



Molecular Simulation HOMEWORK 2: Properties of nitromethane

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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 from ase.data.molecules import molecule
2 import numpy as np
3
4 # Calculate using ase and numpy functions
5 atoms = molecule('CH3NO2')
6 masses = atoms.get_masses()
7 total = masses.sum()
```

```

8 print 'ASE and numpy calculates the molecular weight of nitromethane is {0:1.3f} g/mol'.format(total)
9
10 # Calculate 'by hand' using periodic table
11 C = 12.011
12 H = 1.008
13 N = 14.007
14 O = 15.999
15
16 total = C + 3*H + N + 2*O
17 print 'We calculate "by hand" the molecular weight of nitromethane to be {0:1.3f} g/mol'.format(total)

```

ASE and numpy calculates the molecular weight of nitromethane is 61.040 g/mol
 We calculate "by hand" the molecular weight of nitromethane to be 61.040 g/mol

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`.

The center of mass is defined as

$$R = \frac{1}{M} \sum m_i r_i \quad (1)$$

where M is the total mass and m_i and r_i is each chemical species' mass and distance from a fixed point. Note that R and r_i are given from the same fixed point, which we will define for simplicity as the origin. We will first write a program that calculates this.

```

1 from ase.data.molecules import molecule
2 import numpy as np
3
4 # Prepare the data
5 atoms = molecule('CH3NO2')
6 masses = atoms.get_masses()
7 positions = atoms.get_positions()
8 total_mass = masses.sum()
9
10 # Compute the center of mass (COM). First compute the sums of the m*r values
11 sum = np.array((0., 0., 0.))
12 for mass, pos in zip(masses, positions):
13     sum += mass * pos
14 COM = sum / total_mass
15 print 'We compute the center of mass to be ({0:1.5f}, {1:1.5f}, {2:1.5f})'.format(COM[0], COM[1], COM[2])
16
17 # Use ASE to compute the center of mass
18 COM = atoms.get_center_of_mass()
19 print 'ASE computes the center of mass to be ({0:1.5f}, {1:1.5f}, {2:1.5f})'.format(COM[0], COM[1], COM[2])

```

We compute the center of mass to be (0.00619, 0.07989, 0.00000)
 ASE computes the center of mass to be (0.00619, 0.07989, 0.00000)

3 Moments of Inertia

Compute the moments of inertia for nitromethane

```
1 from ase.data.molecules import molecule
2 atoms = molecule('CH3NO2')
3 I = atoms.get_moments_of_inertia()
4 print 'The moments of inertia are {0:1.3f}, {1:1.3f}, and {2:1.3f} amu*angstroms^2'.format(I[0], I[1], I[2])
```

The moments of inertia are 42.242, 47.838, and 86.868 amu*angstroms²

4 Bond Lengths

Compute the bond length between the C and each H atom

```
1 from ase.data.molecules import molecule
2
3 atoms = molecule('CH3NO2')
4 print 'atom symbol'
5 print '======'
6 for i, atom in enumerate(atoms):
7     print i, ' ', atom.symbol
8
9 # From here we need to find distances between atom indexes 0-2, 0-3, and 0-4
10 indexes = ((0, 2), (0, 3), (0, 4))
11 print 'The C-H bond distances are'
12 for index in indexes:
13     print '{0:1.3f}'.format(atoms.get_distance(index[0], index[1])), 'Angstroms'
```

atom symbol

=====

0 C

1 N

2 H

3 H

4 H

5 O

6 O

The C-H bond distances are

1.090 Angstroms

1.087 Angstroms

1.087 Angstroms

To understand why they are not equal, we can look at the molecule.

