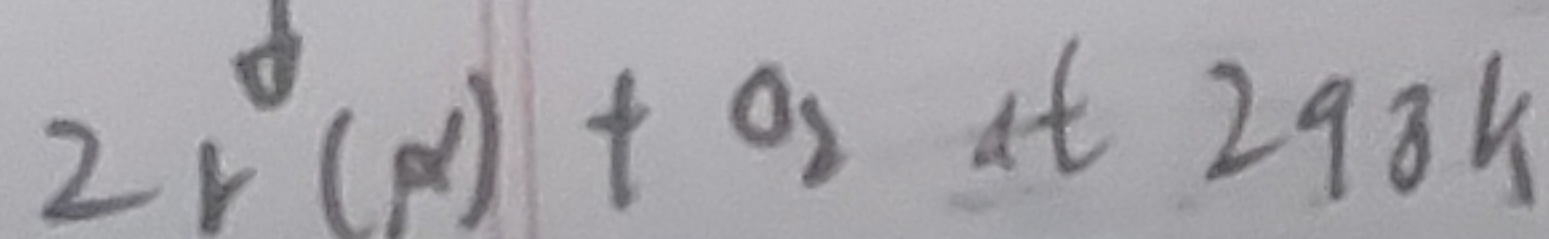


$$\Delta H_1, \Delta S_1$$



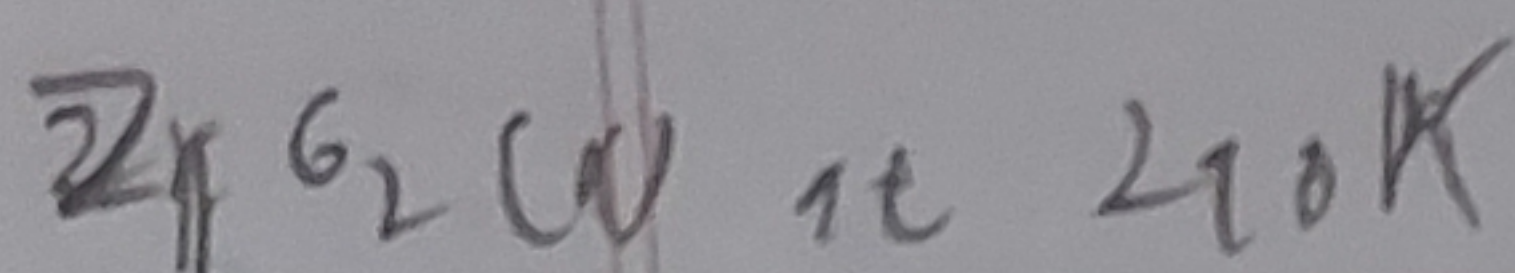
$$\Delta H_2 = -1100100 J/mol$$

$$\Delta S_2 = 56.47 J/K$$

$$C_p(O_2) = 29.96 + 4.12 \times 10^{-3} T - 1.67 \times 10^5 T^{-2}$$

$$\Delta H_1 = \int_{1600}^{1176} C_p(2r(p)) dT + \int_{1176}^{298} C_p(2rO_2(p)) dT - 3960 J/mol + \int_{1600}^{298} C_p(O_2) dT$$

$$\Delta S_1 = \int_{1600}^{1176} \frac{C_p(2r(p))}{T} dT + \int_{1176}^{298} \frac{C_p(2rO_2(p))}{T} dT - \frac{\Delta H_{298}^{2r}}{T_{trans}} + \int_{1600}^{298} \frac{C_p(O_2)}{T} dT$$



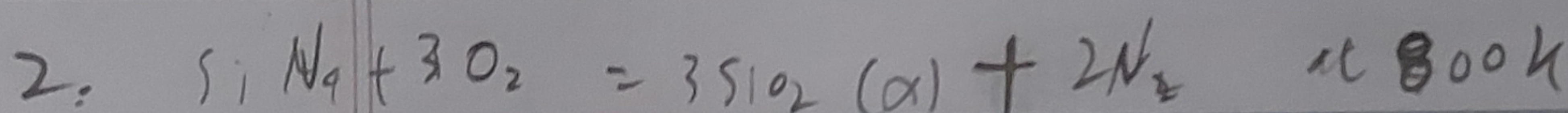
$$C_p(2rO_2(p)) = 21.92, C_p(2rO_2(p)) = 6.762 + 15.34 \times 10^{-3} T - 1.906 \times 10^5 T^{-2}$$

$$\Delta H_3 = \int_{298}^{1418} C_p(2rO_2(p)) dT + 5900 J/mol + \int_{1418}^{1703} + \int_{1703}^{1600} C_p(2rO_2(p)) dT$$

