PROBLEMAS DE DINÂMICA MOLECULAR

(1) $\pi d_{AB}^2 = 0.38\,nm^2$; $\mu_{AB} = 3.32\times10^{-27}\,kg$; $E_a = 183\,kJ/mol$

$$K = \pi d_{AB}^2 \left(\frac{8 K_B T}{\pi \mu_{AB}}\right)^{1/2} \times N_A \times 10^3 \times e^{-E^*/RT}$$

$$K = 3.8\times10^{-19} \times \left(\frac{8\times1.38\times10^{-23}\times 500}{\pi \times 3.32\times10^{-27}}\right)^{1/2} \times 6.023\times10^{23}\times10^3 \times e^{-\frac{183000}{8.314\times500}}$$

$$K \approx \underline{4.1\times10^{-8}\ mol^{-1}.L.s^{-1}}$$

(2) $\sigma(H_2) = 0.27\,nm^2$ e $\sigma(C_2H_4) = 0.64\,nm^2$

$\sigma = \pi d_A^2 \Leftrightarrow d_A = \left(\frac{\sigma}{\pi}\right)^{1/2} = 0.293\,nm$ e $d_B = 0.45\,nm$

$d_{AB} = \frac{1}{2}(d_A + d_B) = 0.372\,nm$, logo $\sigma_{AB} = \pi d_{AB}^2 \approx 0.46\,nm^2$

$M(H_2) = 2.016\,g/mol$, logo $m = 3.35\times10^{-27}\,kg$

$$m' = \frac{28.05\times10^{-3}}{6.022\times10^{23}} \approx 4.66\times10^{-26}\,kg$$

$$\mu_{AB} = \frac{m\times m'}{m+m'} \approx 3.12\times10^{-27}\,kg$$

$$A = 4.6\times10^{-19} \times \left(\frac{8\times1.38\times10^{-23}\times 628}{\pi\times 3.12\times10^{-27}}\right)^{1/2} \times 6.022\times10^{23}\times10^3$$

$$A \approx 7.37\times10^{11}\ M^{-1}s^{-1}$$

Como o $A_{exp} \approx 1.24\times10^{6}\ M^{-1}.s^{-1}$

isso quer dizer que $\underline{P \approx 1.7\times10^{-6}}$, um valor muito baixo. reagentes complexos.

(3) Não é para resolver! Estudar apenas os conceitos teóricos.

(4) $\Delta H^{\neq} = E_a - 2RT$

$\Delta H^{\neq} = 180000 - 2 \times 8.314 \times 628 \approx \underline{169,6 \text{ kJ/mol}}$

$\Delta S^{\neq} = R\left(\ln \frac{A}{B} - 2\right)$

$B = \frac{K_B T}{h} \times \frac{RT}{p^0} = \frac{1.38 \times 10^{-23} \times 628}{6.626 \times 10^{-34}} \times \frac{8.314 \times 628}{10^5}$

$B = 1.31 \times 10^{13} \times 5 \times 10^{-2} \approx 6.8 \times 10^{11} \times \frac{10^3 L}{m^3} \approx 6.8 \times 10^{14}$

$\Delta S^{\neq} = 8,314 \times \left(\ln \frac{1.24 \times 10^6}{6.8 \times 10^{14}} - 2\right) \approx -184 \text{ J.K}^{-1}\text{.mol}^{-1}$

$\Delta G^{\neq} = \Delta H^{\neq} - T\Delta S^{\neq} = 169600 - 628 \times (-184) \approx \underline{285 \text{ kJ/mol}}$

(5) $A = 9.2 \times 10^9 \text{ cm}^3\text{.mol}^{-1}\text{.s}^{-1} \times \frac{1 L}{1000 \text{ cm}^3} \approx 9.2 \times 10^6 \text{ L.mol}^{-1}\text{.s}^{-1}$

$\Delta S^{\neq} = R\left(\ln \frac{9.2 \times 10^6}{5.24 \times 10^{14}} - 2\right) \approx -203 \text{ J/mol} < 0$

(6) Colisões correspondem a um decréscimo de entropia. Colisões com orientações bem definidas correspondem a maior decréscimo de entropia logo $\Delta S^{\neq}$ é ainda mais negativo.