**ANTA**

**Ground state**

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| Bond | Bond length(Å) | Bond | Bond length(Å) |
| C5-N1 | 1.313 | C3-N6 | 1.445 |
| C5-N4 | 1.355 | N4-N9 | 1.399 |
| C5-H10 | 1.079 | N6-O7 | 1.205 |
| N1-N2 | 1.359 | N6-O8 | 1.226 |
| N2-C3 | 1.301 | N9-H11 | 1.018 |
| C3-N4 | 1.368 | N9-H12 | 1.018 |

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| Bond | Bond angle(°) | Bond | Bond angle(°) |
| N1-C5-N4 | 110.843 | C5-N4-N9 | 123.831 |
| N1-C5-H10 | 127.118 | C3-N4-N9 | 133.006 |
| N4-C5-H10 | 122.039 | C3-N6-O8 | 115.920 |
| C5-N1-N2 | 107.612 | C3-N6-O7 | 117.709 |
| N1-N2-C3 | 106.817 | O8-N6-O7 | 126.371 |
| N2-C3-N4 | 111.565 | N4-N9-H11 | 107.148 |
| N2-C3-N6 | 124.911 | N4-N9-H12 | 107.197 |
| N4-C3-N6 | 123.524 | H11-N9-H12 | 105.809 |
| C5-N4-C3 | 103.163 |  |  |

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| Bond | Dihedral angle(°) | Bond | Dihedral angle(°) |
| N4-C5-N1-N2 | -0.010 | N6-C3-N4-C5 | 179.836 |
| H10-C5-N1-N2 | 179.992 | N6-C3-N4-N9 | -0.255 |
| N1-C5-N4-C3 | -0.001 | N2-C3-N6-O8 | 179.227 |
| N1-C5-N4-N9 | 179.921 | N2-C3-N6-O7 | -0.767 |
| H10-C5-N4-C3 | 179.997 | N4-C3-N6-O8 | -0.573 |
| H10-C5-N4-N9 | 0.077 | N4-C3-N6-O7 | 179.433 |
| C5-N1-N2-C3 | 0.018 | C5-N4-N9-H11 | -124.380 |
| N1-N2-C3-N6 | -0.019 | C5-N4-N9-H12 | 122.420 |
| N2-C3-N4-C5 | 179.840 | C3-N4-N9-H11 | 55.727 |
| N2-C3-N4-C5 | 0.013 | C3-N4-N9-H12 | -57.473 |
| N2-C3-N4-N9 | 179.922 |  |  |

**Positively charged**

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| Bond | Bond length(Å) | Bond | Bond length(Å) |
| C5-N1 | 1.323 | C3-N6 | 1.463 |
| C5-N4 | 1.364 | N4-N9 | 1.375 |
| C5-H10 | 1.081 | N9-H11 | 1.018 |
| N1-N2 | 1.244 | N9-H12 | 1.018 |
| N2-C3 | 1.310 | N6-O8 | 1.215 |
| C3-N4 | 1.376 | N6-O7 | 1.199 |

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| Bond | Bond angle(°) | Bond | Bond angle(°) |
| N1-C5-N4 | 105.027 | C5-N4-N9 | 121.877 |
| N1-C5-H10 | 129.176 | C3-N4-N9 | 132.026 |
| N4-C5-H10 | 125.797 | N4-N9-H11 | 110.821 |
| C5-N1-N2 | 112.341 | N4-N9-H12 | 110.821 |
| N1-N2-C3 | 109.791 | H11-N9-H12 | 111.372 |
| N2-C3-N4 | 106.745 | C3-N6-O8 | 114.147 |
| N2-C3-N6 | 126.108 | C3-N6-O7 | 115.817 |
| N4-C3-N6 | 127.147 | O8-N6-O7 | 130.035 |
| C5-N4-C3 | 106.097 |  |  |

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| Bond | Dihedral angle(°) | Bond | Dihedral angle(°) |
| N4-C5-N1-N2 | -0.001 | N6-C3-N4-C5 | 180.000 |
| H10-C5-N1-N2 | -179.000 | N6-C3-N4-N9 | 0.000 |
| N1-C5-N4-C3 | 0.001 | N2-C3-N6-O8 | 179.996 |
| N1-C5-N4-N9 | -179.999 | N2-C3-N6-O7 | 0.005 |
| H10-C5-N4-C3 | -179.000 | N4-C3-N6-O8 | 0.003 |
| H10-C5-N4-N9 | -0.000 | N4-C3-N6-O7 | -179.996 |
| C5-N1-N2-C3 | 0.001 | C5-N4-N9-H11 | -117.907 |
| N1-N2-C3-N4 | 0.000 | C5-N4-N9-H12 | -117.916 |
| N1-N2-C3-N6 | 180.000 | C3-N4-N9-H11 | 62.092 |
| N2-C3-N4-C5 | -0.001 | C3-N4-N9-H12 | -62.084 |
| N2-C3-N4-N9 | 179.999 |  |  |

