

KEY CONCEPTS

A) MECHANISM VS. REACTION

FREE RADICAL HALOGENATION
OF A HYDROCARBON

2-11

3 STEPS!

B) CALC OF ΔH FROM B.D.E

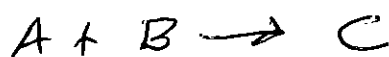
19-21

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$$\Delta H_{\text{RXN}} = \sum \text{BONDS BROKEN} - \sum \text{BONDS FORMED}$$

C) KINETICS, RATE LAWS

FOR A REACTION



$$\text{RATE} = k [A]^m [B]^n$$

DETERMINING m, n

KINETICS CONTINUED

(2)

GIVEN THE FOLLOWING EXPT. DATA

| <u>EXPT.</u> | <u>[A]</u> | <u>[B]</u> | <u>OBSERVED RATE</u> |
|--------------|------------|------------|----------------------|
| 1 | .10 | .10 | 1×10^{-2} |
| 2 | .10 | .20 | 2×10^{-2} |
| 3 | .20 | .10 | 4×10^{-2} |

DETERMINING EXPONENTS (ORDER)

FACTOR BY WHICH CONC CHANGES
RAISED TO X EQUAL TO FACTOR BY
WHICH RATE CHANGES

$$\Delta [\text{REACT}]^x = \Delta \text{RATE}$$

COMPARING EXPTS 1 AND 2

$$\Delta [B] = 2^x = 2 \quad \therefore x = 1$$

COMPARING EXPTS 1 AND 3

$$\Delta [A] = 2^x = 4 \quad \therefore x = 2$$

$$\text{RATE} = k [A]^2 [B]$$

- D) ENERGY DIAGRAMS
 TRANSITION STATES
 INTERMEDIATES
 AXES
 ΔH
 E_a

27 - 29

- E) TEMPERATURE DEPENDENCE
 OF E_a 26
 ARRHENIUS EQN. 25

⚡ WHAT EFFECT DOES
 A , E_a , T HAVE ON
 k AND WHY?

- F) STABILITY OF FREE RADICALS 36
 MOST STABLE IS BENZYL DUE TO
 RESONANCE



- G) HAMMOND POSTULATE 44

KEY CONCEPTS

A) REVIEW EM SPECTRUM 6

B) THEORY 8

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C) KEY FREQUENCIES

sp^3 sp^2 sp "

D) EXAMPLE HYDROLYZATIONS

19-21

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KETONES ALDEHYDES 21-27

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E) INDEX OF HYDROGEN DEFICIENCY
AKA DEGREE OF UNSAT'D

F) MASS SPECTROMETRY

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SPECTRUM 46

SIGNATURES 51 - 53

Br, Cl, I, ALCOHOL
63

INDEX OF HYDROGEN DEFICIENCY

$$= \frac{\# \text{ H ATOMS (REFERENCE COMPOUND)} - \# \text{ H ATOMS (COMPOUND OF INTEREST)}}{2}$$

HOW TO CALCULATE # H ATOMS IN REFERENCE

- FOR ONLY HYDROCARBON (C + H ATOMS)
= $C_n H_{2n+2}$
- FOR EACH HALOGEN (F, Cl, Br, I)
SUBTRACT ONE H FROM REFERENCE COMPD.
- FOR EACH O, Se, S, NO CORRECTION
- FOR EACH N, P, ADD ONE H TO REFERENCE COMPOUND

**IHD = NUMBER OF RINGS
AND/OR PI BONDS IN
COMPOUND OF INTEREST**

EXPT [A] OBSERVED RATE [M·A⁻¹]

1 .10 M 2×10^{-4}

2 .20 M 1×10^{-4}

$$\Delta[A]^x = \Delta \text{RATE}$$

$$2^x = \frac{1 \times 10^{-4}}{2 \times 10^{-4}} = 0.5$$

$$x = -1$$