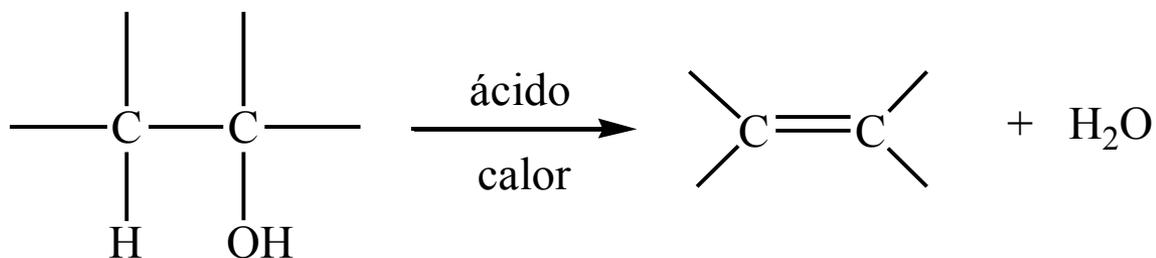


OBTENÇÃO DE ALCENOS

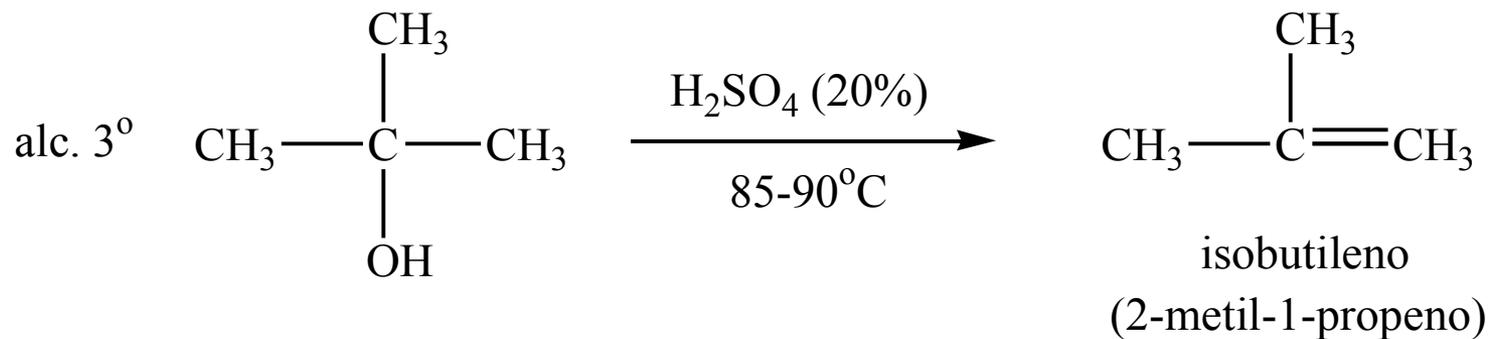
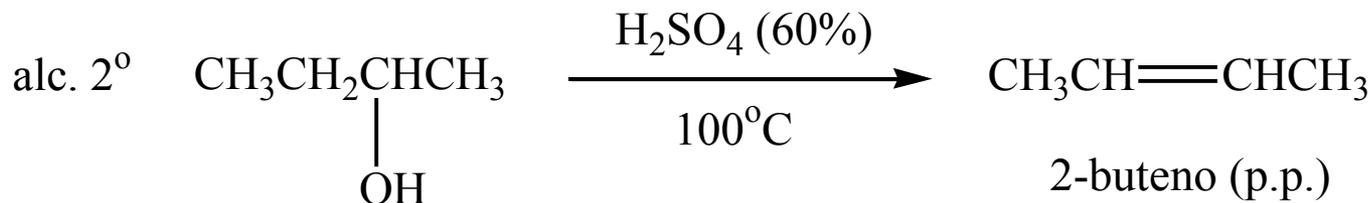
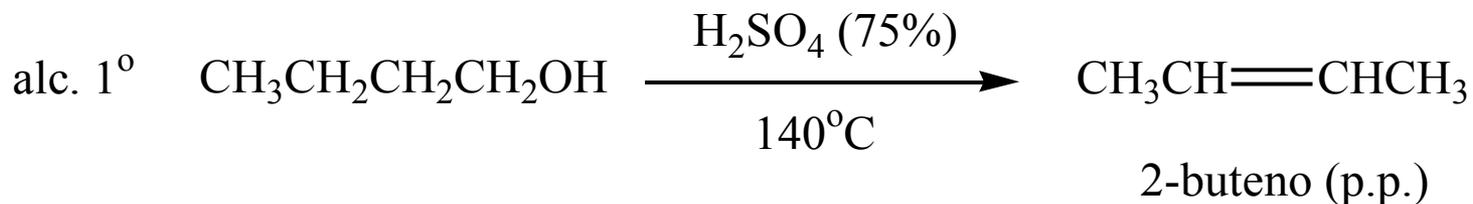
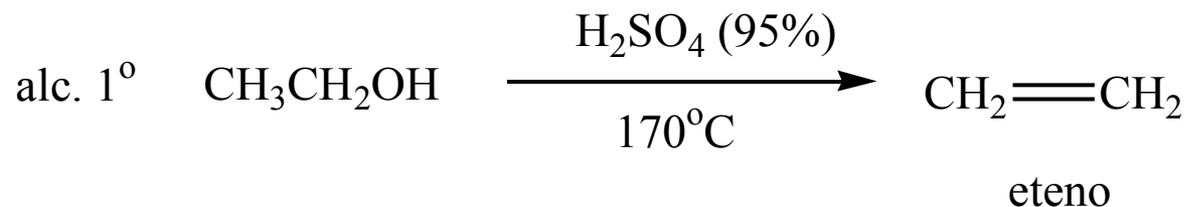
Eliminação 1,2 (β -eliminação)

