

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
- N₂O
- O₃

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

Questions:

- Estimate the rotational constant B for HCl and for CO.
 - Why is B larger for HCl than for CO?
 - Do you have any idea why N₂O behaves like a diatomic molecule – and O₃ not?
 - Calculate the reduced mass of the different molecules from the masses of the individual atoms. (For the diatomic molecules this is trivial. For N₂O, I think the appropriate mass can be found by careful thinking. Ignore O₃.)
 - Calculate the bond length of the various molecules (except O₃) from the reduced mass and the rotational constant. Verify your result with Google. Again N₂O 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 μ 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.