Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# HOMER: A reparameterization of the harmonic oscillator model of aromaticity (HOMA) for excited states†

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## Electronic supplementary information

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## 1. Complementary results

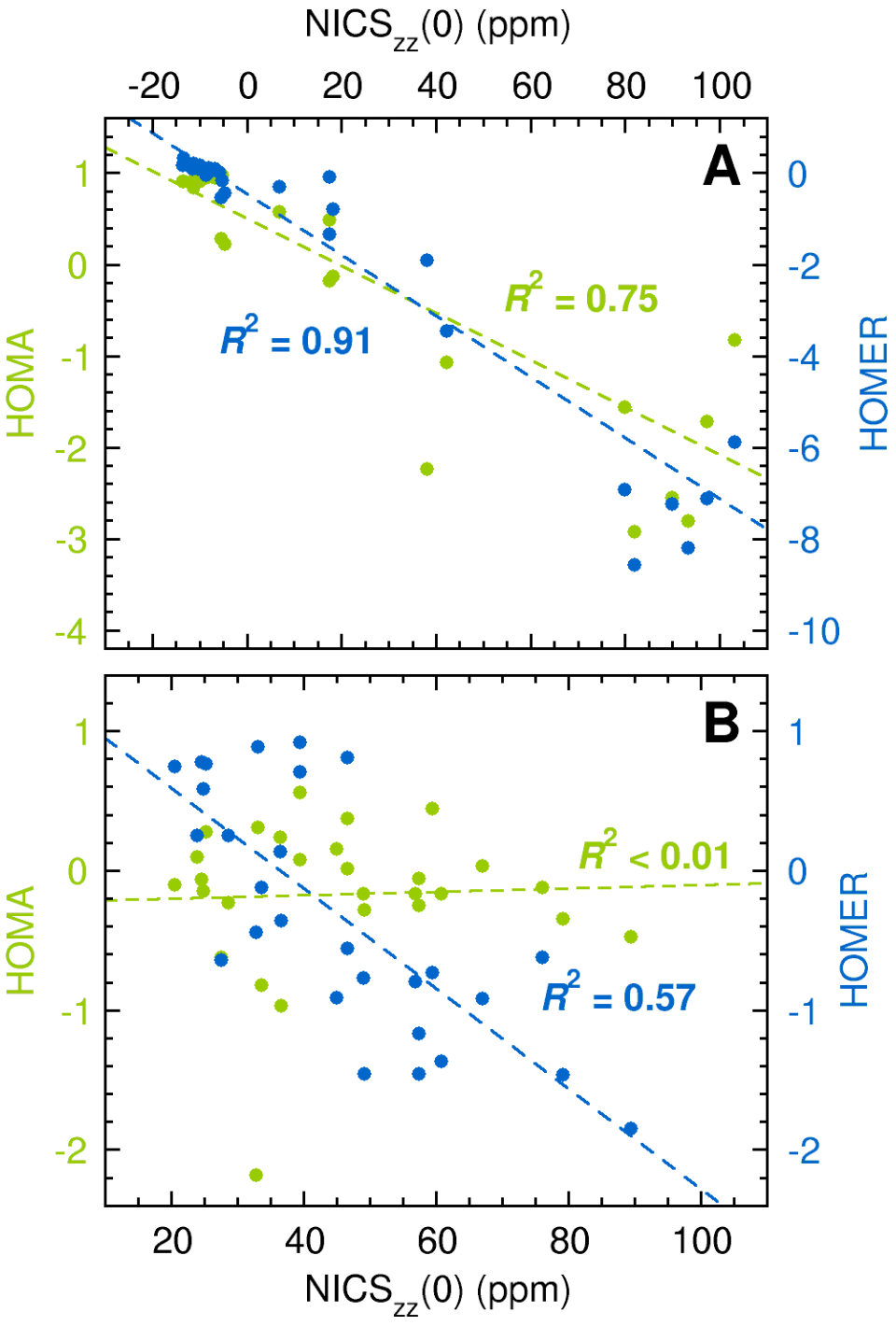


**Fig. S1** Correlation between CASPT2-based HOMA (in green font) / HOMER (in blue font) values and CASSCF-based NICS$_{zz}$(0) values in probing GSA/GSAA (**A**) and ESA/ESAA (**B**).

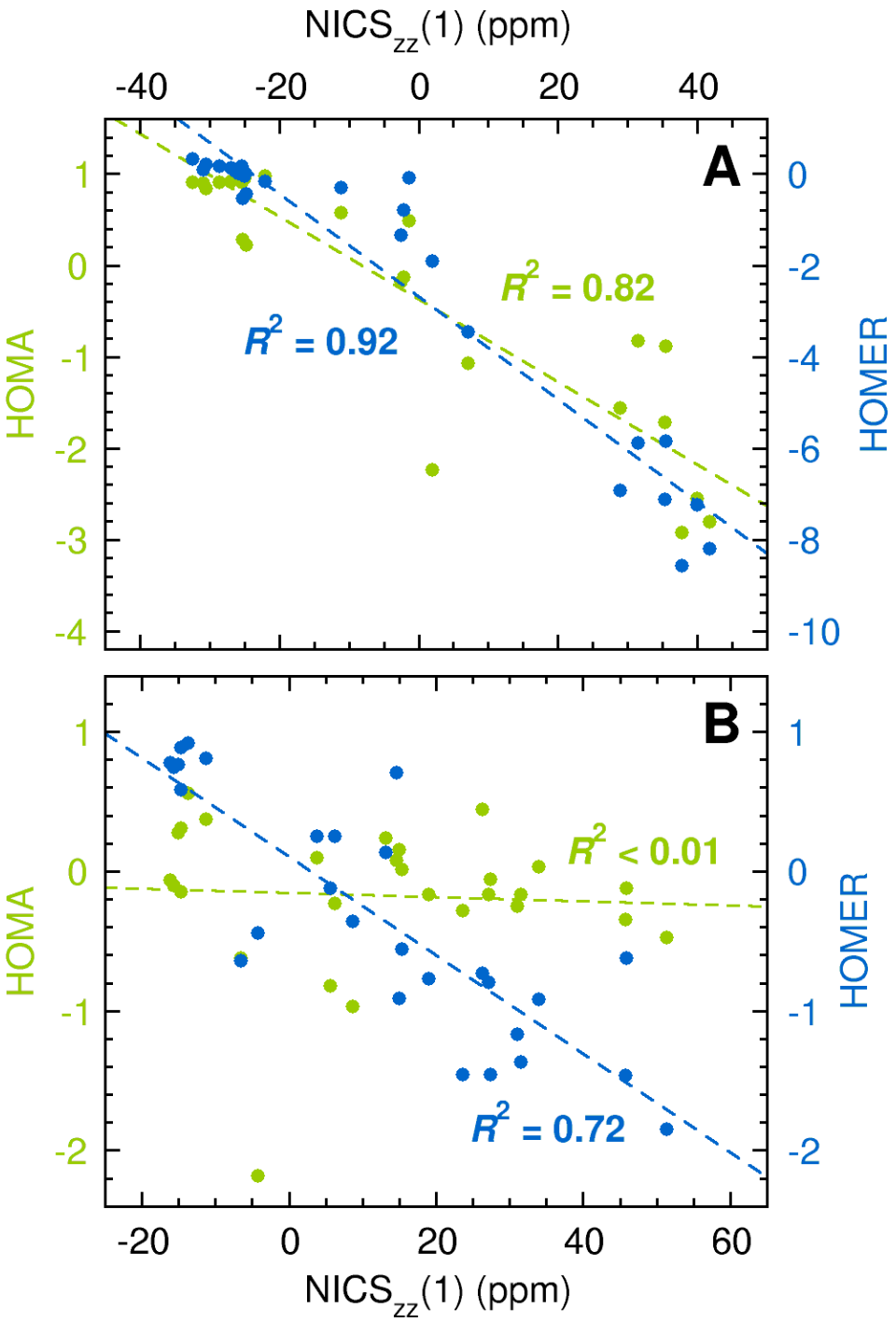


**Fig. S2** Correlation between CASPT2-based HOMA (in green font) / HOMER (in blue font) values and CASSCF-based NICS$_{zz}$(1) values in probing GSA/GSAA (**A**) and ESA/ESAA (**B**).

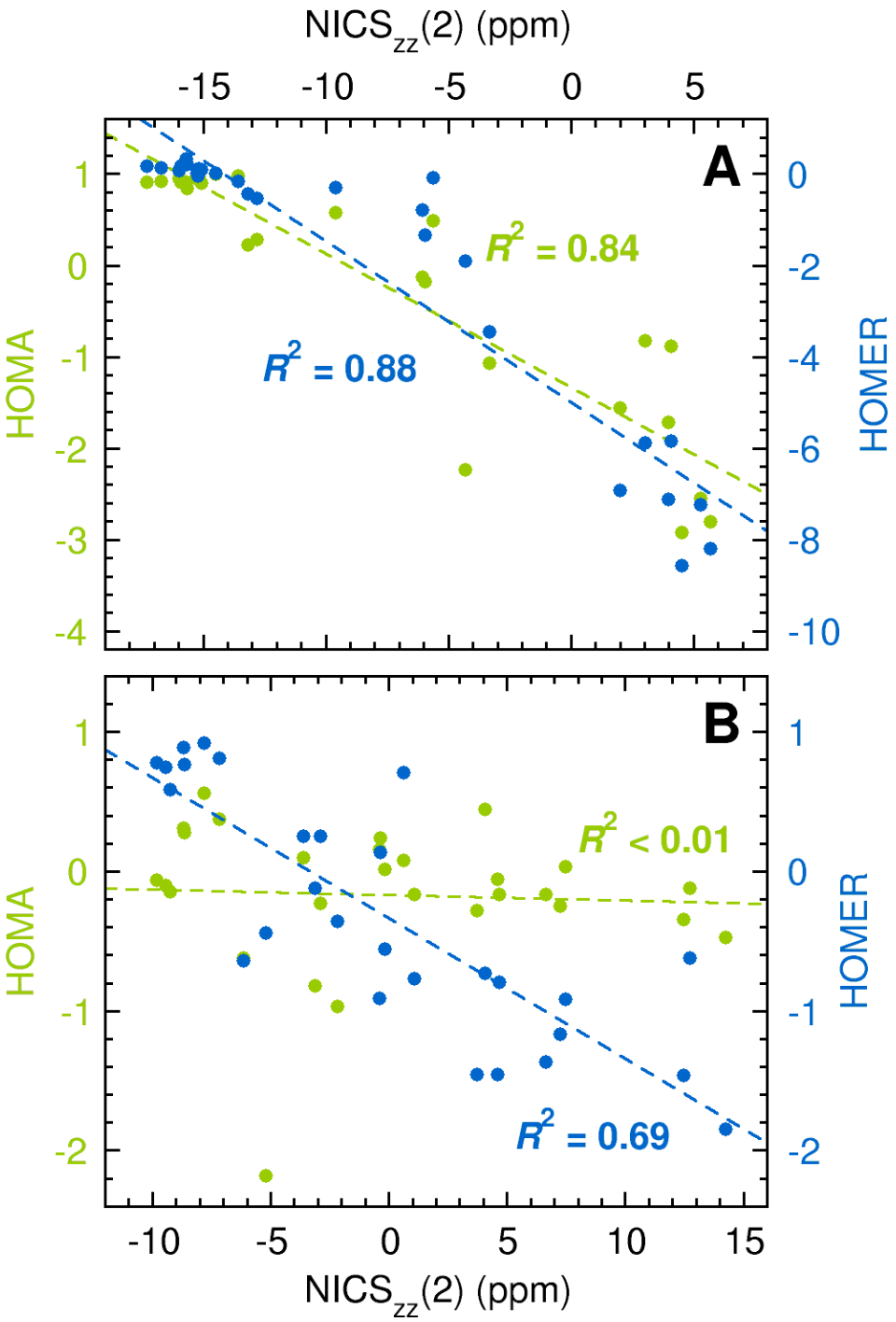


**Fig. S3** Correlation between CASPT2-based HOMA (in green font) / HOMER (in blue font) values and CASSCF-based NICS$_{zz}$(2) values in probing GSA/GSAA (**A**) and ESA/ESAA (**B**).

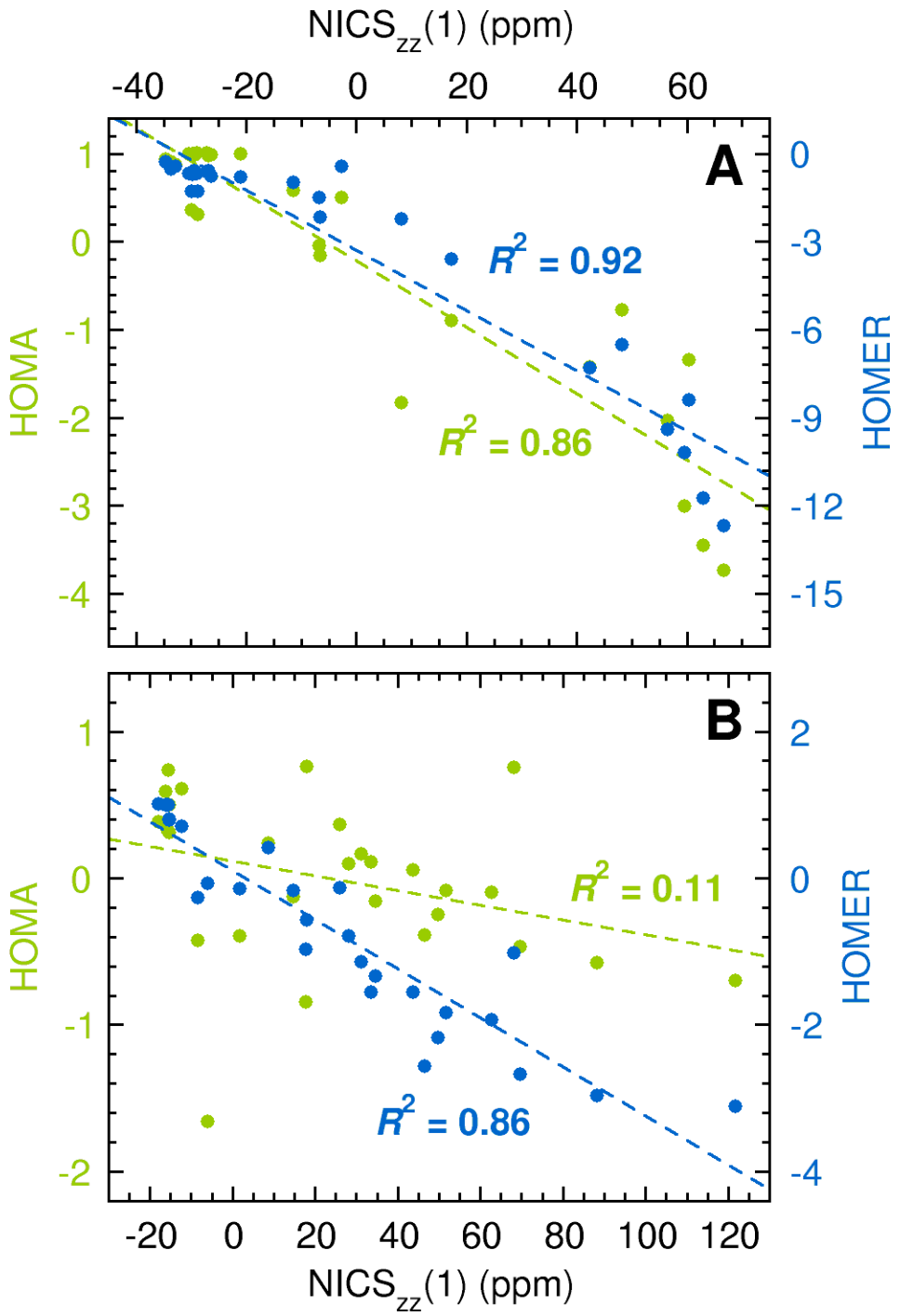


**Fig. S4** Correlation between M06-2X-based HOMA (in green font) / HOMER (in blue font) values and M06-2X-based NICS$_{zz}$(1) values in probing GSA/GSAA (**A**) and ESA/ESAA (**B**).

