**Table II.** Cartesian coordinates of B3LYP/cc-pVTZ optimized geometries of RDX decomposition species on the adiabatic singlet ground state potential energy surface.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | X | Y | Z |  | X | Y | Z |
| **RDX** | | | | **i1** | | | |
| C | 0.529913 | 0.032558 | -1.205285 | N | -1.171339 | 0.123711 | -0.016034 |
| N | 0.336834 | -1.034127 | -0.216854 | N | 1.142694 | 0.099092 | -0.090885 |
| N | 0.385173 | 1.336537 | -0.583245 | N | -0.061225 | 2.190841 | 0.108158 |
| C | -0.473355 | -0.690347 | 0.966317 | C | -1.125033 | 1.520404 | -0.015865 |
| N | 1.375432 | -1.931909 | -0.005291 | C | 1.2189 | 1.542911 | 0.192796 |
| N | -1.444722 | 0.304375 | 0.570509 | C | -0.003589 | -0.63926 | 0.406685 |
| C | -0.909576 | 1.573085 | 0.061730 | H | 1.645678 | 1.724396 | 1.18526 |
| N | -2.627613 | -0.183872 | -0.044390 | H | 1.889345 | 1.989037 | -0.536424 |
| N | 1.527782 | 1.830244 | 0.101891 | H | -2.088449 | 1.9992 | -0.121105 |
| O | -3.316821 | 0.635544 | -0.621185 | H | 0.011335 | -0.740345 | 1.498046 |
| O | -2.876531 | -1.361106 | 0.110633 | H | -0.025762 | -1.624606 | -0.03839 |
| O | 1.363803 | -2.509812 | 1.070391 | N | 2.340336 | -0.59837 | -0.128943 |
| O | 2.164093 | -2.096505 | -0.916614 | N | -2.40162 | -0.541926 | -0.073446 |
| O | 2.586613 | 1.294205 | -0.154919 | O | 2.28007 | -1.815423 | -0.057505 |
| O | 1.352323 | 2.781120 | 0.838309 | O | 3.350473 | 0.072502 | -0.256399 |
| H | -0.235143 | -0.033501 | -1.977722 | O | -2.373262 | -1.73168 | 0.179234 |
| H | 1.506708 | -0.079616 | -1.657253 | O | -3.371747 | 0.12392 | -0.375458 |
| H | 0.143483 | -0.262153 | 1.758855 |  |  |  |  |
| H | -0.971436 | -1.571832 | 1.345219 |  |  |  |  |
| H | -1.622448 | 1.978847 | -0.647871 |  |  |  |  |
| H | -0.761105 | 2.280182 | 0.870932 |  |  |  |  |
| **i2** | | | | **i3** | | | |
| N | -1.460501 | -1.564679 | 0.000000 | N | 1.184773 | 0.684029 | 0.000000 |
| N | 0.000000 | 0.254817 | 0.000000 | N | 0.000000 | -1.368058 | 0.000000 |
| N | 0.909317 | -1.991097 | 0.000000 | N | -1.184773 | 0.684029 | 0.000000 |
| C | -0.303370 | -2.365973 | 0.000000 | C | 0.000000 | 1.291256 | 0.000000 |
| C | 1.225389 | -0.588629 | 0.000000 | C | -1.118260 | -0.645628 | 0.000000 |
| C | -1.256258 | -0.302154 | 0.000000 | C | 1.118260 | -0.645628 | 0.000000 |
| H | -0.507024 | -3.430937 | 0.000000 | H | -2.057208 | -1.187730 | 0.000000 |
| H | -2.071689 | 0.408540 | 0.000000 | H | 0.000000 | 2.375459 | 0.000000 |
| H | 1.823051 | -0.341287 | 0.878646 | H | 2.057208 | -1.187730 | 0.000000 |
