Расчет энтропии смешения в рамках решёточной модели раствора.

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

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

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

$$Z_A = Q_A^{N_A} e^{\left(-\frac{N_A * U_A(0)}{kT} \right)} v_{f,A}^{N_A}$$

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

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

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

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

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

$$\ln \frac{Z_{A-B}}{Z_A Z_B} = \ln \frac{(N_A + N_B)!}{N_A! N_B!} =$$
$$(N_A + N_B) \ln (N_A + N_B) - (N_A) \ln (N_A) - (N_B) \ln (N_B) =$$
$$-N_A \ln \frac{N_A}{(N_A + N_B)} - N_B \ln \frac{N_B}{(N_A + N_B)} \tag{7}$$

$\Delta S = k \ln (Z_{A\text{-}B} / Z_A Z_B) + kT \, \partial \ln (Z_{A\text{-}B} / Z_A Z_B) / \partial T)_V =$

$- R \{ x_A \ln x_A + x_B \ln x_B \}$ (8)