Important Collision Theory and Chain Reactions Formulas PDF

Formulas
Examples
with Units

List of 8
Important Collision Theory and Chain Reactions Formulas

1) Concentration of Radical formed during Chain Propagation Step given kw and kg Formula

Evaluate Formula

Formula

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

Example with Units

$$0.0722\,\text{M} = \frac{70\,\text{L/(mol*s)} \cdot 60.5\,\text{M}}{0.00011\,\text{L/(mol*s)} \cdot (1 - 2.5) \cdot 60.5\,\text{M} + (30.75\,\text{s}^{-1} + 27.89\,\text{s}^{-1})}$$

2) Concentration of Radical formed in Chain Reaction Formula

Evaluate Formula

Formula

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

Example with Units

$$84.6704\,\text{M} = \frac{70\,\text{L/(mol*s)} \cdot 60.5\,\text{M}}{0.00011\,\text{L/(mol*s)} \cdot (1 - 2.5) \cdot 60.5\,\text{M} + 60\,\text{L/(mol*s)}}$$

3) Concentration of Radical in Non-Stationary Chain Reactions Formula

Evaluate Formula

Formula

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

Example with Units

$$0.0722\,\text{M} = \frac{70\,\text{L/(mol*s)} \cdot 60.5\,\text{M}}{-0.00011\,\text{L/(mol*s)} \cdot (2.5 - 1) \cdot 60.5\,\text{M} + (30.75\,\text{s}^{-1} + 27.89\,\text{s}^{-1})}$$

4) Concentration of Radical in Stationary Chain Reactions Formula

Evaluate Formula

Formula

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

Example with Units

$$0.0722\,\text{M} = \frac{70\,\text{L/(mol*s)} \cdot 60.5\,\text{M}}{30.75\,\text{s}^{-1} + 27.89\,\text{s}^{-1}}$$

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

Evaluate Formula

Formula

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

Example with Units

$$2.8\text{E-}20\,\text{1/(m}^3\text{*s)} = \left(3.1416 \cdot \left(\left(2\,\text{m}\right)^2\right) \cdot 12\,\text{1/(m}^3\text{*s)} \cdot \left(\frac{\left(\frac{8 \cdot 1.4\text{E-}23\,\text{J/K} \cdot 85\,\text{K}}{3.1416 \cdot 8\,\text{kg}}\right)^1}{2}\right)\right)$$

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

Evaluate Formula

Formula

$$Z_A = \frac{1 \cdot \pi \cdot \left(\left(\sigma\right)^2\right) \cdot V_{avg} \cdot \left(\left(N^*\right)^2\right)}{1.414}$$

Example with Units

$$1.3\text{E+}6\,\text{1/(m}^3\text{*s)} = \frac{1 \cdot 3.1416 \cdot \left(\left(10\,\text{m}\right)^2\right) \cdot 500\,\text{m/s} \cdot \left(\left(3.4\,\text{1/m}^3\right)^2\right)}{1.414}$$

7) Ratio of Pre-Exponential Factor Formula

Evaluate Formula

Formula

$$A12_{ratio} = \frac{\left(\left(D1\right)^2\right) \cdot \left(\sqrt{\mu 2}\right)}{\left(\left(D2\right)^2\right) \cdot \left(\sqrt{\mu 1}\right)}$$

Example with Units

$$7.3485 = \frac{\left(\left(9\,\text{m}\right)^2\right) \cdot \left(\sqrt{4\,\text{g/mol}}\right)}{\left(\left(3\,\text{m}\right)^2\right) \cdot \left(\sqrt{6\,\text{g/mol}}\right)}$$

8) Ratio of Two Maximum Rate of Biomolecular Reaction Formula

Evaluate Formula

Formula

$$rmax12_{ratio} = \frac{\left(\frac{T_1}{T_2}\right)^1}{2}$$

Example with Units

$$0.3889 = \frac{\left(\frac{350\,K}{450\,K}\right)^1}{2}$$

Variables used in list of Collision Theory and Chain Reactions Formulas above

- **[A]** Concentration of Reactant A *(Molar(M))*
- **$[R]_{CP}$** Concentration of Radical given CP *(Molar(M))*
- **$[R]_{CR}$** Concentration of Radical given CR *(Molar(M))*
- **$[R]_{nonCR}$** Concentration of Radical given nonCR *(Molar(M))*
- **$[R]_{SCR}$** Concentration of Radical given SCR *(Molar(M))*
- **$A12_{ratio}$** Ratio of Pre Exponential Factor
- **D1** Collision Diameter 1 *(Meter)*
- **D2** Collision Diameter 2 *(Meter)*
- **k_1** Reaction Rate Constant for Initiation Step *(Liter per Mole Second)*
- **k_2** Reaction Rate Constant for Propagation Step *(Liter per Mole Second)*
- **k_3** Reaction Rate Constant for Termination Step *(Liter per Mole Second)*
- **k_g** Rate Constant within Gaseous Phase *(1 Per Second)*
- **k_w** Rate Constant at Wall *(1 Per Second)*
- **N^*** Number of A Molecules Per Unit Volume of Vessel *(1 per Cubic Meter)*
- **$rmax12_{ratio}$** Ratio of Two Maximum Rate of Biomolecular Reaction
- **T_1** Temperature 1 *(Kelvin)*
- **T_2** Temperature 2 *(Kelvin)*
- **$T_{Kinetics}$** Temperature_Kinetics *(Kelvin)*
- **V_{avg}** Average Speed of Gas *(Meter per Second)*
- **Z_A** Molecular Collision *(Collisions per Cubic Meter per Second)*
- **Z_{AA}** Molecular Collision per Unit Volume per Unit Time *(Collisions per Cubic Meter per Second)*

Constants, Functions, Measurements used in list of Collision Theory and Chain Reactions Formulas above

- constant(s): **pi**, 3.14159265358979323846264338327950288 *Archimedes' constant*
- constant(s): **[BoltZ]**, 1.38064852E-23 *Boltzmann constant*
- Functions: **sqrt**, sqrt(Number) *A square root function is a function that takes a non-negative number as an input and returns the square root of the given input number.*
- 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 ($1/m^3$) *Carrier Concentration Unit Conversion*
- Measurement: **First Order Reaction Rate Constant** in 1 Per Second (s^{-1}) *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 ($1/(m^3*s)$) *Collision Frequency Unit Conversion*

- Z_{NAB} Number of Collision between A and B *(Collisions per Cubic Meter per Second)*
- α No. of Radicals Formed
- μ Reduced Mass *(Kilogram)*
- μ_1 Reduced Mass 1 *(Gram Per Mole)*
- μ_2 Reduced Mass 2 *(Gram Per Mole)*
- σ Diameter of Molecule A *(Meter)*
- σ_{AB} Closeness of Approach for Collision *(Meter)*

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