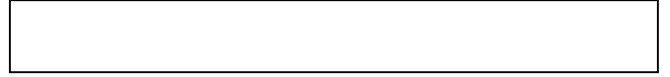


Расчет энтропии смешения в рамках решёточной модели раствора.



$$Z_v = \left(\int_0^{r_{\max}} \left\{ \exp\left(-\frac{U(r)-U(0)}{kT}\right) \times \exp\left(-\frac{U(0)}{kT}\right) \right\} dr_x dr_y dr_z \right)^N =$$

$$\exp\left(-\frac{N \times U(0)}{kT}\right) \left(\int_0^{r_{\max}} \left\{ \exp\left(-\frac{U(r)-U(0)}{kT}\right) \right\} dr_x dr_y dr_z \right)^N \quad (1)$$

$$v_f = \left(\int_0^{r_{\max}} \left\{ \exp\left(-\frac{U(r)-U(0)}{kT}\right) \right\} dr_x dr_y dr_z \right) \quad (2)$$

$$Z_A = Q_{A, \text{пост}}^{N_A} Q_{A, \text{внутр}}^{N_A} e^{\left(\frac{N_A * U_A(0)}{kT}\right)} v_{f,A}^{N_A}$$

$$Z_B = Q_{B, \text{пост}}^{N_B} Q_{B, \text{внутр}}^{N_B} e^{\left(\frac{N_B * U_B(0)}{kT}\right)} v_{f,B}^{N_B} \quad (3)$$

$$Z_{A-B} = Q_{A, \text{пост}}^{N_A} Q_{A, \text{внутр}}^{N_A} Q_{B, \text{пост}}^{N_B} Q_{B, \text{внутр}}^{N_B} \sum_S v_{f,A,S} v_{f,B,S} e^{\left(\sum_{A,B} \frac{U_{f,S}(0)}{kT}\right)} \quad (4)$$

$$\ln \frac{Z_{A-B}}{Z_A Z_B} = \ln \frac{(N_A + N_B)!}{N_A! N_B!} + \ln \frac{v_{f,A,S}^{N_A} v_{f,B,S}^{N_B}}{v_{f,A}^{N_A} v_{f,B}^{N_B}} - \frac{\Delta U(0)}{kT} =$$

$$= \ln \frac{(N_A + N_B)!}{N_A! N_B!} + N_A \ln \frac{v_{f,A,S}}{v_{f,A}} + N_B \ln \frac{v_{f,B,S}}{v_{f,B}} - \frac{\Delta U(0)}{kT} \quad (5)$$

$$\Delta U(0) = N_A (U_{f,A,S}(0) - U_{f,A}(0)) + N_B (U_{f,B,S}(0) - U_{f,B}(0)) \quad (6)$$

$$\begin{aligned} \ln \frac{Z_{A-B}}{Z_A Z_B} &= \ln \frac{(N_A + N_B)!}{N_A! N_B!} = \\ &= (N_A + N_B) \ln(N_A + N_B) - (N_A) \ln(N_A) - (N_B) \ln(N_B) = \\ &= -N_A \ln \frac{N_A}{(N_A + N_B)} - N_B \ln \frac{N_B}{(N_A + N_B)} \end{aligned} \quad (7)$$

$$\begin{aligned} \Delta S &= k \ln (Z_{A-B} / Z_A Z_B) + kT \partial \ln(Z_{A-B} / Z_A Z_B) / \partial T)_V = \\ &= -R \{ x_A \ln x_A + x_B \ln x_B \} \end{aligned} \quad (8)$$