| H | 1.823051 | -0.341287 | -0.878646 |  |  |  |  |
| N | 0.156510 | 1.643540 | 0.000000 |  |  |  |  |
| O | -0.849445 | 2.327696 | 0.000000 |  |  |  |  |
| O | 1.312040 | 2.028234 | 0.000000 |  |  |  |  |
| **i4** | | | | **i5** | | | |
| N | -0.036655 | 1.243721 | 0.000000 | N | -0.271419 | 1.917777 | 0.056034 |
| C | 0.453311 | 0.586473 | 1.214694 | C | -1.333819 | 1.191755 | 0.287139 |
| H | 0.026986 | 1.076929 | 2.080202 | H | -2.287899 | 1.686233 | 0.318874 |
| H | 1.552908 | 0.622196 | 1.275489 | C | 1.092902 | 1.331011 | -0.061801 |
| C | 0.453311 | 0.586473 | -1.214694 | H | 1.488071 | 1.672696 | -1.010935 |
| H | 0.026986 | 1.076929 | -2.080202 | H | 1.681427 | 1.761712 | 0.751038 |
| H | 1.552908 | 0.622196 | -1.275489 | N | -1.233068 | -0.171812 | 0.556355 |
| N | -0.021108 | -0.786169 | 1.161832 | N | 1.031527 | -0.121231 | -0.024693 |
| N | -0.021108 | -0.786169 | -1.161832 | C | 0.064764 | -0.695182 | 0.907232 |
| C | 0.349569 | -1.579675 | 0.000000 | H | 0.063887 | -1.7725 | 0.81391 |
| H | -0.205112 | -2.506477 | 0.000000 | H | 0.284957 | -0.40632 | 1.938886 |
| H | 1.426902 | -1.800576 | 0.000000 | O | -0.274529 | 3.179014 | -0.046337 |
| O | 0.509896 | 2.542260 | 0.000000 | N | -2.111808 | -1.034278 | -0.198845 |
| N | -0.661505 | 3.527247 | 0.000000 | N | 2.257643 | -0.774922 | -0.163612 |
| O | -0.255374 | 4.599973 | 0.000000 | O | -3.025019 | -0.475474 | -0.763799 |
| N | -0.146913 | -1.468792 | 2.367141 | O | -1.898325 | -2.223589 | -0.121152 |
| N | -0.146913 | -1.468792 | -2.367141 | O | 2.297429 | -1.944682 | 0.166943 |
| O | -0.178667 | -0.794000 | 3.381043 | O | 3.164988 | -0.112277 | -0.633638 |
| O | -0.241052 | -2.682001 | 2.300545 |  |  |  |  |
| O | -0.241052 | -2.682001 | -2.300545 |  |  |  |  |
| O | -0.178667 | -0.794000 | -3.381043 |  |  |  |  |
| **i6** | | | | **i7** | | | |
| N | 0.328470 | 1.996846 | -0.419945 | N | 0.446608 | 1.878438 | 0.078788 |
| C | -0.883888 | 1.248973 | -0.515293 | C | -0.801888 | 1.352539 | -0.156945 |
| H | -1.503903 | 1.410372 | -1.385073 | H | 0.478335 | 2.876056 | -0.06146 |
| C | 1.431170 | 1.420364 | 0.370245 | C | 1.508888 | 1.258611 | 0.860309 |
| H | 2.341494 | 1.589366 | -0.193165 | H | 2.474771 | 1.597867 | 0.504441 |
| H | 1.482521 | 1.968864 | 1.308698 | H | 1.418848 | 1.49246 | 1.924407 |
| N | -0.899327 | -0.107702 | -0.075621 | N | -0.860426 | -0.048174 | 0.120497 |
| N | 1.332773 | -0.006177 | 0.653056 | N | 1.431525 | -0.179935 | 0.74635 |
| C | 0.018157 | -0.474759 | 1.011325 | C | 0.112802 | -0.697071 | 1.020346 |
