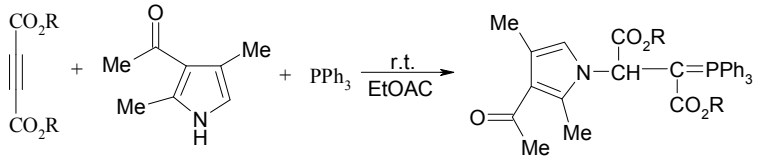
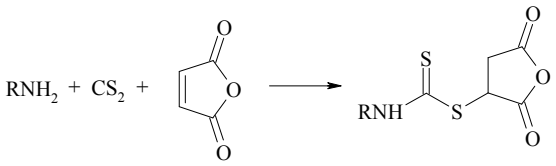
Iranian Journal of Organic Chemistry

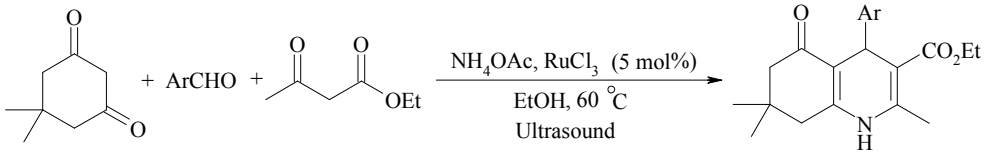
IranJOC Vol.1, No.4, 2009

Contents

Graphical Abstracts







Pure spirooxindol was synthesized and studied by both the experimental and calculation methods of NMR and X-ray spectroscopy. Theoretical methods of substantial quality can be used to calculate NMR data using the gauge including atomic orbital (GIAO) method, yielding data comparable with those of the experiment. *ab initio* and DFT calculations of ^{13}C and ^{1}H NMR chemical shifts of the Novel Spirooxindol Compound were reported. The structure of this molecule at first was optimized with the Gaussian 03 program. After the optimization, ^{13}C and ^{1}H chemical shifts were calculated with GIAO method, using corresponding TMS shielding calculated at the same theoretical levels as the reference. Calculations have been performed with using three different basis sets: 6-31G, 6-31G(d,p) and 6-31+G(d,p) at HF and DFT levels of theories. The results, especially for ^{13}C chemical shifts are in agreement with the experimental values of NMR. In this work the bond lengths of the Spirooxindol was calculated and the results compared with those of the experimental data obtained by X-Ray crystallography. All the computations were done using an IBM x225 Xeon computer that has 2048 MB ram.