A picture containing indoor

Description automatically generated

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| --- | --- | --- | --- | --- | --- |
| C9-N6-C2-C1 | C10-C9-N6-C2 | H17-O7-C2-C1 | H18-O13-C9-N6 | E, kJ/mol | IP, eV |
| -58.7 | -48.7 | -54.1 | -167.4 | 38.84 | 8.266 |
| -87.7 | 62.5 | -47.4 | -56.5 | 30.34 | 8.284 |
| -68.7 | 150.8 | -53.5 | -172.7 | 30.20 | 8.285 |
| -60.0 | -48.6 | -177.5 | -166.4 | 36.74 | 8.335 |
| 154.3 | 69.7 | -71.8 | -63.8 | 24.55 | 8.342 |
| 153.5 | -72.4 | -82.7 | 28.6 | 23.16 | 8.358 |
| 178.7 | -41.0 | -81.0 | -43.0 | 26.07 | 8.398 |
| 159.3 | 91.3 | 72.6 | -165.6 | 18.63 | 8.405 |
| -177.3 | -36.7 | 98.9 | -161.0 | 24.90 | 8.408 |
| -93.7 | -80.1 | 59.8 | 65.0 | 28.92 | 8.417 |
| 167.5 | 171.6 | -83.4 | 172.6 | 16.41 | 8.428 |
| 167.4 | 173.8 | -88.4 | -72.0 | 15.50 | 8.438 |
| 97.1 | -51.2 | 165.7 | 48.6 | 14.47 | 8.440 |
| 90.2 | 172.8 | -41.2 | 178.4 | 21.79 | 8.465 |
| 98.8 | 174.7 | -46.0 | 77.1 | 23.55 | 8.469 |
| 86.4 | 172.8 | -41.8 | -71.0 | 20.18 | 8.483 |
| 152.3 | 69.5 | 78.5 | -64.9 | 10.89 | 8.484 |
| 173.6 | -46.4 | 163.7 | 47.7 | 14.73 | 8.484 |
| 168.1 | -55.7 | 72.2 | -52.3 | 16.62 | 8.494 |
| 151.6 | -79.0 | 69.9 | 24.7 | 16.85 | 8.500 |
| -83.2 | 165.0 | 143.1 | 171.1 | 8.12 | 8.515 |
| 74.9 | 61.3 | 168.8 | -54.6 | 18.05 | 8.525 |
| 161.0 | 171.9 | 72.1 | -72.8 | 4.23 | 8.555 |
| 162.0 | 170.0 | 71.2 | 170.5 | 3.86 | 8.558 |
| 166.3 | 173.5 | 71.7 | 78.8 | 2.82 | 8.608 |
| -57.9 | -44.8 | -55.2 | 43.4 | 25.27 | 8.614 |
| 168.0 | -70.1 | 170.7 | -171.8 | 1.75 | 8.619 |
| -70.2 | 167.9 | -46.5 | 48.9 | 1.66 | 8.620 |
| -61.0 | -46.2 | -178.1 | 42.3 | 23.70 | 8.630 |
| 89.5 | 172.3 | 167.3 | 179.1 | 7.44 | 8.635 |
| -66.6 | 173.9 | -166.7 | 53.7 | 0.00 | 8.637 |
| -175.1 | -52.2 | -65.4 | -52.2 | 2.59 | 8.641 |
| -52.2 | -175.3 | 75.2 | 172.7 | 2.31 | 8.645 |
| 94.0 | 174.3 | 163.8 | 74.9 | 7.92 | 8.646 |
| 87.3 | 173.8 | 169.4 | -70.7 | 5.87 | 8.652 |
| -58.1 | -177.7 | 69.4 | -72.6 | 1.14 | 8.653 |

Relative energies and IPs of trans-C2H4(OH)N=C2H4­ (structure 4) conformers

|  |  |  |
| --- | --- | --- |
| Structure | Rel. Energy (kJ/mol) | IP, eV |
| A picture containing indoor  Description automatically generated | 12.23 | 8.75 |
| A picture containing indoor  Description automatically generated | 0.00 | 8.88 |
| A picture containing icon  Description automatically generated | 3.17 | 8.91 |
| Icon  Description automatically generated | 4.50 | 8.83 |
| Icon  Description automatically generated | 2.21 | 8.86 |
| A picture containing indoor  Description automatically generated | 1.30 | 8.86 |

Relative energies and IPs of cis-C2H4(OH)N=C2H4­ (structure 4) conformers

|  |  |  |
| --- | --- | --- |
| Structure | Rel. Energy (kJ/mol) | IP, eV |
| A picture containing indoor  Description automatically generated | 16.07 | 8.57 |
| Icon  Description automatically generated with medium confidence | 0.00 | 8.74 |
| A picture containing indoor  Description automatically generated | 11.45 | 8.62 |
| A picture containing indoor  Description automatically generated | 4.43 | 8.70 |
| Icon  Description automatically generated | 13.21 | 8.61 |
| A picture containing indoor  Description automatically generated | 17.26 | 8.56 |