| H | 0.013298 | -1.547665 | 1.129888 | H | 0.082903 | -1.764412 | 0.856095 |
| H | -0.266714 | 0.011082 | 1.945013 | H | -0.112332 | -0.489804 | 2.066378 |
| O | -0.873949 | 2.244702 | 0.464407 | O | -1.719509 | 2.002354 | -0.581265 |
| N | -2.135280 | -0.777426 | -0.131014 | N | -2.083349 | -0.74888 | -0.049159 |
| N | 2.082439 | -0.874403 | -0.197326 | N | 2.089951 | -0.748395 | -0.395158 |
| O | -2.975795 | -0.317338 | -0.878123 | O | -2.799099 | -0.421095 | -0.957111 |
| O | -2.231144 | -1.778361 | 0.550496 | O | -2.259459 | -1.658949 | 0.746964 |
| O | 1.729979 | -2.034749 | -0.234926 | O | 1.716689 | -1.847816 | -0.739976 |
| O | 3.048052 | -0.391436 | -0.752738 | O | 3.007441 | -0.107996 | -0.861279 |
| **i8** | | | | **i9** | | | |
| N | 1.758275 | 0.917835 | 0.047897 | C | 1.224291 | -0.923766 | 0.000000 |
| H | 2.280201 | 1.778532 | 0.088054 | N | 0.152703 | -1.780180 | 0.000000 |
| C | 2.388512 | -0.287864 | -0.209414 | C | -0.997656 | -1.180873 | 0.000000 |
| C | 0.378048 | 1.073081 | 0.125486 | C | 0.000000 | 1.028962 | 0.000000 |
| N | 1.822471 | -1.417095 | -0.184025 | N | 1.219942 | 0.373649 | 0.000000 |
| N | -0.267068 | -0.165710 | -0.046807 | H | -1.913982 | -1.761613 | 0.000000 |
| C | 0.432725 | -1.461643 | 0.183212 | N | -1.125073 | 0.156396 | 0.000000 |
| H | -0.083155 | -2.207034 | -0.414474 | H | -2.033751 | 0.597968 | 0.000000 |
| H | 0.341092 | -1.758510 | 1.232020 | O | -0.167365 | 2.222510 | 0.000000 |
| H | 3.446994 | -0.210074 | -0.435508 | H | 2.193837 | -1.411420 | 0.000000 |
| O | -0.141040 | 2.139030 | 0.308586 |  |  |  |  |
| N | -1.683020 | -0.224708 | -0.081579 |  |  |  |  |
| O | -2.279445 | 0.727250 | -0.517352 |  |  |  |  |
| O | -2.153946 | -1.280856 | 0.306991 |  |  |  |  |
| **i10** | | | | **i11** | | | |
| C | 1.152653 | -1.045312 | 0.000000 | C | -0.934665 | 1.604074 | -0.267763 |
| N | 1.197883 | 0.281033 | 0.000000 | N | 0.436019 | 1.974453 | -0.056701 |
| C | 0.000000 | 0.858693 | 0.000000 | N | -1.164805 | 0.162614 | -0.050661 |
| C | -1.079005 | -1.099728 | 0.000000 | C | 1.330672 | 1.129564 | 0.223815 |
| N | 0.052548 | -1.799358 | 0.000000 | N | 1.070206 | -0.224226 | 0.553932 |
| H | 2.104726 | -1.563717 | 0.000000 | C | -0.304506 | -0.472991 | 0.941702 |
| H | -2.008975 | -1.656917 | 0.000000 | N | 1.688507 | -1.246392 | -0.262714 |
| N | -1.174740 | 0.225287 | 0.000000 | N | -2.482255 | -0.260812 | -0.106782 |
| O | -0.015523 | 2.190633 | 0.000000 | O | 1.312304 | -2.377114 | -0.053736 |
| H | -0.943294 | 2.464917 | 0.000000 | O | 2.534594 | -0.878801 | -1.040276 |
|  |  |  |  | O | -3.258321 | 0.477064 | -0.692051 |
