**DFT Study of Interamolecular Double Proton Transfer of 2,5-diaminocyclohexa-2,5-diene-1,4-dione and its derivative and their Aromaticity investigations**

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|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Bond Angle | GS1 | TS1a | Int | TS1b | TS2 | GS2 |
| C1-C2-C3 | 117.67 | 117.59 | 116.36 | 119.82 | 120.92 | 121.86 |
| C2-C3-C4 | 120.85 | 119.61 | 121.56 | 119.12 | 116.64 | 119.87 |
| C3-C4-C5 | 121.48 | 121.09 | 118.84 | 119.35 | 122.36 | 118.27 |
| C4-C5-C6 | 117.67 | 121.20 | 122.86 | 122.89 | 120.99 | 121.86 |
| C5-C6-C1 | 120.84 | 117.15 | 116.79 | 116.76 | 116.64 | 119.87 |
| C6-C1-C2 | 121.48 | 123.36 | 123.59 | 122.07 | 122.36 | 118.27 |
| C1-C2-O8 | 117.68 | 115.59 | 114.89 | 109.42 | 109.78 | 115.13 |
| C4-C5-O9 | 117.68 | 110.82 | 114.22 | 114.42 | 109.78 | 115.13 |
| C4-N10-H11 | 116.87 | 95.92 | 89.09 | 88.00 | 96.04 | 86.19 |
| C1-N7-H12 | 116.87 | 115.44 | 113.79 | 95.53 | 96.04 | 86.19 |
| C5-O9-H11 | 87.37 | 93.74 | 102.21 | 104.07 | 93.86 | 105.11 |

Dihedral angles of the compound A

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Dihedral Angle | GS1 | TS1a | Int | TS1b | TS2 | GS2 |
| C1-C2-C3-C4 | -0.01 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 |
| C2-C3-C4-C5 | -0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| C3-C4-C5-C6 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| C4-C5-C6-C1 | -0.01 | 0.00 | -0.00 | 0.00 | 0.00 | 0.00 |
| C5-C6-C1-C2 | -0.00 | 0.00 | -0.00 | 0.00 | 0.00 | 0.00 |
| C6-C1-C2-C3 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 |
| H11-N10-C4-C5 | -0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 |
| H12-N7-C1-C2 | -0.01 | 0.00 | -0.00 | 0.00 | 0.00 | 0.00 |
| H11-O9-C5-C4 | 0.00 | 0.00 | -0.00 | 0.00 | 0.00 | 0.00 |

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Bond Angle | GS1 | TS1a | Int | TS1b | TS2 | GS2 |
| C1-C2-N3 | 117.93 | 118.59 | 117.77 | 122.28 | 123.05 | 124.41 |
| C2-N3-C4 | 116.66 | 115.31 | 117.89 | 114.78 | 111.94 | 115.99 |
| N3-C4-C5 | 125.40 | 124.42 | 121.06 | 121.19 | 125.01 | 119.60 |
| C4-C5-N6 | 117.93 | 122.56 | 124.67 | 125.27 | 123.05 | 124.41 |
| C5-N6-C1 | 116.66 | 112.65 | 112.80 | 112.38 | 111.94 | 115.99 |
| N6-C1-C2 | 125.40 | 126.46 | 125.81 | 124.10 | 125.01 | 119.60 |
| C1-C2-O8 | 117.81 | 115.48 | 114.70 | 109.02 | 109.58 | 115.21 |
| C4-C5-O9 | 117.81 | 110.09 | 115.18 | 114.72 | 109.58 | 115.21 |
| C4-N10-H11 | 117.94 | 95.35 | 88.24 | 87.21 | 95.27 | 85.13 |
| C1-N7-H12 | 117.94 | 116.84 | 115.62 | 94.57 | 95.27 | 85.13 |
| C5-O9-H11 | 86.98 | 93.27 | 102.71 | 104.45 | 93.66 | 105.58 |

Bond Angles of the compound B

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Dihedral Angle | GS1 | TS1a | Int | TS1b | TS2 | GS2 |
| C1-C2-N3-C4 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| C2-N3-C4-C5 | -0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| N3-C4-C5-N6 | 0.03 | 0.00 | -0.00 | 0.00 | 0.00 | 0.00 |
| C4-C5-N6-C1 | -0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| C5-N6-C1-C2 | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| N6-C1-C2-N3 | -0.01 | 0.00 | -0.00 | 0.00 | 0.00 | 0.00 |
| H11-N10-C4-C5 | 0.01 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 |
| H12-N7-C1-C2 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| H11-O9-C5-C4 | 0.05 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

Dihedral angles of the compound B