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| --- | --- |
|  |  |
| **HPP** | **HNP** |

**Figure 1:** Optimized Chemical Structures of Chalcone derivatives

|  |  |
| --- | --- |
| **Top view of HPP** | **Side view of HPP** |
| **Top view of HNP** | **Side view of HNP** |

**Figure 2:** Al(1 1 0) Metal Surface configuration of adsorbed HPP and HNP molecules

|  |  |
| --- | --- |
| **HPP**  **HOMO ORBITALS** | **HNP** |
| **HPP**  **LUMO ORBITALS** | **HNP** |

**Figure 3:** Orbitals of HOMO and LUMO of HPP and HNP molecules

**Figure 4a:** Second Fukui Function plot for HPP molecule

**Figure 4b:** Second Fukui Function plot for HNP molecule

**List of Tables**

**Table 1:** The two inhibitor’s interaction and binding energy on the Al(110) metal surface

|  |  |  |
| --- | --- | --- |
| **Inhibitor** | **EAl-inhibitor (kJ/mol)** | **Ebinding (kJ/mol)** |
| HPP | -87.953±0.0 | 55.473±0.0 |
| HNP | -63.756±0.0 | 55.825±0.0 |

**Table 2:** Torsion angle, bond length (Å), and bond angle (°) of inhibitor molecules in their optimal neutral form.

|  |  |  |
| --- | --- | --- |
| **Geometry parameters** | **HPP** | **HNP** |
| **Bond length** |  |  |
| C1-C2 | 1.456 | 1.464 |
| C2­­-C3 | 1.348 | 1.355 |
| C3-O4 | 2.808 | 2.820 |
| O4-C5 | 2.384 | 2.378 |
| C5-C6 | 1.400 | 1.402 |
| C6-C7 | 1.388 | 1.386 |
| C7-C8 | 1.398 | 1.395 |
| C8-C9 | 1.397 | 1.393 |
| C9-C10 | 1.395 | 1.393 |
| C10-C11 | 5.326 | - |
| C11-C12 | 1.401 | - |
| C12-C13 | 1.394 | - |
| C13-C14 | 1.399 | - |
| C14-C15 | 1.388 | 1.404 |
| C15-C16 | 1.381 | 1.390 |
| C16-C17 | 3.623 | 1.399 |
| C17- O18 | - | 1.388 |
| C18-C19 | - | 1.380 |
| **Bond angle** |  |  |
| C1-C2-C3 | 120.659 | 118.965 |
| C3-C4-04 | 57.873 | 57.815 |
| C5-C6-C7 | 120.969 | 121.221 |
| C6-C7-C8 | 119.660 | 119.019 |
| C7-C8-C9 | 119.893 | 121.085 |
| C8-C9-C10 | 120.360 | 119.248 |
| C2-C3-C11 | 127.457 | - |
| C3-C11-C12 | 124.387 | - |
| C11-C12-C13 | 120.548 | - |
| C12-C13-C14 | 119.451 | - |
| C13-C14-C15 | 123.692 | - |
| C14-C15-C16 | 118.953 | 120.656 |
| C16-C17-O20 | - | 123.498 |
| C17-C18-C19 | - | 118.856 |

**Table 3:** Calculatedquantum chemical parameters of the studied molecules.

|  |  |  |
| --- | --- | --- |
| **Properties** | **HPP** | **HNP** |
| EHOMO (eV) | -6.019 | -6.206 |
| ELUMO (eV) | -2.307 | -3.687 |
| ΔE (eV) | -3.712 | -2.529 |
| μ (Debye) | 2.110 | 2.310 |
| IE (eV) | 6.019 | 6.206 |
| AE V | 2.307 | 3.687 |
| χ (eV) | 4.163 | 4.947 |
| η (eV) | 1.856 | 1.259 |
| σ (eV)-1 | 0.539 | 0.794 |
| ω (eV) | 4.669 | 9.719 |
| ε (eV)-1 | 0.214 | 0.103 |
| ∆Eb-d (eV) | -0.464 | -0.316 |
| ΔN | 0.387 | 0.259 |
| CosAr(A2) | 259.14 | 289.65 |
| CosVol(A3) | 261.14 | 292.83 |

**Table 4:** Analysed Molecules Fukui indices

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | **Nucleophilic Attack (f+)** | | **Electrophilic Attack (f-)** | |
| Compound | Atom | Milliken | Hirshfield | Milliken | Hirshfield |
| HPP  HNP | O4  O13 | 0.146  0.208 | 0.133  0.191 | 0.073  0.166 | 0.066  0.160 |

**Table 5:** Second Fukui function percentage of the inhibitor Molecules

|  |  |  |
| --- | --- | --- |
| **Molecule** | **F2+%** | **F2-%** |
| **HPP**  **HNP** | 96.55  77.42 | 3.55  22.58 |