**supplement #14: *ELMINATION PATHWAYS***

***CHEMISTRY 3514 Alfred State College***

 **H X**

**| |**KOH or KOR /CCl4 or ROH (solvent)

 ***DEHYDROHALOGENATION:* C-C --------------> C=C**

E1 VS E2-the facts β α

**action or effect E11 E2 (main route)**

**[substrate] increased** Rate increases Rate increases

**[OH-] increased** No Effect On Rate Rate Increases

**Rearrangement ?** YES NO

**Primary H effects ?** NO YES

**halogen (`element’) effect** RI>RBr>RCl>RF RI >>RBr>>RCl>>RF

**on rate ~(25,000:500: 10:1) relative rates**

**effect of order\* on rate** 3o >2o >10 3o >2o >1o

(\*order of α carbon)

**product alkene distribution** follows Zaitsev Rule follows Zaitsev Rule

1(happens **only** if no OH‑)

*other `facts’ on dehydrohalogenation of an alkyl halide:*

0) βC must have at least 1 H for E2; E1 happens even without β-H

1) OH- is consumed

2) E2 is generally the favored route. E1 seen

***The Mechanisms:***(new C—C π bond forms)

 **| | | | | |**

E2: OH- + -C-C- --> -C-C- -------------> -C=C- + H2O + X-

 *one step*  **| |** (C-X breaks)

H XH[+]X(-)

 **OH[-] *both leave ~ simultaneously***

 (C-H breaks)

  *transition state*

 **β position**

 **H OH**

**| | *H+*** (acid)

 ***DEHYDRATION:* C-C --------------> C=C**

E1 VS E2-The facts β α

**action or effect E1 (main route) E2**

**[substrate] increased** Rate increases Rate increases

**[H+] increased**  Rate increases Rate Increases

**Rearrangement ?** YES NO

**Primary H effects ?** NO YES

**effect of order\* on rate** 3o >2o ; both go E1 1o  prefers E21

(\*order of α carbon)

**product alkene distribution**  follows Zaitsev Rule follows Zaitsev Rule

***other `facts’ on dehydration***

0) β C doesn’t need H for E1 to run

1) H+ is NOT consumed

2) E1 is ALMOST always the favored route

3) carbocation can also undergo substitution (a competitive situation)

*acid catalyzed E1*

 **| | rev. | |**

 H+ + -C-C- -C-C- protonation [equilibrium step=>

  **| | | | reversible (rev.)**

**β position**H OH **H OH2 +**

 **| | | | | | fast | |**

 ***E1*** -C-C- --> -C-C- + **H2O****-**C-C------> -C=C- + H+

  **| | | + + |**

H OH2+ **H H**

  *carbocation* *rearranged carbocation*

 ***step 1 step 2***

note: when the β Carbon has no H...step 2 comes after rearrangement to a carbocation with at least one neighboring

Methyl. This explains why dehydration occurs on 2,2,4,4-tetramethyl-3-pentanol to make 2,3,4,4-tetramethyl2-pentene as its chief product.