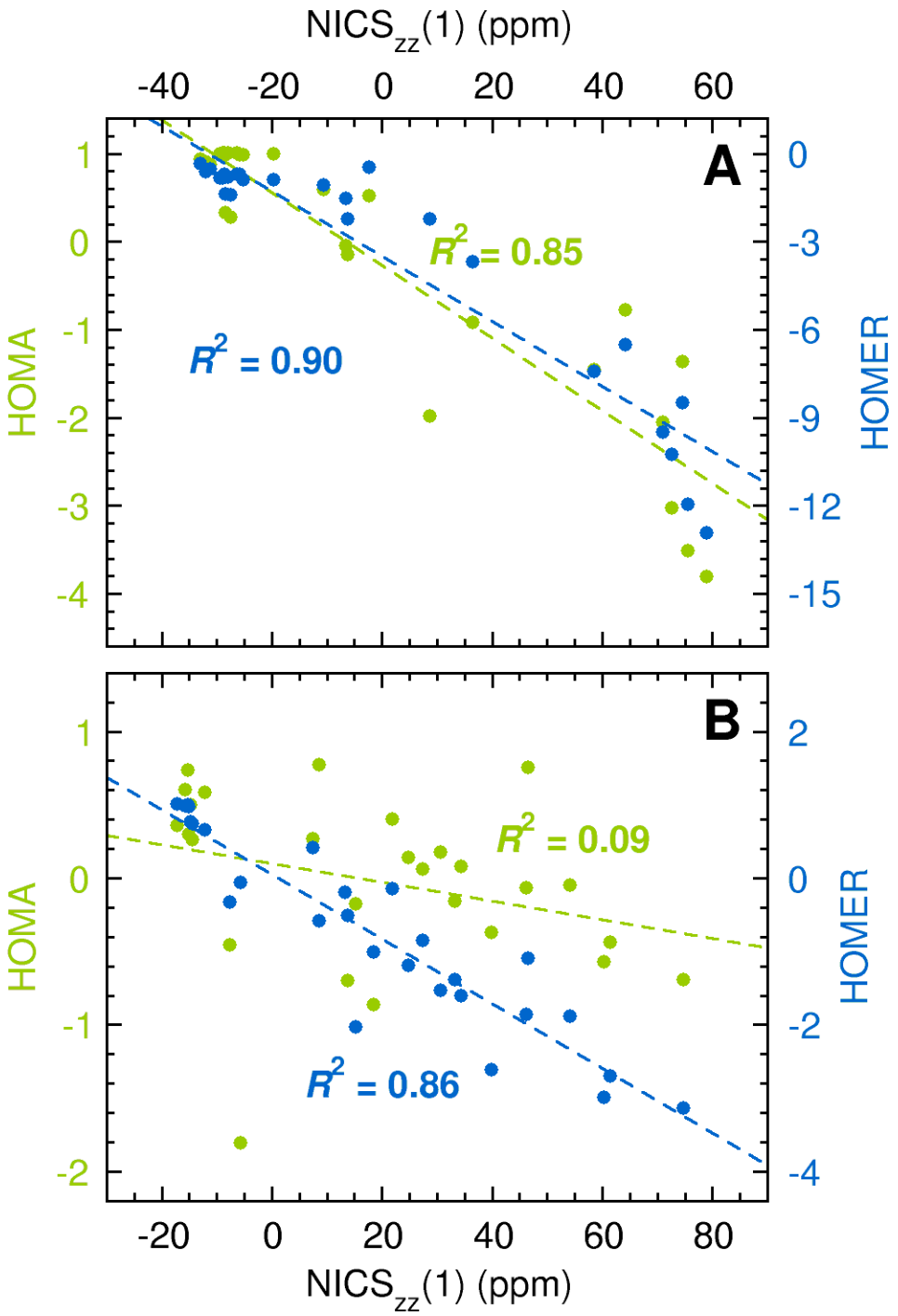


**Fig. S5** Correlation between CAM-B3LYP-based HOMA (in green font) / HOMER (in blue font) values and CAM-B3LYP-based NICS$_{zz}$(1) values in probing GSA/GSAA (**A**) and ESA/ESAA (**B**).

**Table S1** $S_0$ HOMA, HOMER and NICS values for the 28 compounds in Fig. 2 in the main text calculated at the CASPT2/cc-pVDZ (HOMA and HOMER) and CASSCF/cc-pVDZ (NICS) levels of theory[a]

| Compound | HOMA | HOMER | $NICS_{zz}(0)$ (ppm) | $NICS_{zz}(1)$ (ppm) | $NICS_{zz}(2)$ (ppm) |
|---|---|---|---|---|---|
| **1** | 0.912 | 0.114 | -11.103 | -26.884 | -16.683 |
| **2** | 0.944 | 0.059 | -9.645 | -26.389 | -15.951 |
| **3** | 0.937 | 0.083 | -6.726 | -25.280 | -15.222 |
| **4** | 0.971 | 0.010 | -8.037 | -25.792 | -15.224 |
| **5** | 0.960 | 0.091 | -7.911 | -25.604 | -15.167 |
| **6** | 0.988 | -0.001 | -5.614 | -24.826 | -14.446 |
| **7** | 0.572 | -0.310 | 6.978 | -11.084 | -9.570 |
| **8** | 0.942 | -0.053 | -8.602 | -24.886 | -15.182 |
| **9** | 0.485 | -0.099 | 17.630 | -1.342 | -5.608 |
| **10** | 0.972 | -0.168 | -5.080 | -21.978 | -13.551 |
| **11** | 0.901 | 0.151 | -9.782 | -25.342 | -15.870 |
| **12** | 0.899 | 0.154 | -13.398 | -28.569 | -17.288 |
| **13** | -2.812 | -8.200 | 93.412 | 41.783 | 5.733 |
| **14** | -1.728 | -7.134 | 97.477 | 35.423 | 3.996 |
| **15** | -0.895 | -5.861 | 117.188 | 35.549 | 4.099 |
| **16** | -0.834 | -5.899 | 103.329 | 31.603 | 3.040 |
| **17** | -1.076 | -3.458 | 42.309 | 7.218 | -3.290 |
| **18** | -1.569 | -6.934 | 80.078 | 29.058 | 2.038 |
| **19** | -2.924 | -8.581 | 82.046 | 37.826 | 4.546 |
| **20** | -2.556 | -7.254 | 90.012 | 40.073 | 5.308 |
| **21** | 0.837 | 0.206 | -11.101 | -30.475 | -15.633 |
| **22** | 0.894 | 0.313 | -13.215 | -32.383 | -15.666 |
| **23** | 0.892 | 0.079 | -11.366 | -30.857 | -15.047 |
| **24** | 0.218 | -0.446 | -4.666 | -24.652 | -13.149 |
| **25** | 0.272 | -0.549 | -5.272 | -25.231 | -12.780 |
| **26** | -2.241 | -1.914 | 38.153 | 1.995 | -4.288 |
| **27** | -0.132 | -0.799 | 18.385 | -2.044 | -6.022 |
| **28** | -0.187 | -1.347 | 17.536 | -2.483 | -5.939 |

[a] All calculations based on CASPT2/cc-pVDZ geometries.

**Table S2** $T_1$ HOMA, HOMER and NICS values for the 28 compounds in Fig. 2 in the main text calculated at the CASPT2/cc-pVDZ (HOMA and HOMER) and CASSCF/cc-pVDZ (NICS) levels of theory[a]

| Compound | HOMA | HOMER | $NICS_{zz}(0)$ (ppm) | $NICS_{zz}(1)$ (ppm) | $NICS_{zz}(2)$ (ppm) |
|---|---|---|---|---|---|
| **1** | -0.128 | -0.629 | 76.133 | 45.987 | 12.779 |
| **2** | -0.347 | -1.467 | 79.232 | 45.845 | 12.486 |
| **3** | -0.322 | -0.799 | 56.923 | 27.229 | 4.695 |
| **4** | 0.030 | -0.919 | 67.134 | 34.012 | 7.487 |
| **5** | -0.478 | -1.854 | 89.489 | 51.386 | 14.293 |
| **6** | 0.442 | -0.738 | 59.577 | 26.412 | 4.090 |
| **7** | 0.232 | 0.133 | 36.591 | 13.258 | -0.314 |
| **8** | -0.171 | -1.371 | 60.885 | 31.589 | 6.660 |
| **9** | 0.092 | 0.247 | 24.010 | 3.907 | -3.596 |
| **10** | -0.064 | -1.458 | 57.464 | 27.421 | 4.627 |
| **11** | -0.252 | -1.173 | 57.550 | 31.171 | 7.274 |
| **12** | -0.285 | -1.458 | 49.208 | 23.678 | 3.757 |
| **13** | -0.070 | 0.773 | 24.604 | -16.099 | -9.772 |
| **14** | 0.305 | 0.882 | 33.139 | -14.655 | -8.646 |
| **15** | 0.288 | 0.808 | 46.735 | -11.184 | -7.127 |
| **16** | 0.554 | 0.914 | 39.552 | -13.682 | -7.773 |
| **17** | -0.628 | -0.642 | 27.567 | -6.419 | -6.105 |
| **18** | 0.274 | 0.760 | 25.287 | -14.953 | -8.600 |
| **19** | -0.103 | 0.740 | 20.621 | -15.529 | -9.410 |
| **20** | -0.153 | 0.580 | 24.959 | -14.592 | -9.216 |
| **21** | -0.168 | -0.775 | 49.055 | 19.017 | 1.120 |
| **22** | 0.127 | -0.917 | 45.095 | 15.029 | -0.375 |
| **23** | 0.007 | -0.560 | 46.683 | 15.419 | -0.123 |
| **24** | -0.972 | -0.360 | 36.616 | 8.790 | -2.135 |
| **25** | -0.823 | -0.124 | 33.756 | 5.672 | -3.087 |
| **26** | -2.184 | -0.448 | 32.910 | -4.166 | -5.186 |
| **27** | -0.233 | 0.249 | 28.757 | 6.303 | -2.866 |
| **28** | 0.073 | 0.704 | 39.461 | 14.661 | 0.644 |

[a] All calculations based on CASPT2/cc-pVDZ geometries.

**Table S3** $S_0$ HOMA, HOMER and NICS values for the 28 compounds in Fig. 2 in the main text calculated at the M06-2X/cc-pVDZ level of theory

| Compound | HOMA | HOMER | $NICS_{zz}(0)$ (ppm) | $NICS_{zz}(1)$ (ppm) | $NICS_{zz}(2)$ (ppm) |
|---|---|---|---|---|---|
| **1** | 0.989 | -0.706 | -14.501 | -30.265 | -17.828 |
| **2** | 0.995 | -0.708 | -13.316 | -29.771 | -16.995 |
| **3** | 0.985 | -0.642 | -11.158 | -29.281 | -16.424 |
| **4** | 0.999 | -0.695 | -11.597 | -28.824 | -16.050 |
| **5** | 0.995 | -0.597 | -12.186 | -29.324 | -16.249 |
| **6** | 1.000 | -0.630 | -8.587 | -27.159 | -14.960 |
| **7** | 0.573 | -1.004 | 7.087 | -11.326 | -9.440 |
| **8** | 0.983 | -0.787 | -9.823 | -26.317 | -15.487 |
| **9** | 0.500 | -0.452 | 15.935 | -2.580 | -5.818 |
| **10** | 0.988 | -0.798 | -3.536 | -20.937 | -12.954 |
| **11** | 0.976 | -0.601 | -10.696 | -26.847 | -16.215 |
| **12** | 0.982 | -0.650 | -13.764 | -29.312 | -17.337 |
| **13** | -3.742 | -12.706 | 127.588 | 66.717 | 12.056 |
| **14** | -2.035 | -9.403 | 130.087 | 56.622 | 9.131 |
| **15** | -1.377 | -8.402 | 165.947 | 60.523 | 10.040 |
| **16** | -0.781 | -6.537 | 131.268 | 48.230 | 6.913 |
| **17** | -0.906 | -3.608 | 55.800 | 17.271 | -0.963 |
| **18** | -1.429 | -7.317 | 98.894 | 42.438 | 5.010 |
| **19** | -3.010 | -10.216 | 113.069 | 59.735 | 9.613 |
| **20** | -3.453 | -11.760 | 121.882 | 62.994 | 11.031 |
| **21** | 0.875 | -0.462 | -12.748 | -32.710 | -16.254 |
| **22** | 0.933 | -0.298 | -15.499 | -34.589 | -16.197 |
| **23** | 0.904 | -0.534 | -14.457 | -33.569 | -15.737 |
| **24** | 0.305 | -1.303 | -9.123 | -28.798 | -14.354 |
| **25** | 0.359 | -1.292 | -11.323 | -29.784 | -14.000 |
| **26** | -1.837 | -2.227 | 47.058 | 8.181 | -2.910 |
| **27** | -0.051 | -1.500 | 12.987 | -6.680 | -7.579 |
| **28** | -0.166 | -2.180 | 13.086 | -6.515 | -7.227 |

