

Уравнение Траутца-Льюиса.



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

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

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

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

$$V_{цм} = \frac{V_A m_A + V_B m_B}{m_A + m_B} \quad (4)$$

$$V_{отн} = V_A - V_B \quad (5)$$

$$\rho_A \rho_B = \rho_{отн} \rho_{цм} \quad (6)$$

$$dV_A dV_B = dV_{отн} dV_{цм} \quad (7)$$

$$dW(V_{OTH})dW(V_{ЦМ}) = \rho(V_{OTH})\rho(V_{ЦМ})dV_{OTH}dV_{ЦМ} =$$

$$dW(V_A)dW(V_B) = \rho(V_A)\rho(V_B)dV_AdV_B \quad (8)$$

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

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

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

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

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

Количество активных столкновений.

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

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

Интегрирование:

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

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

$$dx = \frac{\mu}{2kT} 2V dV; \quad dV = dx \times \frac{kT}{\mu V} \quad (18)$$

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

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

$$\times \exp\left(-\frac{\mu V_0^2}{2kT}\right) \frac{kT}{\mu V} dx \times n_A n_B$$

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

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

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

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

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

Формула Трауца-Льюиса:

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