

Exercise 12

NAME:	MATRICULATION NUMBER:
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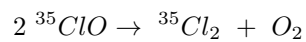
The exercise is due on Wednesday, July 18, 8 am.

12.1 Text book

Read sections 7.3 in G.H. Findenegg, T. Hellweg „Statistische Thermodynamik“

12.2 The activated complex

Calculate the rate constant for the reaction



at 400 K. During the reaction an active complex (ac) is formed (See Fig. 7.5 in G.H. Findenegg, T. Hellweg „Statistische Thermodynamik“). For the calculation you need the values from Table 5.1 in G.H. Findenegg, T. Hellweg „Statistische Thermodynamik“ and the following values:

$$\begin{aligned} I_{\text{ClO}} &= 4.3 \cdot 10^{-46} \text{kgm}^2 \\ I_{\text{ac}} &= I_A I_B I_C = 2.2 \cdot 10^{-135} (\text{kgm}^2)^3 \\ \tilde{\nu}_{\text{vib,ClO}} &= 4.3 \cdot 10^4 \text{m}^{-1} \\ \tilde{\nu}_{\text{vib,ac,1}} &= 15.8 \cdot 10^4 \text{m}^{-1} \\ \tilde{\nu}_{\text{vib,ac,2}} &= 7.6 \cdot 10^4 \text{m}^{-1} \\ \tilde{\nu}_{\text{vib,ac,3}} &= 2.0 \cdot 10^4 \text{m}^{-1} \\ g_{e,0,\text{ClO}} &= 2 \\ \Delta E_0 &= 0 \text{J} \end{aligned}$$