醇到鹵烷的轉換

SN2 Reaction

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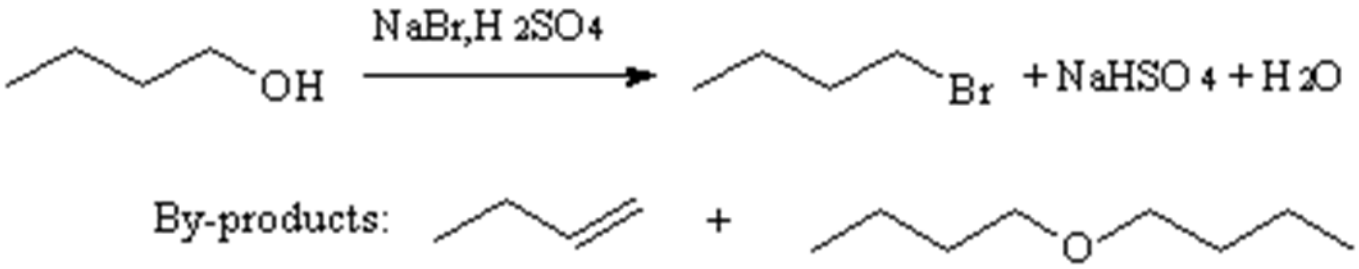
原　理

1. The S_N2 reaction : (sp^3 atom only)



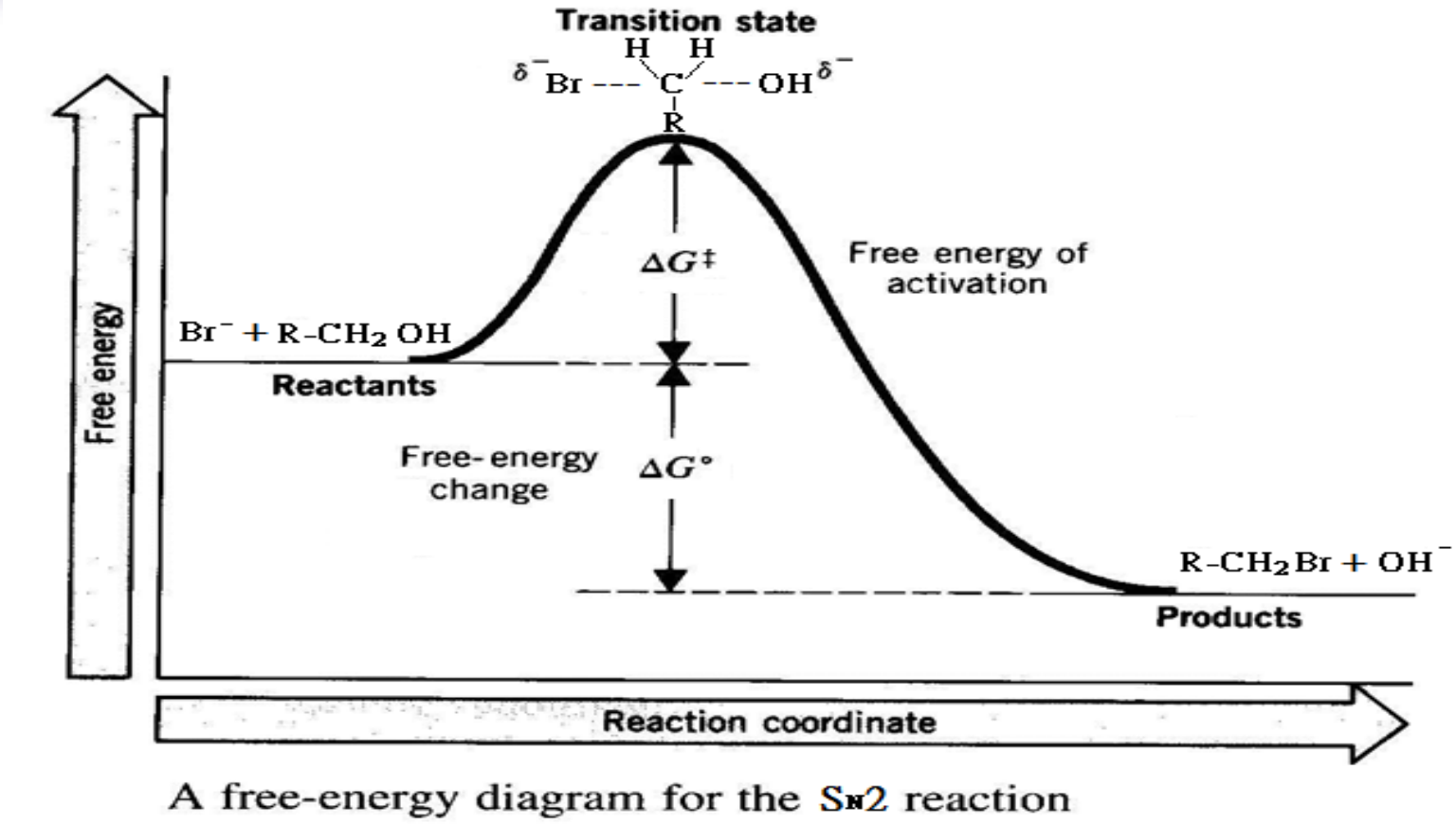
2. Nucleophile : Br^- ; Leaving group : $-OH_2$