**Negatively charged**

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| Bond | Bond length(Å) | Bond | Bond length(Å) |
| C5-N1 | 1.306 | C3-N6 | 1.380 |
| C5-N4 | 1.362 | N4-N9 | 1.404 |
| C5-H10 | 1.080 | N9-H11 | 1.021 |
| N1-N2 | 1.374 | N9-H12 | 1.028 |
| N2-C3 | 1.326 | N6-O8 | 1.309 |
| C3-N4 | 1.380 | N6-O7 | 1.269 |

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| Bond | Bond angle(°) | Bond | Bond angle(°) |
| N1-C5-N4 | 110.588 | C5-N4-N9 | 124.825 |
| N1-C5-H10 | 127.155 | C3-N4-N9 | 130.105 |
| N4-C5-H10 | 122.256 | N4-N9-H11 | 106.297 |
| C5-N1-N2 | 108.105 | N4-N9-H12 | 102.552 |
| N1-N2-C3 | 107.094 | H11-N9-H12 | 104.380 |
| N2-C3-N4 | 109.605 | C3-N6-O8 | 117.126 |
| N2-C3-N6 | 128.010 | C3-N6-O7 | 119.582 |
| N4-C3-N6 | 122.311 | O8-N6-O7 | 123.241 |
| C5-N4-C3 | 104.605 |  |  |

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| Bond | Dihedral angle(°) | Bond | Dihedral angle(°) |
| N4-C5-N1-N2 | 0.468 | N6-C3-N4-C5 | -177.291 |
| H10-C5-N1-N2 | -179.327 | N6-C3-N4-N9 | 10.394 |
| N1-C5-N4-C3 | -0.178 | N2-C3-N6-O8 | -164.844 |
| N1-C5-N4-N9 | 172.665 | N2-C3-N6-O7 | 12.633 |
| H10-C5-N4-C3 | 179.630 | N4-C3-N6-O8 | 11.685 |
| H10-C5-N4-N9 | -7.528 | N4-C3-N6-O7 | -170.838 |
| C5-N1-N2-C3 | -0.577 | C5-N4-N9-H11 | -93.548 |
| N1-N2-C3-N4 | 0.470 | C5-N4-N9-H12 | 157.172 |
| N1-N2-C3-N6 | 177.356 | C3-N4-N9-H11 | 77.382 |
| N2-C3-N4-C5 | -0.193 | C3-N4-N9-H12 | -31.897 |
| N2-C3-N4-N9 | -172.509 |  |  |

**Excited state**

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| Bond | Bond length(Å) | Bond | Bond length(Å) |
| C5-N1 | 1.306 | C3-N6 | 1.413 |
| C5-N4 | 1.365 | N4-N9 | 1.394 |
| C5-H10 | 1.080 | N9-H11 | 1.016 |
| N1-N2 | 1.372 | N9-H12 | 1.017 |
| N2-C3 | 1.300 | N6-O8 | 1.295 |
| C3-N4 | 1.365 | N6-O7 | 1.318 |

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| Bond | Bond angle(°) | Bond | Bond angle(°) |
| N1-C5-N4 | 111.515 | C5-N4-N9 | 125.275 |
| N1-C5-H10 | 127.280 | C3-N4-N9 | 131.373 |
| N4-C5-H10 | 122.205 | N4-N9-H11 | 108.730 |
| C5-N1-N2 | 107.928 | N4-N9-H12 | 109.144 |
| N1-N2-C3 | 106.406 | H11-N9-H12 | 109.087 |
| N2-C3-N4 | 111.806 | C3-N6-O8 | 118.827 |
| N2-C3-N6 | 126.735 | C3-N6-O7 | 117.849 |
| N4-C3-N6 | 121.333 | O8-N6-O7 | 110.571 |
| C5-N4-C3 | 103.338 |  |  |

