# Nitroxidation of H-Terminated Si(111) Surfaces with Nitrobenzene and Nitrosobenzene

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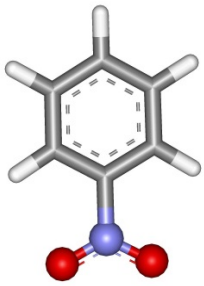
## Supporting Information

**Summary of the Density Functional Theory (DFT) Calculations**

Density functional theory calculations were performed using Gaussian 09 suite of programs with the B3LYP functional and 6-311+G(d,p) basis set.

Nitrobenzene (gas phase)

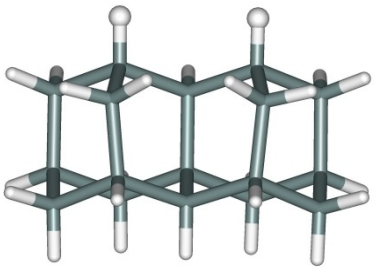


E (RB+HF-LYP) = -436.8746216

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.429825 | -1.218731 | 0.000031 |
| 2 | 6 | 0 | 0.241438 | 0.000003 | 0.000018 |
| 3 | 6 | 0 | -0.429812 | 1.218740 | -0.000015 |
| 4 | 6 | 0 | -1.821209 | 1.210175 | -0.000007 |
| 5 | 6 | 0 | -2.515505 | 0.000006 | -0.000007 |
| 6 | 6 | 0 | -1.821218 | -1.210170 | 0.000000 |
| 7 | 1 | 0 | 0.135238 | -2.140476 | 0.000064 |
| 8 | 1 | 0 | 0.135248 | 2.140485 | -0.000019 |
| 9 | 1 | 0 | -2.362437 | 2.148717 | -0.000012 |
| 10 | 1 | 0 | -3.599426 | 0.000007 | -0.000025 |
| 11 | 1 | 0 | -2.362456 | -2.148706 | 0.000001 |
| 12 | 7 | 0 | 1.722335 | -0.000006 | 0.000002 |
| 13 | 8 | 0 | 2.290912 | 1.084497 | 0.000025 |
| 14 | 8 | 0 | 2.290872 | -1.084512 | -0.000042 |

Si (111) surface (relaxed subsurface)

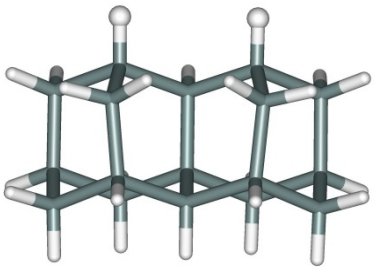


E (RB+HF-LYP) = -4936.40670530

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | -1.957899 | 3.869624 | 0.145897 |
| 2 | 14 | 0 | 1.957899 | 3.869624 | 0.145897 |
| 3 | 14 | 0 | 0.000000 | 3.885245 | 1.473090 |
| 4 | 14 | 0 | 0.000000 | 1.924918 | 2.788068 |
| 5 | 1 | 0 | -3.148816 | 2.008275 | -2.159954 |
| 6 | 1 | 0 | 0.000000 | 3.570180 | -3.259455 |
| 7 | 14 | 0 | 1.930020 | 1.993476 | -1.297651 |
| 8 | 14 | 0 | 0.000000 | 2.210946 | -2.646838 |
| 9 | 14 | 0 | -1.930020 | 1.993476 | -1.297651 |
| 10 | 1 | 0 | 0.000000 | 1.216095 | -3.752065 |
| 11 | 1 | 0 | 2.042587 | 5.116398 | -0.666398 |
| 12 | 1 | 0 | 3.152090 | 3.822928 | 1.035891 |
| 13 | 1 | 0 | 0.000000 | 5.090357 | 2.354469 |
| 14 | 1 | 0 | -2.042587 | 5.116398 | -0.666398 |
| 15 | 1 | 0 | -3.152090 | 3.822928 | 1.035891 |
| 16 | 1 | 0 | 1.203410 | 1.891516 | 3.667062 |
| 17 | 1 | 0 | -1.203410 | 1.891516 | 3.667062 |
| 18 | 14 | 0 | -1.900311 | 0.000000 | -0.011904 |
| 19 | 14 | 0 | 1.900311 | 0.000000 | -0.011904 |
| 20 | 14 | 0 | 0.000000 | 0.000000 | 1.411142 |
| 21 | 14 | 0 | 0.000000 | -1.924918 | 2.788068 |
| 22 | 14 | 0 | 1.957899 | -3.869624 | 0.145897 |
| 23 | 14 | 0 | 0.000000 | -3.885245 | 1.473090 |
| 24 | 14 | 0 | -1.957899 | -3.869624 | 0.145897 |
| 25 | 1 | 0 | 3.152090 | -3.822928 | 1.035891 |
| 26 | 1 | 0 | -3.148816 | -2.008275 | -2.159954 |
| 27 | 1 | 0 | 0.000000 | -1.216095 | -3.752065 |
| 28 | 14 | 0 | 1.930020 | -1.993476 | -1.297651 |
| 29 | 14 | 0 | 0.000000 | -2.210946 | -2.646838 |
| 30 | 14 | 0 | -1.930020 | -1.993476 | -1.297651 |
| 31 | 1 | 0 | 0.000000 | -3.570180 | -3.259455 |
| 32 | 1 | 0 | 2.042587 | -5.116398 | -0.666398 |
| 33 | 1 | 0 | 3.127367 | 0.000000 | 0.841150 |
| 34 | 1 | 0 | -3.127367 | 0.000000 | 0.841150 |
| 35 | 1 | 0 | 1.203410 | -1.891516 | 3.667062 |
| 36 | 1 | 0 | -1.203410 | -1.891516 | 3.667062 |
| 37 | 1 | 0 | -3.152090 | -3.822928 | 1.035891 |
| 38 | 1 | 0 | -2.042587 | -5.116398 | -0.666398 |
| 39 | 1 | 0 | 0.000000 | -5.090357 | 2.354469 |
| 40 | 1 | 0 | 3.148816 | -2.008275 | -2.159954 |
| 41 | 1 | 0 | 3.148816 | 2.008275 | -2.159954 |

Si (111) surface (fixed subsurface)

