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 print 'Atomic weights of species: '
```

```
print masses
mol_weight = masses.sum()
print 'CH3NO2 Molecular weight from Python: {0:3f}'.format(mol_weight)
print 'CH3NO2 Molecualr weight by hand: 61'
```

```
Atomic weights of species:
[ 12.011    14.0067    1.00794   1.00794   1.00794  15.9994   15.9994 ]
Molecular weight from Python: 61.040320
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: ({0:3f},{1:3f},{2:3f})'.format(xpos,ypos,zpos)
print 'CH3NO2 Center of mass from get_center_of_mass: {0}'.format(atoms.get_center_of_mass())
```

```
: Center of mass from Python: (0.006191,0.079887,0.000000)
: Center of mass from get_center_of_mass: [ 0.00619103  0.07988693  0.        ]
```

3 Problem 1.3

```

```

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

```
Bond length between C and H1: 1.090156
Bond length between C and H2: 1.087169
Bond length between C and H3: 1.087169
```

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}'.format(theta_deg)
```

```
Bond angle between O-N-O: 125.728162698
```

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')
```