Exercise 1: Rotational Spectra

Sample Solution

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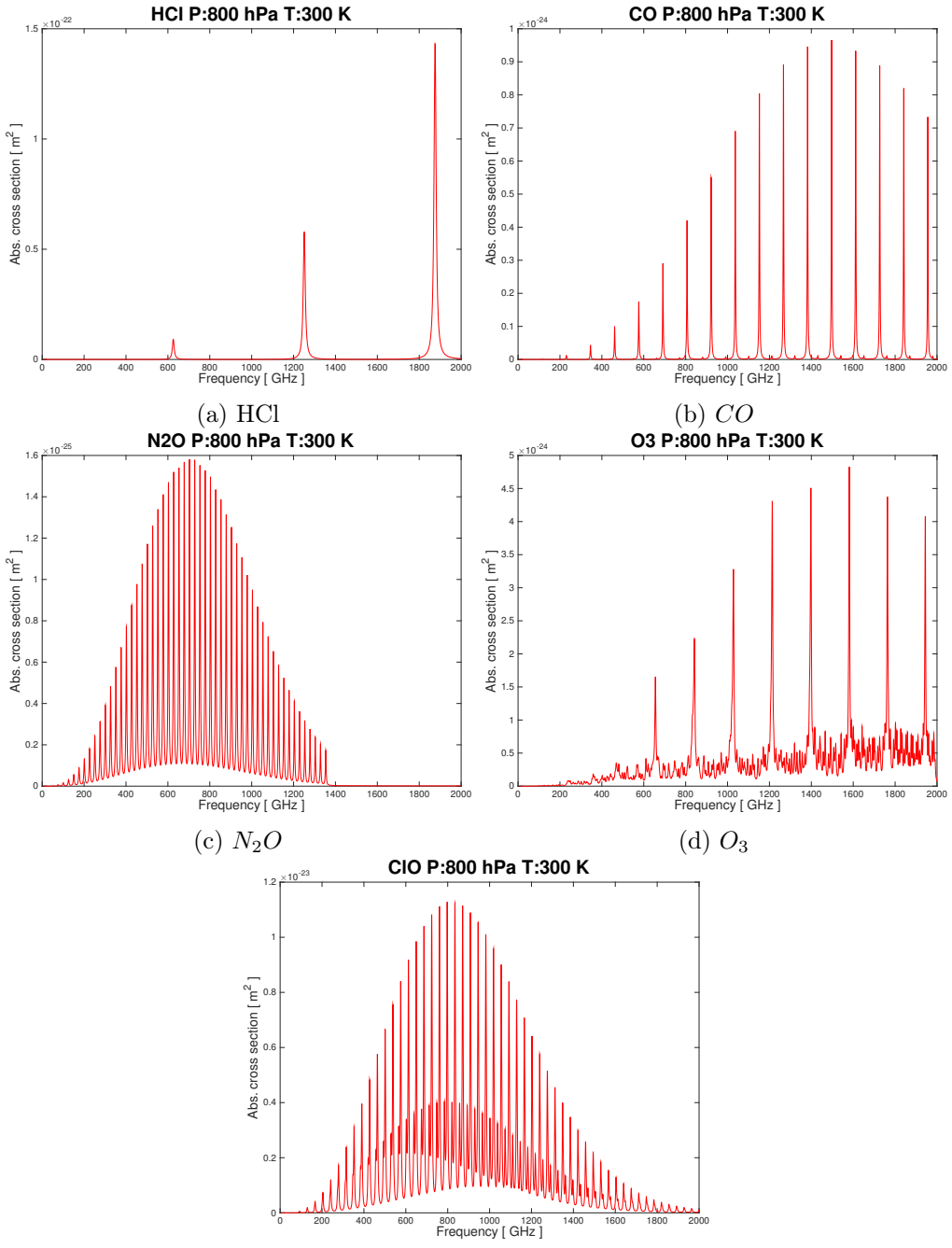
1. Calculate the absorption cross sections in the microwave spectral range for the following molecules:

- HCl
- ClO
- CO
- N_2O
- O_3

Unless otherwise specified use the parameter setting as given in the example file `absorption.arts`.

- Estimate the rotational constant B for HCl and for CO.
  - $B_{HCl} \approx 300\,\mathrm{GHz}$
  - $B_{CO} \approx 100\,\mathrm{GHz}$
- Why is B larger for HCl than for CO?
  - The reduced mass μ is larger for HCl. This is caused by a larger molecule in general and a larger mass difference of the atoms inside the molecule.
- Do you have any idea why N_2O behaves like a diatomic molecule - and O_3 not?
  - The angles between the atoms inside the molecule differ. N_2O has flat angles and therefore momentums of inertia like a linear molecule ($I_A = 0, I_B = I_C$). O_3 has a more complex structure with differing momentums of inertia ($I_A \neq I_B \neq I_C$).

2. Investigate other molecules!



(a) HCl

(b) CO

(c) N_2O

(d) O_3

(e) ClO

Figure 1: Absorption cross sections of the molecules HCl, ClO, CO, N_2O and O_3.

3. Show for a diatomic molecule that the moment of inertia is given by $I = \mu r_0^2$.

$$I = \sum_i m_i r_i^2 = m_1 r_1^2 + m_2 r_2^2$$

The center of gravity is defined as $m_1 r_1 = m_2 r_2$. Insert this and you get

$$\begin{aligned} I &= m_2 r_2 r_1 + m_1 r_1 r_2 \\ &= r_1 r_2 (m_1 + m_2) \end{aligned} \tag{1}$$

We can do more with the center of gravity equation:

$$\begin{aligned} m_1 r_1 = m_2 r_2 = m_2 \overbrace{(r_0 - r_1)}^{\text{from def.}} &= m_2 r_0 - m_2 r_1 \\ (m_1 + m_2) r_1 &= m_2 r_0 \\ r_1 &= \frac{m_2 r_0}{m_1 + m_2} \qquad (2) \\ r_2 &= \frac{m_1 r_0}{m_1 + m_2} \qquad (3) \end{aligned}$$

Insert (2) and (3) into (1):

$$\begin{aligned} I &= \frac{m_2 r_0 \; m_1 r_0 \; (m_1 + m_2)}{(m_1 + m_2)(m_1 + m_2)} \\ &= \frac{m_1 m_2}{m_1 + m_2} r_0^2 = \mu r_0^2 \qquad \square \end{aligned}$$