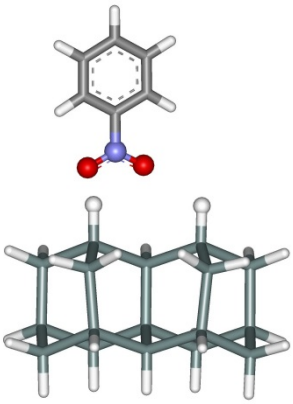


E (RB+HF-LYP) = -4936.40670530

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | -1.956600 | 3.871400 | 0.144799 |
| 2 | 14 | 0 | 1.956600 | 3.871400 | 0.144799 |
| 3 | 14 | 0 | 0.000000 | 3.888300 | 1.472799 |
| 4 | 14 | 0 | 0.000000 | 1.928600 | 2.788599 |
| 5 | 1 | 0 | -3.150000 | 2.010100 | -2.160601 |
| 6 | 1 | 0 | 0.000000 | 3.565700 | -3.264301 |
| 7 | 14 | 0 | 1.930300 | 1.994500 | -1.297501 |
| 8 | 14 | 0 | 0.000000 | 2.207400 | -2.646501 |
| 9 | 14 | 0 | -1.930300 | 1.994500 | -1.297501 |
| 10 | 1 | 0 | 0.000000 | 1.212200 | -3.752801 |
| 11 | 1 | 0 | 2.043800 | 5.119400 | -0.667501 |
| 12 | 1 | 0 | 3.152700 | 3.827000 | 1.034299 |
| 13 | 1 | 0 | 0.000000 | 5.095200 | 2.353999 |
| 14 | 1 | 0 | -2.043800 | 5.119400 | -0.667501 |
| 15 | 1 | 0 | -3.152700 | 3.827000 | 1.034299 |
| 16 | 1 | 0 | 1.202700 | 1.897100 | 3.670399 |
| 17 | 1 | 0 | -1.202700 | 1.897100 | 3.670399 |
| 18 | 14 | 0 | -1.900500 | 0.000000 | -0.011901 |
| 19 | 14 | 0 | 1.900500 | 0.000000 | -0.011901 |
| 20 | 14 | 0 | 0.000000 | 0.000000 | 1.414699 |
| 21 | 14 | 0 | 0.000000 | -1.928600 | 2.788599 |
| 22 | 14 | 0 | 1.956600 | -3.871400 | 0.144799 |
| 23 | 14 | 0 | 0.000000 | -3.888300 | 1.472799 |
| 24 | 14 | 0 | -1.956600 | -3.871400 | 0.144799 |
| 25 | 1 | 0 | 3.152700 | -3.827000 | 1.034299 |
| 26 | 1 | 0 | -3.150000 | -2.010100 | -2.160601 |
| 27 | 1 | 0 | 0.000000 | -1.212200 | -3.752801 |
| 28 | 14 | 0 | 1.930300 | -1.994500 | -1.297501 |
| 29 | 14 | 0 | 0.000000 | -2.207400 | -2.646501 |
| 30 | 14 | 0 | -1.930300 | -1.994500 | -1.297501 |
| 31 | 1 | 0 | 0.000000 | -3.565700 | -3.264301 |
| 32 | 1 | 0 | 2.043800 | -5.119400 | -0.667501 |
| 33 | 1 | 0 | 3.129400 | 0.000000 | 0.840699 |
| 34 | 1 | 0 | -3.129400 | 0.000000 | 0.840699 |
| 35 | 1 | 0 | 1.202700 | -1.897100 | 3.670399 |
| 36 | 1 | 0 | -1.202700 | -1.897100 | 3.670399 |
| 37 | 1 | 0 | -3.152700 | -3.827000 | 1.034299 |
| 38 | 1 | 0 | -2.043800 | -5.119400 | -0.667501 |
| 39 | 1 | 0 | 0.000000 | -5.095200 | 2.353999 |
| 40 | 1 | 0 | 3.150000 | -2.010100 | -2.160601 |
| 41 | 1 | 0 | 3.150000 | 2.010100 | -2.160601 |

Nitrobenzene adsorption (relaxed subsurface)

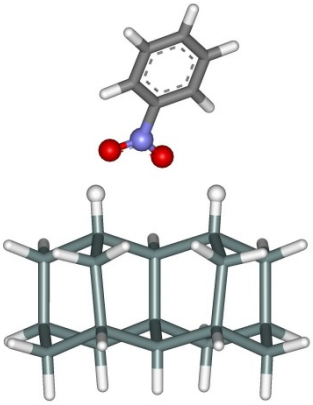


E (RB+HF-LYP) = -5373.28285544

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | -4.419175 | -2.765433 | 1.346471 |
| 2 | 14 | 0 | -1.994300 | -3.820371 | -1.532131 |
| 3 | 14 | 0 | -4.116598 | -2.925395 | -0.994113 |
| 4 | 14 | 0 | -4.237013 | -0.746842 | -1.894261 |
| 5 | 1 | 0 | -2.865263 | -1.391123 | 3.769599 |
| 6 | 1 | 0 | -0.779193 | -3.991736 | 2.210736 |
| 7 | 14 | 0 | -0.289692 | -2.505353 | -0.547438 |
| 8 | 14 | 0 | -0.654269 | -2.567149 | 1.787453 |
| 9 | 14 | 0 | -2.683388 | -1.461015 | 2.288817 |
| 10 | 1 | 0 | 0.484045 | -1.968639 | 2.531385 |
| 11 | 1 | 0 | -1.888209 | -5.222975 | -1.037367 |
| 12 | 1 | 0 | -1.838302 | -3.851623 | -3.014354 |
| 13 | 1 | 0 | -5.188478 | -3.782955 | -1.582624 |
| 14 | 1 | 0 | -4.409407 | -4.123610 | 1.961342 |
| 15 | 1 | 0 | -5.746849 | -2.149247 | 1.627961 |
| 16 | 1 | 0 | -4.078650 | -0.791006 | -3.376124 |
| 17 | 1 | 0 | -5.566642 | -0.140156 | -1.599853 |
| 18 | 14 | 0 | -2.756392 | 0.732269 | 1.386925 |
| 19 | 14 | 0 | -0.396324 | -0.296447 | -1.407238 |
| 20 | 14 | 0 | -2.541385 | 0.624407 | -0.974596 |
| 21 | 14 | 0 | -2.721645 | 2.786929 | -1.920318 |
| 22 | 14 | 0 | 1.046112 | 3.283076 | -1.575618 |
| 23 | 14 | 0 | -1.060814 | 4.213588 | -1.038151 |
| 24 | 14 | 0 | -1.379648 | 4.343178 | 1.301864 |
| 25 | 1 | 0 | 1.162204 | 3.169455 | -3.057733 |
| 26 | 1 | 0 | -1.289844 | 2.298188 | 3.744733 |
| 27 | 1 | 0 | 1.431848 | 0.258568 | 2.532980 |
| 28 | 14 | 0 | 1.278878 | 1.156277 | -0.563029 |
| 29 | 14 | 0 | 1.092075 | 1.486027 | 1.771219 |
| 30 | 14 | 0 | -1.111099 | 2.198477 | 2.265053 |
| 31 | 1 | 0 | 2.027496 | 2.571889 | 2.176935 |
| 32 | 1 | 0 | 2.139232 | 4.181711 | -1.105688 |
| 33 | 1 | 0 | -0.213012 | -0.384160 | -2.888374 |
| 34 | 1 | 0 | -4.098039 | 1.304457 | 1.714033 |
| 35 | 1 | 0 | -2.581068 | 2.681566 | -3.400920 |
| 36 | 1 | 0 | -4.080469 | 3.329333 | -1.633624 |
| 37 | 1 | 0 | -2.743090 | 4.877423 | 1.580526 |
| 38 | 1 | 0 | -0.392809 | 5.285454 | 1.902546 |
| 39 | 1 | 0 | -1.181453 | 5.574361 | -1.641729 |
| 40 | 1 | 0 | 2.619829 | 0.602199 | -0.908242 |
| 41 | 1 | 0 | 1.041206 | -3.098987 | -0.869274 |
| 42 | 6 | 0 | 8.702048 | -1.215012 | -1.080128 |
| 43 | 6 | 0 | 8.426737 | -0.015853 | -0.422151 |
| 44 | 6 | 0 | 7.204776 | 0.166629 | 0.217587 |
| 45 | 6 | 0 | 6.276890 | -0.869870 | 0.183691 |
| 46 | 6 | 0 | 6.529435 | -2.074123 | -0.466283 |
| 47 | 6 | 0 | 7.756080 | -2.240375 | -1.101492 |
| 48 | 1 | 0 | 9.655659 | -1.350750 | -1.577186 |
| 49 | 1 | 0 | 9.162878 | 0.778862 | -0.407246 |
| 50 | 1 | 0 | 6.962984 | 1.084999 | 0.734245 |
| 51 | 1 | 0 | 5.777000 | -2.850433 | -0.466655 |
| 52 | 1 | 0 | 7.972312 | -3.170399 | -1.613356 |
| 53 | 7 | 0 | 4.974006 | -0.683273 | 0.858807 |
| 54 | 8 | 0 | 4.769253 | 0.388392 | 1.416459 |
| 55 | 8 | 0 | 4.172713 | -1.608801 | 0.818741 |

