Superacid Mediated Hydroxyalkylation Reaction of 1,2,3-indanetrione.

A Theoretical Study.

Daniel Romero Nieto, Mikhail G. Zolotukhin, Lioudmila Fomina and Serguei Fomine*

Instituto de Investigaciones en Materiales Universidad Nacional Autonoma de Mexico,
Apartado Postal 70-360, CU, Coyoacan, Mexico DF, 04510, México. E-mail: alit_3@yahoo.com.mx

Abstract:

Energies of mono- and multiprotonation for 1,2,3-indanetrione and ninhydrin in triflic acid media were estimated at PBE0/aug-cc-pvtz//6-31+G** level of theory. The reactivity of formed intermediates in the reaction of aromatic electrophilic substitution has been studied at the same level of theory. It appears that basidity of carbonyl groups in 1,2,3-indanetrione is extremely low due to mutual influences of carbonyl groups. Carbonyl 2 is the least basic but the most reactive in accordance with experiment. Calculations demonstrate that monoprotonated intermediates are the principal reactive species in the reaction of hydroxyalkylation of 1,2,3-indanetrione in triflic acid. New isomerization mechanism of 2,2-diaryl-1,3-indanediones to 3-(diaryl)methylene)isobenzofuranones in triflic acid media involving only monoprotonated intermediates which agrees with experimental and theoretical data has been proposed.