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Important Formulas on Reversible Reaction

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List of 23 Important Formulas on Reversible Reaction

Important Formulas on Reversible Reaction

1) Backward Reaction Rate Constant for 2nd Order Opposed by 1st Order Reaction

Open Calculator

fx $$(k2_b') = (k_f') \cdot \frac{(A_0 - x_{eq}) \cdot (B_0 - x_{eq})}{x_{eq}}$$

ex $$0.026486 m^3/(mol*s) = 0.00618 L/(mol*s) \cdot \frac{(100 mol/L - 70 mol/L) \cdot (80 mol/L - 70 mol/L)}{70 mol/L}$$

2) Backward Reaction Rate Constant for 2nd Order Opposed by 2nd Order Reaction

Open Calculator

fx $$(k_b') = (k_f') \cdot \frac{(A_0 - x_{eq}) \cdot (B_0 - x_{eq})}{x_{eq}^2}$$

ex $$0.000378 L/(mol*s) = 0.00618 L/(mol*s) \cdot \frac{(100 mol/L - 70 mol/L) \cdot (80 mol/L - 70 mol/L)}{(70 mol/L)^2}$$

3) Backward Reaction Rate Constant given Keq and kf

Open Calculator

fx $$(k_{bbr}') = K_{eqm} \cdot (k_f')$$

ex $$0.100734 L/(mol*s) = 16.3 \cdot 0.00618 L/(mol*s)$$

4) Concentration of Product C given kf and kb

Open Calculator

fx $$[C]_{eq} = \frac{k_f'}{k_b'} \cdot \left(\frac{[A]_{eq} \cdot [B]_{eq}}{[D]_{eq}} \right)$$

ex $$19.50758 mol/L = \frac{0.00618 L/(mol*s)}{0.000378 L/(mol*s)} \cdot \left(\frac{0.600 mol/L \cdot 0.700 mol/L}{0.352 mol/L} \right)$$

5) Concentration of Product D given kf and kb

Open Calculator

fx $$[D]_{eq} = \frac{k_f'}{k_b'} \cdot \left(\frac{[A]_{eq} \cdot [B]_{eq}}{[C]_{eq}} \right)$$

ex $$0.353952 mol/L = \frac{0.00618 L/(mol*s)}{0.000378 L/(mol*s)} \cdot \left(\frac{0.600 mol/L \cdot 0.700 mol/L}{19.4 mol/L} \right)$$

6) Concentration of Reactant A given kf and kb

Open Calculator

$$[A]_{eq} = \frac{k_b'}{k_f'} \cdot \left(\frac{[C]_{eq} \cdot [D]_{eq}}{[B]_{eq}} \right)$$

ex $0.596691\text{mol/L} = \frac{0.000378\text{L/(mol*s)}}{0.00618\text{L/(mol*s)}} \cdot \left(\frac{19.4\text{mol/L} \cdot 0.352\text{mol/L}}{0.700\text{mol/L}} \right)$

7) Concentration of Reactant B given kf and kb

Open Calculator

$$[B]_{eq} = \frac{k_b'}{k_f'} \cdot \left(\frac{[C]_{eq} \cdot [D]_{eq}}{[A]_{eq}} \right)$$

ex $0.69614\text{mol/L} = \frac{0.000378\text{L/(mol*s)}}{0.00618\text{L/(mol*s)}} \cdot \left(\frac{19.4\text{mol/L} \cdot 0.352\text{mol/L}}{0.600\text{mol/L}} \right)$

8) Equilibrium Rate Constant given kf and kb

Open Calculator

$$K_{eqm} = \frac{k_f'}{k_b'}$$

ex $16.34921 = \frac{0.00618\text{L/(mol*s)}}{0.000378\text{L/(mol*s)}}$

9) Forward Rate Constant given Keq and kb

Open Calculator

$$(k_{fr}') = K_{eq} \cdot (k_b')$$

ex $0.02268\text{L/(mol*s)} = 60 \cdot 0.000378\text{L/(mol*s)}$

10) Forward Rxn Rate Const for 2nd Order Opposed by 1st Order Rxn given Ini Conc of Reactant B

