

**Exercise No. 1 – Calculation of Absorption Coefficients**

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

- HCl
- ClO
- CO
- N<sub>2</sub>O
- O<sub>3</sub>

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

**Questions:**

- Estimate the rotational constant  $B$  (in GHz) for HCl and for CO.
  - Why is  $B$  larger for HCl than for CO?
  - Do you have any idea why N<sub>2</sub>O behaves like a diatomic molecule – and O<sub>3</sub> not?
  - Calculate the reduced mass (in atomic mass units  $u$ ) of the different molecules from the masses of the individual atoms. (For the diatomic molecules this is trivial. For N<sub>2</sub>O, I think the appropriate mass can be found by careful thinking. Ignore O<sub>3</sub>.)
  - Calculate the bond length (in pm) of the various molecules (except O<sub>3</sub>) from the reduced mass and the rotational constant. Verify your result with Google. Again N<sub>2</sub>O needs some extra thinking.
  - Play with different temperatures. How does the rotational spectrum change? Can you explain the changes?
2. Investigate some other molecules!
3. Show for a diatomic molecule that the moment of inertia is given by

$$I = \mu r_0^2$$

where  $\mu$  is the reduced mass, defined as

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

and  $r_0$  is the distance between the two individual atom's centers of mass.