

# Molecular Dynamics of Benzene

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Repository URL: <https://github.com/ASU-CompMethodsPhysics-PHY494/final-2019-benzene>

# Objectives

1. Develop an MD code that solves Newton's equations of motion for a molecule in a vacuum
2. Generate initial conditions of benzene molecules based on online resources
3. Develop an algorithm that outputs initial positions of all atoms for a single benzene molecule, and assign random velocities (in a specific range) to all atoms in molecule based on initial temperature
4. Develop a total force function that can be integrated over a short time period using velocity Verlet and RK4 algorithms
5. Compile a list of parameters from various existing force-fields for the initial positions and spring constants that produce a stable molecule
6. Implement additional restoring force that creates a stable improper dihedral structure
7. Find parameters that produce a stable, fairly rigid simulation of a benzene molecule
8. Simulate interactions of multiple benzene molecules
9. Deduce heat capacity of benzene from system of molecules

# Background

We simulated the interactions of benzene ( $\text{C}_6\text{H}_6$ ) molecules using a classical approach with molecular dynamics methods to produce a stable simulation of benzene and find the parameters which reproduce experimentally determined properties of benzene. Benzene is made of an inner ring of carbon atoms with one hydrogen atom connected to each carbon atom, which means we must account for bonded (C-C single, C-C double, H-C single) and non-bonded (C-C and H-C) interactions within each molecule. The Morse potential was used to simulate bonded intramolecular interactions,

$$V_M(r_{ij}) = D_{ij} \left( 1 - e^{-\beta_{ij}(r_{ij} - R_{ij})} \right)^2.$$

Intermolecular and non-bonded intramolecular interactions were simulated using the Lennard-Jones Potential,

$$V_{LJ}(r_{ij}) = 4 \left[ (r_{ij}^*)^{-12} - (r_{ij}^*)^{-6} \right], \quad r_{ij} = \sqrt{(\mathbf{x}_j - \mathbf{x}_i)^2}$$

The motivation behind the project was to be able to study benzene or other molecules if a working model was able to be developed. If a realistic model of the molecule was created, it

would be possible to study properties of this or other molecules on length and time scales that are otherwise not accessible.

# Methods

The approach here was to use the velocity Verlet algorithm to create a system of molecules that conserve energy over time. To do this, we first generated a system of molecules that were in their equilibrium positions. This meant using the time-averaged bond lengths of each atom for a typical benzene molecule. With the molecules generated, the atoms were then assigned velocities based on an initial temperature. With initial positions and velocities for each atom in the system,

## Bond Lengths:

- C-C: 0.139 nm
- H-C: 0.109 nm

## Dissociation Energies:

- C-C: 922 kJ/mol
- H-C: 110 kJ/mol

## Force Constants:

- C-C: 1.49E11
- H-C: 9.685E10

## Lennard-Jones Parameters:

- Epsilon = 1.198E-7 Kelvin
- Sigma = 0.341 nm

## Packages Used:

- NumPy

- SciPy

## Results

The main goal of creating a working model of benzene was not accomplished. There were several forces implemented in the code and getting the correct balance to create a stable molecule proved difficult. A seemingly stable molecule becomes unstable after a short period of time and the atoms disperse. The Morse potential was used for the force for bonded interactions and Lennard-Jones (half-weighted Lennard-Jones) interactions were added for fifth (fourth) nearest neighbors. If Lennard-Jones forces are added between all molecules, the physics becomes more realistic but the problem of the instability persists. A harmonic restraint force was added to each atom relative to its' equilibrium position in an attempt to stabilize the molecule. This worked for a short time but again the molecule disintegrated. More fine-tuning needs to be done in order to get the molecule stabilized, which then can be tested for accuracy by comparing the parameters used and observables obtained to experiment.

## Summary

This simulation would likely be improved by implementing more forces, such as the dihedral force to account for torsional angles between the plane that carbon and a hydrogen atom reside in, and the Coulomb force to account for charges between atoms. Our project could be expounded on in the future by implementing quantum mechanical interactions to more accurately simulate the structure of benzene.

# Acknowledgements

Our group would like to thank Ian Kenney for his assistance with developing an approach for tracking individual atoms throughout the calculation process.

# References

<http://manual.gromacs.org/documentation/2016.3/manual-2016.3.pdf>