1. Desidratação de alcoóis



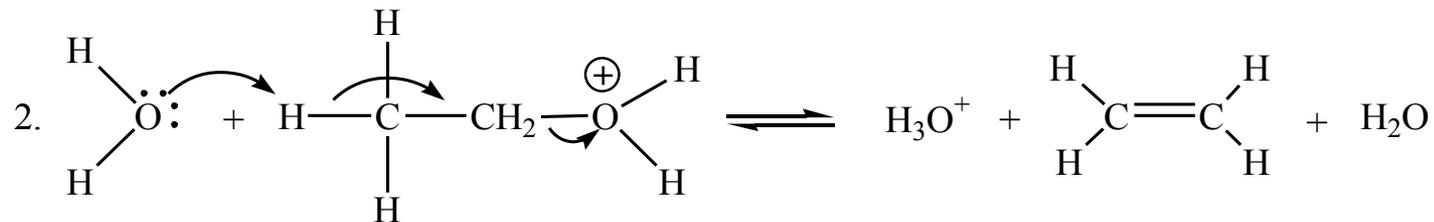
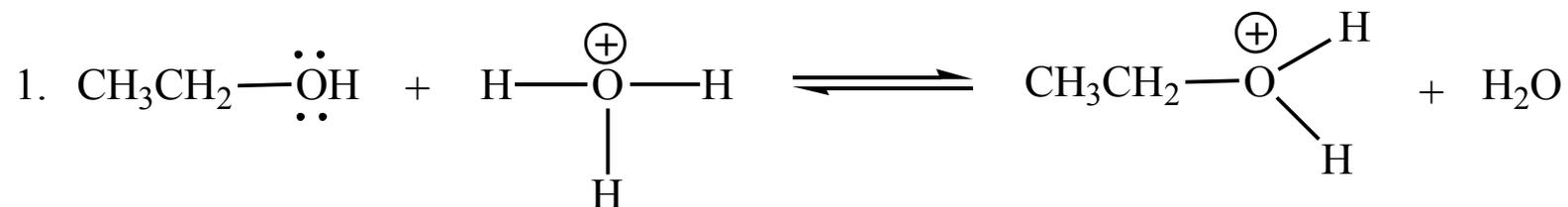
Ordem da facilidade de desidratação: $3^\circ > 2^\circ > 1^\circ$

Exemplos:



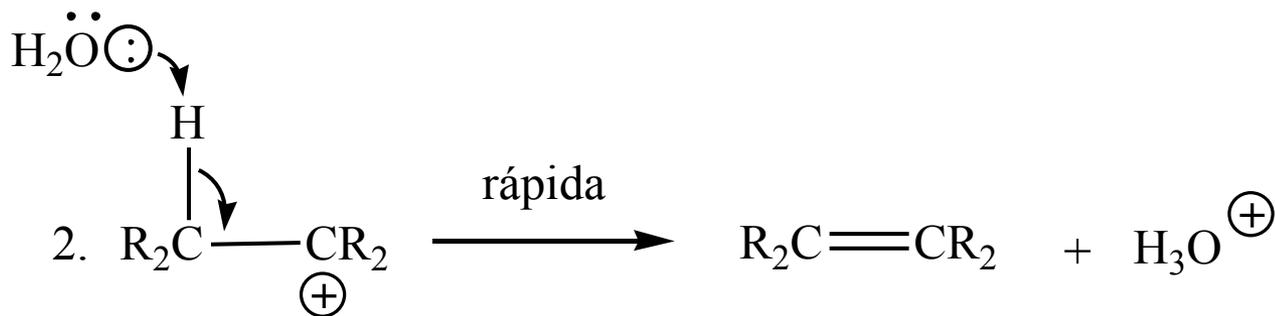
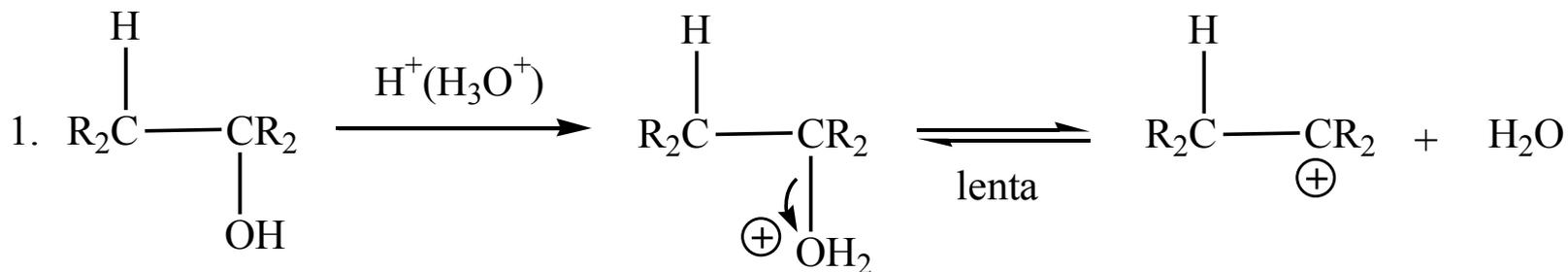
Mecanismo de desidratação de álcoois 1^{os} não ramificados