Nitrobenzene adsorption (fixed subsurface)

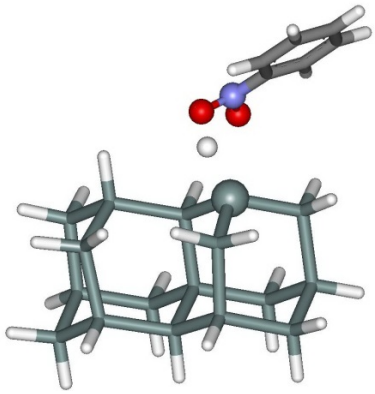


E (RB+HF-LYP) = -5373.28171490

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | 2.694030 | 3.859572 | 1.701137 |
| 2 | 14 | 0 | 0.745411 | 3.927187 | -1.664153 |
| 3 | 14 | 0 | 2.885452 | 3.928467 | -0.647988 |
| 4 | 14 | 0 | 3.950595 | 1.962217 | -1.349623 |
| 5 | 1 | 0 | 1.285203 | 1.988988 | 3.862513 |
| 6 | 1 | 0 | -1.247546 | 3.577396 | 1.730398 |
| 7 | 14 | 0 | -0.529078 | 2.050998 | -0.956215 |
| 8 | 14 | 0 | -0.720802 | 2.222407 | 1.394571 |
| 9 | 14 | 0 | 1.418546 | 1.987607 | 2.377196 |
| 10 | 1 | 0 | -1.672289 | 1.219446 | 1.940546 |
| 11 | 1 | 0 | 0.002350 | 5.171751 | -1.312696 |
| 12 | 1 | 0 | 0.910534 | 3.908390 | -3.145897 |
| 13 | 1 | 0 | 3.683781 | 5.116877 | -1.062249 |
| 14 | 1 | 0 | 2.038232 | 5.098371 | 2.199107 |
| 15 | 1 | 0 | 4.055526 | 3.790667 | 2.296029 |
| 16 | 1 | 0 | 4.129541 | 1.947036 | -2.825746 |
| 17 | 1 | 0 | 5.292311 | 1.837824 | -0.718379 |
| 18 | 14 | 0 | 2.480040 | -0.001472 | 1.665834 |
| 19 | 14 | 0 | 0.551136 | 0.043282 | -1.619333 |
| 20 | 14 | 0 | 2.725497 | 0.046037 | -0.683509 |
| 21 | 14 | 0 | 3.974390 | -1.825922 | -1.428658 |
| 22 | 14 | 0 | 0.795937 | -3.825367 | -1.804084 |
| 23 | 14 | 0 | 2.940896 | -3.832762 | -0.798845 |
| 24 | 14 | 0 | 2.760880 | -3.852530 | 1.551378 |
| 25 | 1 | 0 | 0.954931 | -3.747906 | -3.284625 |
| 26 | 1 | 0 | 1.323589 | -2.094596 | 3.784667 |
| 27 | 1 | 0 | -1.630099 | -1.252274 | 1.906088 |
| 28 | 14 | 0 | -0.507006 | -1.997666 | -1.023555 |
| 29 | 14 | 0 | -0.693839 | -2.245335 | 1.320369 |
| 30 | 14 | 0 | 1.450934 | -2.033013 | 2.300064 |
| 31 | 1 | 0 | -1.214092 | -3.609578 | 1.619900 |
| 32 | 1 | 0 | 0.076158 | -5.094642 | -1.496679 |
| 33 | 1 | 0 | 0.676462 | 0.073255 | -3.108702 |
| 34 | 1 | 0 | 3.863362 | 0.002871 | 2.225125 |
| 35 | 1 | 0 | 4.143469 | -1.749317 | -2.904080 |
| 36 | 1 | 0 | 5.318155 | -1.704503 | -0.801143 |
| 37 | 1 | 0 | 4.123924 | -3.771831 | 2.141556 |
| 38 | 1 | 0 | 2.137863 | -5.122835 | 2.010532 |
| 39 | 1 | 0 | 3.758278 | -4.990630 | -1.259958 |
| 40 | 1 | 0 | -1.851715 | -2.081030 | -1.660697 |
| 41 | 1 | 0 | -1.881011 | 2.143767 | -1.579429 |
| 42 | 6 | 0 | -8.869256 | 0.700244 | -0.178535 |
| 43 | 6 | 0 | -8.587977 | -0.586111 | 0.282525 |
| 44 | 6 | 0 | -7.273084 | -1.037036 | 0.339392 |
| 45 | 6 | 0 | -6.259023 | -0.177980 | -0.072818 |
| 46 | 6 | 0 | -6.515678 | 1.108655 | -0.536303 |
| 47 | 6 | 0 | -7.835982 | 1.544303 | -0.586456 |
| 48 | 1 | 0 | -9.895802 | 1.045596 | -0.220213 |
| 49 | 1 | 0 | -9.392251 | -1.239643 | 0.598278 |
| 50 | 1 | 0 | -7.024713 | -2.028366 | 0.692090 |
| 51 | 1 | 0 | -5.694668 | 1.740046 | -0.846141 |
| 52 | 1 | 0 | -8.057145 | 2.542803 | -0.943878 |
| 53 | 7 | 0 | -4.858066 | -0.649062 | -0.015386 |
| 54 | 8 | 0 | -4.652808 | -1.780614 | 0.405475 |
| 55 | 8 | 0 | -3.982459 | 0.120758 | -0.392930 |

Nitrobenzene adsorption TS (relaxed subsurface)

