**Experiment Code Documentation**

**Introduction**

This document captures the experiment implementation details.

**Code Details**

**A) File Name:** header.html

**File Description:** This is the welcome page. Click ‘start the experiment’ to start.

**B) File Name:** header1.html

**File Description:** This is the start of the experiment. Choose a molecule from the navigation tab to proceed next.

**C) File Name:** water.html

**File Description:** This HTML file contains different elements of the experiment.

1. Header: Logo and navigation bar
2. Image of the molecule
3. Simulation container
4. Radio buttons for the controls – space fill, wireframe, spin (to rotate the molecule)
5. Section for Z-matrix calculation
6. Footer

**1)-Function Name:** molecule

**Function Description:**

This java script function is for the simulation of the molecule. The function uses predefined functions from three.js library. To be able to display anything with three.js, we need three things: scene, camera and renderer, so that we can render the scene with camera.

The camera, scene and renderer objects are initialized. ‘Light’ is focused on the scene with the light objects. The ‘molecule’ function is called by passing three parameters – O radius, H radius, bond radius. These are the JS variables for maintaining the radii of the atoms and bonds. This entire function is used for creating mesh objects (atoms and bonds) and adding them to the scene.

The structure of the molecule (i.e., number and type of atoms and bonds) depends upon a variable ‘calc’. It is initialized and modified in water.js file (according to the z-matrix calculation)

**2)-Function Name:** animate

**Function Description:**

This is a three.js function used for animating the scene. In this function, the renderer is added to the scene and a user defined function called ‘render’ is called.

**3)-Function Name:** render

**Function Description:**

This function is used to rotate the contents (here, water molecule) in the simulator container. The rotation is done only if the check box of the control option ‘spin’ is checked.

**4)-Function Name:** on window resize

**Function Description:**

This function is used to set the simulator dimensions on page resize.

There are similar html files for remaining molecules - ammonia.html, formaldehyde.html, methane.html, benzene.html.

**D) File Name:** water\_z-matrix.html

**File Description:** This HTML file contains the elements for z-matrix calculation of the water molecule. The calculations are displayed step-by-step if a right atom is selected from the drop-down list.

There are similar html files for remaining molecules – ammonia\_z-matrix.html, formaldehyde\_z-matrix.html, methane\_z-matrix.html, benzene\_z-matrix.html.

**E) File Name:** water.js

**File Description:** This file contains functionality regarding z-matrix calculation and simultaneous changes in the simulator container.

**Variables:** Avariable ‘calc’ is for simulation purpose. This is used in the function ‘molecule’ in water.html file. This variable is maintained to know the present structure of the molecule(simulation).

**1)-Function Name:** ready

**Function Description:**

This function is called when the water.html page is loaded. The z-matrix section is loaded with the initial options i.e., ‘select’ and drop-down list of atoms.

**2)-Function Name:** first

**Function Description:**

This function is used to called when an option is selected for the first atom from the drop-down list and ‘render’ button is clicked. The selected options are evaluated and next set of options are displayed (loaded on to the page) if the selected ones are correct. If they are incorrect “Incorrect Option, Try Again!” option is displayed.

**3)-Function Name:** second

**Function Description:**

This function is called when the selection is made from the second list of drop-downs. The selected options are evaluated and corresponding action is taken (As mentioned in the above function)

The functionality of the third () function is similar to second () function.

**4)-Function Name:** submit

**Function Description:**

This function is called when the user clicks the ‘Go to next step’ button (present in water\_z-matrix.html). This function sets a variable called ‘molecule’ (in the local storage -stored for further use in the next pages) with the molecule name (here, it is ‘water’ molecule). Then the page is redirected to “gamessinput.html”

**5)-Function Name:** control changes

**Function Description:**

This function is used to simulation purpose. The controls selected by the user (radio buttons) are retrieved and passed to the function ‘molecule’ in water.html. The scene (of the simulator) is also cleared.