**Table S4** $T_1$ HOMA, HOMER and NICS values for the 28 compounds in Fig. 2 in the main text calculated at the UM06-2X/cc-pVDZ level of theory

| Compound | HOMA | HOMER | $NICS_{zz}(0)$ (ppm) | $NICS_{zz}(1)$ (ppm) | $NICS_{zz}(2)$ (ppm) |
|---|---|---|---|---|---|
| **1** | -0.472 | -2.677 | 106.791 | 69.795 | 22.639 |
| **2** | -0.583 | -2.968 | 134.794 | 88.412 | 29.633 |
| **3** | 0.744 | -1.021 | 105.700 | 68.161 | 22.468 |
| **4** | -0.099 | -1.940 | 105.662 | 62.830 | 18.678 |
| **5** | -0.703 | -3.122 | 183.491 | 121.912 | 41.774 |
| **6** | 0.758 | -0.572 | 37.536 | 18.113 | 2.037 |
| **7** | 0.363 | -0.142 | 53.786 | 26.103 | 4.784 |
| **8** | -0.088 | -1.838 | 87.447 | 51.797 | 14.546 |
| **9** | 0.233 | 0.409 | 30.418 | 8.777 | -1.619 |
| **10** | 0.055 | -1.565 | 79.868 | 43.905 | 10.778 |
| **11** | -0.249 | -2.187 | 80.654 | 49.902 | 14.861 |
| **12** | -0.394 | -2.567 | 77.879 | 46.588 | 12.913 |
| **13** | 0.383 | 1.000 | 25.860 | -17.761 | -10.137 |
| **14** | 0.587 | 0.995 | 35.205 | -16.050 | -8.851 |
| **15** | 0.544 | 0.697 | 50.516 | -12.209 | -7.182 |
| **16** | 0.736 | 0.996 | 40.638 | -15.505 | -8.025 |
| **17** | -0.425 | -0.278 | 26.049 | -8.286 | -6.573 |
| **18** | 0.498 | 0.781 | 27.535 | -15.269 | -8.600 |
| **19** | 0.329 | 0.989 | 24.229 | -15.731 | -9.433 |
| **20** | 0.306 | 0.802 | 27.349 | -15.137 | -9.298 |
| **21** | -0.163 | -1.347 | 69.337 | 34.733 | 6.209 |
| **22** | 0.086 | -1.559 | 68.623 | 33.597 | 5.303 |
| **23** | 0.095 | -0.800 | 63.423 | 28.312 | 3.890 |
| **24** | -0.847 | -0.978 | 48.749 | 17.917 | 0.744 |
| **25** | -0.399 | -0.147 | 27.580 | 1.954 | -4.087 |
| **26** | -1.660 | -0.073 | 31.606 | -6.006 | -5.608 |
| **27** | -0.128 | -0.176 | 40.318 | 14.831 | 0.414 |
| **28** | 0.160 | -1.145 | 61.648 | 31.245 | 7.465 |

**Table S5** $S_0$ HOMA, HOMER and NICS values for the 28 compounds in Fig. 2 in the main text calculated at the CAM-B3LYP/cc-pVDZ level of theory

| Compound | HOMA | HOMER | $NICS_{zz}(0)$ (ppm) | $NICS_{zz}(1)$ (ppm) | $NICS_{zz}(2)$ (ppm) |
|---|---|---|---|---|---|
| **1** | 0.994 | -0.840 | -13.712 | -29.375 | -17.338 |
| **2** | 0.998 | -0.844 | -12.435 | -28.873 | -16.529 |
| **3** | 0.987 | -0.759 | -10.303 | -28.396 | -15.979 |
| **4** | 1.000 | -0.817 | -10.598 | -27.902 | -15.607 |
| **5** | 0.998 | -0.728 | -11.376 | -28.496 | -15.834 |
| **6** | 0.999 | -0.728 | -7.549 | -26.238 | -14.550 |
| **7** | 0.586 | -1.085 | 7.785 | -10.514 | -9.031 |
| **8** | 0.986 | -0.915 | -8.518 | -25.160 | -14.931 |
| **9** | 0.521 | -0.479 | 16.149 | -2.265 | -5.623 |
| **10** | 0.989 | -0.908 | -1.778 | -19.610 | -12.394 |
| **11** | 0.982 | -0.718 | -9.675 | -25.798 | -15.670 |
| **12** | 0.987 | -0.773 | -12.806 | -28.375 | -16.866 |
| **13** | -3.814 | -12.950 | 116.291 | 59.044 | 10.148 |
| **14** | -2.054 | -9.514 | 120.543 | 51.056 | 7.847 |
| **15** | -1.392 | -8.503 | 152.764 | 54.718 | 8.725 |
| **16** | -0.777 | -6.518 | 123.764 | 44.338 | 6.054 |
| **17** | -0.925 | -3.688 | 53.927 | 16.475 | -1.050 |
| **18** | -1.460 | -7.439 | 92.830 | 38.637 | 4.187 |
| **19** | -3.031 | -10.263 | 102.985 | 52.742 | 7.947 |
| **20** | -3.522 | -11.977 | 111.248 | 55.680 | 9.199 |
| **21** | 0.870 | -0.550 | -11.041 | -31.148 | -15.617 |
| **22** | 0.929 | -0.359 | -13.545 | -32.977 | -15.577 |
| **23** | 0.897 | -0.617 | -12.406 | -31.957 | -15.130 |
| **24** | 0.272 | -1.411 | -7.441 | -27.393 | -13.815 |
| **25** | 0.321 | -1.387 | -9.387 | -28.374 | -13.498 |
| **26** | -1.989 | -2.234 | 46.868 | 8.762 | -2.676 |
| **27** | -0.054 | -1.543 | 12.864 | -6.530 | -7.430 |
| **28** | -0.151 | -2.242 | 13.148 | -6.200 | -7.016 |

**Table S6** $T_1$ HOMA, HOMER and NICS values for the 28 compounds in Fig. 2 in the main text calculated at the UCAM-B3LYP/cc-pVDZ level of theory

| Compound | HOMA | HOMER | $NICS_{zz}(0)$ (ppm) | $NICS_{zz}(1)$ (ppm) | $NICS_{zz}(2)$ (ppm) |
|---|---|---|---|---|---|
| **1** | -0.441 | -2.704 | 95.414 | 61.507 | 19.092 |
| **2** | -0.576 | -2.998 | 98.234 | 60.460 | 18.476 |
| **3** | 0.744 | -1.098 | 78.985 | 46.665 | 13.952 |
| **4** | -0.053 | -1.891 | 93.424 | 54.183 | 15.350 |
| **5** | -0.693 | -3.141 | 120.698 | 74.829 | 23.563 |
| **6** | 0.770 | -0.592 | 36.962 | 8.623 | -0.128 |
| **7** | 0.399 | -0.153 | 48.115 | 22.005 | 3.243 |
| **8** | -0.071 | -1.869 | 79.911 | 46.283 | 12.406 |
| **9** | 0.265 | 0.411 | 28.612 | 7.580 | -1.989 |
| **10** | 0.078 | -1.605 | 66.959 | 34.483 | 7.251 |
| **11** | -0.181 | -2.035 | 38.594 | 15.235 | 1.595 |
| **12** | -0.375 | -2.621 | 69.031 | 39.947 | 10.157 |
| **13** | 0.359 | 0.999 | 25.786 | -17.137 | -9.863 |
| **14** | 0.598 | 0.984 | 34.653 | -15.676 | -8.670 |
| **15** | 0.518 | 0.656 | 48.992 | -12.065 | -7.073 |
| **16** | 0.735 | 0.996 | 40.185 | -15.245 | -7.918 |
| **17** | -0.457 | -0.327 | 26.195 | -7.609 | -6.302 |
| **18** | 0.495 | 0.758 | 27.831 | -14.620 | -8.347 |
| **19** | 0.294 | 0.970 | 24.357 | -14.999 | -9.119 |
| **20** | 0.257 | 0.741 | 27.592 | -14.399 | -9.025 |
| **21** | -0.159 | -1.396 | 66.806 | 33.252 | 5.718 |
| **22** | 0.155 | -1.541 | 64.460 | 30.701 | 4.475 |
| **23** | 0.056 | -0.856 | 61.895 | 27.406 | 3.664 |
| **24** | -0.864 | -1.020 | 48.908 | 18.472 | 0.951 |
| **25** | -0.699 | -0.511 | 43.918 | 13.897 | -0.516 |
| **26** | -1.808 | -0.071 | 31.210 | -5.668 | -5.447 |
| **27** | -0.099 | -0.202 | 37.912 | 13.317 | -0.087 |
| **28** | 0.137 | -1.196 | 53.247 | 24.883 | 4.886 |

**Table S7** Comparison of $T_1$ HOMER values for the 28 compounds in Fig. 2 in the main text calculated at the UM06-2X/cc-pVDZ and TD-M06-2X/cc-pVDZ levels of theory, and RMSD (root mean square deviation) values between the corresponding bond lengths

| Compound | HOMER (UM06-2X)[a] | HOMER (TD-M06-2X)[a] | RMSD (Å)[b] |
|---|---|---|---|
| **1** | -2.677 | -2.109 | 0.002 |
| **2** | -2.968 | -2.966 | 0.001 |
| **3** | -1.021 | -1.130 | 0.002 |
| **4** | -1.940 | -1.680 | 0.001 |
| **5** | -3.122 | -3.278 | 0.001 |
| **6** | -0.572 | -0.436 | 0.002 |
| **7** | -0.142 | 0.104 | 0.003 |
| **8** | -1.838 | -1.637 | 0.003 |
| **9** | 0.409 | 0.211 | 0.042 |
| **10** | -1.565 | -1.521 | 0.002 |
| **11** | -2.187 | -2.315 | 0.014 |
| **12** | -2.567 | -2.091 | 0.003 |
| **13** | 1.000 | 0.995 | 0.001 |
| **14** | 0.995 | 0.977 | 0.003 |
| **15** | 0.697 | 0.459 | 0.014 |
| **16** | 0.996 | 0.977 | 0.002 |
| **17** | -0.278 | -6.509 | 0.031 |
| **18** | 0.781 | -0.080 | 0.017 |
| **19** | 0.989 | 0.991 | 0.001 |
| **20** | 0.802 | 0.963 | 0.004 |
| **21** | -1.347 | -1.400 | 0.001 |
| **22** | -1.559 | -2.370 | 0.012 |
| **23** | -0.800 | -0.902 | 0.002 |
| **24** | -0.978 | -1.018 | 0.002 |
| **25** | -0.147 | -1.330 | 0.014 |
| **26** | -0.073 | -5.356 | 0.026 |
| **27** | -0.176 | -0.070 | 0.003 |
| **28** | -1.145 | -1.734 | 0.006 |

[a] As can be seen, the agreement between the two sets of HOMER values is generally good. If one excludes compounds **17** and **26**, which are prominent outliers, the $R^2$ value for the linear correlation between the data sets is 0.92.

[b] The RMSD values consider the bond lengths based upon which the HOMER values are calculated.

## 2. Cartesian coordinates and electronic energies of optimized molecular geometries

Cartesian coordinates in Å and electronic energies ($E$) for $S_0$ and/or $T_1$ states in Hartree atomic units (a.u.).

### 2.1. The 8 compounds in Fig. 1 in the main text (CASPT2/cc-pVQZ)

C4H4. $E(T_1)$ = -154.37079070 a.u.

| | | | |
|---|---|---|---|
| C | 0.000000 | 1.015802 | 0.000000 |
| C | 1.015802 | 0.000000 | 0.000000 |
| C | 0.000000 | -1.015802 | 0.000000 |
| C | -1.015802 | -0.000000 | -0.000000 |
| H | -0.000000 | 2.091366 | -0.000000 |
| H | 2.091366 | 0.000000 | -0.000000 |
| H | 0.000000 | -2.091366 | 0.000000 |
| H | -2.091366 | -0.000000 | -0.000000 |

C6H6. $E(T_1)$ = -231.65725525 a.u.

| | | | |
|---|---|---|---|
| C | -1.202408 | 0.694323 | -0.000000 |
| C | 0.054199 | 1.430900 | 0.000000 |
| C | 1.312709 | 0.697609 | 0.000000 |
| C | 1.314487 | -0.664723 | 0.000000 |
| C | 0.057881 | -1.401300 | -0.000000 |
| C | -1.200630 | -0.668008 | -0.000000 |
| H | -2.132739 | 1.240090 | -0.000000 |
| H | 0.052792 | 2.507559 | -0.000000 |
| H | 2.241611 | 1.245794 | 0.000000 |
| H | 2.244818 | -1.210489 | 0.000000 |
| H | 0.059287 | -2.477958 | -0.000000 |
| H | -2.129531 | -1.216193 | -0.000000 |

C2N2H2. $E(T_1)$ = -186.44113665 a.u.

| | | | |
|---|---|---|---|
| C | 0.000000 | 0.920528 | 0.000000 |
| N | 1.041461 | 0.000000 | 0.000000 |
| C | 0.000000 | -0.920528 | -0.000000 |
| N | -1.041461 | 0.000000 | 0.000000 |
| H | -0.000000 | 1.995743 | 0.000000 |
| H | -0.000000 | -1.995743 | -0.000000 |

C3N3H3. $E(T_1)$ = -279.75140656 a.u.

| | | | |
|---|---|---|---|
| N | 1.291019 | 0.746257 | -0.000000 |
| C | 0.051735 | 1.401950 | -0.000000 |
| N | -1.185990 | 0.743233 | -0.000000 |
| C | -1.131511 | -0.543169 | -0.000000 |
| N | 0.055035 | -1.331921 | 0.000000 |
| C | 1.239679 | -0.540278 | 0.000000 |
| H | 0.050411 | 2.474932 | 0.000000 |
| H | -2.049220 | -1.110930 | -0.000000 |
| H | 2.158771 | -1.105796 | 0.000000 |

N4. $E(T_1)$ = -218.44425059 a.u.

| | | | |
|---|---|---|---|
| N | 0.000000 | 0.972495 | 0.000000 |
| N | 0.972495 | -0.000000 | 0.000000 |
| N | 0.000000 | -0.972495 | -0.000000 |
| N | -0.972495 | -0.000000 | 0.000000 |

N6. $E(T_1)$ = -327.68588725 a.u.

| | | | |
|---|---|---|---|
| N | -1.158567 | 0.729007 | 0.000000 |
| N | -0.036948 | 1.386456 | 0.000000 |
| N | 1.118092 | 0.789679 | -0.000000 |
| N | 1.158567 | -0.729007 | 0.000000 |
| N | 0.036947 | -1.386456 | -0.000000 |
| N | -1.118092 | -0.789679 | 0.000000 |

C2O2H2. $E(T_1)$ = -226.34783782 a.u.

| | | | |
|---|---|---|---|
| C | -0.000000 | 0.966787 | -0.000000 |
| O | 0.983905 | -0.000000 | 0.000000 |
| C | 0.000000 | -0.966787 | -0.000000 |
| O | -0.983905 | -0.000000 | 0.000000 |
| H | 0.000000 | 2.068089 | 0.000000 |
| H | -0.000000 | -2.068089 | -0.000000 |

C3O3H3. $E(T_1)$ = -339.38635396 a.u.