|  |  |  |  | O | -2.747346 | -1.337804 | 0.402768 |
|  |  |  |  | H | -1.224351 | 1.847188 | -1.28759 |
|  |  |  |  | H | -1.568828 | 2.194339 | 0.401235 |
|  |  |  |  | H | -0.491714 | -1.537106 | 0.96707 |
|  |  |  |  | H | -0.453927 | -0.049569 | 1.938272 |
|  |  |  |  | O | 2.614758 | 1.461501 | 0.377757 |
|  |  |  |  | H | 2.708191 | 2.383044 | 0.099279 |
| **i12** | | | |  | | | |
| N | -2.432559 | -0.080269 | -0.600367 |  |  |  |  |
| N | -0.754984 | 1.152353 | 0.448267 |  |  |  |  |
| N | -0.624670 | -1.230307 | 0.490549 |  |  |  |  |
| C | -1.750128 | -1.188219 | -0.125349 |  |  |  |  |
| C | 0.092196 | -0.002620 | 0.634517 |  |  |  |  |
| C | -1.897623 | 1.045066 | -0.258378 |  |  |  |  |
| H | -2.264307 | -2.131563 | -0.279603 |  |  |  |  |
| H | -2.391303 | 1.977717 | -0.512912 |  |  |  |  |
| H | -0.394581 | 2.063522 | 0.680785 |  |  |  |  |
| H | 0.593656 | 0.046688 | 1.600814 |  |  |  |  |
| N | 2.435465 | -0.017083 | 0.261254 |  |  |  |  |
| O | 1.140786 | 0.042560 | -0.368586 |  |  |  |  |
| O | 3.287602 | -0.024383 | -0.530382 |  |  |  |  |
| **tsi1** | | | | **tsi1i2** | | | |
| C | -0.377594 | -1.229808 | 0.982263 | N | -1.047126 | 0.646065 | 0.955238 |
| N | 0.843281 | -0.844964 | 1.380109 | N | 1.080914 | 0.157911 | 0.097057 |
| C | 1.190340 | 0.556695 | 1.477946 | N | 0.079046 | 2.291937 | -0.331369 |
| N | 0.301891 | 1.479555 | 0.775430 | C | -0.986405 | 1.768558 | 0.127101 |
| C | -1.105506 | 1.167200 | 0.941266 | C | 1.323006 | 1.579232 | -0.179937 |
| N | -1.348167 | -0.229684 | 0.613993 | C | -0.005501 | -0.195258 | 0.956048 |
| N | 1.853144 | -1.411048 | -0.344678 | H | 1.920601 | 2.048176 | 0.611124 |
| N | 0.703317 | 1.889337 | -0.525688 | H | 1.889495 | 1.644742 | -1.104817 |
| N | -2.335496 | -0.570701 | -0.298234 | H | -1.937273 | 2.263584 | -0.029396 |
| O | 1.008839 | -2.122990 | -0.929102 | H | 0.263219 | -0.640783 | 1.915732 |
| O | 3.001103 | -1.325556 | -0.643949 | H | -0.659422 | -1.19642 | 0.41346 |
| O | 1.895517 | 1.867294 | -0.755377 | N | 2.068 | -0.769269 | -0.11993 |
| O | -0.173065 | 2.284475 | -1.267365 | N | -2.362031 | -0.588572 | -0.207701 |
| O | -3.132490 | 0.296450 | -0.606695 | O | 1.824089 | -1.914083 | 0.237733 |
| O | -2.335500 | -1.733320 | -0.671748 | O | 3.092266 | -0.372592 | -0.65398 |
| H | 0.032465 | -1.852325 | -0.112549 | O | -1.726041 | -1.661172 | -0.196674 |
| H | -0.795592 | -2.090340 | 1.506335 | O | -3.464669 | -0.452277 | -0.634384 |
| H | 1.138249 | 0.803606 | 2.542691 |  |  |  |  |
| H | 2.209442 | 0.715265 | 1.145118 |  |  |  |  |