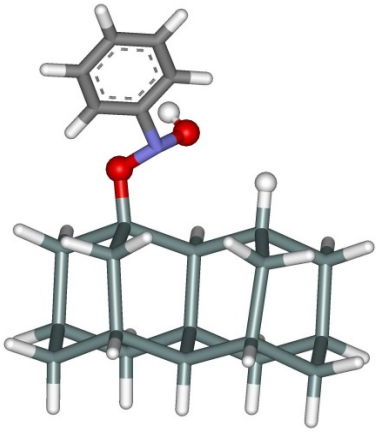


E (RB+HF-LYP) = -5373.22809756

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | -0.177674 | 4.304581 | 1.077896 |
| 2 | 14 | 0 | -2.529940 | 1.937767 | -0.983065 |
| 3 | 14 | 0 | -0.907787 | 3.662553 | -1.077377 |
| 4 | 14 | 0 | 0.964046 | 2.833888 | -2.256148 |
| 5 | 1 | 0 | 1.085079 | 2.803876 | 3.604844 |
| 6 | 1 | 0 | -2.330388 | 1.569556 | 2.869983 |
| 7 | 14 | 0 | -1.663831 | 0.063847 | 0.161102 |
| 8 | 14 | 0 | -1.130551 | 0.867269 | 2.328647 |
| 9 | 14 | 0 | 0.662069 | 2.413827 | 2.225246 |
| 10 | 1 | 0 | -0.816665 | -0.250618 | 3.258869 |
| 11 | 1 | 0 | -3.747735 | 2.428831 | -0.276404 |
| 12 | 1 | 0 | -2.924045 | 1.578982 | -2.373262 |
| 13 | 1 | 0 | -1.468264 | 4.852827 | -1.786696 |
| 14 | 1 | 0 | -1.306362 | 4.890093 | 1.856451 |
| 15 | 1 | 0 | 0.876632 | 5.350674 | 0.952167 |
| 16 | 1 | 0 | 0.573599 | 2.444804 | -3.641324 |
| 17 | 1 | 0 | 2.014916 | 3.886223 | -2.361949 |
| 18 | 14 | 0 | 2.519030 | 1.516107 | 1.056073 |
| 19 | 14 | 0 | 0.235243 | -0.767582 | -0.975717 |
| 20 | 14 | 0 | 1.872321 | 0.947229 | -1.153938 |
| 21 | 14 | 0 | 3.750312 | 0.176926 | -2.377550 |
| 22 | 14 | 0 | 3.049657 | -3.410181 | -1.251191 |
| 23 | 14 | 0 | 4.695716 | -1.713438 | -1.326823 |
| 24 | 14 | 0 | 5.383455 | -1.073639 | 0.843904 |
| 25 | 1 | 0 | 2.619719 | -3.734469 | -2.640827 |
| 26 | 1 | 0 | 3.941565 | 0.000986 | 3.483141 |
| 27 | 1 | 0 | 0.929088 | -1.977715 | 3.167061 |
| 28 | 14 | 0 | 1.202193 | -2.681155 | 0.036478 |
| 29 | 14 | 0 | 2.034249 | -2.217015 | 2.200728 |
| 30 | 14 | 0 | 3.506739 | -0.368570 | 2.102995 |
| 31 | 1 | 0 | 2.800887 | -3.402990 | 2.680576 |
| 32 | 1 | 0 | 3.619137 | -4.650115 | -0.650561 |
| 33 | 1 | 0 | -0.186663 | -1.150489 | -2.355071 |
| 34 | 1 | 0 | 3.563581 | 2.583038 | 0.984840 |
| 35 | 1 | 0 | 3.321870 | -0.162315 | -3.764575 |
| 36 | 1 | 0 | 4.756230 | 1.273657 | -2.470697 |
| 37 | 1 | 0 | 6.381025 | 0.028654 | 0.737894 |
| 38 | 1 | 0 | 6.042945 | -2.218141 | 1.534935 |
| 39 | 1 | 0 | 5.877463 | -2.193609 | -2.103669 |
| 40 | 1 | 0 | 0.188213 | -3.773429 | 0.114397 |
| 41 | 1 | 0 | -2.664211 | -1.476148 | 0.803541 |
| 42 | 6 | 0 | -8.103992 | -0.996638 | 0.018322 |
| 43 | 6 | 0 | -7.424381 | -0.763085 | -1.178603 |
| 44 | 6 | 0 | -6.080961 | -1.094551 | -1.300965 |
| 45 | 6 | 0 | -5.422002 | -1.655503 | -0.202158 |
| 46 | 6 | 0 | -6.091260 | -1.909993 | 0.999223 |
| 47 | 6 | 0 | -7.434722 | -1.568352 | 1.101261 |
| 48 | 1 | 0 | -9.152832 | -0.738338 | 0.105059 |
| 49 | 1 | 0 | -7.943200 | -0.320563 | -2.020730 |
| 50 | 1 | 0 | -5.534291 | -0.923464 | -2.218154 |
| 51 | 1 | 0 | -5.560445 | -2.361409 | 1.825608 |
| 52 | 1 | 0 | -7.961606 | -1.752507 | 2.030047 |
| 53 | 7 | 0 | -4.050490 | -2.018660 | -0.346880 |
| 54 | 8 | 0 | -3.345798 | -1.586971 | -1.285892 |
| 55 | 8 | 0 | -3.380623 | -2.343070 | 0.738712 |

O-Si bond formation, Structure A (relaxed subsurface)