Mecanismo tipo E₂

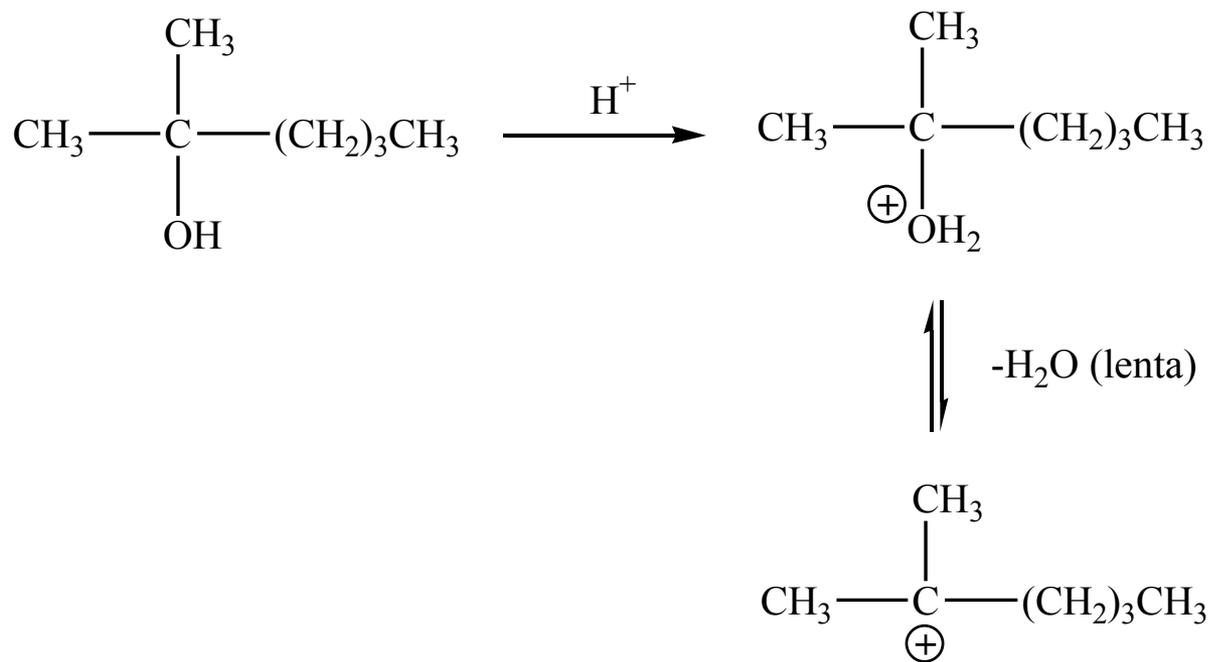


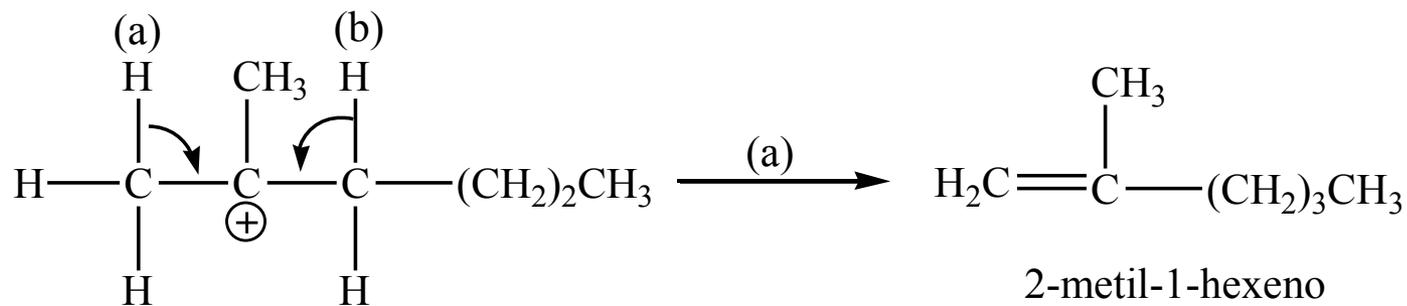
Alcoóis ramificados

Mecanismo E₁

