**ANTA**

**Ground state**

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | X | Y | Z |
| C | -2.040224 | -0.024280 | -0.000070 |
| N | -1.843926 | -1.322714 | -0.000051 |
| N | -0.501214 | -1.535878 | -0.000023 |
| C | 0.065615 | -0.365105 | 0.000032 |
| N | -0.860281 | 0.641667 | -0.000031 |
| N | 1.492398 | -0.137029 | -0.000019 |
| N | 1.847221 | 1.036569 | -0.000270 |
| O | 2.214634 | -1.102061 | 0.000206 |
| O | -0.753484 | 2.036544 | 0.000124 |
| H | -2.988539 | 0.491371 | -0.000061 |
| H | -0.196163 | 2.295416 | -0.811021 |
| H | -0.196930 | 2.295320 | 0.811833 |

**Positively charged**

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | X | Y | Z |
| C | 2.072916 | -0.108895 | -0.000010 |
| N | 1.703676 | -1.379656 | -0.000048 |
| N | 0.467300 | -1.512626 | -0.000037 |
| C | -0.105601 | -0.334304 | -0.000003 |
| N | 0.906175 | 0.598504 | -0.000002 |
| N | 0.890617 | 1.973733 | 0.000016 |
| N | -1.545408 | -0.075797 | 0.000012 |
| O | -1.838630 | 1.102983 | -0.000038 |
| O | -2.250210 | -1.046024 | 0.000086 |
| H | 3.068380 | 0.313126 | -0.000010 |
| H | 0.441039 | 2.330634 | 0.841193 |
| H | 0.440904 | 2.330658 | -0.841078 |

**Negatively charged**

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | X | Y | Z |
| C | 2.050598 | 0.055669 | -0.060025 |
| N | 1.922529 | -1.243747 | -0.051352 |
| N | 0.581095 | -1.540448 | -0.016953 |
| C | -0.072867 | -0.386806 | 0.007091 |
| N | 0.829208 | 0.657654 | -0.021979 |
| N | 0.619851 | 2.038284 | 0.127417 |
| N | -1.437543 | -0.183255 | -0.005246 |
| O | -1.858200 | 1.024954 | -0.281252 |
| O | -2.219107 | -1.162673 | 0.198158 |
| H | 2.970621 | 0.620231 | -0.095255 |
| H | 0.493919 | 2.202383 | 1.126977 |
| H | -0.318449 | 2.166539 | -0.272575 |

**Excited state**

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | X | Y | Z |
| C | -2.065109 | -0.031582 | -0.065479 |
| N | -1.855407 | -1.319860 | -0.105550 |
| N | -0.501042 | -1.529832 | -0.034144 |
| C | 0.049218 | -0.354536 | 0.041818 |
| N | -0.882601 | 0.642612 | 0.039580 |
| N | -0.751462 | 2.026278 | 0.144116 |
| N | 1.425390 | -0.074076 | 0.199982 |
| O | 1.923805 | 0.962877 | -0.394884 |
| O | 2.269532 | -1.085682 | 0.152487 |
| H | -3.015950 | 0.477829 | -0.108936 |
| H | -0.110480 | 2.348558 | -0.575413 |
| H | -0.369066 | 2.256907 | 1.057605 |

**AHNTA**

**Ground state**

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | X | Y | Z |
| C | 1.263531 | -0.162928 | -0.037152 |
| N | 0.992710 | -1.458689 | -0.014952 |
| N | -0.361251 | -1.583213 | -0.006850 |
| C | -0.873034 | -0.392564 | -0.031645 |
| N | 0.116689 | 0.571486 | -0.037133 |
| N | 0.109245 | 1.965712 | -0.085679 |
| N | -2.272721 | -0.085927 | 0.031514 |
| O | -2.555456 | 1.099958 | 0.205374 |
| O | -3.065071 | -0.990882 | -0.085018 |
| N | 2.474392 | 0.455619 | -0.111629 |
| N | 3.607824 | -0.324058 | 0.114062 |
| H | -0.567630 | 2.294461 | 0.598050 |
| H | -0.225792 | 2.254890 | -1.002703 |
| H | 2.466701 | 1.438748 | 0.139502 |
| H | 3.960513 | -0.215084 | 1.059063 |
| H | 4.319230 | -0.099184 | -0.569312 |

**Positively charged**

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | X | Y | Z |
| C | -1.242223 | -0.120819 | -0.007911 |
| N | -1.026632 | -1.414402 | -0.012134 |
| N | 0.315994 | -1.577337 | -0.007144 |
| C | 0.852425 | -0.387160 | -0.000846 |
| N | -0.097307 | 0.600694 | -0.000724 |
| N | -0.109727 | 1.998394 | 0.005560 |
| N | 2.282690 | -0.104253 | 0.001959 |
| O | 2.561086 | 1.086323 | -0.008981 |
| O | 3.027610 | -1.044013 | 0.014256 |
| N | -2.482729 | 0.464163 | -0.014203 |
| N | -3.558293 | -0.290518 | 0.036198 |
| H | 0.410323 | 2.326056 | -0.808490 |
| H | 0.394673 | 2.319154 | 0.832142 |
| H | -2.559150 | 1.484093 | -0.004978 |
| H | -3.416596 | -1.300540 | -0.003969 |
| H | -4.467999 | 0.143455 | -0.070940 |

**Negatively charged**

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | X | Y | Z |
| C | 1.270236 | -0.183970 | -0.098874 |
| N | 1.038243 | -1.464275 | -0.078504 |
| N | -0.344672 | -1.628988 | -0.037845 |
| C | -0.887436 | -0.429092 | -0.043924 |
| N | 0.112407 | 0.532699 | -0.082619 |
| N | 0.050379 | 1.934826 | -0.132965 |
| N | -2.220552 | -0.082850 | 0.049218 |
| O | -2.492046 | 1.171903 | 0.323916 |
| O | -3.114314 | -0.975791 | -0.070705 |
| N | 2.482453 | 0.509738 | -0.162150 |
| N | 3.597899 | -0.277795 | 0.195091 |
| H | -0.883666 | 2.120338 | 0.264645 |
| H | -0.028376 | 2.186313 | -1.119523 |
| H | 2.382406 | 1.383534 | 0.354268 |
| H | 3.637758 | -0.443247 | 1.199428 |
| H | 4.432863 | 0.199055 | -0.119309 |

**Excited state**

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | X | Y | Z |
| C | 1.263736 | -0.169437 | -0.054861 |
| N | 0.992143 | -1.464486 | -0.040493 |
| N | -0.362718 | -1.587344 | -0.017625 |
| C | -0.872860 | -0.396106 | -0.025537 |
| N | 0.117703 | 0.565135 | -0.039793 |
| N | 0.110408 | 1.961861 | -0.041053 |
| N | -2.269631 | -0.081852 | 0.029917 |
| O | -2.547126 | 1.112903 | 0.125527 |
| O | -3.063074 | -0.990983 | -0.019549 |
| N | 2.472675 | 0.453547 | -0.133937 |
| N | 3.604209 | -0.319061 | 0.131595 |
| H | -0.551495 | 2.256489 | 0.674427 |
| H | -0.283229 | 2.268935 | -0.930109 |
| H | 2.448892 | 1.435973 | 0.125826 |
| H | 3.939768 | -0.162389 | 1.078465 |
| H | 4.328880 | -0.075711 | -0.534315 |