| | | | |
|---|---|---|---|
| O | 0.000000 | 1.130491 | 0.741646 |
| C | 0.000000 | -0.006907 | 1.413336 |
| O | -0.000000 | -1.137730 | 0.730533 |
| C | 0.000001 | -1.152549 | -0.800721 |
| O | 0.000000 | 0.006585 | -1.343687 |
| C | -0.000000 | 1.160322 | -0.789351 |
| H | 0.000000 | -0.012371 | 2.529711 |
| H | 0.000001 | -2.156985 | -1.278264 |
| H | -0.000001 | 2.169389 | -1.257019 |

**2.2. The 28 compounds in Fig. 2 in the main text (CASPT2/cc-pVDZ)**

Compound **1** $S_0$ geometry. $E(S_0)$ = -231.50001024 a.u.

| | | | |
|---|---|---|---|
| C | -1.218035 | 0.703233 | 0.000000 |
| C | -0.000000 | 1.406465 | 0.000000 |
| C | 1.218035 | 0.703233 | -0.000000 |
| C | 1.218035 | -0.703232 | 0.000000 |
| C | 0.000000 | -1.406465 | -0.000000 |
| C | -1.218034 | -0.703233 | 0.000000 |
| H | -2.164977 | 1.249950 | 0.000000 |
| H | -0.000000 | 2.499901 | -0.000000 |
| H | 2.164977 | 1.249950 | -0.000000 |
| H | 2.164978 | -1.249950 | 0.000000 |
| H | 0.000000 | -2.499901 | 0.000000 |
| H | -2.164977 | -1.249951 | -0.000000 |

Compound **1** $T_1$ geometry. $E(T_1)$ = -231.36399600 a.u.

| | | | |
|---|---|---|---|
| C | -1.214650 | 0.700934 | 0.000000 |
| C | 0.050965 | 1.446504 | 0.000000 |
| C | 1.321828 | 0.709935 | 0.000000 |
| C | 1.326729 | -0.671333 | 0.000000 |
| C | 0.061115 | -1.416903 | -0.000000 |
| C | -1.209748 | -0.680334 | -0.000000 |
| H | -2.158489 | 1.252423 | 0.000000 |
| H | 0.047094 | 2.537915 | -0.000000 |
| H | 2.261731 | 1.268105 | 0.000000 |
| H | 2.270569 | -1.222822 | 0.000000 |
| H | 0.064986 | -2.508315 | -0.000000 |
| H | -2.149651 | -1.238505 | 0.000000 |

Compound **2** $S_0$ geometry. $E(S_0)$ = -247.51656287 a.u.

| | | | |
|---|---|---|---|
| N | -1.215022 | -0.769257 | 0.000000 |
| C | -0.000797 | -1.356464 | 0.000000 |
| C | 1.217726 | -0.654782 | -0.000000 |
| C | 1.182203 | 0.748479 | 0.000000 |
| C | -0.071031 | 1.380779 | -0.000000 |
| C | -1.226469 | 0.579454 | 0.000000 |
| H | -0.002371 | -2.451991 | -0.000000 |
| H | 2.165892 | -1.198581 | -0.000000 |
| H | 2.106290 | 1.333537 | 0.000000 |
| H | -0.157043 | 2.470430 | 0.000000 |
| H | -2.217405 | 1.046602 | 0.000000 |

Compound **2** $T_1$ geometry. $E(T_1)$ = -247.37915129 a.u.

| | | | |
|---|---|---|---|
| N | -1.251019 | -0.792047 | 0.000000 |
| C | -0.044931 | -1.387445 | 0.000000 |
| C | 1.263924 | -0.630416 | 0.000000 |
| C | 1.221054 | 0.773076 | 0.000000 |
| C | -0.029258 | 1.412115 | -0.000000 |

C -1.273355 0.552804 -0.000000
H -0.034221 -2.480755 -0.000000
H 2.205088 -1.183338 0.000000
H 2.145208 1.358182 0.000000
H -0.126510 2.499338 -0.000000
H -2.257036 1.030103 -0.000000

Compound **3** $S_0$ geometry. $E(S_0)$ = -263.49986054 a.u.
N 1.206321 -0.735521 0.000000
N 1.276759 0.605051 0.000000
C 0.136774 1.321815 0.000000
C -1.152880 0.758889 0.000000
C -1.226061 -0.633892 -0.000000
C -0.002502 -1.328871 -0.000000
H 0.281144 2.406364 0.000000
H -2.043747 1.391906 0.000000
H -2.178363 -1.170060 -0.000000
H 0.027412 -2.422577 -0.000000

Compound **3** $T_1$ geometry. $E(T_1)$ = -263.36341698 a.u.
N 1.244436 -0.758760 0.000000
N 1.258989 0.734115 0.000000
C 0.079851 1.370190 0.000000
C -1.189478 0.762480 0.000000
C -1.204182 -0.738969 -0.000000
C 0.053306 -1.371449 -0.000000
H 0.166031 2.463093 0.000000
H -2.109376 1.348261 0.000000
H -2.135227 -1.306651 -0.000000
H 0.117614 -2.465703 -0.000000

Compound **4** $S_0$ geometry. $E(S_0)$ = -263.53697452 a.u.
N -1.211186 -0.723915 0.000000
C 0.001496 -1.310872 0.000000
N 1.212830 -0.721155 -0.000000
C 1.191597 0.626393 -0.000000
C -0.001552 1.363363 0.000000
C -1.193022 0.623673 0.000000
H 0.002742 -2.405695 0.000000
H 2.165703 1.127632 -0.000000
H -0.002800 2.455518 0.000000
H -2.168267 1.122693 0.000000

Compound **4** $T_1$ geometry. $E(T_1)$ = -263.39626221 a.u.
N -1.248455 -0.746190 0.000000
C 0.045812 -1.331489 0.000000
N 1.296849 -0.658522 -0.000000
C 1.235153 0.645597 0.000000
C -0.047555 1.381808 0.000000

C -1.276645 0.559104 0.000000
H 0.083280 -2.419627 0.000000
H 2.180014 1.201551 -0.000000
H -0.085117 2.472157 0.000000
H -2.257520 1.048783 -0.000000

Compound **5** $S_0$ geometry. $E(S_0)$ = -263.52941264 a.u.
N -0.000003 1.430482 0.000000
C 1.134424 0.703044 0.000000
C 1.134427 -0.703039 0.000000
N 0.000003 -1.430481 -0.000000
C -1.134424 -0.703044 -0.000000
C -1.134427 0.703039 0.000000
H 2.077534 1.259189 -0.000000
H 2.077539 -1.259180 0.000000
H -2.077535 -1.259188 0.000000
H -2.077540 1.259179 -0.000000

Compound **5** $T_1$ geometry. $E(T_1)$ = -263.39233865 a.u.
N -0.000003 1.477956 0.000000
C 1.135334 0.759494 0.000000
C 1.135363 -0.759435 0.000000
N 0.000003 -1.477956 0.000000
C -1.135334 -0.759494 -0.000000
C -1.135363 0.759435 0.000000
H 2.083763 1.303410 -0.000000
H 2.083806 -1.303324 0.000000
H -2.083763 -1.303410 -0.000000
H -2.083806 1.303324 0.000000

Compound **6** $S_0$ geometry. $E(S_0)$ = -279.56107646 a.u.
N -1.202474 -0.694256 0.000000
C -1.124132 0.649013 0.000000
N -0.000006 1.388501 -0.000000
C 1.124127 0.649020 -0.000000
N 1.202480 -0.694245 -0.000000
C 0.000005 -1.298033 0.000000
H -2.072448 1.196515 -0.000000
H 2.072436 1.196535 0.000000
H 0.000012 -2.393050 -0.000000

Compound **6** $T_1$ geometry. $E(T_1)$ = -279.40647057 a.u.
N 1.306932 0.754850 0.000000
C 0.053010 1.410329 0.000000
N -1.200614 0.754218 -0.000000
C -1.137218 -0.547222 -0.000000
N 0.053674 -1.349389 0.000001
C 1.244192 -0.546618 0.000000
H 0.052730 2.498447 0.000000

H -2.068252 -1.121999 -0.000001
H 2.175509 -1.120931 -0.000000

Compound **7** $S_0$ geometry. $E(S_0)$ = -322.57633255 a.u.
N -1.137186 -0.241817 0.000000
C -0.000302 -1.076061 0.000000
C 1.248696 -0.319424 -0.000000
C 1.270385 1.058606 -0.000000
C 0.055792 1.817477 -0.000000
C -1.133618 1.126544 0.000000
H 2.168014 -0.909251 -0.000000
H 2.231028 1.582816 -0.000000
H 0.057529 2.907578 -0.000000
H -2.111811 1.612145 0.000000
O -0.126152 -2.299637 0.000000
H -2.020959 -0.746328 0.000000

Compound **7** $T_1$ geometry. $E(T_1)$ = -322.47806954 a.u.
N -1.184806 -0.251943 0.000000
C -0.042691 -1.060461 0.000000
C 1.245281 -0.366553 -0.000000
C 1.317220 1.092799 -0.000000
C 0.141884 1.804631 -0.000000
C -1.147304 1.137906 0.000000
H 2.131225 -1.003112 -0.000000
H 2.285958 1.595887 -0.000000
H 0.146942 2.897642 0.000000
H -2.097793 1.667766 0.000000
O -0.148795 -2.286925 0.000000
H -2.068663 -0.749111 0.000000

Compound **8** $S_0$ geometry. $E(S_0)$ = -322.57832759 a.u.
N -1.197524 -0.304150 0.000000
C -0.005079 -0.908955 0.000000
C 1.234712 -0.234651 -0.000000
C 1.210115 1.162170 0.000000
C -0.031667 1.828391 0.000000
C -1.194151 1.048549 0.000000
H 2.163721 -0.807563 -0.000000
H 2.146596 1.727167 -0.000000
H -0.094918 2.918498 0.000000
H -2.181419 1.522206 0.000000
O 0.000719 -2.262452 -0.000000
H -0.940641 -2.504685 -0.000000

Compound **8** $T_1$ geometry. $E(T_1)$ = -322.44827736 a.u.
N -1.245277 -0.316278 0.000000
C -0.099489 -0.919795 0.000000
C 1.244538 -0.275553 0.000000

C 1.274854 1.180512 -0.000000
C 0.077875 1.846859 -0.000000
C -1.198105 1.086761 0.000000
H 2.136230 -0.901973 0.000000
H 2.229696 1.710813 -0.000000
H 0.035516 2.939144 -0.000000
H -2.157582 1.604230 0.000000
O -0.043471 -2.263500 -0.000000
H -0.977190 -2.542976 -0.000000

Compound **9** $S_0$ geometry. $E(S_0)$ = -413.68209873 a.u.
N -1.144530 1.029748 0.000000
C -1.240839 -0.357335 0.000000
N -0.001600 -0.981727 -0.000000
C 1.283631 -0.401121 -0.000000
C 1.249494 1.065472 0.000000
C 0.052598 1.713739 0.000000
H 2.194337 1.607003 0.000000
H -0.028375 2.802799 0.000000
O -2.305601 -0.949600 0.000000
O 2.286754 -1.099453 -0.000000
H -2.030520 1.521869 0.000000
H -0.031056 -1.999926 -0.000000

Compound **9** $T_1$ geometry. $E(T_1)$ = -413.56215627 a.u.
N -1.151672 1.036173 0.000000
C -1.226392 -0.353233 0.000000
N -0.001536 -1.004916 -0.000000
C 1.283265 -0.414483 -0.000000
C 1.283525 1.023033 0.000000
C -0.002106 1.802307 0.000000
H 2.249569 1.528394 0.000000
H -0.083454 2.884091 0.000000
O -2.298464 -0.936816 0.000000
O 2.296352 -1.118014 -0.000000
H -2.064125 1.482105 0.000000
H -0.042383 -2.020505 -0.000000

Compound **10** $S_0$ geometry. $E(S_0)$ = -413.66764118 a.u.
N 1.215536 1.075945 0.000000
C 1.113996 -0.261948 0.000000
N 0.002049 -1.014569 0.000000
C -1.144121 -0.326685 0.000000
C -1.204293 1.081243 0.000000
C 0.030666 1.726937 0.000000
H -2.155801 1.612047 0.000000
H 0.086645 2.820454 0.000000
O 2.261787 -0.958461 -0.000000
O -2.285246 -1.033739 -0.000000

H 2.955258 -0.278004 -0.000000
H -1.999014 -1.963805 0.000000

Compound **10** $T_1$ geometry. $E(T_1)$ = -413.52445198 a.u.
N 1.239528 1.097182 0.000000
C 1.135796 -0.226627 0.000000
N -0.031493 -1.058825 -0.000000
C -1.144899 -0.374310 -0.000000
C -1.226232 1.063414 -0.000000
C 0.103476 1.805723 -0.000000
H -2.194138 1.564773 -0.000000
H 0.148695 2.894416 -0.000000
O 2.250327 -0.972242 0.000000
O -2.316089 -1.032718 -0.000000
H 2.974565 -0.322562 0.000000
H -2.068118 -1.974651 0.000000

Compound **11** $S_0$ geometry. $E(S_0)$ = -286.70400445 a.u.
C -1.235287 0.713193 0.000406
C -0.004518 1.405232 0.000028
C 1.209363 0.700380 -0.029804
C 1.221612 -0.705340 -0.053033
C -0.002198 -1.397417 -0.047704
C -1.219565 -0.698592 -0.018028
H -0.003346 2.500063 0.023272
H 2.151314 1.256856 -0.033477
H 2.167938 -1.251682 -0.076195
H -0.013400 -2.491276 -0.065457
H -2.167398 -1.246944 -0.008930
N -2.452119 1.415116 0.106717
H -2.396068 2.340763 -0.314317
H -3.222847 0.909156 -0.325919

Compound **11** $T_1$ geometry. $E(T_1)$ = -286.57496684 a.u.
C -1.257513 0.726026 0.000929
C 0.040003 1.440038 0.000213
C 1.202794 0.755447 -0.247688
C 1.169437 -0.690386 -0.471167
C -0.056549 -1.429216 -0.168018
C -1.223935 -0.752493 0.080069
H 0.050698 2.519226 0.186553
H 2.160409 1.282339 -0.277673
H 2.078547 -1.224815 -0.754184
H -0.032750 -2.521987 -0.139570
H -2.145703 -1.290733 0.324980
N -2.360655 1.382347 0.556580
H -2.416364 2.367244 0.300340
H -3.247875 0.923285 0.354657

Compound **12** $S_0$ geometry. $E(S_0)$ = -323.50254727 a.u.