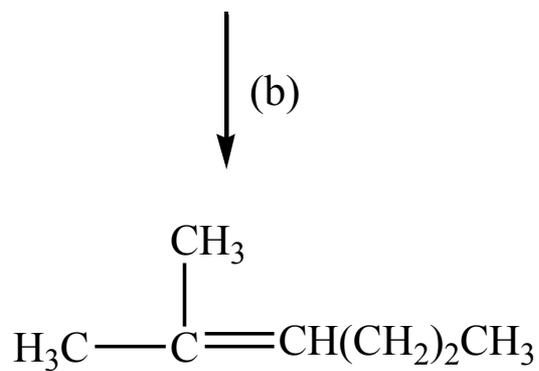


Exemplo:





~20%



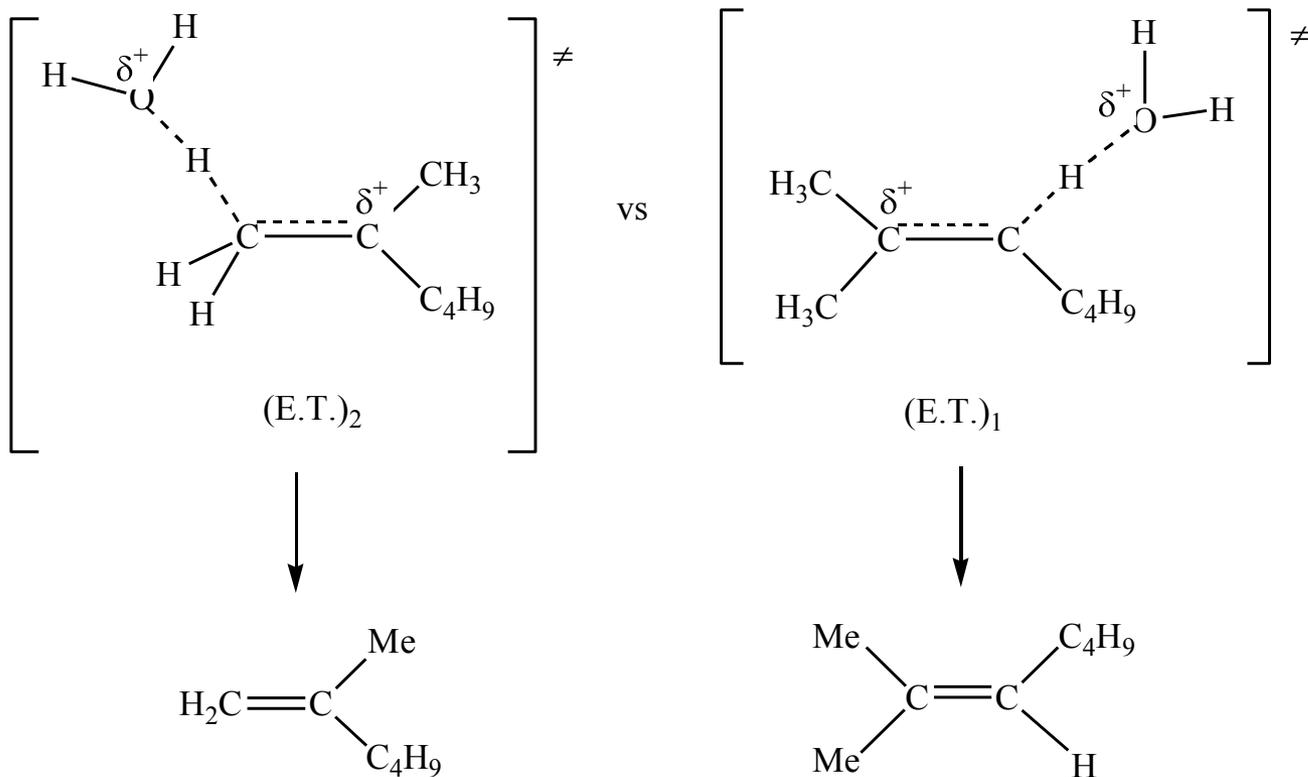
2-metil-2-hexeno
(produto principal)