Open Calculator

$$(k_{fB}') = \left(\frac{1}{t} \right) \cdot \left(\frac{x_{eq}}{B_0^2 - x_{eq}^2} \right) \cdot \ln \left(\frac{x_{eq} \cdot \left(B_0^2 - x \cdot x_{eq} \right)}{B_0^2 \cdot (x_{eq} - x)} \right)$$

ex

$$1.8E\text{^}\text{-}6\text{L/(mol*s)} = \left(\frac{1}{3600\text{s}} \right) \cdot \left(\frac{70\text{mol/L}}{(80\text{mol/L})^2 - (70\text{mol/L})^2} \right) \cdot \ln \left(\frac{70\text{mol/L} \cdot \left((80\text{mol/L})^2 - 27.5\text{mol/L} \right.}{(80\text{mol/L})^2 \cdot (70\text{mol/L} - 27.5\text{m}} \right.$$

11) Forward Rxn Rate Const for 2nd Order Opposed by 2nd Order Rxn given Ini Conc of Reactant A

Open Calculator

fx $$(k_{fA}') = \left(\frac{1}{t}\right) \cdot \left(\frac{x_{eq}^2}{2 \cdot A_0 \cdot (A_0 - x_{eq})}\right) \cdot \ln\left(\frac{x \cdot (A_0 - 2 \cdot x_{eq}) + A_0 \cdot x_{eq}}{A_0 \cdot (x_{eq} - x)}\right)$$

ex $$0.074415\text{L/(mol*s)} = \left(\frac{1}{3600\text{s}}\right) \cdot \left(\frac{(70\text{mol/L})^2}{2 \cdot 100\text{mol/L} \cdot (100\text{mol/L} - 70\text{mol/L})}\right) \cdot \ln\left(\frac{27.5\text{mol/L} \cdot (100\text{mol/L} -}{100\text{mol/L} \cdot (}\right.$$

12) Product Conc for 1st Order Opposed by 1st Order Rxn given Initial Conc of B greater than 0

Open Calculator

fx $$x = x_{eq} \cdot \left(1 - \exp\left(-k_f \cdot \left(\frac{A_0 + B_0}{B_0 + x_{eq}}\right) \cdot t\right)\right)$$

ex $$24.04203\text{mol/L} = 70\text{mol/L} \cdot \left(1 - \exp\left(-0.0000974\text{s}^{-1} \cdot \left(\frac{100\text{mol/L} + 80\text{mol/L}}{80\text{mol/L} + 70\text{mol/L}}\right) \cdot 3600\text{s}\right)\right)$$

13) Product Conc of First Order Opposed by First Order Reaction given Initial Conc of Reactant

Open Calculator

fx $$x = x_{eq} \cdot \left(1 - \exp\left(-k_f \cdot t \cdot \left(\frac{A_0}{x_{eq}}\right)\right)\right)$$

ex $$27.58165\text{mol/L} = 70\text{mol/L} \cdot \left(1 - \exp\left(-0.0000974\text{s}^{-1} \cdot 3600\text{s} \cdot \left(\frac{100\text{mol/L}}{70\text{mol/L}}\right)\right)\right)$$

14) Product Concentration of 1st Order Opposed by 1st Order Reaction at given Time t

Open Calculator

fx $$x = x_{eq} \cdot (1 - \exp(-(k_f + k_b) \cdot t))$$

ex $$27.59038\text{mol/L} = 70\text{mol/L} \cdot (1 - \exp(-(0.0000974\text{s}^{-1} + 0.0000418\text{s}^{-1}) \cdot 3600\text{s}))$$

15) Rate Constant for Backward Reaction

Open Calculator

fx $$(k_{brc}') = k_f \cdot \frac{A_0 - x_{eq}}{x_{eq}^2}$$

ex $$6\text{E\^{}-7L/(mol*s)} = 0.0000974\text{s}^{-1} \cdot \frac{100\text{mol/L} - 70\text{mol/L}}{(70\text{mol/L})^2}$$

