Problem 1

The code for all subproblems are in file `hw02.py`.

Subproblem 1.1

The molecular weight of nitromethane is 61.04 u.

```
import numpy as np
from ase.data.molecules import molecule

atoms = molecule('CH3NO2')
masses = atoms.get_masses()

#MW from database
mw_db = np.sum(masses)

#MW "by hand"
mw_bh = 0.0
for i,atom in enumerate(atoms):
    mw_bh += atom.mass

# Print molecular weights
print 'Molecular weight (database) = {0} u'.format(mw_db)
print 'Molecular weight (by hand) = {0} u'.format(mw_bh)
```

Output:
Molecular weight (database) = 61.04032 u
Molecular weight (by hand) = 61.04032 u

Subproblem 1.2

The center of mass of nitromethane is [0.0062, 0.0799, 0].

```
# Suproblem 1.1 here

# COM from database
com_db = atoms.get_center_of_mass()

# COM "by hand"
com_bh = 0.0
for i,atom in enumerate(atoms):
    com_bh += atom.mass*atom.position
com_bh /= mw_bh

# Print centers of mass
print 'Center of mass (database) = {0}'.format(com_db)
print 'Center of mass (by hand) = {0}'.format(com_bh)
```

Output:
Center of mass (database) = [0.00619103 0.07988693 0.]
Center of mass (by hand) = [0.00619103 0.07988693 0.]

Subproblem 1.3

The moments of inertia of nitromethane are $[42.2416, 47.8379, 86.8675]$. The coordinates obtained using the calculation described in OpenMD have the same values but in different positions.

```
# Suproblems 1.1 and 1.2 here

# MOI from database
moi_db = atoms.get_moments_of_inertia()

# MOI "by hand"
# Inertia tensor matrix
I = np.zeros((3,3))
for i,atom in enumerate(atoms):
    dx = atom.position[0] - com_bh[0]
    dy = atom.position[1] - com_bh[1]
    dz = atom.position[2] - com_bh[2]
    I[0,0] += atom.mass*(dy*dy + dz*dz)
    I[1,1] += atom.mass*(dx*dx + dz*dz)
    I[2,2] += atom.mass*(dx*dx + dy*dy)

    I[0,1] -= atom.mass*(dx*dy)
    I[0,2] -= atom.mass*(dx*dz)
    I[1,2] -= atom.mass*(dy*dz)

    I[1,0] = I[0,1]
    I[2,0] = I[0,2]
    I[2,1] = I[1,2]

(moi_bh, evects) = np.linalg.eig(I)

# Print centers of mass
print 'Moment of inertia (database) = {0}'.format(moi_db)
print 'Moment of inertia (by hand) = {0}'.format(moi_bh)
```

Output:
Moment of inertia (database) = [42.24164093 47.83785675 86.86751504]
Moment of inertia (by hand) = [86.86751504 42.24164093 47.83785675]

Subproblem 1.4

The bond lengths are as follows:

Atom 1	Atom 2	Distance [Å]
C	H	1.0902
C	H	1.0872
C	H	1.0872

```
# Suproblem 1.1 here

# Print bonds lengths
Cind = 0
for i,atom1 in enumerate(atoms):
    if (atom1.symbol == 'C'):
        Cind = i # Store index for C atom
        k = 1
        for j,atom2 in enumerate(atoms):
            if (atom2.symbol == 'H'):
                print 'Distance C - H{0} = {1} Ang'.format(k,atoms.
                    get_distance(i, j))
                k += 1
        break
```

Output:
Distance C - H1 = 1.09015550124 Ang
Distance C - H2 = 1.08716892196 Ang
Distance C - H3 = 1.08716892196 Ang

Subproblem 1.5

The bond angle between O – N – O is 125.7282 °.

```
# Suproblem 1.1 here

# Get indices for N and O atoms
Nind = 0
Oind = np.zeros(2, np.int)
k = 0
for i,atom1 in enumerate(atoms):
    if (atom1.symbol == 'N'):
        Nind = i
    elif (atom1.symbol == 'O'):
        Oind[k] = i
        k += 1
    if (k == 2):
        break

# Compute vectors of difference of positions
a = atoms.positions[Nind] - atoms.positions[Oind[0]]
b = atoms.positions[Nind] - atoms.positions[Oind[1]]

# Compute angle in degrees
```

```
theta_rad = np.arccos(np.dot(a,b)/(np.linalg.norm(a)*np.linalg.norm(b)))
theta_deg = theta_rad*180./np.pi

# Print angle
print 'Angle O - N - O = {0} deg'.format(theta_deg)
```

Output:
Angle O - N - O = 125.728162698 deg

Subproblem 1.6

The XYZ file `nitromethane.xyz` was generated.

```
# Suproblem 1.1 here

# Generate XYZ file
write('nitromethane.xyz', atoms)
```

Subproblem 1.7

The graphic picture of nitromethane rotated by 45 ° in both x and y axes is given below:

```
# Suproblem 1.1 here

# Display nitromethane
atoms.set_cell([10, 11.5, 12.1])
atoms.center(vacuum=13)
write('nitromethane.png', atoms, show_unit_cell=2,rotation='45x,45y,0z')
```

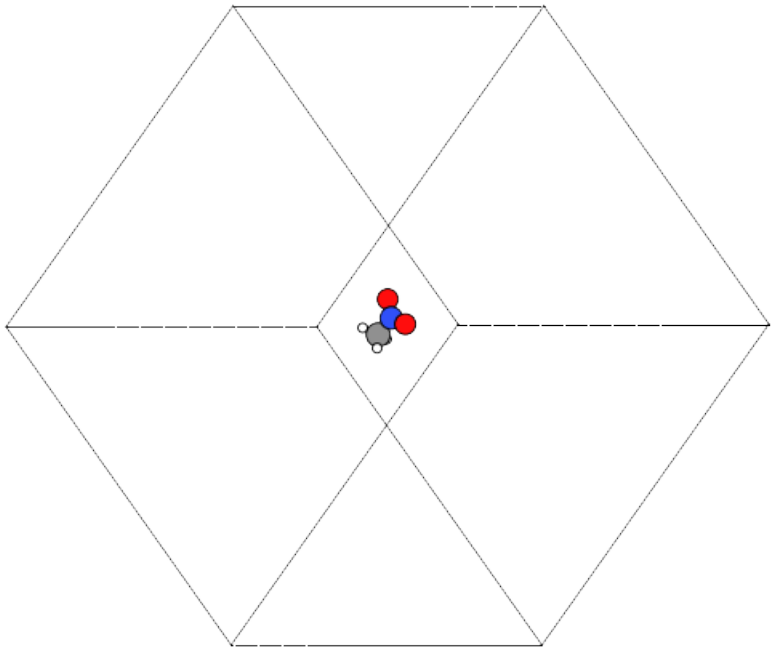

Figure 1: Graphic image of nitromethane for Subproblem 1.7.

Problem 2

Annotations (in red) were added to Section 10 in file `dft.pdf` and the new file is `dft-bacalfa.pdf`.