$$\Delta S_3 = \int_{298}^{1418} \frac{C_p(2rO_2(p))}{T} dT + \frac{\Delta H_{298}^{2rO_2}}{T_{trans}} + \int_{1418}^{1600} \frac{C_p(2rO_2(p))}{T} dT$$



$$\Delta H = \Delta H_1 + \Delta H_2 + \Delta H_3 = -1.080 \times 10^6 J/mol \quad \Delta S = \Delta S_1 + \Delta S_2 + \Delta S_3 = -198.5 J/K \cdot mol$$



$$H_{SiN_4, 800} = \Delta H_{f, SiN_4} + \int_{298}^{800} C_p(SiN_4) dT$$

$$H_{O_2, 800} = \int_{298}^{800} C_p(O_2) dT$$

$$H_{SiO_2, 800} = \Delta H_{f, SiO_2} + \int_{298}^{800} C_p(SiO_2) dT$$

$$H_{N_2, 800} = \int_{298}^{800} C_p(N_2) dT$$

$$C_p(SiN_4) = 70.56 + 90.94 \times 10^{-3} T$$

$$C_p(O_2) = 29.96 + 4.12 \times 10^{-3} T - 1.67 \times 10^5 T^{-2}$$

$$C_p(SiO_2) = 43.01 + 1 \times 10^{-3} T - 6.2 \times 10^5 T^{-2}$$

$$C_p(N_2) = 29.07 + 4.29 \times 10^{-3} T$$

$$\Delta H_{800} = 3H_{SiO_2, 800} + 2H_{N_2, 800} - H_{SiN_4, 800} - 3H_{O_2, 800} = -2004.59 kJ/mol$$

$$S_{SiN_4, 800} = S_{298, SiN_4} + \int_{298}^{800} \frac{C_p(SiN_4)}{T} dT$$

$$\Delta S = 3S_{SiO_2, 800} + 2S_{N_2, 800} - S_{SiN_4, 800} - 3S_{O_2, 800} = 232.22 kJ/K \cdot mol$$

$$S_{O_2} = S_{298, O_2} + \int_{298}^{800} \frac{C_p(O_2)}{T} dT$$

$$\Delta G = \Delta H - T\Delta S = +1804.54 kJ/mol$$

$$S_{SiO_2} = S_{298, SiO_2} + \int_{298}^{800} \frac{C_p(SiO_2)}{T} dT$$

$$\Delta G' = \Delta H' - T\Delta S' = -1811.26 kJ/mol$$

$$S_{N_2} = S_{298, N_2} + \int_{298}^{800} \frac{C_p(N_2)}{T} dT$$

$$\begin{aligned} &= 3H_{SiO_2} + 2H_{N_2} - H_{SiN_4} - 3H_{O_2} \text{ at } 298 \\ &= -1909.94 kJ/mol \end{aligned}$$

$$\begin{aligned} \Delta S' &= \Delta S_{298} = 3S_{SiO_2} + 2S_{N_2} - S_{SiN_4} - 3S_{O_2} \text{ at } 298 \\ &= -220.37 J/K \cdot mol \end{aligned}$$

$$\Delta G' = \Delta H' - T\Delta S' = -1811.26 kJ/mol$$

$$\text{error} = \left| \frac{\Delta G - \Delta G'}{\Delta G} \right| \times 100 = 0.34\%$$

$$1) Z = \sum e^{-\frac{\epsilon_i}{kT}} \quad \left\{ \begin{array}{l} 0 \\ \epsilon_{UV} \end{array} \right. \text{ (atom)} \quad 2) Z = e^{-\frac{0}{kT}} + e^{-\frac{\epsilon_{UV}}{kT}} = 1 + e^{-\frac{\epsilon_{UV}}{kT}}$$

$$n = \frac{N e^{-\frac{\epsilon_{UV}}{kT}}}{Z} \Rightarrow \frac{n}{N} = \frac{e^{-\frac{\epsilon_{UV}}{kT}}}{1 + e^{-\frac{\epsilon_{UV}}{kT}}} = \frac{1}{1 + e^{\frac{\epsilon_{UV}}{kT}}}$$

$$1) \text{ Van't Hoff; } \Delta E = n \epsilon_{UV} \quad \Delta S = k \ln \frac{N!}{n!(N-n)!}$$

$$= k (n \ln N! - \ln(n!) - \ln(N-n)!)$$

$$= k (N \ln N - N - (n \ln n + n) - ((N-n) \ln(N-n) - (N-n)))$$

$$= k (N \ln N - n \ln n - (N-n) \ln(N-n))$$

$$k (N (\ln N - \ln(N-n)) - n (\ln n - \ln(N-n))) = k (N \ln \frac{N}{N-n} + n \ln \frac{n}{N-n})$$