**VIT Bhopal University**

**Final Practical Examination**

**Computation Chemistry (CHY-1005)**

Max. Marks: 50

|  |  |  |  |
| --- | --- | --- | --- |
| **Registration No.** |  | **Branch** |  |
| **Name of Student** |  | **Date** |  |
| **Slot** |  | **Name of Faculty** |  |

**Note: Applicable to registration number ending with even number (i.e. 0, 2, 4, 6, and 8) only.**

**Exercise: Build Ethane Molecule and calculate the following using suitable software:-**

**1) Geometry optimization and calculate minimum energy**

**2) Calculate the IR frequency and Molecular Orbital Energy.**

**3) Calculate the Minimum Potential Energy from Potential Energy Curve.**

**Strike out whatever is not applicable and use observation table which is applicable as per your registration number.**

**(Report images and values wherever applicable)**

**Results:**

Observation Table – o1 – Visualization of Ethane Molecule

|  |  |  |
| --- | --- | --- |
| **S.No.** | **Name of Molecule** | **Image of build Ethane Molecule** |
| 1 |  | Bond Length:  C-C Bond Length:  C-H Bond Length: |

Observation Table – o2 – Optimization of Ethane Molecule

|  |  |  |
| --- | --- | --- |
| **S.No.** | **Description** | **Image of optimized Ethane Molecule** |
| 1 |  |  |
| 2 | Minimum Energy |  |

Observation Table – o3 – Calculation of IR Frequency and Molecular Orbital

|  |  |  |
| --- | --- | --- |
| **S.No.** | **Description** | **Results** |
| 1 | IR Spectrograph |  |
| 2 | IR Frequency |  |
| 3 | Molecular Orbital Values | Least unoccupied molecular orbital:  Highest occupied molecular orbital: |

Observation Table – o4 – Potential Energy Curve

|  |  |  |
| --- | --- | --- |
| **S.No.** | **Description** | **Results** |
| 1 | Potential Energy Curve |  |
| 2 | Minimum Energy |  |

**VIT Bhopal University**

**Final Practical Examination**

**Computation Chemistry (CHY-1005)**

Max. Marks: 50

|  |  |  |  |
| --- | --- | --- | --- |
| **Registration No.** | 22BAI10051 | **Branch** | Cse ai and ml |
| **Name of Student** | nishant | **Date** | 30-2-23 |
| **Slot** | A11-a12-a13 | **Name of Faculty** | Manoj acharya |

**Note: Applicable to registration number ending with even number (i.e. 1, 3, 5, 7, and 9) only.**

**Exercise: Build Butane Molecule and calculate the following using suitable software:-**

**1) Geometry optimization and calculate minimum energy**

**2) Calculate the IR frequency and Molecular Orbital Energy.**

**3) Calculate the Minimum Potential Energy from Potential Energy Curve.**

**Strike out whatever is not applicable and use observation table which is applicable as per your registration number.**

**(Report images and values wherever applicable)**

**Results:**

Observation Table – o1 – Visualization of Butane Molecule

|  |  |  |
| --- | --- | --- |
| **S.No.** | **Name of Molecule** | **Image of build Butane Molecule** |
| 1 | butane | Bond Length:  C-C Bond Length:1.54 angstom  C-H Bond Length:1.07 angstrom |

Observation Table – o2 – Optimization of Butane Molecule

|  |  |  |
| --- | --- | --- |
| **S.No.** | **Description** | **Image of optimized Butane Molecule** |
| 1 |  |  |
| 2 | Minimum Energy | -156.42949447 a.u |

Observation Table – o3 – Calculation of IR Frequency and Molecular Orbital

|  |  |  |
| --- | --- | --- |
| **S.No.** | **Description** | **Results** |
| 1 | IR Spectrograph |  |
| 2 | IR Frequency |  |
| 3 | Molecular Orbital Values | Least unoccupied molecular orbital:  Highest occupied molecular orbital: |

Observation Table – o4 – Potential Energy Curve

|  |  |  |
| --- | --- | --- |
| **S.No.** | **Description** | **Results** |
| 1 | Potential Energy Curve |  |
| 2 | Minimum Energy |  |