

pm-hw2

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Contents

1	Properties of Nitromethane	1
1.1	Molecular Weight	1
1.2	Center of Mass	2
1.3	Moments of Inertia	2
1.4	Bond Lengths	2
1.5	Bond angle in the nitro group	3
1.6	Generate an xyz file	3
1.7	Create a graphic of Nitromethane	3
2	Chapter 2 of dft-book	4

1 Properties of Nitromethane

1.1 Molecular Weight

```
1 from ase.data.molecules import molecule
2 from ase import Atoms, Atom
3 from ase.io import write
4
5 atoms1 = molecule('CH3NO2')
6 atoms2= Atoms([Atom('C'),Atom('H'),Atom('H'),Atom('H'),Atom('N'), Atom('O'), Atom('O')])
7
8 masses1 = atoms1.get_masses()
9 masses2 =atoms2.get_masses()
10 molecular_weight1 = masses1.sum()
11 molecular_weight2 = masses2.sum()
12
13 print 'The molecular weight of nitromehtane computed by ase is {0} gm/mol'.format(molecular_weight1)
14 print 'The molecular weight of nitromethane computed by hand is {0} gm/mol'.format(molecular_weight2)
```

The molecular weight of nitromethane computed by ase is 61.04032 gm/mol
The molecular weight of nitromethane computed by hand is 61.04032 gm/mol

1.2 Center of Mass

```
1 from ase.structure import molecule
2 from ase.io import write
3 import numpy as np
4
5 def fn_com(atoms):
6     pos= atoms.positions
7     masses=atoms.get_masses()
8     COM = np.array([0., 0.,0.])
9
10    for m,p in zip(masses, pos):
11        COM +=m*p
12    COM /=masses.sum()
13    return COM
14
15 atoms= molecule('CH3NO2')
16 COM1= fn_com(atoms)
17
18 print 'COM1={0}'.format(COM1)
19 print 'COM2={0}'.format(atoms.get_center_of_mass())
```

```
COM1=[ 0.00619103  0.07988693  0.          ]
COM2=[ 0.00619103  0.07988693  0.          ]
```

1.3 Moments of Inertia

```
1 from ase.structure import molecule
2
3 atoms=molecule('CH3NO2')
4 molecular_formula=atoms.get_chemical_symbols(reduce=True)
5 print 'The Moments of Inertia for {0} are {1}'.format(molecular_formula, atoms.get_moments_of_inertia())
```

The Moments of Inertia for CNH3O2 are [42.24164093 47.83785675 86.86751504]

1.4 Bond Lengths

```
1 from ase.structure import molecule
2 from ase.io import write
3
4 atoms= molecule('CH3NO2')
5 print 'atom symbol'
6 print '-----'
7 for i,atom in enumerate(atoms):
8     print '{0} {1}'.format(i,atom.symbol)
```

```

9
10 s='The C-H bond lengths are {0:1.3f},{1:1.3f}, and {2:1.3f} Angstroms'
11 print s.format(atoms.get_distance(0,2),atoms.get_distance(0,3),atoms.get_distance(0,4))

```

atom symbol

0 C

1 N

2 H

3 H

4 H

5 O

6 O

The C-H bond lengths are 1.090,1.087, and 1.087 Angstroms

1.5 Bond angle in the nitro group

```

1 from ase.structure import molecule
2 from numpy import pi
3
4 atoms= molecule('CH3NO2')
5 print 'The O-N-O bond angle is {0:1.3F} degrees'.format(atoms.get_angle([5,4,6])*180/pi)

```

The O-N-O bond angle is 44.117 degrees

1.6 Generate an xyz file

```

1 from ase.io import read,write
2 from ase.data.molecules import molecule
3
4 atoms= molecule('CH3NO2')
5
6 write('CH3NO2.xyz', atoms)

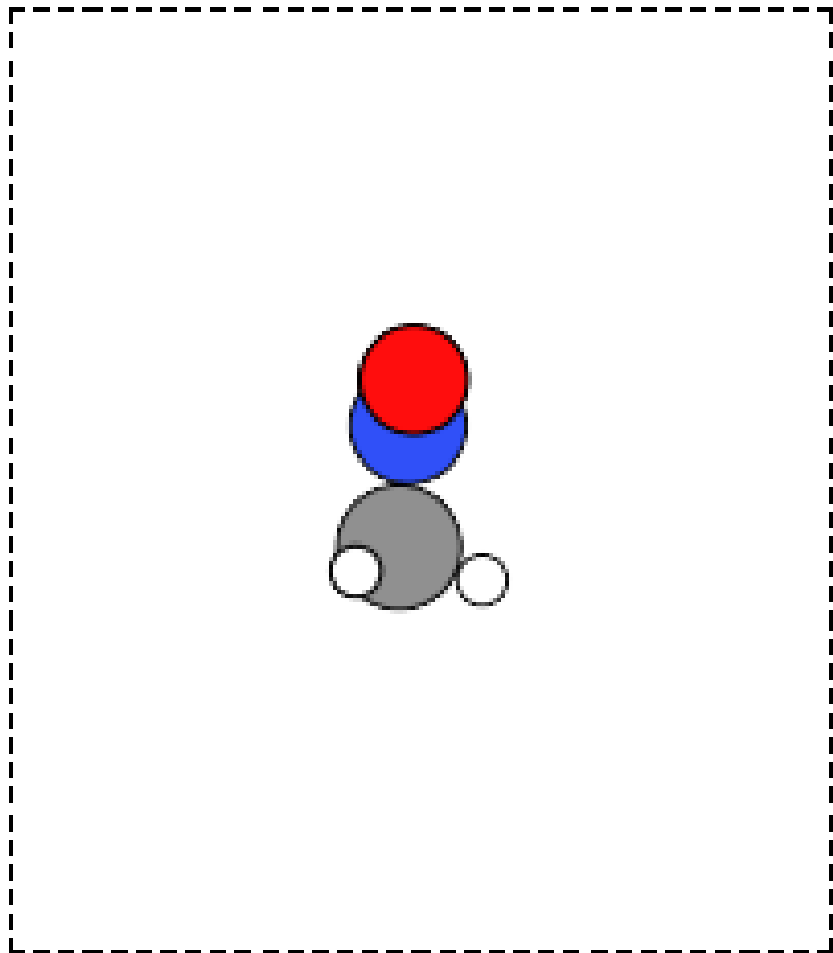
```

1.7 Create a graphic of Nitromethane

```

1 from ase.structure import molecule
2 from ase.io import write
3 atoms= molecule('CH3NO2', cell=(10,11.5,12.1))
4
5 atoms.center()
6 write('CH3NO2.png',atoms,show_unit_cell=2)

```



2 Chapter 2 of dft-book

See attached.