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| Bond | Dihedral angle(°) | Bond | Dihedral angle(°) |
| N4-C5-N1-N2 | -0.349 | N6-C3-N4-C5 | -177.043 |
| H10-C5-N1-N2 | 179.463 | N6-C3-N4-N9 | 1.651 |
| N1-C5-N4-C3 | 0.724 | N2-C3-N6-O8 | 144.487 |
| N1-C5-N4-N9 | -178.076 | N2-C3-N6-O7 | 6.379 |
| H10-C5-N4-C3 | -179.100 | N4-C3-N6-O8 | -39.945 |
| H10-C5-N4-N9 | 2.100 | N4-C3-N6-O7 | -178.052 |
| C5-N1-N2-C3 | -0.200 | C5-N4-N9-H11 | -126.795 |
| N1-N2-C3-N4 | 0.683 | C5-N4-N9-H12 | 114.310 |
| N1-N2-C3-N6 | 176.606 | C3-N4-N9-H11 | 54.761 |
| N2-C3-N4-C5 | -0.868 | C3-N4-N9-H12 | -64.134 |
| N2-C3-N4-N9 | 177.827 |  |  |

**AHNTA**

**Ground state**

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| Bond | Bond length(Å) | Bond | Bond length(Å) |
| C5-N1 | 1.324 | N9-H12 | 1.017 |
| C5-N4 | 1.362 | N9-H13 | 1.018 |
| C5-N10 | 1.362 | N6-O8 | 1.231 |
| N1-N2 | 1.360 | N6-O7 | 1.208 |
| N2-C3 | 1.296 | N10-N11 | 1.394 |
| C3-N4 | 1.382 | N10-H14 | 1.015 |
| C3-N6 | 1.434 | N11-H15 | 1.015 |
| N4-N9 | 1.395 | N11-H16 | 1.012 |

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| Bond | Bond angle(°) | Bond | Bond angle(°) |
| N1-C5-N4 | 110.826 | N4-N9-H13 | 108.477 |
| N1-C5-N10 | 128.856 | H12-N9-H13 | 107.143 |
| N4-C5-N10 | 120.256 | C3-N6-O8 | 115.859 |
| C5-N1-N2 | 107.063 | C3-N6-O7 | 118.393 |
| N1-N2-C3 | 107.994 | O8-N6-O7 | 125.748 |
| N2-C3-N4 | 110.988 | C5-N10-N11 | 117.390 |
| N2-C3-N6 | 125.510 | C5-N10-H14 | 114.823 |
| N4-C3-N6 | 123.371 | N11-N10-H14 | 120.528 |
| C5-N4-C3 | 103.118 | N10-N11-H15 | 111.923 |
| C5-N4-N9 | 122.918 | N10-N11-H16 | 109.756 |
| C3-N4-N9 | 133.918 | H15-N11-H16 | 111.151 |
| N4-N9-H12 | 107.656 |  |  |

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| Bond | Dihedral angle(°) | Bond | Dihedral angle(°) |
| N4-C5-N1-N2 | 0.304 | N6-C3-N4-C5 | 177.075 |
| N10-C5-N1-N2 | -176.810 | N6-C3-N4-N9 | -5.422 |
| N1-C5-N4-C3 | -0.795 | N2-C3-N6-O8 | 169.051 |
| N1-C5-N4-N9 | -178.652 | N2-C3-N6-O7 | -10.826 |
| N10-C5-N4-C3 | 176.604 | N4-C3-N6-O8 | -6.407 |
| N10-C5-N4-N9 | -1.253 | N4-C3-N6-O7 | 173.716 |
| N1-C5-N10-N11 | -13.473 | C5-N4-N9-H12 | -135.466 |
| N1-C5-N10-H14 | -163.930 | C5-N4-N9-H13 | 108.908 |
| N4-C5-N10-N11 | 169.650 | C3-N4-N9-H12 | 47.432 |
| N4-C5-N10-H14 | 19.193 | C3-N4-N9-H13 | -68.194 |
| C5-N1-N2-C3 | 0.363 | C5-N10-N11-H15 | -99.447 |
| N1-N2-C3-N4 | -0.892 | C5-N10-N11-H16 | 136.647 |
| N1-N2-C3-N6 | -176.830 | H14-N10-N11-H15 | 49.251 |
| N2-C3-N4-C5 | 1.034 | H14-N10-N11-H16 | -74.654 |
| N2-C3-N4-N9 | 178.537 |  |  |

**Positively charged**

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| Bond | Bond length(Å) | Bond | Bond length(Å) |
| C5-N1 | 1.311 | N9-H12 | 1.020 |
| C5-N4 | 1.353 | N9-H13 | 1.020 |
| C5-N10 | 1.372 | N6-O8 | 1.223 |
| N1-N2 | 1.352 | N6-O7 | 1.199 |
| N2-C3 | 1.305 | N10-N11 | 1.315 |
| C3-N4 | 1.370 | N10-H14 | 1.023 |
| C3-N6 | 1.458 | N11-H15 | 1.021 |
| N4-N9 | 1.398 | N11-H16 | 1.014 |