```
1 from ase.data.molecules import molecule
2 from ase.visualize import view
3 from ase.io import write
4
5 atoms = molecule('CH3NO2')
6 atoms.set_cell((10, 10, 10))
7 atoms.center()
8 write('CH3NO2.png', atoms, show_unit_cell=2)
9 write('CH3NO2_rot.png', atoms, show_unit_cell=2, rotation='-90x, -90y, 90z')
```

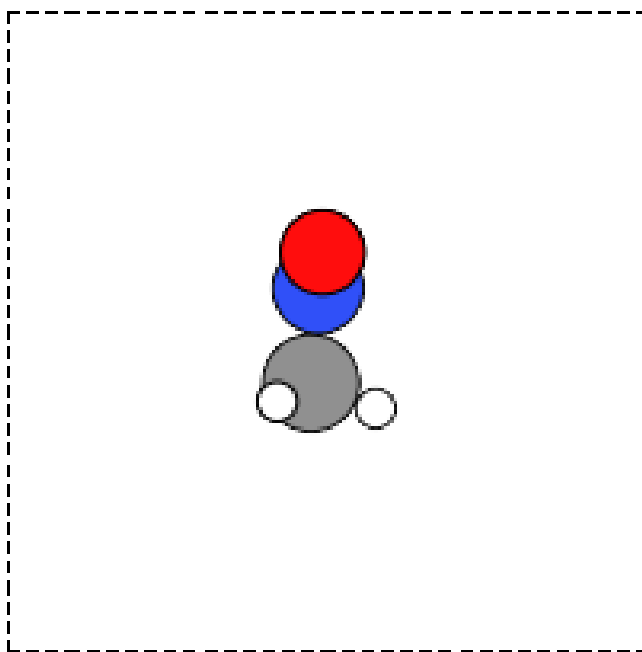


Figure 1: Side view of CH₃NO₂

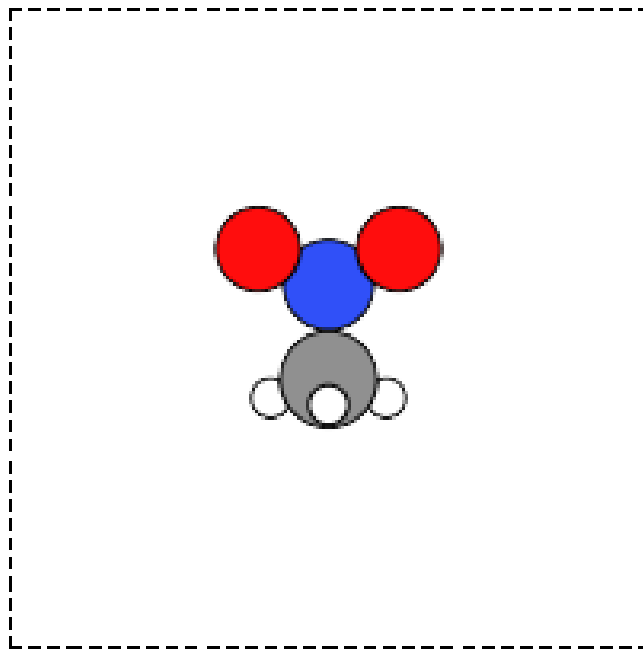


Figure 2: Side view of CH_3NO_2

We can see that the molecule is symmetric along a plane that **splites** the two oxygens. These therefore will have the same bond length.

5 Bond angle in the nitro group

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

From the previous problem, we know the indexes of the O-N-O bond are 6, 1, and 5

```

1 from ase.data.molecules import molecule
2 from numpy import pi
3
4 atoms = molecule('CH3NO2')
5 s = 'The angle between O-N-O is {0:1.1f} degrees'
6 print s.format(atoms.get_angle([6,1,5])*180/pi)

```

The angle between O-N-O is 125.7 degrees

6 Generate an xyz file

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

```
1 from ase.data.molecules import molecule
2 from ase.io import write
3
4 atoms = molecule('CH3NO2')
5 write('CH3NO2.xyz', atoms)
6 file = open('CH3NO2.xyz', 'r')
7 lines = file.readlines()
8 for line in lines:
9     print line[0:-1] #We want this to avoid the extra new line at the end of each line
```

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

7 Create a graphic of nitromethane

The molecule should be centered in a unit cell with dimensions $10 \times 11.52.1 \text{ \AA}$. *The unit cell should be visible*

```
1 from ase.data.molecules import molecule
2 from ase.visualize import view
3 from ase.io import write
4
5 atoms = molecule('CH3NO2')
6 atoms.set_cell((10, 11.5, 12.1))
7 atoms.center()
8 write('CH3NO2_image.png', atoms, show_unit_cell=2, rotation='-45x, -45y, 45z')
```

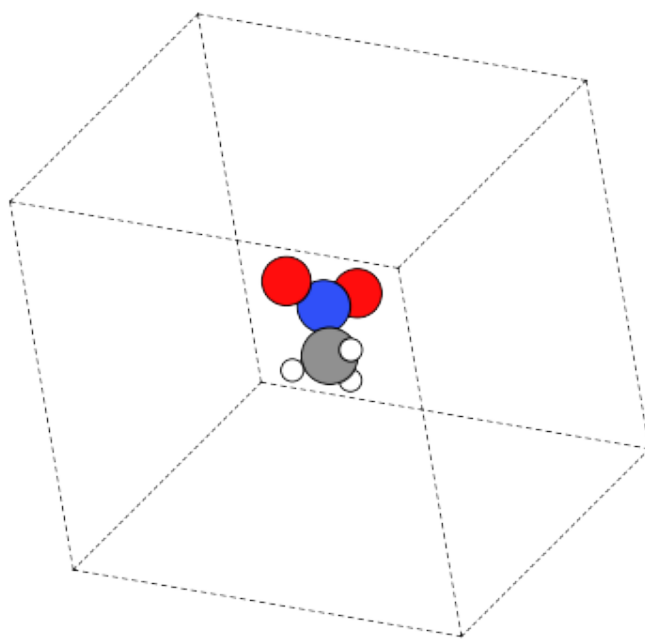


Figure 3: Graphic of nitromethane