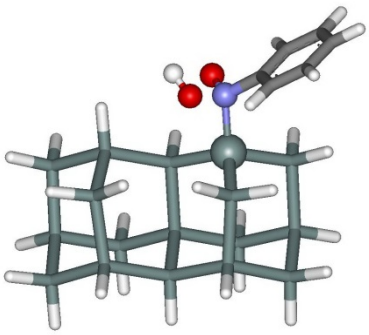


E (RB+HF-LYP) = -5373.33833303

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | -4.437246 | -2.256480 | 1.457407 |
| 2 | 14 | 0 | -2.211782 | -3.615496 | -1.458620 |
| 3 | 14 | 0 | -4.183399 | -2.442953 | -0.886557 |
| 4 | 14 | 0 | -4.001572 | -0.265087 | -1.775384 |
| 5 | 1 | 0 | -2.667473 | -1.133941 | 3.869164 |
| 6 | 1 | 0 | -0.985409 | -3.982774 | 2.248958 |
| 7 | 14 | 0 | -0.319728 | -2.560639 | -0.501430 |
| 8 | 14 | 0 | -0.670742 | -2.584308 | 1.837056 |
| 9 | 14 | 0 | -2.522300 | -1.220072 | 2.385389 |
| 10 | 1 | 0 | 0.545134 | -2.159126 | 2.579528 |
| 11 | 1 | 0 | -2.290455 | -5.020627 | -0.966165 |
| 12 | 1 | 0 | -2.089171 | -3.661042 | -2.943400 |
| 13 | 1 | 0 | -5.373566 | -3.134052 | -1.466358 |
| 14 | 1 | 0 | -4.615494 | -3.604956 | 2.067034 |
| 15 | 1 | 0 | -5.657679 | -1.456018 | 1.758844 |
| 16 | 1 | 0 | -3.863936 | -0.320542 | -3.258775 |
| 17 | 1 | 0 | -5.222786 | 0.531442 | -1.464635 |
| 18 | 14 | 0 | -2.303814 | 0.964421 | 1.492500 |
| 19 | 14 | 0 | -0.124394 | -0.358211 | -1.364321 |
| 20 | 14 | 0 | -2.117165 | 0.847819 | -0.870758 |
| 21 | 14 | 0 | -2.063328 | 3.032518 | -1.779690 |
| 22 | 14 | 0 | 1.728580 | 3.084604 | -1.515440 |
| 23 | 14 | 0 | -0.238943 | 4.245955 | -0.905875 |
| 24 | 14 | 0 | -0.478260 | 4.374504 | 1.442838 |
| 25 | 1 | 0 | 1.802780 | 2.981578 | -2.999632 |
| 26 | 1 | 0 | -0.593159 | 2.284346 | 3.850383 |
| 27 | 1 | 0 | 1.798745 | -0.073065 | 2.532835 |
| 28 | 14 | 0 | 1.703649 | 0.924846 | -0.544437 |
| 29 | 14 | 0 | 1.603423 | 1.208762 | 1.806787 |
| 30 | 14 | 0 | -0.475394 | 2.195592 | 2.364368 |
| 31 | 1 | 0 | 2.695662 | 2.138717 | 2.215260 |
| 32 | 1 | 0 | 2.936517 | 3.816164 | -1.039710 |
| 33 | 1 | 0 | 0.008135 | -0.442215 | -2.849262 |
| 34 | 1 | 0 | -3.548660 | 1.720803 | 1.827501 |
| 35 | 1 | 0 | -1.956950 | 2.945405 | -3.264021 |
| 36 | 1 | 0 | -3.346257 | 3.718535 | -1.455313 |
| 37 | 1 | 0 | -1.754085 | 5.072229 | 1.768220 |
| 38 | 1 | 0 | 0.638891 | 5.167306 | 2.030504 |
| 39 | 1 | 0 | -0.199125 | 5.621112 | -1.486195 |
| 40 | 7 | 0 | 3.408717 | -1.077713 | -0.684841 |
| 41 | 8 | 0 | 3.235661 | 0.297217 | -1.030596 |
| 42 | 6 | 0 | 4.766059 | -1.293933 | -0.250550 |
| 43 | 6 | 0 | 5.247851 | -2.607980 | -0.224181 |
| 44 | 6 | 0 | 5.555030 | -0.245388 | 0.225160 |
| 45 | 6 | 0 | 6.523292 | -2.861987 | 0.268594 |
| 46 | 1 | 0 | 4.622145 | -3.414147 | -0.583228 |
| 47 | 6 | 0 | 6.830081 | -0.517445 | 0.719426 |
| 48 | 1 | 0 | 5.177941 | 0.766152 | 0.197053 |
| 49 | 6 | 0 | 7.320429 | -1.820228 | 0.743562 |
| 50 | 1 | 0 | 6.892989 | -3.880995 | 0.285066 |
| 51 | 1 | 0 | 7.441922 | 0.300466 | 1.082901 |
| 52 | 1 | 0 | 8.312745 | -2.023972 | 1.128624 |
| 53 | 8 | 0 | 3.124794 | -1.833146 | -1.842324 |
| 54 | 1 | 0 | 3.767358 | -1.552363 | -2.519910 |
| 55 | 1 | 0 | 0.895947 | -3.352101 | -0.833744 |

N-Si bond formation (relaxed subsurface)

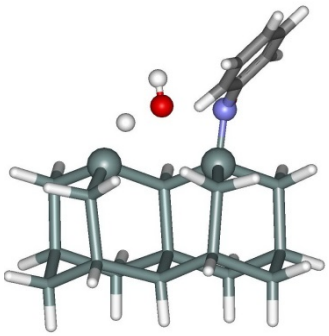


E (RB+HF-LYP) = -5373.27227312

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | -1.080124 | 4.003496 | 1.216147 |
| 2 | 14 | 0 | -2.867782 | 1.570043 | -1.282793 |
| 3 | 14 | 0 | -1.487620 | 3.481961 | -1.054092 |
| 4 | 14 | 0 | 0.592584 | 3.027334 | -2.069968 |
| 5 | 1 | 0 | 0.103467 | 2.451173 | 3.745000 |
| 6 | 1 | 0 | -2.983268 | 0.853136 | 2.570133 |
| 7 | 14 | 0 | -1.801232 | -0.233187 | -0.175643 |
| 8 | 14 | 0 | -1.651918 | 0.363883 | 2.113929 |
| 9 | 14 | 0 | -0.099985 | 2.141734 | 2.298233 |
| 10 | 1 | 0 | -1.264224 | -0.791176 | 2.961843 |
| 11 | 1 | 0 | -4.197405 | 1.825966 | -0.664103 |
| 12 | 1 | 0 | -3.063654 | 1.265053 | -2.725414 |
| 13 | 1 | 0 | -2.156339 | 4.638647 | -1.720815 |
| 14 | 1 | 0 | -2.351791 | 4.362341 | 1.905817 |
| 15 | 1 | 0 | -0.170992 | 5.181725 | 1.289513 |
| 16 | 1 | 0 | 0.407070 | 2.724270 | -3.517277 |
| 17 | 1 | 0 | 1.481545 | 4.218958 | -1.962728 |
| 18 | 14 | 0 | 1.975889 | 1.607278 | 1.286896 |
| 19 | 14 | 0 | 0.263231 | -0.757383 | -1.209323 |
| 20 | 14 | 0 | 1.634221 | 1.180091 | -1.019570 |
| 21 | 14 | 0 | 3.715402 | 0.818284 | -2.089353 |
| 22 | 14 | 0 | 3.462766 | -2.922434 | -1.389824 |
| 23 | 14 | 0 | 4.834314 | -1.016446 | -1.114247 |
| 24 | 14 | 0 | 5.187259 | -0.529869 | 1.172804 |
| 25 | 1 | 0 | 3.236453 | -3.153890 | -2.844274 |
| 26 | 1 | 0 | 3.333177 | 0.033032 | 3.711805 |
| 27 | 1 | 0 | 0.677714 | -2.262054 | 2.848946 |
| 28 | 14 | 0 | 1.398119 | -2.615310 | -0.271824 |
| 29 | 14 | 0 | 1.905349 | -2.262051 | 2.010814 |
| 30 | 14 | 0 | 3.105296 | -0.237557 | 2.260852 |
| 31 | 1 | 0 | 2.777161 | -3.376819 | 2.480998 |
| 32 | 1 | 0 | 4.142373 | -4.128536 | -0.836727 |
| 33 | 1 | 0 | 0.026002 | -0.985360 | -2.659920 |
| 34 | 1 | 0 | 2.857369 | 2.805979 | 1.426745 |
| 35 | 1 | 0 | 3.477082 | 0.568577 | -3.539390 |
| 36 | 1 | 0 | 4.537673 | 2.056031 | -1.971225 |
| 37 | 1 | 0 | 6.010334 | 0.706507 | 1.294525 |
| 38 | 1 | 0 | 5.934196 | -1.641116 | 1.827711 |
| 39 | 1 | 0 | 6.148211 | -1.235150 | -1.789089 |
| 40 | 1 | 0 | 0.580302 | -3.852101 | -0.424682 |
| 41 | 1 | 0 | -2.191745 | -3.542041 | 0.032051 |
| 42 | 6 | 0 | -7.044228 | -1.383442 | 0.243493 |
| 43 | 6 | 0 | -6.556541 | -1.453895 | -1.059531 |
| 44 | 6 | 0 | -5.190664 | -1.606521 | -1.293278 |
| 45 | 6 | 0 | -4.328085 | -1.688361 | -0.206909 |
| 46 | 6 | 0 | -4.796678 | -1.627531 | 1.102669 |
| 47 | 6 | 0 | -6.163401 | -1.473918 | 1.321345 |
| 48 | 1 | 0 | -8.107146 | -1.265870 | 0.420601 |
| 49 | 1 | 0 | -7.238016 | -1.393625 | -1.900291 |
| 50 | 1 | 0 | -4.782457 | -1.678568 | -2.291806 |
| 51 | 1 | 0 | -4.113278 | -1.735811 | 1.933071 |
| 52 | 1 | 0 | -6.539880 | -1.436219 | 2.337032 |
| 53 | 7 | 0 | -2.870943 | -1.790957 | -0.493176 |
| 54 | 8 | 0 | -2.590414 | -2.233678 | -1.684001 |
| 55 | 8 | 0 | -2.309149 | -2.760385 | 0.597113 |

