Wittig reaction essay

ObjectiveTo synthesize 3-phenylpropenoic acid from Wittig reaction.

IntroductionThe Wittig reaction is a chemical reaction of an aldehyde or ketone with a triphenyl phosphonium ylide (often called a Wittig reagent) to give an alkene and triphenylphosphine oxide. Wittig reaction is widely used in organic synthesis for the preparation of alkenes. Scheme 1Triphenylphosphine (1) reacts with an alkyl halide (2) to form a phosphonium halide (3). Subsequently, addition of a strong base eliminates the hydrogen halide to form an ylide, alkylidenephosphorane (4).

Scheme 2The carbon of the ylide acts as a nucleophile and adds to the carbonyl group (5) to form a betaine intermediate which undergo an in situ 1, 2-elimination to give the triphenylphosphine oxide (6) and an alkene (7) as the product. Scheme 3Triphenylphosphine react with methyl bromoethanoate to form phosphonium salt. Addition of NaOH eliminates the hydrogen halide to form ylide, methyltriphenylphosphoranyl-ethanoate. Ester formed from the reaction of the ylide, methyltriphenylphosphoranyl-ethanoate (9) and benzaldehyde. (E)-3-phenylpropenoate (10) which is formed then hydrolyzed with base and 3-phenylprepenoic acid (11) is then isolated as crystalline solids.

Results & Calculations(I) Preparation of triphenylphosphoranyl ethanoate (4) from methoxycarbonyl – methylenyltriphenylphosphonium bromide. Mass of triphenylphosphine= 5. 00gNumber of mol of triphenylphosphine= 5. 00 g262. 3 g/mol = 0.

019 molMass of methyl bromoethanoate = 3. 00gNumber of mol of methyl bromoethanoate= 3. 00 g152. 98 g/mol = 0.

0196 mol1 mol of triphenylphosphine = 1 mol of methyl bromoethanoate0. 019 mol of triphenylphosphine = 0. 019 mol of methyl bromoethanoate? triphenylphosphine is limiting reagent. Mass of phosphorium salt (Theoretical)= 0.

019 mol x 415. 23 g/mol= 7. 92 gMass of plastic= 0. 57 gMass of plastic + phosphorium salt= 4.

65 gMass of...