There are similar html files for remaining molecules – ammonia.js, formaldehyde.js, methane.js, benzene\_z-matrix.js. These files contain various functions for the functionality of the simulator.

**F) File Name:** gamessinput.html

**File Description:** The contents of this file give the description of the method, Basis set, Procedure used as GAMESS input.

**1)-Function Name:** submit

**Function Description:**

On clicking ‘go to next step’ step button, this function is invoked. The page is redirected to inp.html page**.**

**G) File Name:** inp.html

**File Description:** This file contains functionality regarding input for the GAMESS software.

**1)-Function Name:** ready

**Function Description:**

On the page loading, the GAMESS input information is taken from inp\_bk.html file (according to the molecule\_name variable from the local storage)

**2)-Function Name:** submit

**Function Description:**

When ‘run gamess’ button is clicked, this function redirects the current page to output.html.

**H) File Name:** inp\_bk.html

**File Description:** This file contains information regarding input to be displayed on the inp.html page.

**I) File Name:** output.html

**File Description:** This file contains functionality regarding output of the GAMESS software.

**1)-Function Name:** ready

**Function Description:**

On the page loading, the GAMESS output is taken from output\_bk.html file (according to the molecule\_name variable from the local storage) and displayed.

**2)-Function Name:** submit

**Function Description:**

When ‘next’ button is clicked, this function redirects the current page to final\_latest.html.

**J) File Name:** output\_bk.html

**File Description:** This file contains information regarding output to be displayed on the output.html page.

**K) File Name:** final\_latest.html

**File Description:** This file contains a simulator container and graph plotted as energy difference vs optimization step number.

**Other details:**

**1)**- What is the browser Compatibility?

Experiment works fine on Chrome. But since three.js library is used, to include the three.js into the project,

1. the installation is done via npm

Run “npm install three”

1. using python http server (if python is installed in the system)

run “python -m http.server 8000”

(to run on the local server port 8000)

Run the file as” <http://localhost:8000/filename.html>”

**2)**- Explain the abstracted working of experiment?

Steps to follow:

* Run header.html file
* Click the “Start the Experiment”
* Select a molecule from the navigation tab to procced.
* For example, choose water. Select the atom from the drop-down list (according to the order in the molecule image)
* Simultaneously, the simulation appears on the simulator container.
* Select the different control options present on the right side of the simulator to see the corresponding changes in the simulation (the different options are space fill, wireframe, spin).
* If the selection of the atoms is wrong, the message “Incorrect Option, Try Again!” is displayed.
* After the whole molecule is completed, click the “Go to next step” button to go to the next page where the method, Basis set, Procedure used for the GAMESS calculations are displayed. Click “Go to next step” button.
* The page displays input file for GAMESS software. Click on “RUN GAMESS”.
* The page displays output of the calculations. Click “next” button.
* This final page displays the simulator along with the graph plotted as energy difference vs optimization step number.
* Click on another molecule in the navigation tab to continue the experiment with that molecule.

**3)** How is the Z-matrix calculated for the molecules?

Z-matrix calculation is different for different molecules. Select the atoms from the drop-down lists according to the following:

1. Water (H2O):

atom-number atom

1. O

2. H 1

3. H 1 2

2. Ammonia (NH3):

1. N

2. H 1

3. H 1 2

4. H 1 2 3

3. Formaldehyde (CH2O):

1. O

2. C 1

3. H 2 1

4. H 2 1 3

4. Methane (CH4):

1. C

2. H 1

3. H 1 2

4. H 1 2 3

5. H 1 2 3

5. Benzene (C6H6):

1. C

2. C 1

3. C 2 1

4. C 3 2 1

5. C 4 3 2

6. C 1 2 3

7. H 1 6 5

8. H 2 1 6

9. H 3 2 1

10. H 4 3 2

11. H 5 4 3

12. H 6 1 2