pm-hw2

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Contents

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 nitromehtane 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

```
from ase.structure import molecule
from ase.io import write
import numpy as np

def fn_com(atoms):
    pos= atoms.positions
    masses=atoms.get_masses()
    COM = np.array([0., 0.,0.])

    for m,p in zip(masses, pos):
        COM +=m*p
    COM /=masses.sum()
    return COM

atoms= molecule('CH3NO2')
COM1= fn_com(atoms)

print 'COM1={0}'.format(COM1)
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

```
from ase.structure import molecule

atoms=molecule('CH3NO2')
molecular_formula=atoms.get_chemical_symbols(reduce=True)
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

```
from ase.structure import molecule
from ase.io import write

atoms= molecule('CH3NO2')
print 'atom symbol'
print '-----------'
for i,atom in enumerate(atoms):
    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)
```

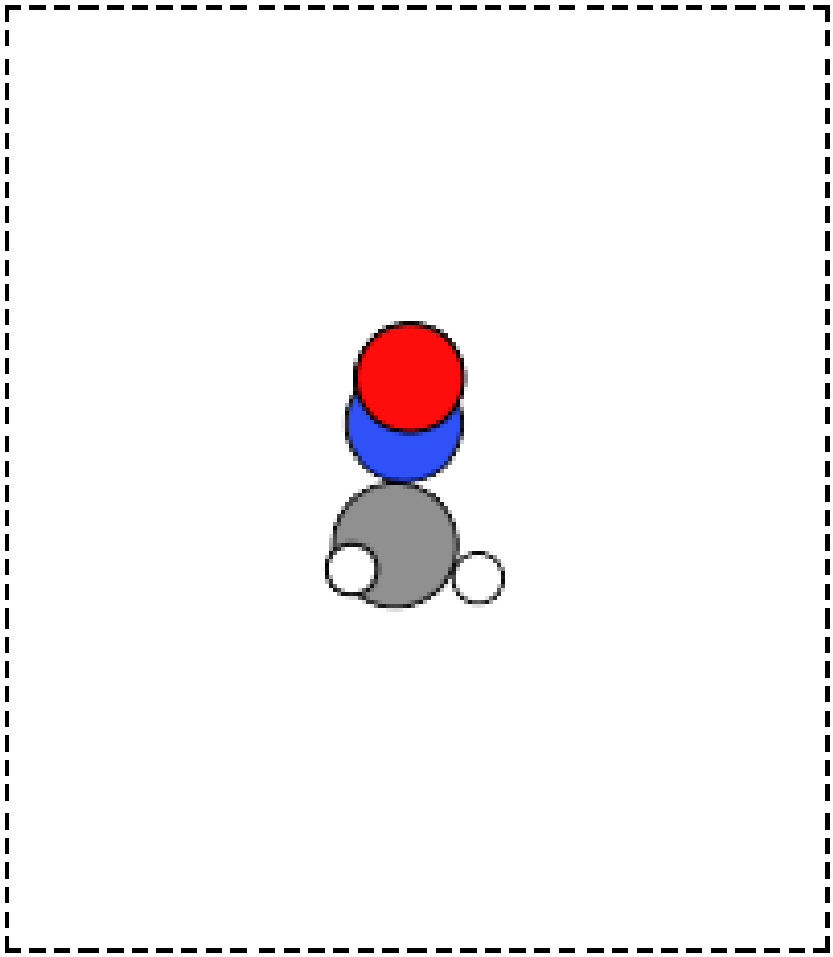
```
The O-N-O bond angle is 44.117 degrees
```

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 9 of dft-book

See attached.