| | | | |
|---|---|---|---|
| C | -1.232177 | 0.711398 | 0.000000 |
| C | -0.019033 | 1.422895 | 0.000000 |
| C | 1.196902 | 0.722904 | 0.000000 |
| C | 1.201200 | -0.688535 | 0.000000 |
| C | -0.015004 | -1.395279 | 0.000000 |
| C | -1.235455 | -0.701828 | 0.000000 |
| H | -0.034182 | 2.516263 | -0.000000 |
| H | 2.140382 | 1.276021 | 0.000000 |
| H | 2.150732 | -1.231374 | 0.000000 |
| H | -0.014477 | -2.488580 | 0.000000 |
| H | -2.186909 | -1.239129 | 0.000000 |
| C | -2.484979 | 1.430039 | -0.000000 |
| N | -3.509099 | 2.017047 | -0.000000 |

Compound **12** $T_1$ geometry. $E(T_1)$ = -323.37648224 a.u.

| | | | |
|---|---|---|---|
| C | 0.050845 | 1.480334 | 0.000000 |
| C | 1.332734 | 0.739226 | 0.000000 |
| C | 1.327510 | -0.625022 | -0.000000 |
| C | 0.074587 | -1.376607 | -0.000000 |
| C | -1.190020 | -0.661338 | -0.000000 |
| C | -1.226673 | 0.708786 | 0.000000 |
| H | 2.266159 | 1.307611 | -0.000000 |
| H | 2.276349 | -1.169827 | -0.000000 |
| H | 0.090150 | -2.468046 | -0.000000 |
| H | -2.124205 | -1.229545 | -0.000000 |
| H | -2.168375 | 1.262040 | 0.000000 |
| C | 0.033726 | 2.874091 | 0.000000 |
| N | 0.016130 | 4.072922 | 0.000000 |

Compound **13** $S_0$ geometry. $E(S_0)$ = -154.18538258 a.u.

| | | | |
|---|---|---|---|
| C | 0.670819 | 0.791911 | 0.000000 |
| C | -0.699252 | 0.766917 | 0.000000 |
| C | -0.670819 | -0.791911 | -0.000000 |
| C | 0.699252 | -0.766917 | 0.000000 |
| H | 1.428665 | 1.576545 | 0.000000 |
| H | -1.485193 | 1.523408 | 0.000000 |
| H | -1.428665 | -1.576545 | -0.000000 |
| H | 1.485193 | -1.523408 | 0.000000 |

Compound **13** $T_1$ geometry. $E(T_1)$ = -154.17429621 a.u.

| | | | |
|---|---|---|---|
| C | -0.000000 | 1.027035 | 0.000000 |
| C | 1.027035 | 0.000000 | 0.000000 |
| C | -0.000000 | -1.027035 | 0.000000 |
| C | -1.027035 | 0.000000 | 0.000000 |
| H | 0.000000 | 2.117901 | 0.000000 |
| H | 2.117901 | 0.000000 | 0.000000 |
| H | -0.000000 | -2.117901 | 0.000000 |
| H | -2.117901 | 0.000000 | 0.000000 |

Compound **14** $S_0$ geometry. $E(S_0)$ = -170.21083210 a.u.

| | | | |
|---|---|---|---|
| N | -1.061631 | -0.238590 | 0.000000 |
| C | 0.024091 | -0.970508 | 0.000000 |
| C | 1.019309 | 0.211650 | -0.000000 |
| C | -0.105472 | 0.979467 | -0.000000 |
| H | 0.089233 | -2.064082 | 0.000000 |
| H | 2.097966 | 0.376029 | -0.000000 |
| H | -0.383348 | 2.034535 | -0.000000 |

Compound **14** $T_1$ geometry. $E(T_1)$ = -170.19362934 a.u.

| | | | |
|---|---|---|---|
| N | -1.033601 | -0.232291 | 0.000000 |
| C | 0.170036 | -0.960604 | 0.000000 |
| C | 0.999855 | 0.224776 | -0.000000 |
| C | -0.257150 | 0.940969 | 0.000000 |
| H | 0.298150 | -2.043628 | -0.000000 |
| H | 2.065445 | 0.464212 | -0.000000 |
| H | -0.604834 | 1.974608 | 0.000000 |

Compound **15** $S_0$ geometry. $E(S_0)$ = -186.20489223 a.u.

| | | | |
|---|---|---|---|
| N | -1.022865 | -0.183384 | 0.000000 |
| N | -0.058107 | -1.037571 | 0.000000 |
| C | 0.983688 | 0.085430 | -0.000000 |
| C | -0.034376 | 0.986790 | 0.000000 |
| H | 2.074675 | 0.048130 | -0.000000 |
| H | -0.203747 | 2.065233 | 0.000000 |

Compound **15** $T_1$ geometry. $E(T_1)$ = -186.19461475 a.u.

| | | | |
|---|---|---|---|
| N | -1.017808 | -0.182477 | 0.000000 |
| N | 0.122420 | -1.026723 | 0.000000 |
| C | 0.960598 | 0.101210 | 0.000000 |
| C | -0.183443 | 0.948405 | 0.000000 |
| H | 2.051684 | 0.158120 | 0.000000 |
| H | -0.446903 | 2.008591 | 0.000000 |

Compound **16** $S_0$ geometry. $E(S_0)$ = -186.24186245 a.u.

| | | | |
|---|---|---|---|
| C | 0.590727 | 0.697362 | 0.000000 |
| N | -0.704286 | 0.827792 | 0.000000 |
| C | -0.590727 | -0.697362 | 0.000000 |
| N | 0.704286 | -0.827792 | -0.000000 |
| H | 1.392886 | 1.444726 | -0.000000 |
| H | -1.392886 | -1.444726 | 0.000000 |

Compound **16** $T_1$ geometry. $E(T_1)$ = -186.21171510 a.u.

| | | | |
|---|---|---|---|
| C | 0.598357 | 0.706369 | 0.000000 |
| N | -0.804412 | 0.681537 | 0.000000 |
| C | -0.598357 | -0.706369 | -0.000000 |
| N | 0.804412 | -0.681537 | 0.000000 |
| H | 1.303709 | 1.537274 | 0.000000 |

H -1.303709 -1.537274 -0.000000

Compound **17** $S_0$ geometry. $E(S_0)$ = -245.32471992 a.u.
N 0.011925 0.000000 0.031889
C -0.030806 0.000000 1.458469
C 1.515401 -0.000000 1.468956
C 1.442640 -0.000000 0.105437
H 2.296905 0.000000 2.221770
H 2.134576 -0.000000 -0.736569
O -0.939784 0.000000 2.242284
H -0.674061 -0.000000 -0.710150

Compound **17** $T_1$ geometry. $E(T_1)$ = -245.25396704 a.u.
N 0.023698 0.000000 0.063372
C 0.010232 0.000000 1.513248
C 1.480592 0.000000 1.458254
C 1.411099 0.000000 -0.038858
H 2.272205 0.000000 2.206673
H 2.045443 0.000000 -0.915998
O -0.911161 -0.000000 2.304716
H -0.719754 -0.000000 -0.634148

Compound **18** $S_0$ geometry. $E(S_0)$ = -245.27978534 a.u.
N 1.100455 -0.273859 0.000000
C 0.002651 0.424898 0.000000
C -1.007430 -0.735046 0.000000
C 0.130485 -1.475339 -0.000000
H -2.085546 -0.885895 -0.000000
H 0.419848 -2.526783 -0.000000
O -0.187275 1.739117 -0.000000
H 0.706470 2.129674 -0.000000

Compound **18** $T_1$ geometry. $E(T_1)$ = -245.24980616 a.u.
N 1.091498 -0.271630 0.000000
C -0.108015 0.422066 0.000000
C -0.946120 -0.745367 0.000000
C 0.324853 -1.465331 -0.000000
H -2.014709 -0.964729 0.000000
H 0.683861 -2.491139 -0.000000
O -0.313350 1.743293 0.000000
H 0.572850 2.142720 -0.000000

Compound **19** $S_0$ geometry. $E(S_0)$ = -209.39474477 a.u.
C 0.678783 0.802353 0.000760
C -0.691266 0.857039 0.006637
C -0.717341 -0.691947 -0.174837
C 0.647587 -0.748433 -0.191937
H -1.440121 1.628850 0.181284
H -1.513023 -1.433240 -0.265964

H 1.398240 -1.534918 -0.278844
N 1.752244 1.642158 0.250402
H 2.545416 1.448872 -0.360224
H 1.500223 2.627482 0.184394

Compound **19** $T_1$ geometry. $E(T_1)$ = -209.38240787 a.u.
C 0.000000 1.041631 0.000863
C 1.025963 0.015578 0.000857
C 0.003300 -1.007049 -0.164965
C -1.023550 0.024724 -0.153595
H 2.113830 0.019962 0.090890
H 0.008031 -2.088099 -0.292070
H -2.112520 0.038770 -0.227087
N -0.011320 2.409253 0.234653
H 0.848403 2.864969 -0.066056
H -0.812785 2.872402 -0.190021

Compound **20** $S_0$ geometry. $E(S_0)$ = -246.19579054 a.u.
C 0.670728 0.820250 0.000000
C -0.645683 0.403538 0.000000
C -0.178828 -1.068235 0.000000
C 1.134042 -0.672165 0.000000
H -1.605686 0.920894 -0.000000
H -0.692956 -2.029377 0.000000
H 2.107282 -1.163787 0.000000
C 1.322769 2.076841 -0.000000
N 1.887806 3.124241 -0.000000

Compound **20** $T_1$ geometry. $E(T_1)$ = -246.18762301 a.u.
C 0.000022 1.068693 -0.000000
C 1.032007 0.026773 0.000000
C -0.000505 -0.978145 0.000001
C -1.032499 0.027304 0.000001
H 2.121980 0.032537 -0.000001
H -0.000786 -2.069083 0.000002
H -2.122469 0.033630 0.000002
C 0.000383 2.472890 -0.000001
N 0.000690 3.667341 -0.000001

Compound **21** $S_0$ geometry. $E(S_0)$ = -209.52042114 a.u.
C 1.130204 0.334480 0.000000
C 0.712353 -0.993885 0.000000
C -0.717707 -0.990026 0.000000
C -1.128383 0.340575 0.000000
N 0.003038 1.125713 -0.000000
H 0.005768 2.137550 0.000000
H 2.125783 0.772992 -0.000000
H 1.366061 -1.864626 -0.000000
H -1.376110 -1.857224 0.000000

H -2.121579 0.784459 0.000000

Compound **21** $T_1$ geometry. $E(T_1)$ = -209.37798844 a.u.
C 1.157489 0.342555 0.000000
C 0.670720 -1.053804 0.000000
C -0.698000 -1.035910 -0.000000
C -1.148127 0.372582 0.000000
N 0.015550 1.192767 0.000000
H 0.028652 2.198839 -0.000000
H 2.170926 0.734344 -0.000000
H 1.317352 -1.930421 0.000000
H -1.367302 -1.895328 -0.000000
H -2.150982 0.790663 0.000000

Compound **22** $S_0$ geometry. $E(S_0)$ = -225.53434058 a.u.
N -0.000000 1.086821 0.000000
N -1.153250 0.390202 0.000000
C -0.747485 -0.894434 -0.000000
C 0.665618 -1.010854 0.000000
C 1.118863 0.309012 -0.000000
H -0.042676 2.099194 0.000000
H -1.494084 -1.687302 0.000000
H 1.270187 -1.914655 0.000000
H 2.117352 0.741256 -0.000000

Compound **22** $T_1$ geometry. $E(T_1)$ = -225.38281943 a.u.
N -0.000000 1.144818 0.000000
N -1.184936 0.453621 0.000000
C -0.727480 -0.951105 -0.000000
C 0.636871 -1.057972 0.000000
C 1.156807 0.288738 -0.000000
H -0.019111 2.153143 -0.000000
H -1.486088 -1.731145 -0.000000
H 1.231890 -1.969200 0.000000
H 2.170676 0.680160 0.000000

Compound **23** $S_0$ geometry. $E(S_0)$ = -225.55036117 a.u.
N 0.000000 1.110076 0.000000
C -1.091039 0.284380 0.000000
N -0.747107 -0.998612 -0.000000
C 0.634189 -0.988953 -0.000000
C 1.125733 0.308141 0.000000
H -0.014423 2.122989 0.000000
H -2.108909 0.670947 0.000000
H 1.207754 -1.914315 0.000000
H 2.132024 0.718722 0.000000

Compound **23** $T_1$ geometry. $E(T_1)$ = -225.40377573 a.u.
N 0.000000 1.177097 0.000000

C -1.119035 0.276349 0.000000
N -0.708313 -1.064522 0.000000
C 0.601720 -1.032518 -0.000000
C 1.146932 0.360040 -0.000000
H -0.034496 2.183310 0.000000
H -2.152856 0.608052 0.000000
H 1.203917 -1.943027 -0.000000
H 2.163921 0.740416 0.000000

Compound **24** $S_0$ geometry. $E(S_0)$ = -229.34792703 a.u.
O 0.000010 -1.169326 0.000565
C -1.094373 -0.353145 -0.000270
C -0.719531 0.970421 -0.000821
C 0.719513 0.970434 -0.000208
C 1.094379 -0.353125 0.000689
H -2.057494 -0.855846 -0.000341
H -1.387403 1.829361 -0.001605
H 1.387370 1.829386 -0.000464
H 2.057509 -0.855810 0.001550

Compound **24** $T_1$ geometry. $E(T_1)$ = -229.22033220 a.u.
O 0.000011 -1.242766 0.000600
C -1.108047 -0.375911 -0.000264
C -0.683952 1.031033 0.000026
C 0.683934 1.031045 -0.000073
C 1.108053 -0.375892 -0.000445
H -2.086837 -0.845932 -0.000113
H -1.357985 1.886139 0.000227
H 1.357953 1.886162 -0.000007
H 2.086851 -0.845897 -0.000375

Compound **25** $S_0$ geometry. $E(S_0)$ = -245.37973637 a.u.
O 0.387249 1.085549 0.000029
C 1.096632 -0.071660 -0.000094
N 0.385345 -1.168060 -0.000094
C -0.928183 -0.699957 0.000039
C -0.920903 0.670941 0.000108
H 2.179548 0.024440 -0.000175
H -1.780557 -1.375242 0.000067
H -1.679673 1.446895 0.000213

Compound **25** $T_1$ geometry. $E(T_1)$ = -245.24744412 a.u.
O 0.411761 1.154263 0.000031
C 1.116853 -0.080302 -0.000096
N 0.315838 -1.222564 0.000099
C -0.910129 -0.760508 0.000057
C -0.910669 0.722973 -0.000162
H 2.200425 -0.038829 0.000136
H -1.789076 -1.406203 0.000168