| H | -1.348624 | 1.348876 | 1.989034 |  |  |  |  |
| H | -1.720400 | 1.792103 | 0.307883 |  |  |  |  |
| **tsi2i3** | | | | **tsi2i12** | | | |
| N | 1.748607 | 1.190567 | -0.363890 | N | -1.45966 | -1.290583 | 0.39817 |
| N | 0.097716 | 0.247041 | 1.041857 | N | -0.157684 | -0.083967 | -1.204857 |
| N | 1.601630 | -1.181381 | -0.239246 | N | -1.508369 | 1.108615 | 0.442911 |
| C | 2.113268 | -0.089108 | -0.705956 | C | -1.825685 | -0.053134 | 0.913357 |
| C | 0.567655 | -1.006659 | 0.693287 | C | -0.746497 | 1.077972 | -0.699453 |
| C | 0.721997 | 1.286483 | 0.437401 | C | -0.60409 | -1.243348 | -0.567719 |
| H | 2.922309 | -0.168024 | -1.423193 | H | -2.438695 | -0.090887 | 1.806018 |
| H | 0.347507 | 2.275048 | 0.679336 | H | -0.164411 | -2.15753 | -0.946324 |
| H | -0.460199 | -1.433591 | 0.162681 | H | -1.142634 | 0.385542 | -1.810184 |
| H | 0.602951 | -1.714307 | 1.526768 | H | -0.439829 | 2.003201 | -1.161448 |
| N | -1.770268 | 0.072611 | -0.130520 | N | 1.668577 | -0.018608 | 0.096011 |
| O | -2.657392 | 0.841138 | -0.355172 | O | 1.608713 | 1.16889 | 0.380769 |
| O | -1.789343 | -1.141799 | -0.351252 | O | 2.571681 | -0.773572 | 0.382879 |
| **tsi4** | | | | **tsi4i5** | | | |
| C | 0.683815 | 1.273659 | 0.820197 | N | 0.362884 | -1.539778 | 0.513595 |
| N | -0.621768 | 1.030237 | 1.292655 | C | 1.166515 | -0.419850 | 0.523159 |
| C | -0.965153 | -0.316969 | 1.614508 | H | 1.862901 | -0.419053 | -0.495832 |
| N | -2.147832 | 1.909228 | -0.670747 | H | 1.984760 | -0.545817 | 1.242222 |
| O | -3.118534 | 1.419198 | -0.197009 | C | -0.995306 | -1.569036 | -0.045095 |
| O | -1.233709 | 1.460602 | -1.293409 | H | -0.950322 | -1.977103 | -1.054482 |
| H | 0.683693 | 2.121377 | 0.134149 | H | -1.578423 | -2.248338 | 0.579857 |
| H | 1.280937 | 1.61293 | 1.692924 | N | 0.424425 | 0.811299 | 0.687112 |
| H | -2.040268 | -0.450885 | 1.589568 | N | -1.540995 | -0.216703 | -0.069170 |
| H | -0.643992 | -0.49356 | 2.656258 | C | -0.998973 | 0.723833 | 0.905063 |
| N | -0.334099 | -1.365403 | 0.808866 | H | -1.450978 | 1.694822 | 0.756148 |
| N | 1.357978 | 0.14996 | 0.160401 | H | -1.172913 | 0.378986 | 1.928251 |
| C | 1.090222 | -1.206536 | 0.643553 | O | 0.899473 | -2.685947 | 0.671076 |
| H | 1.556792 | -1.379214 | 1.618037 | N | 3.202503 | -0.667595 | -1.181601 |
| H | 1.473754 | -1.922263 | -0.068859 | O | 3.977091 | -0.791653 | -0.345050 |
| N | -1.053098 | -1.778675 | -0.347874 | N | 0.933674 | 1.952425 | 0.050436 |
| N | 2.634131 | 0.399925 | -0.318081 | N | -2.890288 | -0.123099 | -0.387890 |
