2\_aminoethanol Ionisation potentials

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Name | Image | Abs. energy, hartree | Rel. energy among neutrals, kJ/mol | Geometry | | | Ionization energy, eV | Name | Image | Abs. energy, hartree | Rel. energy among ions, kJ/mol | Geometry | | |
| 4-3-2-1 | 5-1-2-3 | 11-4-3-2 | 4-3-2-1 | 5-1-2-3 | 11-4-3-2 |
| Neutral 1 |  | -210.03764 | 5.4 | -65° 59° 166° | | | 8.79 | Ion 1 |  | -209.714585 | 0.0 | -30° 27° -159° | | |
| Neutral 2 |  | -210.037219 | 6.51 | -60° -64° 174° | | | 8.81 | Ion 2 |  | -209.71361 | 2.56 | 64° 88° 92° | | |
| Neutral 3 |  | -210.036731 | 7.79 | -62° 54° -69° | | | 8.79 |
| Neutral 4 |  | -210.036602 | 8.13 | -57° -68° -68° | | | 8.79 |
| Neutral 5 |  | -210.033176 | 17.12 | 73° 79° -168° | | | 8.7 |
| Neutral 6 |  | -210.039697 | 0.0 | 54° 80° -40° | | | 8.91 | Ion 3 |  | -209.712363 | 5.83 | 72° 89° -100° | | |
| Neutral 7 |  | -210.036108 | 9.42 | 60° -65° -65° | | | 8.81 |
| Neutral 8 |  | -210.035473 | 11.09 | -180° 75° -178° | | | 8.79 | Ion 4 |  | -209.712299 | 6.0 | -173° 86° -91° | | |
| Neutral 9 |  | -210.035356 | 11.4 | 180° -59° -180° | | | 8.79 |
| Neutral 10 |  | -210.035234 | 11.72 | -177° -58° -63° | | | 8.79 |
| Neutral 11 |  | -210.035152 | 11.93 | -178° 72° -67° | | | 8.79 |
| Neutral 12 |  | -210.035076 | 12.13 | -177° 169° -64° | | | 8.78 |