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| Bond | Bond angle(°) | Bond | Bond angle(°) |
| N1-C5-N4 | 112.757 | N4-N9-H13 | 108.281 |
| N1-C5-N10 | 124.707 | H12-N9-H13 | 107.072 |
| N4-C5-N10 | 122.535 | C3-N6-O8 | 114.348 |
| C5-N1-N2 | 106.380 | C3-N6-O7 | 117.214 |
| N1-N2-C3 | 107.343 | O8-N6-O7 | 128.439 |
| N2-C3-N4 | 111.865 | C5-N10-N11 | 119.661 |
| N2-C3-N6 | 125.451 | C5-N10-H14 | 119.528 |
| N4-C3-N6 | 122.684 | N11-N10-H14 | 120.721 |
| C5-N4-C3 | 101.654 | N10-N11-H15 | 116.929 |
| C5-N4-N9 | 121.710 | N10-N11-H16 | 118.971 |
| C3-N4-N9 | 136.636 | H15-N11-H16 | 122.964 |
| N4-N9-H12 | 108.245 |  |  |

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| Bond | Dihedral angle(°) | Bond | Dihedral angle(°) |
| N4-C5-N1-N2 | 0.022 | N6-C3-N4-C5 | 179.823 |
| N10-C5-N1-N2 | 179.827 | N6-C3-N4-N9 | -0.236 |
| N1-C5-N4-C3 | -0.004 | N2-C3-N6-O8 | 179.127 |
| N1-C5-N4-N9 | -179.958 | N2-C3-N6-O7 | -0.865 |
| N10-C5-N4-C3 | -179.814 | N4-C3-N6-O8 | -0.689 |
| N10-C5-N4-N9 | 0.232 | N4-C3-N6-O7 | 179.319 |
| N1-C5-N10-N11 | 3.085 | C5-N4-N9-H12 | -122.472 |
| N1-C5-N10-H14 | 179.664 | C5-N4-N9-H13 | 121.778 |
| N4-C5-N10-N11 | -177.129 | C3-N4-N9-H12 | 57.595 |
| N4-C5-N10-H14 | -0.550 | C3-N4-N9-H13 | -58.155 |
| C5-N1-N2-C3 | -0.031 | C5-N10-N11-H15 | -5.204 |
| N1-N2-C3-N4 | 0.030 | C5-N10-N11-H16 | -173.383 |
| N1-N2-C3-N6 | -179.803 | H14-N10-N11-H15 | 178.258 |
| N2-C3-N4-C5 | -0.016 | H14-N10-N11-H16 | 10.080 |
| N2-C3-N4-N9 | 179.926 |  |  |

**Negatively charged**

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| Bond | Bond length(Å) | Bond | Bond length(Å) |
| C5-N1 | 1.301 | N9-H12 | 1.032 |
| C5-N4 | 1.362 | N9-H13 | 1.021 |
| C5-N10 | 1.398 | N6-O8 | 1.313 |
| N1-N2 | 1.393 | N6-O7 | 1.269 |
| N2-C3 | 1.317 | N10-N11 | 1.411 |
| C3-N4 | 1.388 | N10-H14 | 1.020 |
| C3-N6 | 1.380 | N11-H15 | 1.019 |
| N4-N9 | 1.404 | N11-H16 | 1.012 |

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| Bond | Bond angle(°) | Bond | Bond angle(°) |
| N1-C5-N4 | 111.470 | N4-N9-H13 | 106.494 |
| N1-C5-N10 | 130.049 | H12-N9-H13 | 104.961 |
| N4-C5-N10 | 118.464 | C3-N6-O8 | 116.970 |
| C5-N1-N2 | 107.081 | C3-N6-O7 | 119.818 |
| N1-N2-C3 | 107.531 | O8-N6-O7 | 123.135 |
| N2-C3-N4 | 109.549 | C5-N10-N11 | 113.386 |
| N2-C3-N6 | 128.770 | C5-N10-H14 | 108.489 |
| N4-C3-N6 | 121.585 | N11-N10-H14 | 115.303 |
| C5-N4-C3 | 104.368 | N10-N11-H15 | 111.784 |
| C5-N4-N9 | 124.232 | N10-N11-H16 | 108.096 |
| C3-N4-N9 | 131.380 | H15-N11-H16 | 110.529 |
| N4-N9-H12 | 101.867 |  |  |

