Problem 1

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

Subproblem 1.1

The molecular weight of nitromethane is 61.04 u.

Subproblem 1.2

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

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

Subproblem 1.5

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

Subproblem 1.6

The XYZ file `nitromethane.xyz` was generated.

Subproblem 1.7

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

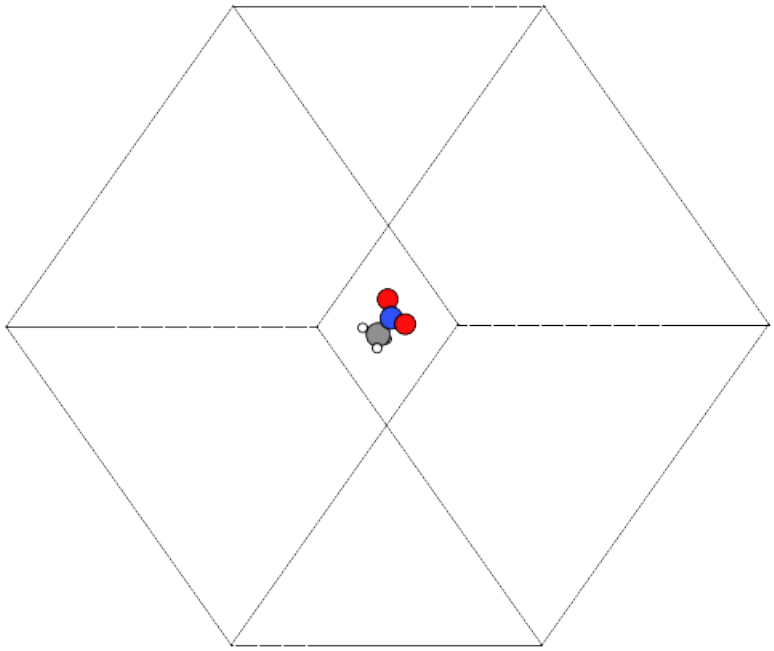

Figure 1: Graphic image of nitromethane for Subproblem 1.7.

Problem 2

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