$H_2O$ formation TS (relaxed subsurface)

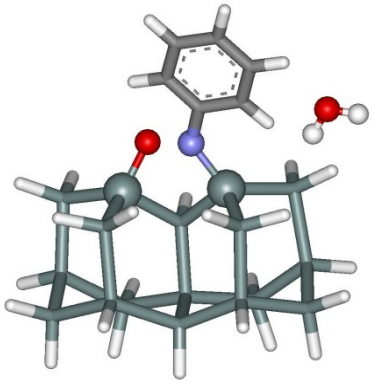


E (RB+HF-LYP) = -5373.23903597

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | -0.738782 | 4.060233 | 1.545980 |
| 2 | 14 | 0 | -2.551478 | 2.210560 | -1.357867 |
| 3 | 14 | 0 | -0.992902 | 3.901353 | -0.797217 |
| 4 | 14 | 0 | 1.086367 | 3.327371 | -1.760334 |
| 5 | 1 | 0 | 0.045877 | 2.031992 | 3.879030 |
| 6 | 1 | 0 | -3.091105 | 1.011371 | 2.347821 |
| 7 | 14 | 0 | -1.836600 | 0.128917 | -0.455841 |
| 8 | 14 | 0 | -1.799139 | 0.423262 | 1.894550 |
| 9 | 14 | 0 | -0.055424 | 1.959642 | 2.390272 |
| 10 | 1 | 0 | -1.601178 | -0.858697 | 2.618171 |
| 11 | 1 | 0 | -3.900046 | 2.542177 | -0.813790 |
| 12 | 1 | 0 | -2.662246 | 2.111677 | -2.837944 |
| 13 | 1 | 0 | -1.488611 | 5.199612 | -1.343877 |
| 14 | 1 | 0 | -2.027186 | 4.462762 | 2.178583 |
| 15 | 1 | 0 | 0.277521 | 5.099427 | 1.872653 |
| 16 | 1 | 0 | 0.949897 | 3.239155 | -3.241736 |
| 17 | 1 | 0 | 2.093008 | 4.384055 | -1.456522 |
| 18 | 14 | 0 | 2.051276 | 1.383027 | 1.456270 |
| 19 | 14 | 0 | 0.277111 | -0.513501 | -1.298087 |
| 20 | 14 | 0 | 1.815685 | 1.249586 | -0.899507 |
| 21 | 14 | 0 | 3.842600 | 0.597533 | -1.940257 |
| 22 | 14 | 0 | 2.973642 | -3.167735 | -1.474796 |
| 23 | 14 | 0 | 4.595977 | -1.476176 | -1.091540 |
| 24 | 14 | 0 | 5.005612 | -1.129219 | 1.212227 |
| 25 | 1 | 0 | 2.772038 | -3.297988 | -2.946127 |
| 26 | 1 | 0 | 3.225641 | -0.442603 | 3.780443 |
| 27 | 1 | 0 | 0.314710 | -2.332627 | 2.767359 |
| 28 | 14 | 0 | 0.956923 | -2.597989 | -0.382008 |
| 29 | 14 | 0 | 1.525144 | -2.439467 | 1.907439 |
| 30 | 14 | 0 | 2.976355 | -0.621541 | 2.317695 |
| 31 | 1 | 0 | 2.234002 | -3.691426 | 2.304407 |
| 32 | 1 | 0 | 3.505492 | -4.468292 | -0.975644 |
| 33 | 1 | 0 | 0.113307 | -0.656179 | -2.774467 |
| 34 | 1 | 0 | 2.970171 | 2.513715 | 1.790704 |
| 35 | 1 | 0 | 3.608913 | 0.520558 | -3.410738 |
| 36 | 1 | 0 | 4.879967 | 1.642905 | -1.705505 |
| 37 | 1 | 0 | 5.985579 | -0.016564 | 1.369464 |
| 38 | 1 | 0 | 5.602229 | -2.347031 | 1.831763 |
| 39 | 1 | 0 | 5.881164 | -1.833253 | -1.766612 |
| 40 | 1 | 0 | -0.605224 | -3.125837 | -0.586363 |
| 41 | 1 | 0 | -2.419221 | -3.408052 | -1.013380 |
| 42 | 6 | 0 | -6.713968 | -2.146464 | 0.973460 |
| 43 | 6 | 0 | -6.799887 | -1.715086 | -0.349575 |
| 44 | 6 | 0 | -5.650553 | -1.361844 | -1.048780 |
| 45 | 6 | 0 | -4.410945 | -1.441760 | -0.407154 |
| 46 | 6 | 0 | -4.311992 | -1.882822 | 0.915407 |
| 47 | 6 | 0 | -5.468787 | -2.231108 | 1.600515 |
| 48 | 1 | 0 | -7.612207 | -2.422242 | 1.513648 |
| 49 | 1 | 0 | -7.764575 | -1.647262 | -0.838682 |
| 50 | 1 | 0 | -5.695175 | -1.016124 | -2.072528 |
| 51 | 1 | 0 | -3.338817 | -2.012272 | 1.365925 |
| 52 | 1 | 0 | -5.396933 | -2.587281 | 2.621367 |
| 53 | 7 | 0 | -3.236466 | -1.013534 | -1.141989 |
| 54 | 8 | 0 | -3.340014 | -0.952730 | -2.375105 |
| 55 | 8 | 0 | -1.899743 | -2.668323 | -0.662951 |

Nitroso adduct, Structure B (relaxed subsurface)



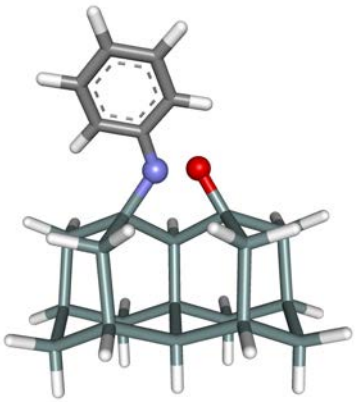
Nitroso adduct: E (RB+HF-LYP) = -5296.88606667

