Homework 2

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Contents

1 Problem 1.1

```
1  from ase import Atoms, Atom
2  from ase.data.molecules import molecule
3  from ase.io import write
4
5  atoms = molecule('CH3NO2')
6  masses = atoms.get_masses()
7  masses2 = [12, 14, 1, 1, 1, 16, 16]
```

```
print 'Atomic weights of species from ase: '
print masses
print 'Atomic weights of species (for hand calculation):'
print masses2
mol_weight = masses.sum()
print 'CH3NO2 Molecular weight from Python and ase: {0:1.4f}'.format(mol_weight)
print 'CH3NO2 Molecualr weight by hand: ',sum(masses2)
```

```
Atomic weights of species from ase:
[ 12.011    14.0067    1.00794   1.00794   1.00794  15.9994   15.9994 ]
Atomic weights of species (for hand calculation):
[12, 14, 1, 1, 1, 16, 16]
CH3NO2 Molecular weight from Python and ase: 61.0403
CH3NO2 Molecualr weight by hand:  61
```

2 Problem 1.2

```
from ase import Atoms, Atom
from ase.data.molecules import molecule
from ase.io import write

atoms = molecule('CH3NO2')

masses = atoms.get_masses()
pos = atoms.get_positions()
mol_weight = masses.sum()

xpos = 0
ypos = 0
zpos = 0

for i,t in zip(pos,masses):
    xpos = xpos + (i[0]*t)
    ypos = ypos + (i[1]*t)
    zpos = zpos + (i[2]*t)

xpos = xpos/mol_weight
ypos = ypos/mol_weight
zpos = zpos/mol_weight

print 'CH3NO2 Center of mass from Python: ({0:1.5f},{1:1.5f},{2:1.5f})'.format(xpos,ypos,zpos)
print 'CH3NO2 Center of mass from get_center_of_mass: {0}'.format(atoms.get_center_of_mass())
```

```
CH3NO2 Center of mass from Python: (0.00619,0.07989,0.00000)
CH3NO2 Center of mass from get_center_of_mass: [ 0.00619103  0.07988693  0.
```

3 Problem 1.3

```
from ase import Atoms, Atom
from ase.data.molecules import molecule
from ase.io import write
import numpy as np

atoms = molecule('CH3NO2')

print 'CH3NO2 Moments of inertia: ',atoms.get_moments_of_inertia()
```

```
CH3NO2 Moments of inertia:  [ 42.24164093  47.83785675  86.86751504]
```

4 Problem 1.4

```
from ase import Atoms, Atom
from ase.data.molecules import molecule
from ase.io import write

atoms = molecule('CH3NO2')

print 'Bond length between C and H1: {0:1.4f}'.format(atoms.get_distance(0,2))
print 'Bond length between C and H2: {0:1.4f}'.format(atoms.get_distance(0,3))
print 'Bond length between C and H3: {0:1.4f}'.format(atoms.get_distance(0,4))
```

```
Bond length between C and H1: 1.0902
Bond length between C and H2: 1.0872
Bond length between C and H3: 1.0872
```

5 Problem 1.5

```
from ase import Atoms, Atom
from ase.data.molecules import molecule
from ase.io import write
from numpy import arccos, dot, pi
from numpy.linalg import norm

atoms = molecule('CH3NO2')

a = atoms.positions[1] - atoms.positions[5]
b = atoms.positions[1] - atoms.positions[6]

theta_deg = arccos(dot(a,b)/(norm(a)*norm(b)))*180./pi

print 'Bond angle between O-N-O: {0:1.4f}'.format(theta_deg)
```

Bond angle between O-N-O: 125.7282

6 Problem 1.6

```
from ase import Atoms, Atom
from ase.data.molecules import molecule
from ase.io import write

atoms = molecule('CH3NO2')
pos = atoms.get_positions()
sym = atoms.get_chemical_symbols()

f_xyz = open('hw2_coord.xyz','w')

f_xyz.write('7 Atoms\nAtoms\n')

for i,j in zip(sym,pos):
    f_xyz.write('{0} {1} {2} {3}\n'.format(i,j[0],j[1],j[2]))
f_xyz.close()
```

7 Problem 1.7

```
from ase import Atoms, Atom
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('hw2_fig.png',atoms,show_unit_cell=2,rotation='45x,45y,0z')
```