| O | -2.258497 | -1.634816 | -0.309907 | O | 2.100391 | 1.885282 | -0.297007 |
| O | -0.41226 | -2.297226 | -1.237536 | O | 0.203552 | 2.918394 | -0.038739 |
| O | 2.944778 | 1.572014 | -0.456518 | O | -3.452442 | 0.925250 | -0.128872 |
| O | 3.326796 | -0.570548 | -0.576641 | O | -3.374798 | -1.102454 | -0.929196 |
| **tsi5i6** | | | | **tsi6i7** | | | |
| N | 0.472752 | 1.764522 | -0.350276 | N | -0.060330 | 2.090214 | -0.346970 |
| C | -0.684169 | 1.133534 | -0.535731 | C | -1.224395 | 1.293489 | -0.172171 |
| H | -1.391194 | 1.535413 | -1.241452 | H | -1.575459 | 1.412237 | -1.254717 |
| C | 1.45547 | 1.211158 | 0.591908 | C | 1.210335 | 1.608472 | -0.014008 |
| H | 2.461905 | 1.4393 | 0.26384 | H | 1.911713 | 1.727069 | -0.851954 |
| H | 1.268498 | 1.652832 | 1.57097 | H | 1.580841 | 2.361773 | 0.711127 |
| N | -0.988822 | -0.016857 | 0.092337 | N | -0.859122 | -0.141957 | -0.024238 |
| N | 1.290951 | -0.228131 | 0.708716 | N | 1.354916 | 0.270150 | 0.538782 |
| C | -0.042681 | -0.642854 | 1.047851 | C | 0.137311 | -0.367509 | 1.010237 |
| H | -0.143686 | -1.71719 | 0.987891 | H | 0.301935 | -1.428829 | 1.144368 |
| H | -0.26762 | -0.298299 | 2.055231 | H | -0.156269 | 0.095722 | 1.954362 |
| O | -0.196103 | 2.943432 | 0.138504 | O | -2.078941 | 1.742292 | 0.685239 |
| N | -2.276879 | -0.626195 | -0.09506 | N | -1.854973 | -1.091876 | -0.247220 |
| N | 1.9699 | -1.037977 | -0.259112 | N | 2.313643 | -0.559737 | -0.099777 |
| O | -2.996127 | -0.123731 | -0.922519 | O | -2.742298 | -0.751814 | -1.005152 |
| O | -2.489111 | -1.583615 | 0.614276 | O | -1.719255 | -2.176090 | 0.289163 |
| O | 1.499708 | -2.138335 | -0.4716 | O | 2.266570 | -1.743132 | 0.145521 |
| O | 2.984764 | -0.574079 | -0.725771 | O | 3.141275 | 0.010965 | -0.788716 |
| **tsi7i8** | | | | **tsi7i11** | | | |
| N | 0.150055 | 2.021302 | 0.118191 | C | -1.258422 | 1.564977 | 0.159182 |
| H | 0.152605 | 2.973456 | -0.210211 | N | 0.119817 | 1.987240 | 0.170821 |
| C | 1.356344 | 1.451297 | 0.644603 | N | -1.268151 | 0.108147 | -0.038541 |
| C | -0.968878 | 1.30616 | -0.235263 | C | 1.167459 | 1.199546 | 0.073667 |
| N | 1.311439 | 0.252931 | 1.235929 | N | 1.051628 | -0.160989 | 0.236478 |
| N | -0.843104 | -0.051322 | 0.177784 | C | -0.252745 | -0.662774 | 0.663436 |
| C | 0.032002 | -0.392137 | 1.316302 | N | 2.083501 | -1.092363 | -0.099292 |
| H | 2.125738 | 1.055455 | -0.333061 | N | -2.516673 | -0.490535 | -0.181441 |
| H | 0.149821 | -1.469208 | 1.344604 | O | 1.817631 | -2.252231 | 0.138977 |
| H | -0.415692 | -0.0741 | 2.267035 | O | 3.093703 | -0.638697 | -0.565310 |
