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# Collision Theory and Chain Reactions Formulas

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# List of 8 Collision Theory and Chain Reactions Formulas

## Collision Theory and Chain Reactions

1) Concentration of Radical formed during Chain Propagation Step given  $k_w$  and  $k_g$  

$$\text{fx } [R]_{\text{CP}} = \frac{k_1 \cdot [A]}{k_2 \cdot (1 - \alpha) \cdot [A] + (k_w + k_g)}$$

Open Calculator 

ex

$$0.072233\text{M} = \frac{70\text{L}/(\text{mol}\cdot\text{s}) \cdot 60.5\text{M}}{0.00011\text{L}/(\text{mol}\cdot\text{s}) \cdot (1 - 2.5) \cdot 60.5\text{M} + (30.75\text{s}^{-1} + 27.89\text{s}^{-1})}$$


2) Concentration of Radical formed in Chain Reaction 

$$\text{fx } [R]_{\text{CR}} = \frac{k_1 \cdot [A]}{k_2 \cdot (1 - \alpha) \cdot [A] + k_3}$$

Open Calculator 

ex

$$84.67037\text{M} = \frac{70\text{L}/(\text{mol}\cdot\text{s}) \cdot 60.5\text{M}}{0.00011\text{L}/(\text{mol}\cdot\text{s}) \cdot (1 - 2.5) \cdot 60.5\text{M} + 60\text{L}/(\text{mol}\cdot\text{s})}$$

3) Concentration of Radical in Non-Stationary Chain Reactions 


$$\text{fx } [R]_{\text{nonCR}} = \frac{k_1 \cdot [A]}{-k_2 \cdot (\alpha - 1) \cdot [A] + (k_w + k_g)}$$

Open Calculator 

ex

$$0.072233\text{M} = \frac{70\text{L}/(\text{mol}\cdot\text{s}) \cdot 60.5\text{M}}{-0.00011\text{L}/(\text{mol}\cdot\text{s}) \cdot (2.5 - 1) \cdot 60.5\text{M} + (30.75\text{s}^{-1} + 27.89\text{s}^{-1})}$$




4) Concentration of Radical in Stationary Chain Reactions 

$$\text{fx } [R]_{\text{SCR}} = \frac{k_1 \cdot [A]}{k_w + k_g}$$

Open Calculator 

$$\text{ex } 0.07222\text{M} = \frac{70\text{L}/(\text{mol}\cdot\text{s}) \cdot 60.5\text{M}}{30.75\text{s}^{-1} + 27.89\text{s}^{-1}}$$

5) Number of Collision per Unit Volume per Unit Time between A and B 

fx

Open Calculator 

$$Z_{\text{NAB}} = \left( \pi \cdot ((\sigma_{\text{AB}})^2) \cdot Z_{\text{AA}} \cdot \left( \frac{\left( \frac{8 \cdot [\text{BoltZ}] \cdot T_{\text{Kinetics}}}{\pi \cdot \mu} \right)^1}{2} \right) \right)$$

$$\text{ex } 2.8\text{E}^{-20}/(\text{m}^3\cdot\text{s}) = \left( \pi \cdot ((2\text{m})^2) \cdot 12/(\text{m}^3\cdot\text{s}) \cdot \left( \frac{\left( \frac{8 \cdot [\text{BoltZ}] \cdot 85\text{K}}{\pi \cdot 8\text{kg}} \right)^1}{2} \right) \right)$$

6) Number of Collision per Unit Volume per Unit Time between Same Molecule 

$$\text{fx } Z_{\text{A}} = \frac{1 \cdot \pi \cdot ((\sigma)^2) \cdot V_{\text{avg}} \cdot ((N^*)^2)}{1.414}$$

Open Calculator 

$$\text{ex } 1.3\text{E}^6/(\text{m}^3\cdot\text{s}) = \frac{1 \cdot \pi \cdot ((10\text{m})^2) \cdot 500\text{m/s} \cdot ((3.4/\text{m}^3)^2)}{1.414}$$



7) Ratio of Pre-Exponential Factor 

$$\text{fx } A_{12\text{ratio}} = \frac{\left((D1)^2\right) \cdot \left(\sqrt{\mu 2}\right)}{\left((D2)^2\right) \cdot \left(\sqrt{\mu 1}\right)}$$

Open Calculator 

$$\text{ex } 7.348469 = \frac{\left((9\text{m})^2\right) \cdot \left(\sqrt{4\text{g/mol}}\right)}{\left((3\text{m})^2\right) \cdot \left(\sqrt{6\text{g/mol}}\right)}$$

8) Ratio of Two Maximum Rate of Biomolecular Reaction 

$$\text{fx } r_{\text{max}12\text{ratio}} = \frac{\left(\frac{T_1}{T_2}\right)^1}{2}$$