3. Relative nucleophilicity in protic

$^-SH > {}^-CN > I^- > {}^-OH > N3^- > Br^- > CH_3CO_2^- > Cl^- > F^- > H_2O$

原　理

S_N2 Reaction



A free-energy diagram for the S_N2 reaction

Reaction rate for S_N2 : $CH_3X > 1^o > 2^o > 3^o$

合 成 步 驟

6.65g NaBr + 7.5mL H_2O + 5mL n-butyl alcoho
in 50mL R.B. flask

↓ (ice-water bath)

add 5.75mL conc. H_2SO_4 (dropwise)

↓

reflux for 30 min (stirring bar)

↓

cool the flask near the room temp.

↓

distillation

↓

collect all the distillate (5~10mL)

純 化 步 驟

pour the distillate into the separatory funnel that contains 5mL H_2O

↓(shake and pour the organic layer)

wash with the 10mL 10% $NaHSO_{3(aq)}$

↓(shake and pour the organic layer)

wash with the 5mL conc. H_2SO_4 (carefully)

↓(shake and pour the upper layer)

wash with the 10mL 10% $NaOH_{(aq)}$

↓ (shake and pour the organic layer)

wash with the 10mL H_2O

↓ (shake and pour the organic layer)

純 化 步 驟

dry it with $MgSO_{4(anhy)}$

↓

filter and collect the filtrate

↓

distillation (不做)

↓

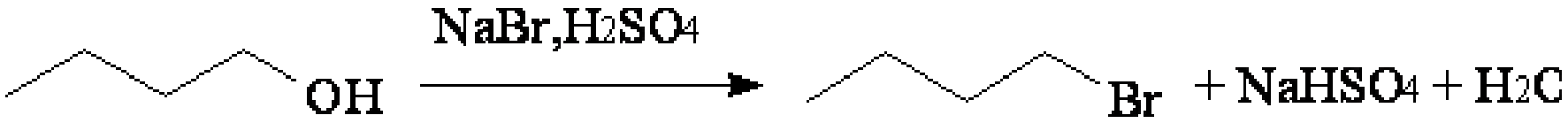
collect the b.p.=99~103℃ material (不做)

↓

weight (過濾前收集瓶先烘乾、秤重)

產 率 計 算

Calculate the % yield :



量取 5.0mL
Mass: 4.05 g
MW:74.12 g/mol
mole數= 0.0546 mol
NaBr: 0.0646 mol

理論mole數 = 0.0546 mol (∵係數比 1:1)
MW: 137.03 g/mol
理論產量: 7.48 g
實際產量: 5.00 g
%yeild = 66.84%

Check out

1. 繳交產物並告知產物淨重。

2. 實驗問題：3, 4, 5

The End !

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