the formation of glycine– C_{60} and glycine– C_{80} complexes were investigated by the Density Functional based Tight Binding (DFTB) treatment. It was found that the binding of glycine to C_{80} generated the most stable complexes via its amino nitrogen active site. We have also tested the stability of these complexes with density functional based tight binding molecular dynamics simulation which have been carried out at room temperature. These indicate that proteins might be able to form stable bindings to fullerenes, especially C_{80} , via their active sites.