| H | 2.013158 | 2.185199 | 1.11282 | O | -3.440988 | 0.257998 | -0.445200 |
| O | -1.920131 | 1.784469 | -0.791525 | O | -2.572626 | -1.702128 | -0.061437 |
| N | -1.919287 | -0.946673 | -0.066763 | H | -1.798368 | 2.025843 | -0.663642 |
| N | 2.149478 | -0.835918 | -0.391721 | H | -1.762915 | 1.835183 | 1.093837 |
| O | -2.491915 | -0.847917 | -1.120398 | H | -0.340164 | -1.706252 | 0.396239 |
| O | -2.119964 | -1.763283 | 0.817202 | H | -0.345461 | -0.552323 | 1.748360 |
| O | 2.319228 | -1.999195 | -0.589137 | O | 2.207096 | 1.906431 | -0.128345 |
| O | 2.652469 | 0.082807 | -1.072265 | H | 1.179777 | 2.755569 | -0.078163 |
| **tsi8i9** | | | | **tsi9i10** | | | |
| N | 1.746057 | 0.790055 | -0.325357 | C | 1.161058 | 1.037054 | 0.000037 |
| H | 2.365972 | 1.58038 | -0.42406 | N | 1.755693 | -0.169034 | 0.000041 |
| C | 2.272378 | -0.509809 | -0.394577 | C | 0.931107 | -1.208187 | 0.000020 |
| C | 0.50848 | 1.102899 | 0.156923 | C | -0.903425 | 0.220005 | -0.000021 |
| N | 1.632105 | -1.521487 | 0.054322 | N | -0.136857 | 1.315491 | 0.000008 |
| N | -0.289069 | -0.117427 | 0.253229 | H | 1.340483 | -2.211075 | 0.000024 |
| C | 0.345488 | -1.39362 | 0.458933 | N | -0.381558 | -1.052761 | -0.000004 |
| H | -1.321792 | -1.914406 | -0.130675 | H | -1.658759 | -1.208315 | -0.000053 |
| H | 0.025968 | -1.938447 | 1.338202 | O | -2.163248 | 0.072593 | -0.000069 |
| H | 3.270277 | -0.589498 | -0.799179 | H | 1.830868 | 1.889540 | 0.000059 |
| O | 0.122599 | 2.186956 | 0.49762 |  |  |  |  |
| N | -1.559715 | -0.082227 | -0.135631 |  |  |  |  |
| O | -2.206547 | 0.895232 | -0.430191 |  |  |  |  |
| O | -2.14157 | -1.309343 | -0.097167 |  |  |  |  |
| **tsi9i12** | | | | **HNO** | | | |
| N | -2.387631 | 0.439084 | 0.431366 | N | 0.062942 | 0.577891 | 0.000000 |
| N | -0.322951 | 0.939266 | -0.511661 | O | 0.062942 | -0.620459 | 0.000000 |
| N | -0.817749 | -1.337903 | 0.013796 | H | -0.944133 | 0.918438 | 0.000000 |
| C | -1.971023 | -0.877576 | 0.360589 | **HONO** | | | |
| C | 0.205221 | -0.39417 | -0.26217 | O | 0.890457 | -0.603908 | 0.000000 |
| C | -1.545779 | 1.283764 | -0.080246 | H | 1.760520 | -0.180168 | 0.000000 |
| H | -2.742631 | -1.603767 | 0.596138 | N | 0.000000 | 0.519635 | 0.000000 |
| H | -1.83393 | 2.323198 | -0.203873 | O | -1.110522 | 0.171748 | 0.000000 |
| H | 0.261993 | 1.583271 | -1.021639 |  |  |  |  |
| H | 0.80583 | -0.289668 | 0.877717 |  |  |  |  |
| N | 2.277227 | -0.316367 | 0.569705 |  |  |  |  |
| O | 1.226092 | -0.716516 | -1.001961 |  |  |  |  |
| O | 2.790901 | 0.697303 | 0.516985 |  |  |  |  |