# A Radiation Course based upon Numerical Methods

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# 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?

1. Investigate some other molecules!
2. Show for a diatomic molecule that the moment of inertia is given by

where is the reduced mass, defined as

and is the distance between the two individual atom’s centers of mass.