Open Calculator 

$$\text{ex } 0.388889 = \frac{\left(\frac{350\text{K}}{450\text{K}}\right)^1}{2}$$



## Variables Used











- **[A]** Concentration of Reactant A (*Molar(M)*)
- **[R]<sub>CP</sub>** Concentration of Radical given CP (*Molar(M)*)
- **[R]<sub>CR</sub>** Concentration of Radical given CR (*Molar(M)*)
- **[R]<sub>nonCR</sub>** Concentration of Radical given nonCR (*Molar(M)*)
- **[R]<sub>SCR</sub>** Concentration of Radical given SCR (*Molar(M)*)
- **A<sub>12ratio</sub>** Ratio of Pre Exponential Factor
- **D<sub>1</sub>** Collision Diameter 1 (*Meter*)
- **D<sub>2</sub>** Collision Diameter 2 (*Meter*)
- **k<sub>1</sub>** Reaction Rate Constant for Initiation Step (*Liter per Mole Second*)
- **k<sub>2</sub>** Reaction Rate Constant for Propagation Step (*Liter per Mole Second*)
- **k<sub>3</sub>** Reaction Rate Constant for Termination Step (*Liter per Mole Second*)
- **k<sub>g</sub>** Rate Constant within Gaseous Phase (*1 Per Second*)
- **k<sub>w</sub>** Rate Constant at Wall (*1 Per Second*)
- **N<sup>\*</sup>** Number of A Molecules Per Unit Volume of Vessel (*1 per Cubic Meter*)
- **r<sub>max12ratio</sub>** Ratio of Two Maximum Rate of Biomolecular Reaction
- **T<sub>1</sub>** Temperature 1 (*Kelvin*)
- **T<sub>2</sub>** Temperature 2 (*Kelvin*)
- **T<sub>Kinetics</sub>** Temperature\_Kinetics (*Kelvin*)
- **V<sub>avg</sub>** Average Speed of Gas (*Meter per Second*)
- **Z<sub>A</sub>** Molecular Collision (*Collisions per Cubic Meter per Second*)
- **Z<sub>AA</sub>** Molecular Collision per Unit Volume per Unit Time (*Collisions per Cubic Meter per Second*)



- $Z_{NAB}$  Number of Collision between A and B (Collisions per Cubic Meter per Second)
- $\alpha$  No. of Radicals Formed
- $\mu$  Reduced Mass (Kilogram)
- $\mu_1$  Reduced Mass 1 (Gram Per Mole)
- $\mu_2$  Reduced Mass 2 (Gram Per Mole)
- $\sigma$  Diameter of Molecule A (Meter)
- $\sigma_{AB}$  Closeness of Approach for Collision (Meter)













## Constants, Functions, Measurements used

- **Constant:** **pi**, 3.14159265358979323846264338327950288  
*Archimedes' constant*
- **Constant:** **[BoltZ]**, 1.38064852E-23 Joule/Kelvin  
*Boltzmann constant*
- **Function:** **sqrt**, sqrt(Number)  
*Square root function*
- **Measurement:** **Length** in Meter (m)  
*Length Unit Conversion* 
- **Measurement:** **Weight** in Kilogram (kg)  
*Weight Unit Conversion* 
- **Measurement:** **Temperature** in Kelvin (K)  
*Temperature Unit Conversion* 
- **Measurement:** **Speed** in Meter per Second (m/s)  
*Speed Unit Conversion* 
- **Measurement:** **Molar Concentration** in Molar(M) (M)  
*Molar Concentration Unit Conversion* 
- **Measurement:** **Molar Mass** in Gram Per Mole (g/mol)  
*Molar Mass Unit Conversion* 
- **Measurement:** **Carrier Concentration** in 1 per Cubic Meter (1/m<sup>3</sup>)  
*Carrier Concentration Unit Conversion* 
- **Measurement:** **First Order Reaction Rate Constant** in 1 Per Second (s<sup>-1</sup>)  
*First Order Reaction Rate Constant Unit Conversion* 
- **Measurement:** **Second Order Reaction Rate Constant** in Liter per Mole Second (L/(mol\*s))  
*Second Order Reaction Rate Constant Unit Conversion* 
- **Measurement:** **Collision Frequency** in Collisions per Cubic Meter per Second (1/(m<sup>3</sup>\*s))  
*Collision Frequency Unit Conversion* 



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- [Collision Theory Formulas](#) 
- [Collision Theory and Chain Reactions Formulas](#) 
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- [First Order Reaction Formulas](#) 
- [Important Formulas on Enzyme Kinetics](#) 
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