16) Rate Constant for Forward Reaction

Open Calculator

fx $$k_f = \left(\frac{1}{t}\right) \cdot \left(\frac{x_{eq}}{2 \cdot A_0 - x_{eq}}\right) \cdot \ln\left(\frac{A_0 \cdot x_{eq} + x \cdot (A_0 - x_{eq})}{A_0 \cdot (x_{eq} - x)}\right)$$

ex $$9.1E\hat{}\text{-}5s^{-1} = \left(\frac{1}{3600s}\right) \cdot \left(\frac{70mol/L}{2 \cdot 100mol/L - 70mol/L}\right) \cdot \ln\left(\frac{100mol/L \cdot 70mol/L + 27.5mol/L \cdot (100mol/L -}{100mol/L \cdot (70mol/L - 27.5mol/L)}\right)$$

17) Reactant Concentration at given Time t

Open Calculator

fx $$A = A_0 \cdot \left(\frac{k_f}{k_f + k_b}\right) \cdot \left(\left(\frac{k_b}{k_f}\right) + \exp(-(k_f + k_b) \cdot t)\right)$$

ex $$72.42095mol/L = 100mol/L \cdot \left(\frac{0.0000974s^{-1}}{0.0000974s^{-1} + 0.0000418s^{-1}}\right) \cdot \left(\left(\frac{0.0000418s^{-1}}{0.0000974s^{-1}}\right) + \exp(-(0.0000974s^{-1} + ($$

18) Time taken for 1st Order Opposed by 1st Order Reaction

Open Calculator

fx $$t = \frac{\ln\left(\frac{x_{eq}}{x_{eq} - x}\right)}{k_f + k_b}$$

ex $$3584.707s = \frac{\ln\left(\frac{70mol/L}{70mol/L - 27.5mol/L}\right)}{0.0000974s^{-1} + 0.0000418s^{-1}}$$

19) Time taken for 1st Order Opposed by 1st Order Reaction given Initial Concentration of Reactant

Open Calculator

fx $$t = \left(\frac{1}{k_f}\right) \cdot \left(\frac{x_{eq}}{A_0}\right) \cdot \ln\left(\frac{x_{eq}}{x_{eq} - x}\right)$$

ex $$3586.179s = \left(\frac{1}{0.0000974s^{-1}}\right) \cdot \left(\frac{70mol/L}{100mol/L}\right) \cdot \ln\left(\frac{70mol/L}{70mol/L - 27.5mol/L}\right)$$

20) Time taken for 2nd Order Opposed by 1st Order Reaction given Initial Conc of Reactant A

Open Calculator

fx $$t = \left(\frac{1}{k_f{}'}\right) \cdot \left(\frac{x_{eq}}{(A_0^2) - (x_{eq}^2)}\right) \cdot \ln\left(\frac{x_{eq} \cdot (A_0^2 - x \cdot x_{eq})}{A_0^2 \cdot (x_{eq} - x)}\right)$$

ex $$0.633369s = \left(\frac{1}{0.00618L/(mol*s)}\right) \cdot \left(\frac{70mol/L}{\left((100mol/L)^2\right) - \left((70mol/L)^2\right)}\right) \cdot \ln\left(\frac{70mol/L \cdot \left((100mol/L)^2 -}{(100mol/L)^2 \cdot (70mo}\right)$$

21) Time taken for 2nd Order Opposed by 2nd Order Reaction given Initial Conc of Reactant B

Open Calculator

fx $$t_{2nd} = \left(\frac{1}{k_f{}'}\right) \cdot \left(\frac{x_{eq}^2}{2 \cdot B_0 \cdot (B_0 - x_{eq})}\right) \cdot \ln\left(\frac{x \cdot (B_0 - 2 \cdot x_{eq}) + B_0 \cdot x_{eq}}{B_0 \cdot (x_{eq} - x)}\right)$$

ex $$74302.86\text{s} = \left(\frac{1}{0.00618\text{L}/(\text{mol*s})}\right) \cdot \left(\frac{(70\text{mol/L})^2}{2 \cdot 80\text{mol/L} \cdot (80\text{mol/L} - 70\text{mol/L})}\right) \cdot \ln\left(\frac{27.5\text{mol/L} \cdot (80\text{mol/L} -}{80\text{mol/L} \cdot (7}\right.$$