H -1.692636 1.475910 -0.000035

Compound **26** $S_0$ geometry. $E(S_0)$ = -265.17961756 a.u.
O 0.375708 -1.041837 -0.000193
C -0.576157 0.068563 -0.000201
C 0.555328 1.061744 0.000556
C 1.354792 -0.035948 0.000519
O -1.759690 -0.010426 -0.000723
H 0.654498 2.142934 0.000964
H 2.413576 -0.290990 0.001118

Compound **26** $T_1$ geometry. $E(T_1)$ = -265.08501524 a.u.
O 0.363228 -1.007229 -0.000186
C -0.583924 0.106559 -0.000192
C 0.525158 1.053377 0.000647
C 1.433968 -0.144540 0.000469
O -1.779391 0.034815 -0.000732
H 0.607568 2.140072 0.000401
H 2.470518 -0.453131 0.001407

Compound **27** $S_0$ geometry. $E(S_0)$ = -342.39569508 a.u.
O 0.332419 -1.169445 -0.000005
C 1.058432 0.028232 -0.000026
C 0.258604 1.256162 -0.000009
C -1.109295 1.221483 0.000023
C -1.788252 -0.051007 0.000043
C -1.024077 -1.178353 0.000028
O 2.265044 -0.039594 -0.000054
H 0.825230 2.188983 -0.000024
H -1.684246 2.151800 0.000035
H -2.875265 -0.131286 0.000069
H -1.417896 -2.196282 0.000039

Compound **27** $T_1$ geometry. $E(T_1)$ = -342.30721606 a.u.
O 0.344177 -1.210812 -0.000005
C 1.044206 -0.007043 -0.000025
C 0.306112 1.237545 -0.000010
C -1.155849 1.265183 0.000032
C -1.787500 0.044976 0.000044
C -1.028677 -1.175683 0.000015
O 2.263200 -0.080192 -0.000054
H 0.915811 2.142060 -0.000026
H -1.700052 2.210086 0.000053
H -2.876890 -0.042436 0.000072
H -1.467649 -2.171540 0.000034

Compound **28** $S_0$ geometry. $E(S_0)$ = -342.38096311 a.u.
O 1.782246 -0.000008 0.000029
C 1.065471 1.158858 -0.000054

C -0.291972 1.223036 -0.000079
C -1.112210 0.000004 -0.000014
C -0.291984 -1.223035 0.000056
C 1.065461 -1.158865 0.000077
H 1.726603 2.026671 -0.000091
H -0.784928 2.197142 -0.000154
O -2.343735 0.000012 -0.000017
H -0.784938 -2.197142 0.000103
H 1.726582 -2.026687 0.000134

Compound **28** $T_1$ geometry. $E(T_1)$ = -342.25671917 a.u.
O 1.807208 -0.000008 0.000029
C 1.087961 1.180900 -0.000055
C -0.318573 1.211451 -0.000061
C -1.082921 -0.000004 -0.000009
C -0.318546 -1.211446 0.000050
C 1.087851 -1.180844 0.000067
H 1.739414 2.052241 -0.000074
H -0.831668 2.175486 -0.000121
O -2.375964 -0.000038 -0.000023
H -0.831606 -2.175494 0.000087
H 1.739285 -2.052207 0.000106

**2.3. The 28 compounds in Fig. 2 in the main text (M06-2X/cc-pVDZ)**

Compound **1** $S_0$ geometry. $E(S_0)$ = -232.162455637 a.u.

| | | | |
|---|---|---|---|
| C | -0.000000 | 1.394638 | -0.000000 |
| C | -1.207792 | 0.697319 | -0.000000 |
| C | -1.207792 | -0.697319 | -0.000000 |
| C | 0.000000 | -1.394638 | -0.000000 |
| C | 1.207792 | -0.697319 | -0.000000 |
| C | 1.207792 | 0.697319 | -0.000000 |
| H | -0.000000 | 2.485503 | -0.000000 |
| H | -2.152509 | 1.242751 | -0.000000 |
| H | -2.152509 | -1.242751 | -0.000000 |
| H | 0.000000 | -2.485503 | -0.000000 |
| H | 2.152509 | -1.242751 | -0.000000 |
| H | 2.152509 | 1.242751 | -0.000000 |

Compound **1** $T_1$ geometry. $E(T_1)$ = -232.012431653 a.u.

| | | | |
|---|---|---|---|
| C | 1.270244 | -0.671871 | 0.000000 |
| C | -0.000003 | -1.421829 | 0.000000 |
| C | -1.270244 | -0.671871 | -0.000000 |
| C | -1.270244 | 0.671871 | 0.000000 |
| C | 0.000003 | 1.421829 | 0.000000 |
| C | 1.270244 | 0.671871 | 0.000000 |
| H | 2.208101 | -1.228590 | 0.000000 |
| H | -0.000003 | -2.509051 | 0.000000 |
| H | -2.208103 | -1.228588 | -0.000000 |
| H | -2.208101 | 1.228590 | 0.000000 |
| H | 0.000003 | 2.509051 | 0.000000 |
| H | 2.208103 | 1.228588 | 0.000000 |

Compound **2** $S_0$ geometry. $E(S_0)$ = -248.199244315 a.u.

| | | | |
|---|---|---|---|
| N | -1.199920 | 0.760138 | 0.000000 |
| C | -0.000000 | 1.347254 | 0.000000 |
| C | 1.207778 | 0.650488 | -0.000000 |
| C | 1.169940 | -0.741132 | -0.000000 |
| C | -0.072118 | -1.369923 | 0.000000 |
| C | -1.218161 | -0.575548 | 0.000000 |
| H | -0.003483 | 2.440890 | 0.000000 |
| H | 2.153518 | 1.192335 | -0.000000 |
| H | 2.091465 | -1.325021 | -0.000000 |
| H | -0.158168 | -2.456512 | 0.000000 |
| H | -2.208528 | -1.039489 | 0.000000 |

Compound **2** $T_1$ geometry. $E(T_1)$ = -248.046912897 a.u.

| | | | |
|---|---|---|---|
| N | -1.206285 | -0.835329 | 0.000000 |
| C | -1.293658 | 0.486147 | 0.000000 |
| C | -0.075707 | 1.401629 | 0.000000 |
| C | 1.179505 | 0.816771 | -0.000000 |
| C | 1.285365 | -0.563974 | -0.000000 |

| | | | |
|---|---|---|---|
| C | -0.000000 | -1.381939 | -0.000000 |
| H | -2.292158 | 0.925514 | 0.000000 |
| H | -0.218756 | 2.480225 | 0.000000 |
| H | 2.076989 | 1.438231 | -0.000000 |
| H | 2.244748 | -1.077250 | -0.000000 |
| H | 0.060148 | -2.471215 | -0.000000 |

Compound **3** $S_0$ geometry. $E(S_0)$ = -264.202211956 a.u.

| | | | |
|---|---|---|---|
| N | -1.261553 | -0.596368 | -0.000000 |
| N | -1.191778 | 0.725829 | 0.000000 |
| C | -0.000000 | 1.319702 | 0.000000 |
| C | 1.213987 | 0.627682 | 0.000000 |
| C | 1.141214 | -0.751919 | -0.000000 |
| C | -0.138941 | -1.312396 | -0.000000 |
| H | -0.031871 | 2.411390 | 0.000000 |
| H | 2.163851 | 1.162509 | 0.000000 |
| H | 2.029447 | -1.383885 | -0.000000 |
| H | -0.285669 | -2.394647 | -0.000000 |

Compound **3** $T_1$ geometry. $E(T_1)$ = -264.098385811 a.u.

| | | | |
|---|---|---|---|
| N | 1.117791 | 0.763936 | -0.000000 |
| N | 0.000000 | 1.353902 | -0.000000 |
| C | -1.187971 | 0.696605 | 0.000000 |
| C | -1.175149 | -0.673101 | 0.000000 |
| C | 0.107347 | -1.350012 | 0.000000 |
| C | 1.245437 | -0.587725 | -0.000000 |
| H | -2.089562 | 1.306449 | 0.000000 |
| H | -2.113996 | -1.222670 | 0.000000 |
| H | 0.183368 | -2.435238 | 0.000000 |
| H | 2.257664 | -0.988013 | -0.000000 |

Compound **4** $S_0$ geometry. $E(S_0)$ = -264.239642586 a.u.

| | | | |
|---|---|---|---|
| N | 1.196783 | 0.714991 | 0.000000 |
| C | 0.000000 | 1.305303 | 0.000000 |
| N | -1.196781 | 0.714993 | 0.000000 |
| C | -1.181901 | -0.620104 | 0.000000 |
| C | -0.000001 | -1.353858 | 0.000000 |
| C | 1.181900 | -0.620105 | 0.000000 |
| H | 0.000002 | 2.399026 | 0.000000 |
| H | -2.156505 | -1.116706 | 0.000000 |
| H | -0.000001 | -2.442908 | 0.000000 |
| H | 2.156503 | -1.116709 | 0.000000 |

Compound **4** $T_1$ geometry. $E(T_1)$ = -264.087271937 a.u.

| | | | |
|---|---|---|---|
| N | 1.264014 | 0.689060 | 0.000000 |
| C | 0.000000 | 1.327448 | 0.000000 |
| N | -1.264051 | 0.689015 | 0.000000 |
| C | -1.256483 | -0.588695 | 0.000000 |
| C | 0.000007 | -1.378119 | 0.000000 |

| | | | |
|---|---|---|---|
| C | 1.256512 | -0.588651 | 0.000000 |
| H | -0.000029 | 2.412883 | 0.000000 |
| H | -2.218667 | -1.113029 | 0.000000 |
| H | 0.000020 | -2.465330 | 0.000000 |
| H | 2.218711 | -1.112952 | 0.000000 |

Compound **5** $S_0$ geometry. $E(S_0)$ = -264.232591807 a.u.

| | | | |
|---|---|---|---|
| N | 0.000000 | 1.409902 | -0.000000 |
| C | -1.128096 | 0.697885 | -0.000000 |
| C | -1.128096 | -0.697885 | -0.000000 |
| N | 0.000000 | -1.409902 | 0.000000 |
| C | 1.128096 | -0.697885 | 0.000000 |
| C | 1.128096 | 0.697885 | 0.000000 |
| H | -2.067622 | 1.256204 | -0.000000 |
| H | -2.067622 | -1.256204 | -0.000000 |
| H | 2.067622 | -1.256204 | 0.000000 |
| H | 2.067622 | 1.256204 | 0.000000 |

Compound **5** $T_1$ geometry. $E(T_1)$ = -264.081762751 a.u.

| | | | |
|---|---|---|---|
| N | -0.000116 | -1.460995 | 0.000000 |
| C | -1.125989 | -0.764273 | 0.000000 |
| C | -1.125989 | 0.764279 | 0.000000 |
| N | 0.000116 | 1.460995 | 0.000000 |
| C | 1.125989 | 0.764273 | 0.000000 |
| C | 1.125989 | -0.764279 | 0.000000 |
| H | -2.072585 | -1.306501 | 0.000000 |
| H | -2.072586 | 1.306494 | 0.000000 |
| H | 2.072585 | 1.306501 | 0.000000 |
| H | 2.072586 | -1.306494 | 0.000000 |

Compound **6** $S_0$ geometry. $E(S_0)$ = -280.283393912 a.u.

| | | | |
|---|---|---|---|
| N | 1.188591 | 0.686249 | 0.000000 |
| C | 0.000000 | 1.290268 | 0.000000 |
| N | -1.188605 | 0.686225 | 0.000000 |
| C | -1.117405 | -0.645134 | 0.000000 |
| N | 0.000014 | -1.372475 | 0.000000 |
| C | 1.117405 | -0.645134 | 0.000000 |
| H | -0.000009 | 2.384439 | 0.000000 |
| H | -2.064980 | -1.192227 | 0.000000 |
| H | 2.064989 | -1.192212 | 0.000000 |

Compound **6** $T_1$ geometry. $E(T_1)$ = -280.141277545 a.u.

| | | | |
|---|---|---|---|
| N | -1.209189 | 0.649548 | 0.080718 |
| C | 0.000002 | 1.259771 | -0.155074 |
| N | 1.209190 | 0.649545 | 0.080718 |
| C | 1.162153 | -0.643934 | 0.134474 |
| N | -0.000002 | -1.250461 | -0.362479 |
| C | -1.162155 | -0.643931 | 0.134473 |
| H | 0.000003 | 2.346050 | -0.217493 |

| | | | |
|---|---|---|---|
| H | 1.998866 | -1.258957 | 0.470781 |
| H | -1.998869 | -1.258952 | 0.470780 |

Compound **7** $S_0$ geometry. $E(S_0)$ = -323.417969762 a.u.

| | | | |
|---|---|---|---|
| N | -1.135251 | 0.240456 | -0.000000 |
| C | 0.000000 | 1.067231 | -0.000000 |
| C | 1.248024 | 0.317480 | -0.000000 |
| C | 1.263097 | -1.043396 | 0.000000 |
| C | 0.052275 | -1.804210 | 0.000000 |
| C | -1.123621 | -1.120659 | 0.000000 |
| H | 2.161356 | 0.910387 | -0.000000 |
| H | 2.219922 | -1.569194 | 0.000000 |
| H | 0.058659 | -2.890917 | 0.000000 |
| H | -2.098487 | -1.607737 | 0.000000 |
| O | -0.127242 | 2.278568 | -0.000000 |
| H | -2.015403 | 0.747051 | -0.000000 |

Compound **7** $T_1$ geometry. $E(T_1)$ = -323.314278615 a.u.

| | | | |
|---|---|---|---|
| N | -1.170434 | 0.287495 | 0.000000 |
| C | 0.000000 | 1.052603 | -0.000000 |
| C | 1.252022 | 0.329845 | -0.000000 |
| C | 1.271767 | -1.133663 | -0.000000 |
| C | 0.084353 | -1.791139 | 0.000000 |
| C | -1.173680 | -1.095262 | 0.000000 |
| H | 2.153662 | 0.937119 | -0.000000 |
| H | 2.219586 | -1.667281 | -0.000000 |
| H | 0.050912 | -2.881382 | 0.000000 |
| H | -2.136029 | -1.596067 | 0.000000 |
| O | -0.083639 | 2.275259 | -0.000000 |
| H | -2.032754 | 0.818768 | 0.000000 |

Compound **8** $S_0$ geometry. $E(S_0)$ = -323.421268797 a.u.

| | | | |
|---|---|---|---|
| N | -1.182842 | 0.303569 | -0.000000 |
| C | 0.000000 | 0.902689 | -0.000000 |
| C | 1.228190 | 0.225124 | -0.000000 |
| C | 1.192998 | -1.158799 | 0.000000 |
| C | -0.042397 | -1.815666 | 0.000000 |
| C | -1.191265 | -1.036160 | 0.000000 |
| H | 2.156767 | 0.793265 | -0.000000 |
| H | 2.123569 | -1.728332 | 0.000000 |
| H | -0.110398 | -2.902317 | 0.000000 |
| H | -2.180077 | -1.502000 | 0.000000 |
| O | 0.010825 | 2.249131 | -0.000000 |
| H | -0.921727 | 2.518222 | -0.000000 |