Water: E (RB+HF-LYP) = -76.45846272

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | -0.072766 | 4.389204 | 1.183531 |
| 2 | 14 | 0 | -2.209315 | 2.521417 | -1.681581 |
| 3 | 14 | 0 | -0.370174 | 3.966450 | -1.130202 |
| 4 | 14 | 0 | 1.786264 | 3.212973 | -1.790900 |
| 5 | 1 | 0 | 0.297280 | 2.611184 | 3.817120 |
| 6 | 1 | 0 | -2.919829 | 2.212039 | 2.027763 |
| 7 | 14 | 0 | -1.747868 | 0.556730 | -0.441983 |
| 8 | 14 | 0 | -1.815596 | 1.227131 | 1.840313 |
| 9 | 14 | 0 | 0.201067 | 2.348182 | 2.350218 |
| 10 | 1 | 0 | -2.076065 | 0.073879 | 2.738104 |
| 11 | 1 | 0 | -3.476408 | 3.223085 | -1.329009 |
| 12 | 1 | 0 | -2.198192 | 2.283025 | -3.151105 |
| 13 | 1 | 0 | -0.625484 | 5.274300 | -1.806711 |
| 14 | 1 | 0 | -1.246596 | 5.099420 | 1.765112 |
| 15 | 1 | 0 | 1.117968 | 5.273877 | 1.329547 |
| 16 | 1 | 0 | 1.863687 | 2.957398 | -3.256653 |
| 17 | 1 | 0 | 2.772915 | 4.279157 | -1.458099 |
| 18 | 14 | 0 | 2.133856 | 1.139466 | 1.665114 |
| 19 | 14 | 0 | 0.344822 | -0.029018 | -1.290589 |
| 20 | 14 | 0 | 2.249584 | 1.162856 | -0.698843 |
| 21 | 14 | 0 | 3.891938 | -0.237033 | -1.681231 |
| 22 | 14 | 0 | 1.521590 | -3.517078 | -1.610166 |
| 23 | 14 | 0 | 3.582699 | -2.480340 | -0.949580 |
| 24 | 14 | 0 | 3.913617 | -2.361711 | 1.393863 |
| 25 | 1 | 0 | 1.387965 | -3.423976 | -3.089051 |
| 26 | 1 | 0 | 2.347000 | -1.136254 | 3.889727 |
| 27 | 1 | 0 | -0.968643 | -1.973901 | 2.581379 |
| 28 | 14 | 0 | -0.061884 | -2.174293 | -0.512328 |
| 29 | 14 | 0 | 0.242642 | -2.387190 | 1.830496 |
| 30 | 14 | 0 | 2.165285 | -1.127663 | 2.407314 |
| 31 | 1 | 0 | 0.522546 | -3.813651 | 2.161318 |
| 32 | 1 | 0 | 1.545930 | -4.953843 | -1.219568 |
| 33 | 1 | 0 | 0.199635 | -0.076994 | -2.777312 |
| 34 | 1 | 0 | 3.332803 | 1.810874 | 2.249565 |
| 35 | 1 | 0 | 3.751996 | -0.123302 | -3.160229 |
| 36 | 1 | 0 | 5.277805 | 0.175654 | -1.320058 |
| 37 | 1 | 0 | 5.237078 | -1.719067 | 1.631281 |
| 38 | 1 | 0 | 3.946374 | -3.722196 | 2.001183 |
| 39 | 1 | 0 | 4.684418 | -3.306170 | -1.530076 |
| 40 | 6 | 0 | -6.496528 | -2.094980 | 0.261780 |
| 41 | 6 | 0 | -5.563406 | -3.089596 | -0.024095 |
| 42 | 6 | 0 | -4.242715 | -2.775984 | -0.332501 |
| 43 | 6 | 0 | -3.826745 | -1.434384 | -0.359583 |
| 44 | 6 | 0 | -4.776132 | -0.429272 | -0.093085 |
| 45 | 6 | 0 | -6.088447 | -0.762336 | 0.221830 |
| 46 | 1 | 0 | -7.521760 | -2.350331 | 0.501110 |
| 47 | 1 | 0 | -5.863084 | -4.132092 | -0.009071 |
| 48 | 1 | 0 | -3.530477 | -3.555197 | -0.557944 |
| 49 | 1 | 0 | -4.496196 | 0.617551 | -0.146658 |
| 50 | 1 | 0 | -6.798297 | 0.031765 | 0.425950 |
| 51 | 7 | 0 | -2.507478 | -1.066400 | -0.632626 |
| 52 | 8 | 0 | -1.703606 | -2.199162 | -1.036690 |

Nitroso adduct, (fixed subsurface)



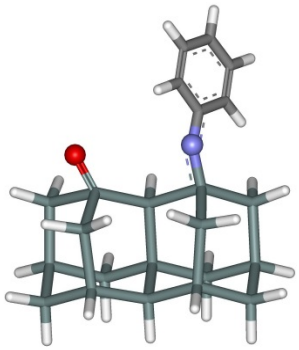
Nitroso adduct: E (RB+HF-LYP) = -5296.84449678

Water: E (RB+HF-LYP) = -76.45846272

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | 2.046633 | 2.827731 | -1.573560 |
| 2 | 14 | 0 | -0.046607 | 4.408382 | 1.441140 |
| 3 | 14 | 0 | 0.128435 | 4.294998 | -0.914420 |
| 4 | 14 | 0 | -1.769835 | 3.152185 | -1.728216 |
| 5 | 1 | 0 | 3.066553 | 2.125610 | 1.903163 |
| 6 | 14 | 0 | -0.058394 | 2.222724 | 2.350230 |
| 7 | 14 | 0 | 1.954059 | 1.148997 | 1.728310 |
| 8 | 14 | 0 | 1.844799 | 0.548394 | -0.564780 |
| 9 | 1 | 0 | 2.221776 | -0.016766 | 2.608531 |
| 10 | 1 | 0 | 1.098613 | 5.175832 | 2.010735 |
| 11 | 1 | 0 | -1.299703 | 5.129991 | 1.805652 |
| 12 | 1 | 0 | 0.175732 | 5.676225 | -1.482839 |
| 13 | 1 | 0 | 3.321487 | 3.500010 | -1.186823 |
| 14 | 1 | 0 | 2.025176 | 2.752640 | -3.063177 |
| 15 | 1 | 0 | -3.014607 | 3.883924 | -1.353850 |
| 16 | 1 | 0 | -1.727600 | 3.073025 | -3.217181 |
| 17 | 14 | 0 | -0.092626 | -0.179767 | -1.552383 |
| 18 | 14 | 0 | -1.938908 | 1.028109 | 1.532742 |
| 19 | 14 | 0 | -1.868123 | 0.958732 | -0.841556 |
| 20 | 14 | 0 | -3.788647 | -0.134326 | -1.692370 |
| 21 | 14 | 0 | -4.099087 | -2.188825 | 1.513097 |
| 22 | 14 | 0 | -3.941731 | -2.331007 | -0.842145 |
| 23 | 14 | 0 | -1.838916 | -3.484248 | -1.496794 |
| 24 | 1 | 0 | -5.305707 | -1.391558 | 1.876786 |
| 25 | 1 | 0 | 0.943203 | -2.039859 | 2.519077 |
| 26 | 14 | 0 | -2.146190 | -1.176090 | 2.387306 |
| 27 | 14 | 0 | -0.253160 | -2.454147 | 1.743588 |
| 28 | 14 | 0 | 0.063961 | -2.249023 | -0.601092 |
| 29 | 1 | 0 | -0.509176 | -3.893290 | 2.036720 |
| 30 | 1 | 0 | -4.260241 | -3.548080 | 2.105892 |
| 31 | 1 | 0 | -3.161849 | 1.783831 | 1.945590 |
| 32 | 1 | 0 | 0.057006 | -0.253143 | -3.031904 |
| 33 | 1 | 0 | -5.000442 | 0.651096 | -1.318588 |
| 34 | 1 | 0 | -3.713433 | -0.159800 | -3.181919 |
| 35 | 1 | 0 | -1.790868 | -3.499504 | -2.985569 |
| 36 | 1 | 0 | -1.892055 | -4.898427 | -1.029327 |
| 37 | 1 | 0 | -5.157791 | -3.006450 | -1.388133 |
| 38 | 1 | 0 | -2.234574 | -1.123834 | 3.878035 |
| 39 | 1 | 0 | -0.130456 | 2.301550 | 3.840672 |
| 40 | 7 | 0 | 2.553630 | -1.140563 | -0.690325 |
| 41 | 8 | 0 | 1.751372 | -2.298799 | -1.089025 |
| 42 | 6 | 0 | 3.871163 | -1.513397 | -0.413356 |
| 43 | 6 | 0 | 4.848216 | -0.505369 | -0.325908 |
| 44 | 6 | 0 | 4.253801 | -2.844711 | -0.180705 |
| 45 | 6 | 0 | 6.151005 | -0.813457 | 0.049220 |
| 46 | 1 | 0 | 4.595790 | 0.519594 | -0.581332 |
| 47 | 6 | 0 | 5.566442 | -3.137539 | 0.171920 |
| 48 | 1 | 0 | 3.519390 | -3.629550 | -0.280454 |
| 49 | 6 | 0 | 6.522657 | -2.131794 | 0.302616 |
| 50 | 1 | 0 | 6.883569 | -0.016832 | 0.116153 |
| 51 | 1 | 0 | 5.842671 | -4.171346 | 0.349607 |
| 52 | 1 | 0 | 7.542179 | -2.372412 | 0.578880 |