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| Bond | Dihedral angle(°) | Bond | Dihedral angle(°) |
| N4-C5-N1-N2 | -0.386 | N6-C3-N4-C5 | 176.737 |
| N10-C5-N1-N2 | -178.839 | N6-C3-N4-N9 | -4.890 |
| N1-C5-N4-C3 | 0.241 | N2-C3-N6-O8 | 164.957 |
| N1-C5-N4-N9 | -178.282 | N2-C3-N6-O7 | -11.961 |
| N10-C5-N4-C3 | 178.894 | N4-C3-N6-O8 | -11.087 |
| N10-C5-N4-N9 | 0.371 | N4-C3-N6-O7 | 171.996 |
| N1-C5-N10-N11 | -18.205 | C5-N4-N9-H12 | -158.555 |
| N1-C5-N10-H14 | -147.670 | C5-N4-N9-H13 | 91.730 |
| N4-C5-N10-N11 | 163.433 | C3-N4-N9-H12 | 23.352 |
| N4-C5-N10-H14 | 33.968 | C3-N4-N9-H13 | -86.363 |
| C5-N1-N2-C3 | 0.381 | C5-N10-N11-H15 | -73.744 |
| N1-N2-C3-N4 | -0.236 | C5-N10-N11-H16 | 164.392 |
| N1-N2-C3-N6 | -176.660 | H14-N10-N11-H15 | 52.173 |
| N2-C3-N4-C5 | 0.010 | H14-N10-N11-H16 | -69.690 |
| N2-C3-N4-N9 | 178.383 |  |  |

**Excited state**

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| Bond | Bond length(Å) | Bond | Bond length(Å) |
| C5-N1 | 1.355 | N9-H12 | 1.023 |
| C5-N4 | 1.389 | N9-H13 | 1.021 |
| C5-N10 | 1.328 | N6-O8 | 1.285 |
| N1-N2 | 1.330 | N6-O7 | 1.263 |
| N2-C3 | 1.410 | N10-N11 | 1.390 |
| C3-N4 | 1.357 | N10-H14 | 1.019 |
| C3-N6 | 1.352 | N11-H15 | 1.015 |
| N4-N9 | 1.399 | N11-H16 | 1.014 |

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| Bond | Bond angle(°) | Bond | Bond angle(°) |
| N1-C5-N4 | 111.156 | N4-N9-H13 | 107.179 |
| N1-C5-N10 | 129.784 | H12-N9-H13 | 104.999 |
| N4-C5-N10 | 119.059 | C3-N6-O8 | 117.330 |
| C5-N1-N2 | 108.307 | C3-N6-O7 | 117.144 |
| N1-N2-C3 | 107.138 | O8-N6-O7 | 125.526 |
| N2-C3-N4 | 109.179 | C5-N10-N11 | 120.263 |
| N2-C3-N6 | 127.315 | C5-N10-H14 | 116.337 |
| N4-C3-N6 | 123.394 | N11-N10-H14 | 123.198 |
| C5-N4-C3 | 104.142 | N10-N11-H15 | 110.260 |
| C5-N4-N9 | 122.483 | N10-N11-H16 | 109.814 |
| C3-N4-N9 | 133.364 | H15-N11-H16 | 110.884 |
| N4-N9-H12 | 105.105 |  |  |

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| Bond | Dihedral angle(°) | Bond | Dihedral angle(°) |
| N4-C5-N1-N2 | -1.628 | N6-C3-N4-C5 | 173.681 |
| N10-C5-N1-N2 | 178.024 | N6-C3-N4-N9 | -7.560 |
| N1-C5-N4-C3 | 2.720 | N2-C3-N6-O8 | 168.617 |
| N1-C5-N4-N9 | -176.211 | N2-C3-N6-O7 | -11.714 |
| N10-C5-N4-C3 | -176.974 | N4-C3-N6-O8 | -7.117 |
| N10-C5-N4-N9 | 4.095 | N4-C3-N6-O7 | 172.552 |
| N1-C5-N10-N11 | -1.979 | C5-N4-N9-H12 | -141.987 |
| N1-C5-N10-H14 | -176.978 | C5-N4-N9-H13 | 106.665 |
| N4-C5-N10-N11 | 177.650 | C3-N4-N9-H12 | 39.440 |
| N4-C5-N10-H14 | 2.651 | C3-N4-N9-H13 | -71.908 |
| C5-N1-N2-C3 | -0.142 | C5-N10-N11-H15 | -110.374 |
| N1-N2-C3-N4 | 1.885 | C5-N10-N11-H16 | 127.154 |
| N1-N2-C3-N6 | -174.345 | H14-N10-N11-H15 | 64.270 |
| N2-C3-N4-C5 | -2.728 | H14-N10-N11-H16 | -58.202 |
| N2-C3-N4-N9 | 176.031 |  |  |