Compound **8** $T_1$ geometry. $E(T_1)$ = -323.282951629 a.u.

| | | | |
|---|---|---|---|
| N | -1.193285 | 0.445104 | -0.000000 |
| C | 0.000000 | 0.918478 | -0.000000 |
| C | 1.262646 | 0.144147 | 0.000000 |

| | | | |
|---|---|---|---|
| C | 1.131068 | -1.311782 | 0.000000 |
| C | -0.114990 | -1.824879 | -0.000000 |
| C | -1.298030 | -0.946987 | -0.000000 |
| H | 2.210432 | 0.674550 | 0.000000 |
| H | 2.017892 | -1.943258 | 0.000000 |
| H | -0.278654 | -2.903752 | -0.000000 |
| H | -2.302742 | -1.361291 | -0.000000 |
| O | 0.190362 | 2.239063 | 0.000000 |
| H | -0.700992 | 2.631654 | -0.000000 |

Compound **9** $S_0$ geometry. $E(S_0)$ = -414.705324094 a.u.

| | | | |
|---|---|---|---|
| N | -1.139147 | -1.024430 | -0.000000 |
| C | -1.231772 | 0.362087 | -0.000000 |
| N | 0.000000 | 0.986067 | -0.000000 |
| C | 1.275216 | 0.395565 | 0.000000 |
| C | 1.240540 | -1.067071 | 0.000000 |
| C | 0.053714 | -1.703501 | 0.000000 |
| H | 2.185036 | -1.602641 | 0.000000 |
| H | -0.029079 | -2.790244 | 0.000000 |
| O | -2.289629 | 0.946442 | -0.000000 |
| O | 2.270077 | 1.084554 | 0.000000 |
| H | -2.026757 | -1.511561 | -0.000000 |
| H | -0.024938 | 2.002542 | -0.000000 |

Compound **9** $T_1$ geometry. $E(T_1)$ = -414.580314211 a.u.

| | | | |
|---|---|---|---|
| N | -1.149632 | -1.030189 | -0.000000 |
| C | -1.219673 | 0.359092 | 0.000000 |
| N | -0.000000 | 1.006409 | 0.000000 |
| C | 1.276131 | 0.405815 | 0.000000 |
| C | 1.277139 | -1.022910 | -0.000000 |
| C | -0.002555 | -1.795245 | -0.000000 |
| H | 2.241515 | -1.524095 | -0.000000 |
| H | -0.081388 | -2.873981 | -0.000000 |
| O | -2.282956 | 0.936913 | 0.000000 |
| O | 2.282829 | 1.104745 | 0.000000 |
| H | -2.064035 | -1.469715 | -0.000000 |
| H | -0.033896 | 2.020474 | 0.000000 |

Compound **10** $S_0$ geometry. $E(S_0)$ = -414.690738921 a.u.

| | | | |
|---|---|---|---|
| N | 1.203680 | -1.063591 | -0.000000 |
| C | 1.108618 | 0.263667 | -0.000000 |
| N | -0.000000 | 1.003555 | 0.000000 |
| C | -1.136903 | 0.322027 | 0.000000 |
| C | -1.194785 | -1.079139 | 0.000000 |
| C | 0.032526 | -1.715045 | -0.000000 |
| H | -2.144133 | -1.607532 | 0.000000 |
| H | 0.093610 | -2.806413 | -0.000000 |
| O | 2.251418 | 0.955850 | -0.000000 |
| O | -2.273696 | 1.023273 | 0.000000 |

| | | | |
|---|---|---|---|
| H | 2.959519 | 0.292715 | -0.000000 |
| H | -2.013265 | 1.959442 | 0.000000 |

Compound **10** $T_1$ geometry. $E(T_1)$ = -414.541627133 a.u.

| | | | |
|---|---|---|---|
| N | 1.195382 | -1.110430 | 0.000000 |
| C | 1.129134 | 0.200543 | 0.000000 |
| N | -0.000000 | 1.050175 | -0.000000 |
| C | -1.124267 | 0.401735 | -0.000000 |
| C | -1.249304 | -1.025986 | -0.000000 |
| C | 0.053912 | -1.805457 | 0.000000 |
| H | -2.231857 | -1.491293 | -0.000000 |
| H | 0.076080 | -2.890848 | 0.000000 |
| O | 2.263418 | 0.898367 | 0.000000 |
| O | -2.267514 | 1.090586 | -0.000000 |
| H | 2.976208 | 0.237712 | 0.000000 |
| H | -2.012196 | 2.029575 | -0.000000 |

Compound **11** $S_0$ geometry. $E(S_0)$ = -287.503561528 a.u.

| | | | |
|---|---|---|---|
| C | -0.938473 | 0.000001 | -0.010720 |
| C | -0.221796 | -1.206017 | -0.005955 |
| C | 1.169528 | -1.200730 | 0.003735 |
| C | 1.878608 | 0.000001 | 0.008876 |
| C | 1.169529 | 1.200729 | 0.003734 |
| C | -0.221797 | 1.206017 | -0.005949 |
| H | -0.767300 | -2.152159 | -0.013882 |
| H | 1.705360 | -2.151203 | 0.008949 |
| H | 2.968262 | 0.000001 | 0.017410 |
| H | 1.705360 | 2.151203 | 0.008950 |
| H | -0.767298 | 2.152161 | -0.013865 |
| N | -2.333438 | -0.000006 | -0.083007 |
| H | -2.761953 | -0.834232 | 0.305635 |
| H | -2.761953 | 0.834271 | 0.305525 |

Compound **11** $T_1$ geometry. $E(T_1)$ = -287.363100899 a.u.

| | | | |
|---|---|---|---|
| C | 0.922381 | -0.000017 | 0.037961 |
| C | 0.197975 | 1.257952 | -0.148926 |
| C | -1.146559 | 1.262064 | -0.065934 |
| C | -1.836057 | 0.000009 | 0.250768 |
| C | -1.146553 | -1.262076 | -0.065940 |
| C | 0.197987 | -1.257955 | -0.148903 |
| H | 0.759111 | 2.163647 | -0.398291 |
| H | -1.719951 | 2.172955 | -0.247411 |
| H | -2.830666 | 0.000009 | 0.694220 |
| H | -1.719948 | -2.172952 | -0.247473 |
| H | 0.759117 | -2.163675 | -0.398204 |
| N | 2.307427 | 0.000023 | 0.075792 |
| H | 2.732626 | 0.840701 | 0.456310 |
| H | 2.732675 | -0.840705 | 0.456141 |

Compound **12** $S_0$ geometry. $E(S_0)$ = -324.390136574 a.u.

| | | | |
|---|---|---|---|
| C | 0.000000 | 0.604071 | -0.000000 |
| C | 1.215573 | -0.090722 | -0.000000 |
| C | 1.209658 | -1.482052 | 0.000000 |
| C | 0.000258 | -2.177258 | 0.000000 |
| C | -1.209302 | -1.482262 | 0.000000 |
| C | -1.215521 | -0.090980 | 0.000000 |
| H | 2.152632 | 0.465562 | -0.000000 |
| H | 2.154190 | -2.026224 | -0.000000 |
| H | 0.000395 | -3.267765 | 0.000000 |
| H | -2.153725 | -2.026633 | 0.000000 |
| H | -2.152595 | 0.465269 | 0.000000 |
| C | -0.000514 | 2.046003 | -0.000000 |
| N | -0.000258 | 3.204142 | -0.000000 |

Compound **12** $T_1$ geometry. $E(T_1)$ = -324.255721243 a.u.

| | | | |
|---|---|---|---|
| C | 0.000000 | 0.643503 | 0.000000 |
| C | 1.278361 | -0.112387 | 0.000000 |
| C | 1.260346 | -1.457231 | 0.000000 |
| C | 0.003433 | -2.196378 | 0.000000 |
| C | -1.254331 | -1.462420 | 0.000000 |
| C | -1.277372 | -0.117393 | 0.000000 |
| H | 2.209545 | 0.452441 | 0.000000 |
| H | 2.197410 | -2.014930 | 0.000000 |
| H | 0.006131 | -3.283610 | 0.000000 |
| H | -2.189960 | -2.022664 | 0.000000 |
| H | -2.209960 | 0.444974 | 0.000000 |
| C | -0.003836 | 2.031760 | 0.000000 |
| N | -0.007540 | 3.206723 | 0.000000 |

Compound **13** $S_0$ geometry. $E(S_0)$ = -154.620014697 a.u.

| | | | |
|---|---|---|---|
| C | -0.667104 | 0.786077 | -0.000000 |
| C | 0.667104 | 0.786077 | -0.000000 |
| C | 0.667104 | -0.786077 | -0.000000 |
| C | -0.667104 | -0.786077 | -0.000000 |
| H | -1.436994 | 1.555911 | -0.000000 |
| H | 1.436990 | 1.555916 | -0.000000 |
| H | 1.436994 | -1.555911 | -0.000000 |
| H | -1.436990 | -1.555916 | -0.000000 |

Compound **13** $T_1$ geometry. $E(T_1)$ = -154.602042821 a.u.

| | | | |
|---|---|---|---|
| C | 0.000000 | 1.016072 | -0.000000 |
| C | 1.016072 | -0.000000 | -0.000000 |
| C | -0.000000 | -1.016072 | -0.000000 |
| C | -1.016072 | 0.000000 | -0.000000 |
| H | 0.000000 | 2.103251 | -0.000000 |
| H | 2.103251 | -0.000000 | -0.000000 |
| H | -0.000000 | -2.103251 | -0.000000 |
| H | -2.103251 | 0.000000 | -0.000000 |

Compound **14** $S_0$ geometry. $E(S_0)$ = -170.666163420 a.u.

| | | | |
|---|---|---|---|
| N | -1.054924 | 0.236768 | -0.000000 |
| C | -0.000000 | 0.959646 | -0.000000 |
| C | 1.014112 | -0.212194 | 0.000000 |
| C | -0.082196 | -0.967743 | 0.000000 |
| H | 0.052525 | 2.054884 | -0.000000 |
| H | 2.090830 | -0.366323 | 0.000000 |
| H | -0.350384 | -2.024188 | 0.000000 |

Compound **14** $T_1$ geometry. $E(T_1)$ = -170.640365966 a.u.

| | | | |
|---|---|---|---|
| N | -1.044411 | 0.050199 | 0.000000 |
| C | -0.092611 | -0.960764 | 0.000000 |
| C | 1.014172 | -0.048720 | 0.000000 |
| C | -0.000000 | 0.965196 | 0.000000 |
| H | -0.258198 | -2.035839 | 0.000000 |
| H | 2.101364 | -0.101017 | 0.000000 |
| H | -0.061658 | 2.051196 | 0.000000 |

Compound **15** $S_0$ geometry. $E(S_0)$ = -186.677011287 a.u.

| | | | |
|---|---|---|---|
| N | -1.013346 | -0.181434 | 0.000000 |
| N | -0.098357 | -1.024699 | 0.000000 |
| C | 0.977088 | 0.079774 | 0.000000 |
| C | -0.000000 | 0.980334 | 0.000000 |
| H | 2.065260 | 0.022039 | 0.000000 |
| H | -0.145865 | 2.060241 | 0.000000 |

Compound **15** $T_1$ geometry. $E(T_1)$ = -186.658886870 a.u.

| | | | |
|---|---|---|---|
| N | -0.073104 | -1.020765 | 0.000000 |
| N | -1.023313 | 0.011577 | 0.000000 |
| C | -0.000000 | 0.953798 | 0.000000 |
| C | 0.950531 | -0.078902 | 0.000000 |
| H | -0.058439 | 2.041979 | 0.000000 |
| H | 2.030169 | -0.227037 | 0.000000 |

Compound **16** $S_0$ geometry. $E(S_0)$ = -186.718765059 a.u.

| | | | |
|---|---|---|---|
| C | 0.747644 | 0.500102 | -0.000000 |
| N | 0.747644 | -0.777379 | -0.000000 |
| C | -0.747644 | -0.500102 | -0.000000 |
| N | -0.747644 | 0.777379 | -0.000000 |
| H | 1.575039 | 1.220623 | -0.000000 |
| H | -1.575039 | -1.220623 | -0.000000 |

Compound **16** $T_1$ geometry. $E(T_1)$ = -186.676845920 a.u.

| | | | |
|---|---|---|---|
| C | 0.687936 | 0.605524 | 0.000000 |
| N | -0.687936 | 0.781584 | 0.000000 |
| C | -0.687936 | -0.605524 | 0.000000 |
| N | 0.687936 | -0.781584 | 0.000000 |
| H | 1.504788 | 1.324241 | 0.000000 |

| | | | |
|---|---|---|---|
| H | -1.504788 | -1.324241 | 0.000000 |

Compound **17** $S_0$ geometry. $E(S_0)$ = -245.945310000 a.u.

| | | | |
|---|---|---|---|
| N | -0.961434 | -0.458096 | 0.000000 |
| C | 0.000000 | 0.593339 | 0.000000 |
| C | 1.109611 | -0.468624 | -0.000000 |
| C | 0.121711 | -1.382233 | -0.000000 |
| H | 2.191483 | -0.469542 | -0.000000 |
| H | 0.038688 | -2.467129 | -0.000000 |
| O | -0.114915 | 1.776018 | 0.000000 |
| H | -1.968745 | -0.519690 | 0.000000 |

Compound **17** $T_1$ geometry. $E(T_1)$ = -245.868214052 a.u.

| | | | |
|---|---|---|---|
| N | -0.881682 | -0.534934 | 0.000000 |
| C | -0.000000 | 0.605483 | 0.000000 |
| C | 1.122057 | -0.336273 | -0.000000 |
| C | 0.144079 | -1.464795 | -0.000000 |
| H | 2.203196 | -0.238162 | -0.000000 |
| H | 0.108775 | -2.543800 | -0.000000 |
| O | -0.230389 | 1.790626 | 0.000000 |
| H | -1.893907 | -0.624996 | 0.000000 |

Compound **18** $S_0$ geometry. $E(S_0)$ = -245.898684013 a.u.

| | | | |
|---|---|---|---|
| N | -1.090105 | -0.262890 | -0.000000 |
| C | -0.000000 | 0.418181 | 0.000000 |
| C | 0.998706 | -0.743831 | -0.000000 |
| C | -0.133825 | -1.451035 | -0.000000 |
| H | 2.071641 | -0.904221 | -0.000000 |
| H | -0.432235 | -2.498950 | -0.000000 |
| O | 0.187460 | 1.721644 | 0.000000 |
| H | -0.697639 | 2.130364 | 0.000000 |

Compound **18** $T_1$ geometry. $E(T_1)$ = -245.857238718 a.u.

