

عنوان مقاله:

AIM analysis for the ylide rotamers from the reaction between triphenylphosphine and dialkyl acetylenedicarboxylates in the presence of 2-pyrrolicarbaldehyde

محل انتشار:

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خلاصه مقاله:

A facile synthesis and kinetic investigation of the reaction between triphenylphosphine 1, dialkyl acetylenedicarboxylates 2 and 2- pyrrolicarbaldehyde 3 (as a NH-acid) have been earlier reported[1], [2] and depicted in Figure 1. Recently, different reports have been published on the synthesis of stable phosphorus ylides from the reaction between triphenylphosphine and reactive acetylenic esters in the presence of N-H, C- or S-H heterocyclic compounds.[3], [4] These ylides usually exist as a mixture of two geometrical isomers, although some ylides exhibit one geometrical isomer. It is important to remember that in medicinal chemistry sometimes only one of the two geometrical isomers shows biological and pharmacological activity. For this reason quantum mechanical calculations have been performed in order to gain a better understanding of most important geometrical parameters and also relative energies of both geometrical isomers in the case of ylides which have two or only one geometrical isomer. The Z and E isomers were optimized for all ylide structures at HF/6-31G level of theory by Gaussian 98 package program.

کلمات کلیدی:

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