~80%

Porque???

ESTADOS DE TRANSIÇÃO

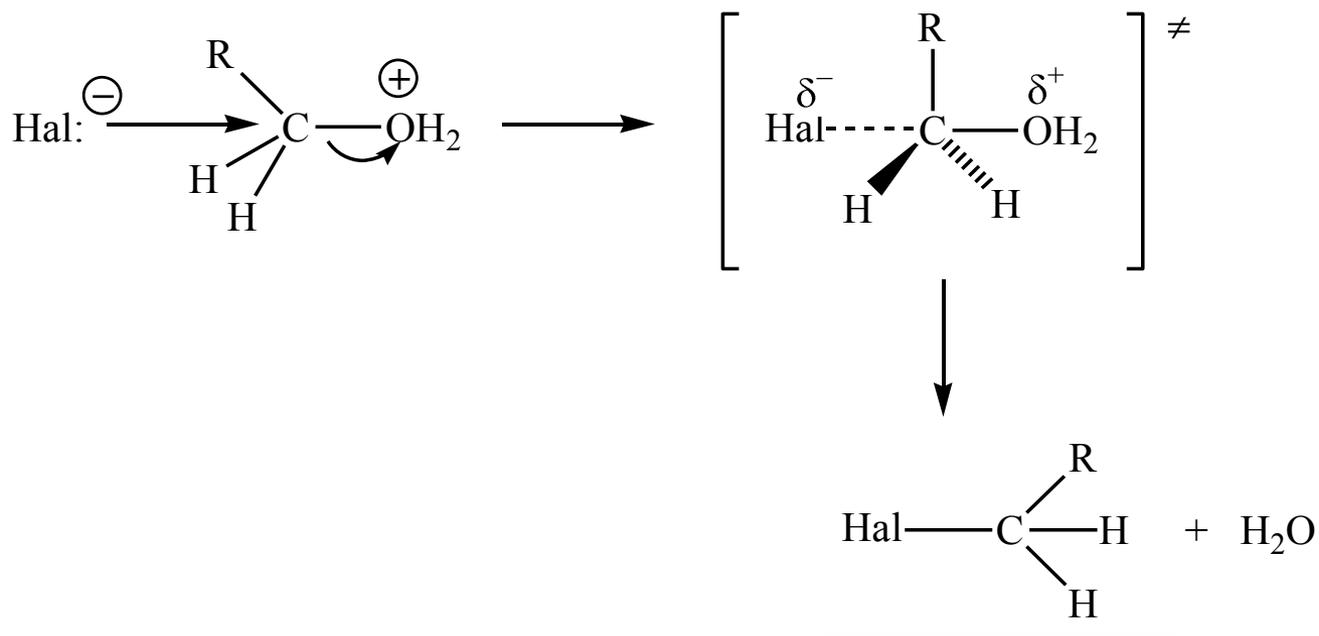
Regra de Saytzeff (Zaitzev)

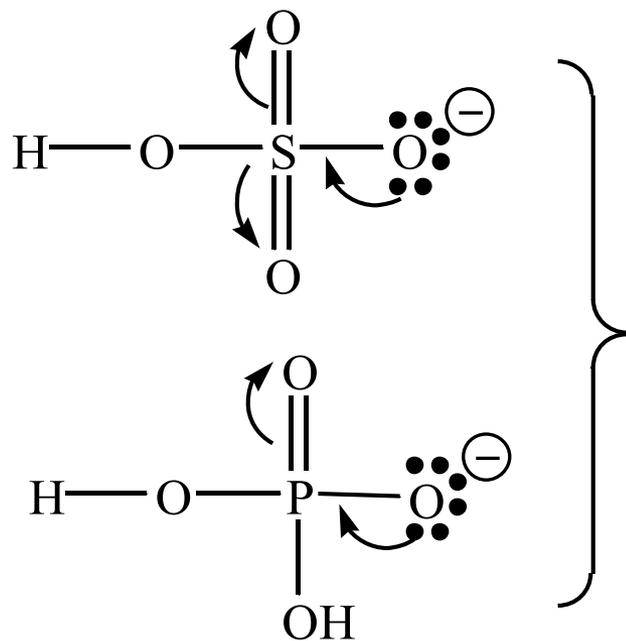


Qual E.T. é o mais estável e porque??

