

Programming Project 0: Geometry

Object-oriented programming basics

Write a class to store the geometry, masses, and nuclear charges of a molecule. Afterwards, write a small program to test your class. Make sure each class method is called at least once.

Extra Files

<u>file name</u>	<u>description</u>
molecule.xyz	sample .xyz file for testing out your program
masses.py	provides functions <code>get_mass</code> and <code>get_charge</code> which return the mass and charge of an atom, e.g.: <pre>>>> import masses >>> masses.get_mass("O") 15.99491461956 >>> masses.get_charge("O") 8</pre>

Class description

Member variables.

<u>name</u>	<u>type</u>	<u>description</u>
units	str	either "Angstrom" or "Bohr", specifying the distance units used for spatial coordinates
natom	int	the number of atoms
labels	list of strs	a list of uppercase atomic symbols, following the order of the .xyz file
masses	list of floats	a list of atomic masses, following the order of the .xyz file
charges	list of ints	a list of atomic charges, following the order of the .xyz file
geom	numpy.matrix	an $\text{natom} \times 3$ matrix containing the Cartesian coordinates of each atom, following the order of the .xyz file

Methods.

<u>method</u>	<u>description</u>
Constructor (<code>__init__</code>)	takes <code>str</code> contents of an .xyz file as input; initializes all member variables and fills them with their correct values
<code>to_bohr</code>	converts the distance units to Bohr, changing member variables <code>units</code> and <code>geom</code> if necessary
<code>to_angstrom</code>	converts the distance units to Angstroms, changing member variables <code>units</code> and <code>geom</code> if necessary