Homework 2 - Due 9/18/2012

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Contents

1 Properties of nitromethane

Use the `ase.data.molecules` database to answer these questions.

1.1 Molecular weight

Use `ase` and python to compute the molecular weight of nitromethane (CH3NO2). Compare your answer to what you compute "by hand".

1.2 Center of mass

Write a python function to compute the center of mass of nitromethane. Compare your answer to the output of `ase.Atoms.get_center_of_mass`.

1.3 Moments of inertia

Compute the moments of inertia for nitromethane

1.4 bond lengths

Compute the bond length between the C and each H atom.

1.5 bond angle in the nitro group

Compute the bond angle in degrees between O-N-O in the nitro group.

1.6 Generate an xyz file

Use `ase` to generage an xyz file of the coordinates of the nitromethane molecule. Include the output of your xyz file in your homework.

1.7 Create a graphic of nitromethane

The molecule should be centered in a unit cell with dimensions $10 \times 11.5 \times 12.1$ Å. The unit cell should be visible in the figure. Create a png file and embed it in the file you turn in.

2 Read chapter 10 of dft-book

Annotate the chapter using Acrobat Reader with sticky notes indicating any areas that are confusing, typos, or other types of errors. Click on all the links. Turn this in with your homework assignment.