Por que na obtenção de alcenos via reação de desidratação de alcoóis não são empregados ácidos halogenídricos concentrados, mas sim H_3PO_4 de (85%) ou H_2SO_4 (98%)??

Exemplo:



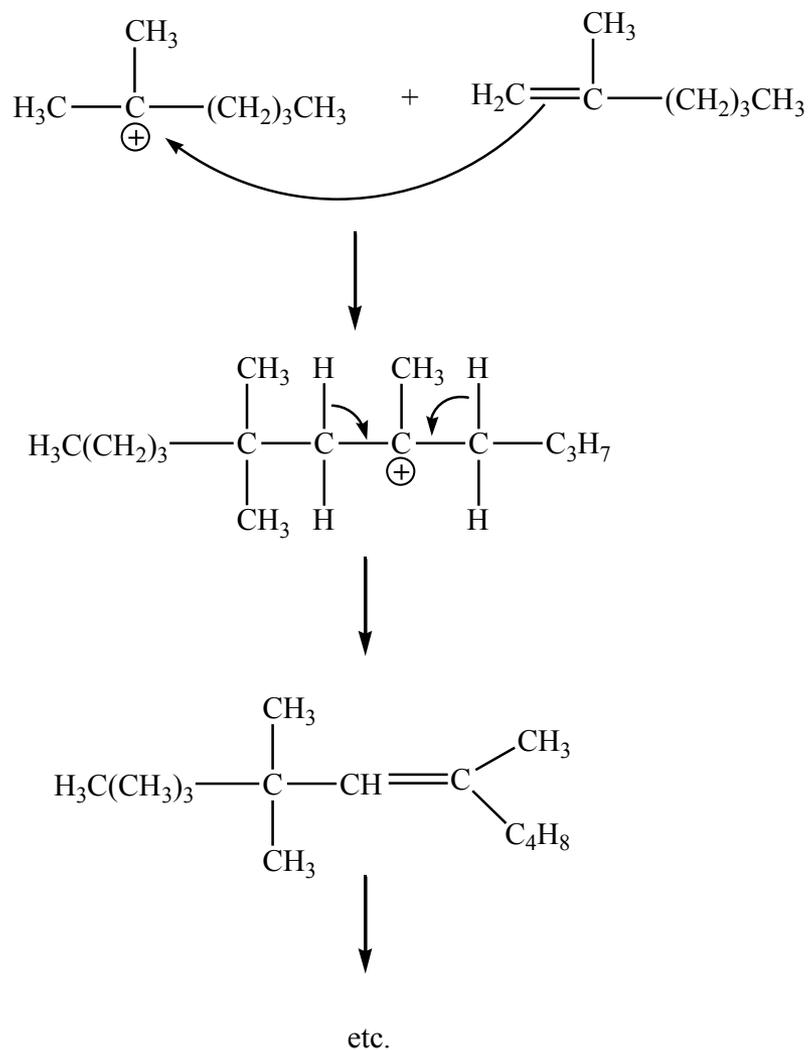


São fracos nucleófilos

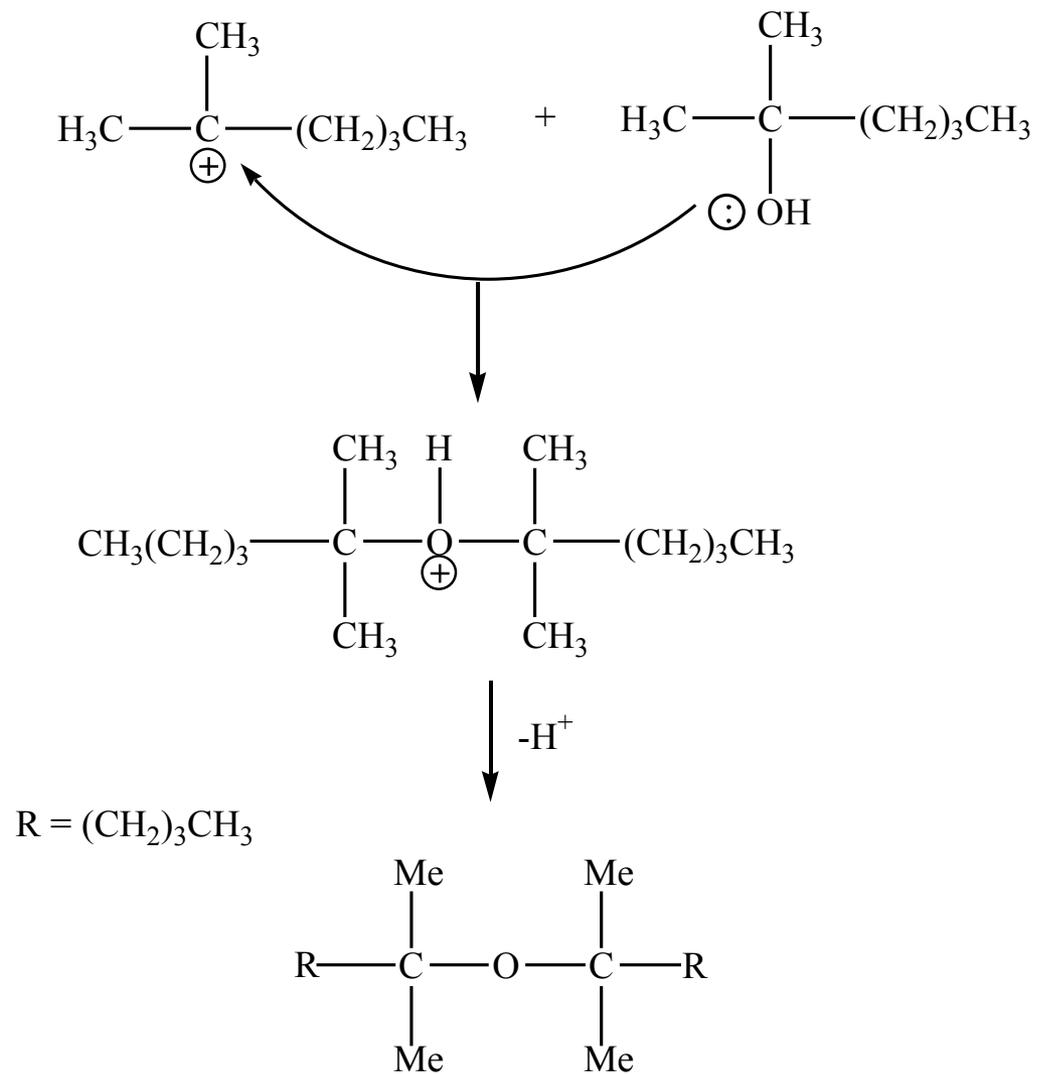
e a reação de $\text{S}_{\text{N}}2$ ocorre em
menor extensão (ou não ocorre)

Reações secundárias que podem ocorrer no caso da formação de carbocátion:

