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 23

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

C) KINETICS, RATE LAWS

FOR A REACTION

$A + B \rightarrow C$

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

DETERMINING n, m

KINETICS CONTINUED

GIVEN THE FOLLOWING EXPT. DATA

EXPT.	[A]	[B]	OBSERVED RATE
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

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

COMPARING EXPTS 1 AND 3

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

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

D) ENERGY DIAGRAMS

TRANSITION STATES
/INTERMEDIATES
AXES
ΔH
E_a

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~~6~~ WHAT EFFECT DOES

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k AND WHY?

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UNIT TWO

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INDEX OF HYDROGEN DEFICIENCY

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

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 CMPD.
- 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·s^{-1}]
1	.10 M	2×10^{-4}
2	.20 M	1×10^{-4}

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

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

$$x = -1$$