22) Time Taken for Completion of Reaction

Open Calculator

fx $$t = \left(\frac{1}{k_f}\right) \cdot \left(\frac{x_{eq}}{2 \cdot A_0 - x_{eq}}\right) \cdot \ln\left(\frac{A_0 \cdot x_{eq} + x \cdot (A_0 - x_{eq})}{A_0 \cdot (x_{eq} - x)}\right)$$

ex $$3374.533\text{s} = \left(\frac{1}{0.0000974\text{s}^{-1}}\right) \cdot \left(\frac{70\text{mol/L}}{2 \cdot 100\text{mol/L} - 70\text{mol/L}}\right) \cdot \ln\left(\frac{100\text{mol/L} \cdot 70\text{mol/L} + 27.5\text{mol/L} \cdot (100\text{m}}{100\text{mol/L} \cdot (70\text{mol/L} - 27.5\text{m}}\right.$$

23) Time taken when Initial Concentration of Reactant B greater than 0

Open Calculator

fx $$t = \frac{1}{k_f} \cdot \ln\left(\frac{x_{eq}}{x_{eq} - x}\right) \cdot \left(\frac{B_0 + x_{eq}}{A_0 + B_0}\right)$$

ex $$4269.26\text{s} = \frac{1}{0.0000974\text{s}^{-1}} \cdot \ln\left(\frac{70\text{mol/L}}{70\text{mol/L} - 27.5\text{mol/L}}\right) \cdot \left(\frac{80\text{mol/L} + 70\text{mol/L}}{100\text{mol/L} + 80\text{mol/L}}\right)$$

Variables Used

- $[A]_{eq}$ Concentration of Reactant A at Equilibrium *(Mole per Liter)*
- $[B]_{eq}$ Concentration of Reactant B at Equilibrium *(Mole per Liter)*
- $[C]_{eq}$ Concentration of Product C at Equilibrium *(Mole per Liter)*
- $[D]_{eq}$ Concentration of Product D at Equilibrium *(Mole per Liter)*
- **A** Concentration of A at Time t *(Mole per Liter)*
- A_0 Initial Concentration of Reactant A *(Mole per Liter)*
- B_0 Initial Concentration of Reactant B *(Mole per Liter)*
- k_b Backward Reaction Rate Constant *(1 Per Second)*
- k_b' Backward Reaction Rate Constant for 2nd Order *(Liter per Mole Second)*
- k_{bbr}' Backward Reaction Rate Constant given kf and Keq *(Liter per Mole Second)*
- k_{brc}' Rate Constant of Backward Reaction *(Liter per Mole Second)*
- K_{eq} Equilibrium Constant for Second Order Reaction
- K_{eqm} Equilibrium Constant
- k_f Forward Reaction Rate Constant *(1 Per Second)*
- k_f' Forward Reaction Rate Constant for 2nd Order *(Liter per Mole Second)*
- k_{fA}' Forward Reaction Rate Constant given A *(Liter per Mole Second)*
- k_{fB}' Forward Reaction Rate Constant given B *(Liter per Mole Second)*
- k_{fr}' Forward Reaction Rate Constant given kf and Keq *(Liter per Mole Second)*
- $k2_b'$ Rate Constant for Backward Reaction *(Cubic Meter per Mole Second)*
- **t** Time *(Second)*
- t_{2nd} Time for 2nd Order *(Second)*
- **x** Concentration of Product at Time t *(Mole per Liter)*
- x_{eq} Concentration of Reactant at Equilibrium *(Mole per Liter)*

Constants, Functions, Measurements used

- Function: **exp**, exp(Number)
  n an exponential function, the value of the function changes by a constant factor for every unit change in the independent variable.
- Function: **ln**, ln(Number)
  The natural logarithm, also known as the logarithm to the base e, is the inverse function of the natural exponential function.
- Measurement: **Time** in Second (s)
  Time Unit Conversion
- Measurement: **Molar Concentration** in Mole per Liter (mol/L)
  Molar 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 Cubic Meter per Mole Second ($m^3/(mol*s)$), Liter per Mole Second (L/(mol*s))
  Second Order Reaction Rate Constant Unit Conversion

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