1. Dimerização e eventual polimerização:

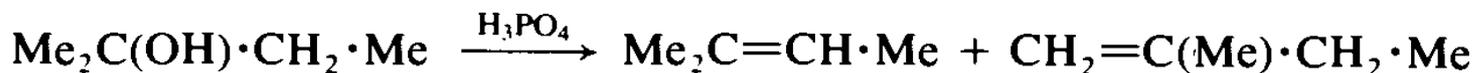


2. Obtenção de éter:

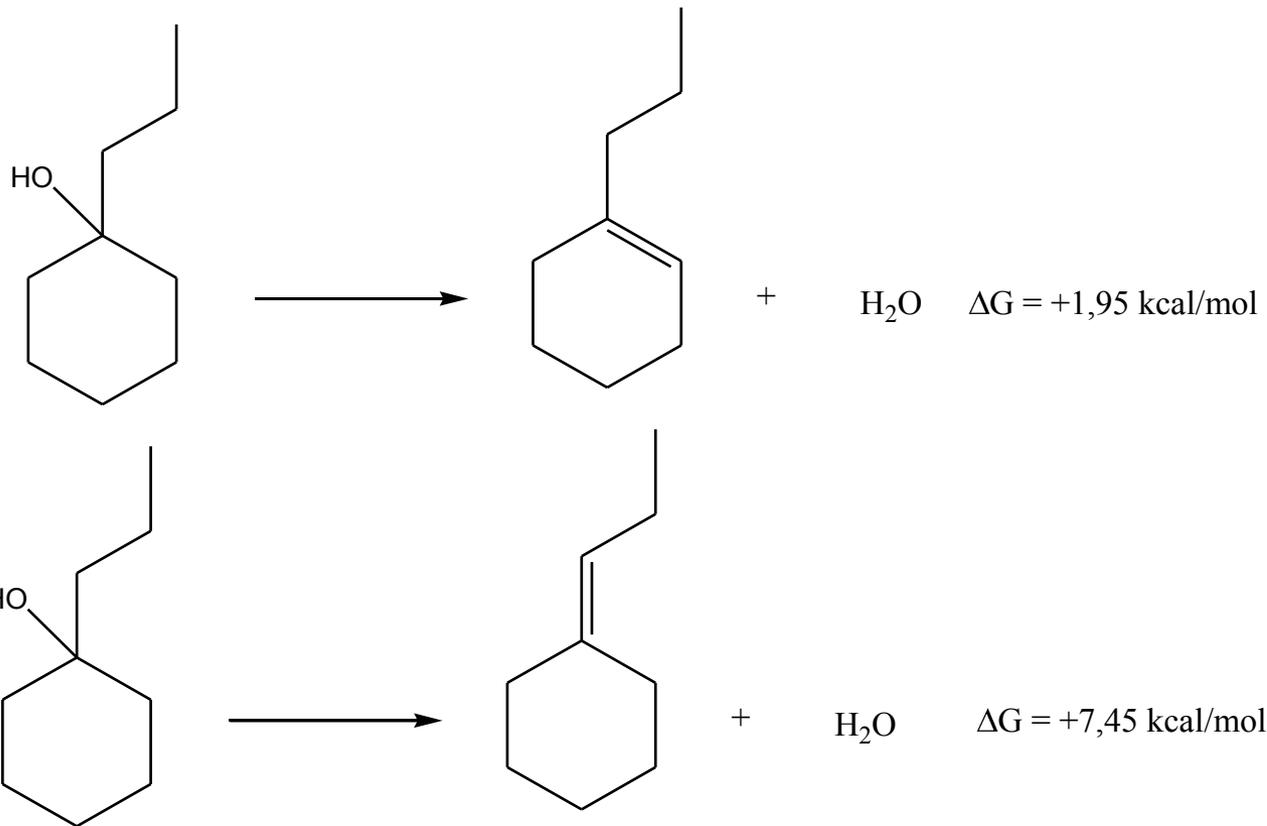


Eliminação de água a partir de 1-butilciclo-hexanol

Experiment 5.12 2-METHYLBUT-2-ENE (*in admixture with 2-METHYLBUT-1-ENE*)



Place 25.0 g (31 ml, 0.28 mol) of 2-methylbutan-2-ol and 10 ml of 85 per cent orthophosphoric acid in a 100-ml, round-bottomed flask and swirl to mix thoroughly. Fit the flask with a 20-cm fractionating column filled with glass helices, a Claisen still-head and a condenser leading to a 50-ml receiving flask cooled in a beaker of iced water (Fig. 2.104). Add a few pieces of porous porcelain and heat the reaction mixture gently with a Bunsen burner. Collect the alkene fraction which distils in the range 35–38 °C during a period of 30 minutes. Dry the distillate with 1–2 g of magnesium sulphate. Wash and dry the distillation apparatus, decant the dried distillate into a 50-ml flask and redistil in the reassembled apparatus. Collect the fraction boiling at 37–38 °C; the yield is 12.5 g (64%). Record the infrared spectrum of the product using a fixed path-length cell (0.025 mm). The stretching bands of the terminal (1645 cm⁻¹) and non-terminal (1670 cm⁻¹) carbon–carbon double bonds can both be observed; bands at 890 and 805 cm⁻¹ (=C–H deformation) also establish the presence of both terminal and non-terminal olefinic systems. Analyse the product by g.l.c. on a Silicone oil column at 30 °C; 2-methylbut-1-ene appears first, closely followed by 2-methylbut-2-ene; the areas under the peaks are in the ratio of 1:4.



Resultados calculados em B3LYP/6-31G(d,p), sendo $\Delta G = \Sigma G_{\text{prod}} - \Sigma G_{\text{reag}}$

Energia Livre do *exo* é $5,5 \text{ kcal.mol}^{-1}$ maior que do *endo*

Execução do Experimento em 16 de Novembro 2015 (2ª feira)

Lab. A:

04; 08; 12; 16; 20; 24; 28; 32; 36; 40.

Lab. B:

44; 48; 52; 56; 60; 64; 68; 72; 76; 78.

Execução do Experimento em 17 de Novembro 2015 (3ª feira)

Lab. A:

02; 06; 10; 14; 18; 22; 26; 30; 34; 38.

Lab. B:

42; 46; 50; 54; 58; 62; 66; 74; 80.