Homework 2 - Due 9/18/2012

John Kitchin

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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".

1.1.1 solution :noexport:

```
from ase.data.molecules import molecule
atoms = molecule('CH3NO2')
print 'CH3NO2 molecular weight = {0} gm/mol'.format(atoms.get_masses().sum())
```

```
CH3NO2 molecular weight = 61.04032 gm/mol
```

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`.

1.2.1 solution :noexport:

```
from ase.data.molecules import molecule
import numpy as np
atoms = molecule('CH3NO2')

masses = atoms.get_masses()
positions = atoms.positions

COM = np.array([0.0, 0.0, 0.0])
for m,p in zip(masses, positions):
    COM += m*p

COM /= masses.sum()

print 'COM-1          = {0}'.format(COM)

P = [0,0,0]
M = 0
for i,atom in enumerate(atoms):
    P = P + masses[i]*atom.position
    M = M + masses[i]
print 'COM-2          = {0}'.format(P/M)



print 'center of mass = {0} gm/mol'.format(atoms.get_center_of_mass())
```

```
COM-1          = [ 0.00619103  0.07988693  0.        ]
COM-2          = [ 0.00619103  0.07988693  0.        ]
center of mass = [ 0.00619103  0.07988693  0.        ] gm/mol
```

1.3 Moments of inertia

Compute the moments of inertia for nitromethane

1.3.1 solution :noexport:

```
from ase.data.molecules import molecule
atoms = molecule('CH3NO2')
print 'CH3NO2 moments of inertia = {0}'.format(atoms.get_moments_of_inertia())
```

```
CH3NO2 moments of inertia = [ 42.24164093  47.83785675  86.86751504]
```

1.4 bond lengths

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

1.4.1 solution :noexport:

```
from ase.data.molecules import molecule
atoms = molecule('CH3NO2')
for i,atom in enumerate(atoms):
    print i, atom

print
print atoms.get_distance(0,2)
print atoms.get_distance(0,3)
print atoms.get_distance(0,4)
```

```
0 Atom('C', [-0.11428199999999999, -1.314565, 0.0], index=0)
1 Atom('N', [0.0, 0.16647999999999999, 0.0], index=1)
2 Atom('H', [0.89956499999999995, -1.7152559999999999, 0.0], index=2)
3 Atom('H', [-0.64092099999999996, -1.6072120000000001, 0.90495599999999998], index=3
4 Atom('H', [-0.64092099999999996, -1.6072120000000001, -0.90495599999999998], index=
5 Atom('O', [0.066748000000000002, 0.72823199999999999, -1.103775], index=5)
6 Atom('O', [0.066748000000000002, 0.72823199999999999, 1.103775], index=6)
1.09015550124
1.08716892196
1.08716892196
```

1.5 bond angle in the nitro group

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

1.5.1 solution :noexport:

```
from ase.data.molecules import molecule
import numpy as np
atoms = molecule('CH3NO2')
for i,atom in enumerate(atoms):
    print i, atom

print
print atoms.get_angle([5,1,6])*180./np.pi
```

```
0 Atom('C', [-0.11428199999999999, -1.314565, 0.0], index=0)
1 Atom('N', [0.0, 0.16647999999999999, 0.0], index=1)
2 Atom('H', [0.89956499999999995, -1.7152559999999999, 0.0], index=2)
3 Atom('H', [-0.64092099999999996, -1.6072120000000001, 0.90495599999999998], index=
4 Atom('H', [-0.64092099999999996, -1.6072120000000001, -0.90495599999999998], index
5 Atom('O', [0.066748000000000002, 0.72823199999999999, -1.103775], index=5)
6 Atom('O', [0.066748000000000002, 0.72823199999999999, 1.103775], index=6)

125.728162698
```

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.

1.6.1 solution :noexport:

```
from ase.data.molecules import molecule
from ase.io import write
atoms = molecule('CH3NO2')

write('ch3no2.xyz', atoms)
```

```
7

C      -0.114282000000000     -1.314565000000000      0.000000000000000
N       0.000000000000000      0.166480000000000      0.000000000000000
H       0.899565000000000     -1.715256000000000      0.000000000000000
H      -0.640921000000000     -1.607212000000000      0.904956000000000
H      -0.640921000000000     -1.607212000000000     -0.904956000000000
O       0.066748000000000      0.728232000000000     -1.103775000000000
O       0.066748000000000      0.728232000000000      1.103775000000000
```

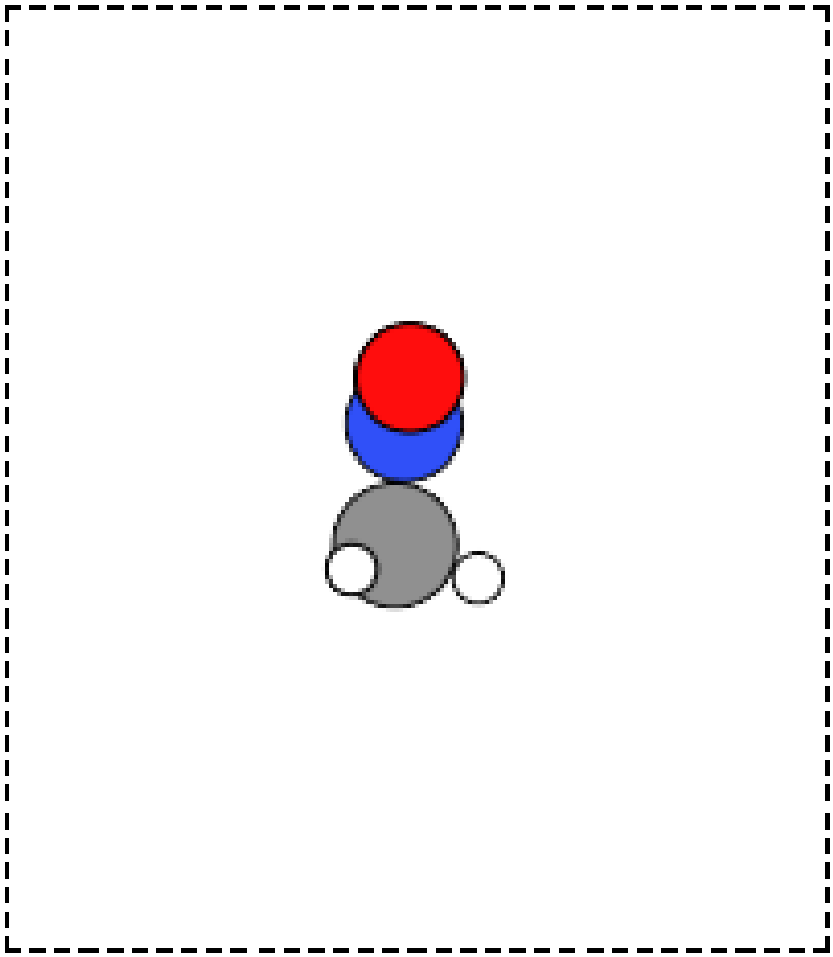
1.7 Create a graphic of nitromethane

The molecule should be centered in a unit cell with dimensions 10× 11.5 × 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.

1.7.1 solution :noexport:

```
from ase.data.molecules import molecule
from ase.io import write
atoms = molecule('CH3NO2')
atoms.set_cell([10, 11.5, 12.1])
atoms.center()

write('ch3no2.png', atoms, show_unit_cell=2)
```



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.