Уравнение Траутца-Льюиса.

$$dw_A(A)dw_B(B) = \rho(V_A)\rho(V_B)dV_A dV_B =$$

$$\left(\frac{m_A}{2\pi kT}\right)^{\frac{3}{2}} \exp\left(-\frac{m_A V_A^2}{2kT}\right)\left(\frac{m_B}{2\pi kT}\right)^{\frac{3}{2}} \exp\left(-\frac{m_B V_B^2}{2kT}\right) dV_A dV_B \qquad (1)$$

$$\frac{m_A V_A^2}{2} + \frac{m_B V_B^2}{2} = \frac{\mu V_{отн}^2}{2} + \frac{\left(m_A + m_B\right) V_{ц.м.}^2}{2} \qquad (2)$$

$$\mu = \frac{m_A m_B}{m_A + m_B} \qquad (3)$$

$$V_{ЦМ} = \frac{V_A m_A + V_B m_B}{m_A + m_B} \qquad (4)$$

$$V_{ОТН} = V_A - V_B \qquad (5)$$

$$\rho_A \rho_B = \rho_{ОТН} \rho_{ЦМ} \qquad (6)$$

$$dV_A dV_B = dV_{ОТН} dV_{ЦМ} \qquad (7)$$

$$dW(V_{OTH})dW(V_{ЦМ}) = \rho(V_{OTH})\rho(V_{ЦМ})dV_{OTH}dV_{ЦМ} = \\ dW(V_A)dW(V_B) = \rho(V_A)\rho(V_B)dV_A dV_B \quad (8)$$

$$dW^*(V_{OTH}) = \left(\int_{-\infty}^{\infty} \rho_{ц.м.} dV_{ц.м.}\right)\rho_{OTH}dV_{OTH} = \rho_{OTH}dV_{OTH} \quad (9)$$

$$dV_{OTH} = dV_{X,OTH}dV_{Y,OTH}dV_{Z,OTH} = V^2 dV \sin\theta d\theta d\varphi \quad (10)$$

$$dW(V,\theta,\varphi) = V^2 dV \sin\theta d\theta d\varphi \quad (11)$$

$$dW(V) = \rho(V)V^2 dV \times \int_0^{\pi} \sin\theta d\theta \times \int_0^{2\pi} d\varphi \quad (12)$$

$$dW(V) = 4\pi \times \rho(V)V^2 dV \quad (13)$$

<u>Количество активных столкновений.</u>

$$dr = \pi d^2 \times \left(\frac{V^2 - V_0^2}{V^2}\right) \times V \times \left(\frac{\mu}{2\pi kT}\right)^{\frac{3}{2}} \times \exp\left(-\frac{\mu V^2}{2kT}\right) V^2 4\pi n_B dV \quad (14)$$

$$dr = \pi \times \pi^{-\frac{1}{2}} d^2 \times \left(V^2 - V_0^2\right) \times V \times \left(\frac{2^{\frac{1}{3}}\mu}{kT}\right)^{\frac{3}{2}} \times \exp\left(-\frac{\mu V^2}{2kT}\right) n_B dV \quad (15)$$

Интегрирование:

$$-\frac{dn_B}{dt}=\int_{V_0}^{\infty}\pi d^2(V^2-V_0^2)\times V\times\left(\frac{2^{\frac{1}{3}}\mu}{\pi kT}\right)^{\frac{3}{2}}\times\exp\left(\frac{-\mu V^2}{2kT}\right)dV\times n_A n_B \tag{16}$$

$$x=\frac{\mu}{2kT}\left(V^2-V_0^2\right);\ -\frac{\mu V^2}{2kT}=-x+\frac{-\mu V_0^2}{2kT} \tag{17}$$

$$dx=\frac{\mu}{2kT}2VdV;\quad dV=dx\times\frac{kT}{\mu} \tag{18}$$

$$\exp\left(-\frac{\mu V^2}{2kT}\right)=\exp\left(-\frac{\mu V_0{}^2}{2kT}\right)\times\exp\left(-x\right) \tag{19}$$

$$-\frac{dn_B}{dt}=\int_{V_0}^{\infty}\pi\pi^{-\frac{1}{2}}d^2\frac{2kT}{\mu}x\times\left(\frac{2^{\frac{1}{3}}\mu}{kT}\right)^{\frac{3}{2}}V\times\exp\left(-x\right)\times$$
$$\times\exp\left(\frac{-\mu V_0^2}{2kT}\right)\frac{kT}{\mu V}dx\times n_A n_B \tag{20}$$

$$-\frac{dn_B}{dt}=\pi d^2 n_A n_B\exp\left(\frac{-\mu V_0^2}{kT}\right)\left(\frac{8kT}{\pi\mu}\right)^{\frac{1}{2}}\int_0^{\infty}x\times\exp(-x)dx \tag{21}$$

$$\int_0^\infty x\exp(-x)\,dx = -x\exp(-x)\Big|_0^\infty - \int_0^\infty -\exp(-x)\,dx =$$

$$-x\exp(-x)\Big|_0^\infty - \exp(-x)\Big|_0^\infty = (-0+0)-(0-1) = 1 \qquad (22)$$

$$-\frac{dn_B}{dt} = \pi d^2\left(\frac{8kT}{\pi\mu}\right)^{\frac{1}{2}}\exp\left(\frac{-\mu V_0^2}{2kT}\right)n_A n_B$$

$$r = -\frac{d[B]}{dt} = N_A\pi d^2\left(\frac{8kT}{\pi\mu}\right)^{\frac{1}{2}}\exp\left(\frac{-\mu V_0^2}{2kT}\right)[A][B] \qquad (23)$$

<u>Формула Трауца-Льюиса:</u>

$$\boxed{k = N_A\pi d^2\left(\frac{8kT}{\pi\mu}\right)^{\frac{1}{2}}\exp\left(\frac{-\mu V_0^2}{2kT}\right) = N_A\pi d^2\left(\frac{8kT}{\pi\mu}\right)^{\frac{1}{2}}\exp\left(-\frac{E_{TAC}}{kT}\right)}$$