| | | | |
|---|---|---|---|
| N | -0.973802 | -0.525941 | -0.000000 |
| C | 0.000000 | 0.428083 | 0.000000 |
| C | 1.096186 | -0.482094 | 0.000000 |
| C | 0.046189 | -1.488588 | 0.000000 |
| H | 2.182026 | -0.427300 | 0.000000 |
| H | -0.050357 | -2.567947 | -0.000000 |
| O | -0.135048 | 1.750068 | -0.000000 |
| H | -1.088924 | 1.931888 | -0.000000 |

Compound **19** $S_0$ geometry. $E(S_0)$ = -209.969997273 a.u.

| | | | |
|---|---|---|---|
| C | -0.455159 | 0.064710 | 0.011571 |
| C | 0.433287 | 1.080233 | 0.021068 |
| C | 1.560608 | 0.014254 | -0.000907 |
| C | 0.690648 | -1.001566 | 0.000248 |
| H | 0.386895 | 2.163393 | -0.007930 |
| H | 2.649292 | 0.069775 | -0.018061 |

| | | | |
|---|---|---|---|
| H | 0.742796 | -2.086677 | -0.031447 |
| N | -1.802978 | -0.117680 | -0.083591 |
| H | -2.158770 | -0.966817 | 0.342471 |
| H | -2.375668 | 0.698296 | 0.108224 |

Compound **19** $T_1$ geometry. $E(T_1)$ = -209.948094862 a.u.

| | | | |
|---|---|---|---|
| C | -0.451957 | 0.000003 | 0.001268 |
| C | 0.562313 | -1.016832 | 0.000583 |
| C | 1.584376 | -0.000005 | 0.005692 |
| C | 0.562321 | 1.016833 | 0.000580 |
| H | 0.550633 | -2.104677 | -0.008701 |
| H | 2.668423 | -0.000008 | 0.031411 |
| H | 0.550650 | 2.104678 | -0.008704 |
| N | -1.825222 | 0.000003 | -0.087527 |
| H | -2.267731 | -0.839144 | 0.274954 |
| H | -2.267739 | 0.839130 | 0.274992 |

Compound **20** $S_0$ geometry. $E(S_0)$ = -246.851762839 a.u.

| | | | |
|---|---|---|---|
| C | 0.000000 | 0.103906 | 0.000000 |
| C | 1.321815 | -0.117397 | 0.000000 |
| C | 1.071351 | -1.654153 | 0.000000 |
| C | -0.247495 | -1.452584 | -0.000000 |
| H | 2.197560 | 0.529350 | 0.000000 |
| H | 1.717349 | -2.528573 | 0.000000 |
| H | -1.139869 | -2.074587 | -0.000000 |
| C | -0.826244 | 1.255416 | -0.000000 |
| N | -1.527372 | 2.180383 | -0.000000 |

Compound **20** $T_1$ geometry. $E(T_1)$ = -246.837121306 a.u.

| | | | |
|---|---|---|---|
| C | -0.082293 | 0.000000 | 0.000000 |
| C | 0.949805 | 1.021700 | -0.000000 |
| C | 1.940973 | -0.000000 | 0.000001 |
| C | 0.949805 | -1.021700 | 0.000001 |
| H | 0.944254 | 2.107445 | -0.000001 |
| H | 3.028382 | -0.000000 | 0.000002 |
| H | 0.944254 | -2.107445 | 0.000002 |
| C | -1.485540 | 0.000000 | -0.000001 |
| N | -2.650484 | 0.000000 | -0.000001 |

Compound **21** $S_0$ geometry. $E(S_0)$ = -210.099030530 a.u.

| | | | |
|---|---|---|---|
| C | -0.332729 | -1.121387 | 0.000000 |
| C | 0.982647 | -0.712123 | 0.000000 |
| C | 0.982647 | 0.712123 | 0.000000 |
| C | -0.332729 | 1.121387 | 0.000000 |
| N | -1.118235 | -0.000000 | 0.000000 |
| H | -2.127666 | 0.000000 | 0.000000 |
| H | -0.771333 | -2.113861 | 0.000000 |
| H | 1.849485 | -1.365793 | 0.000000 |
| H | 1.849485 | 1.365793 | 0.000000 |

| | | | |
|---|---|---|---|
| H | -0.771333 | 2.113861 | 0.000000 |

Compound **21** $T_1$ geometry. $E(T_1)$ = -209.946458302 a.u.

| | | | |
|---|---|---|---|
| C | 1.149069 | 0.355688 | 0.000000 |
| C | 0.672690 | -1.040828 | 0.000000 |
| C | -0.672703 | -1.040803 | 0.000000 |
| C | -1.149052 | 0.355680 | 0.000000 |
| N | 0.000000 | 1.190763 | 0.000000 |
| H | -0.000007 | 2.194896 | 0.000000 |
| H | 2.156142 | 0.754353 | 0.000000 |
| H | 1.326411 | -1.908700 | 0.000000 |
| H | -1.326442 | -1.908663 | 0.000000 |
| H | -2.156125 | 0.754347 | 0.000000 |

Compound **22** $S_0$ geometry. $E(S_0)$ = -226.130816260 a.u.

| | | | |
|---|---|---|---|
| N | 0.000000 | 1.080390 | 0.000000 |
| N | -1.139039 | 0.384331 | 0.000000 |
| C | -0.748131 | -0.883983 | 0.000000 |
| C | 0.661928 | -1.002112 | 0.000000 |
| C | 1.109649 | 0.303106 | 0.000000 |
| H | -0.042025 | 2.090577 | 0.000000 |
| H | -1.495631 | -1.672844 | 0.000000 |
| H | 1.263389 | -1.904249 | 0.000000 |
| H | 2.106861 | 0.731404 | 0.000000 |

Compound **22** $T_1$ geometry. $E(T_1)$ = -225.971127813 a.u.

| | | | |
|---|---|---|---|
| N | 0.000000 | 1.145179 | 0.000000 |
| N | -1.177058 | 0.446796 | 0.000000 |
| C | -0.716802 | -0.948389 | 0.000000 |
| C | 0.621807 | -1.054877 | 0.000000 |
| C | 1.154429 | 0.290312 | 0.000000 |
| H | -0.022390 | 2.151777 | 0.000000 |
| H | -1.475020 | -1.725719 | 0.000000 |
| H | 1.212600 | -1.965773 | 0.000000 |
| H | 2.167608 | 0.673615 | 0.000000 |

Compound **23** $S_0$ geometry. $E(S_0)$ = -226.148571393 a.u.

| | | | |
|---|---|---|---|
| N | 0.000000 | 1.102295 | 0.000000 |
| C | -1.086217 | 0.280623 | 0.000000 |
| N | -0.741065 | -0.985149 | 0.000000 |
| C | 0.632602 | -0.982335 | 0.000000 |
| C | 1.117179 | 0.301991 | 0.000000 |
| H | -0.013484 | 2.112860 | 0.000000 |
| H | -2.103386 | 0.663836 | 0.000000 |
| H | 1.201173 | -1.907908 | 0.000000 |
| H | 2.121770 | 0.709513 | 0.000000 |

Compound **23** $T_1$ geometry. $E(T_1)$ = -225.992426307 a.u.

| | | | |
|---|---|---|---|
| N | 1.141212 | 0.279190 | 0.000000 |

| | | | |
|---|---|---|---|
| C | -0.000000 | 1.156681 | 0.000000 |
| N | -1.198998 | 0.416223 | 0.000000 |
| C | -0.852470 | -0.821971 | -0.000000 |
| C | 0.617548 | -1.018738 | -0.000000 |
| H | 2.109802 | 0.546944 | 0.000000 |
| H | 0.068023 | 2.236736 | 0.000000 |
| H | -1.585570 | -1.630027 | -0.000000 |
| H | 1.221780 | -1.917371 | -0.000000 |

Compound **24** $S_0$ geometry. *E*($S_0$) = -229.949870463 a.u.

| | | | |
|---|---|---|---|
| O | -0.000000 | 1.154234 | 0.000051 |
| C | 1.088580 | 0.349776 | -0.000023 |
| C | 0.718052 | -0.958674 | -0.000013 |
| C | -0.718052 | -0.958674 | 0.000034 |
| C | -1.088580 | 0.349776 | -0.000056 |
| H | 2.048922 | 0.853588 | -0.000028 |
| H | 1.381801 | -1.817137 | -0.000016 |
| H | -1.381801 | -1.817138 | 0.000064 |
| H | -2.048923 | 0.853588 | -0.000078 |

Compound **24** $T_1$ geometry. *E*($T_1$) = -229.812526157 a.u.

| | | | |
|---|---|---|---|
| O | 1.231524 | 0.000000 | -0.000760 |
| C | 0.376566 | 1.105753 | 0.000502 |
| C | -1.024851 | 0.672411 | -0.000059 |
| C | -1.024850 | -0.672411 | 0.000053 |
| C | 0.376567 | -1.105753 | 0.000702 |
| H | 0.843632 | 2.082838 | -0.000317 |
| H | -1.880025 | 1.341849 | -0.000476 |
| H | -1.880024 | -1.341850 | -0.000252 |
| H | 0.843633 | -2.082837 | -0.000066 |

Compound **25** $S_0$ geometry. *E*($S_0$) = -246.000962583 a.u.

| | | | |
|---|---|---|---|
| O | -0.356092 | -1.079887 | 0.000023 |
| C | -1.094859 | 0.045994 | -0.000090 |
| N | -0.413135 | 1.142531 | -0.000092 |
| C | 0.907884 | 0.713497 | 0.000037 |
| C | 0.931935 | -0.641992 | 0.000112 |
| H | -2.173884 | -0.076468 | -0.000172 |
| H | 1.738316 | 1.412082 | 0.000068 |
| H | 1.706490 | -1.399234 | 0.000215 |

Compound **25** $T_1$ geometry. *E*($T_1$) = -245.864926306 a.u.

| | | | |
|---|---|---|---|
| O | 1.193307 | -0.074689 | -0.128176 |
| C | 0.246172 | -1.131470 | -0.001471 |
| N | -1.090663 | -0.622041 | -0.090303 |
| C | -0.942326 | 0.661486 | 0.024972 |
| C | 0.440129 | 1.039926 | 0.063562 |
| H | 0.463913 | -1.802639 | 0.842670 |
| H | -1.787499 | 1.351125 | 0.057933 |

| | | | |
|---|---|---|---|
| H | 0.947930 | 1.983669 | 0.234548 |

Compound **26** $S_0$ geometry. $E(S_0)$ = -265.821613726 a.u.

| | | | |
|---|---|---|---|
| O | 0.334979 | -1.043103 | 0.000256 |
| C | -0.568399 | 0.088920 | -0.000403 |
| C | 0.590396 | 1.035118 | 0.000179 |
| C | 1.336869 | -0.078778 | -0.000222 |
| O | -1.743292 | 0.042061 | 0.000049 |
| H | 0.728845 | 2.108571 | 0.000485 |
| H | 2.384464 | -0.371788 | -0.000247 |

Compound **26** $T_1$ geometry. $E(T_1)$ = -265.722419717 a.u.

| | | | |
|---|---|---|---|
| O | 0.404123 | -0.977676 | 0.000595 |
| C | -0.582260 | 0.075846 | -0.000068 |
| C | 0.472519 | 1.073507 | 0.000230 |
| C | 1.429312 | -0.077168 | -0.001745 |
| O | -1.767131 | -0.054632 | 0.000001 |
| H | 0.508684 | 2.158891 | 0.001427 |
| H | 2.477959 | -0.333534 | 0.003294 |

Compound **27** $S_0$ geometry. $E(S_0)$ = -343.263584942 a.u.

| | | | |
|---|---|---|---|
| O | 0.329125 | -1.153856 | -0.000003 |
| C | 1.054781 | 0.039330 | -0.000004 |
| C | 0.250570 | 1.256236 | -0.000007 |
| C | -1.101190 | 1.204464 | 0.000024 |
| C | -1.775796 | -0.065291 | 0.000044 |
| C | -1.012486 | -1.176389 | 0.000025 |
| O | 2.250581 | -0.036680 | -0.000070 |
| H | 0.810089 | 2.189786 | -0.000031 |
| H | -1.685493 | 2.126161 | 0.000030 |
| H | -2.859631 | -0.145767 | 0.000066 |
| H | -1.397896 | -2.195988 | 0.000031 |

Compound **27** $T_1$ geometry. $E(T_1)$ = -343.165621714 a.u.

| | | | |
|---|---|---|---|
| O | 0.418803 | -1.174302 | -0.000007 |
| C | 1.042424 | 0.071103 | -0.000028 |
| C | 0.221277 | 1.251435 | -0.000008 |
| C | -1.239069 | 1.170690 | 0.000032 |
| C | -1.771447 | -0.076061 | 0.000044 |
| C | -0.939050 | -1.238512 | 0.000022 |
| O | 2.251159 | 0.069495 | -0.000054 |
| H | 0.762904 | 2.194352 | -0.000025 |
| H | -1.847255 | 2.071542 | 0.000050 |
| H | -2.849506 | -0.240629 | 0.000071 |
| H | -1.310647 | -2.258732 | 0.000031 |

Compound **28** $S_0$ geometry. $E(S_0)$ = -343.249547092 a.u.

| | | | |
|---|---|---|---|
| O | 1.756674 | 0.000000 | -0.000023 |
| C | 1.056403 | -1.157078 | 0.000052 |

| | | | |
|---|---|---|---|
| C | -0.285458 | -1.223116 | 0.000073 |
| C | -1.102924 | 0.000000 | 0.000017 |
| C | -0.285458 | 1.223116 | -0.000066 |
| C | 1.056403 | 1.157077 | -0.000080 |
| H | 1.723886 | -2.017641 | 0.000091 |
| H | -0.785370 | -2.190506 | 0.000134 |
| O | -2.320526 | -0.000000 | 0.000029 |
| H | -0.785369 | 2.190506 | -0.000115 |
| H | 1.723886 | 2.017641 | -0.000138 |

Compound **28** $T_1$ geometry. $E(T_1)$ = -343.125198664 a.u.

| | | | |
|---|---|---|---|
| O | 1.785705 | 0.000013 | -0.000024 |
| C | 1.059383 | -1.168565 | 0.000043 |
| C | -0.295792 | -1.213067 | 0.000062 |
| C | -1.040069 | -0.000016 | 0.000012 |
| C | -0.295804 | 1.213062 | -0.000051 |
| C | 1.059365 | 1.168568 | -0.000066 |
| H | 1.703162 | -2.043795 | 0.000082 |
| H | -0.799364 | -2.177908 | 0.000114 |
| O | -2.376959 | 0.000000 | 0.000024 |
| H | -0.799394 | 2.177892 | -0.000086 |
| H | 1.703126 | 2.043813 | -0.000112 |