O insertion TS (relaxed subsurface)

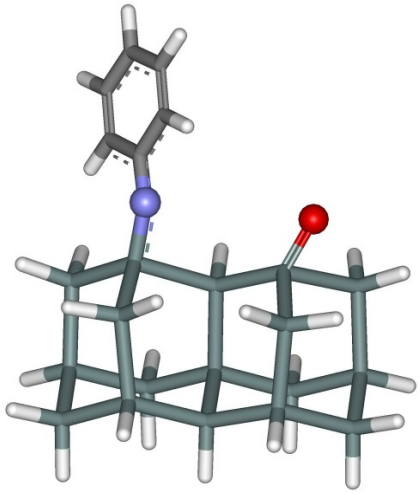


E (RB+HF-LYP) = -5296.84599279

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | -0.261506 | 4.549962 | 0.876781 |
| 2 | 14 | 0 | -2.903412 | 2.255256 | -0.894390 |
| 3 | 14 | 0 | -1.183414 | 3.850417 | -1.184261 |
| 4 | 14 | 0 | 0.498388 | 2.790914 | -2.452093 |
| 5 | 1 | 0 | 1.114801 | 3.125670 | 3.375284 |
| 6 | 1 | 0 | -2.387056 | 2.123233 | 3.141263 |
| 7 | 14 | 0 | -2.197252 | 0.422844 | 0.479361 |
| 8 | 14 | 0 | -1.330887 | 1.284869 | 2.503993 |
| 9 | 14 | 0 | 0.539467 | 2.672679 | 2.073750 |
| 10 | 1 | 0 | -0.991057 | 0.180711 | 3.437754 |
| 11 | 1 | 0 | -4.091665 | 2.874962 | -0.237807 |
| 12 | 1 | 0 | -3.342204 | 1.771550 | -2.235380 |
| 13 | 1 | 0 | -1.723509 | 5.030038 | -1.923627 |
| 14 | 1 | 0 | -1.296412 | 5.253851 | 1.685920 |
| 15 | 1 | 0 | 0.846137 | 5.510747 | 0.612372 |
| 16 | 1 | 0 | -0.047961 | 2.343785 | -3.764513 |
| 17 | 1 | 0 | 1.626758 | 3.726603 | -2.720750 |
| 18 | 14 | 0 | 2.236500 | 1.601386 | 0.808295 |
| 19 | 14 | 0 | -0.350313 | -0.665551 | -0.757047 |
| 20 | 14 | 0 | 1.346914 | 0.918429 | -1.281527 |
| 21 | 14 | 0 | 3.030368 | -0.095025 | -2.603086 |
| 22 | 14 | 0 | 2.088739 | -3.504284 | -1.129823 |
| 23 | 14 | 0 | 3.900259 | -1.988231 | -1.506316 |
| 24 | 14 | 0 | 4.878184 | -1.242504 | 0.514718 |
| 25 | 1 | 0 | 1.376071 | -3.757783 | -2.403493 |
| 26 | 1 | 0 | 3.907041 | 0.253436 | 3.158349 |
| 27 | 1 | 0 | 0.760349 | -1.517291 | 3.536929 |
| 28 | 14 | 0 | 0.534198 | -2.478209 | 0.442401 |
| 29 | 14 | 0 | 1.683155 | -1.929198 | 2.445630 |
| 30 | 14 | 0 | 3.248439 | -0.236856 | 1.911059 |
| 31 | 1 | 0 | 2.419982 | -3.144519 | 2.889625 |
| 32 | 1 | 0 | 2.596561 | -4.755710 | -0.523527 |
| 33 | 1 | 0 | -0.990876 | -1.169585 | -2.007258 |
| 34 | 1 | 0 | 3.303993 | 2.614621 | 0.549734 |
| 35 | 1 | 0 | 2.471144 | -0.451935 | -3.937034 |
| 36 | 1 | 0 | 4.111715 | 0.910179 | -2.807593 |
| 37 | 1 | 0 | 5.948306 | -0.257450 | 0.190324 |
| 38 | 1 | 0 | 5.508856 | -2.380480 | 1.241168 |
| 39 | 1 | 0 | 4.935218 | -2.650240 | -2.361091 |
| 40 | 6 | 0 | -6.523140 | -2.941929 | -0.685765 |
| 41 | 6 | 0 | -5.739470 | -3.476725 | 0.344369 |
| 42 | 6 | 0 | -4.647666 | -2.778593 | 0.822250 |
| 43 | 6 | 0 | -4.285119 | -1.503835 | 0.279654 |
| 44 | 6 | 0 | -5.108764 | -0.984990 | -0.771373 |
| 45 | 6 | 0 | -6.199642 | -1.693267 | -1.235681 |
| 46 | 1 | 0 | -7.379911 | -3.491388 | -1.058180 |
| 47 | 1 | 0 | -5.988725 | -4.444096 | 0.765445 |
| 48 | 1 | 0 | -4.022300 | -3.178475 | 1.610724 |
| 49 | 1 | 0 | -4.867809 | -0.018711 | -1.197448 |
| 50 | 1 | 0 | -6.811138 | -1.281474 | -2.030861 |
| 51 | 7 | 0 | -3.217638 | -0.883882 | 0.791499 |
| 52 | 8 | 0 | -0.006204 | -3.956703 | 0.186030 |

O insertion TS (fixed subsurface)

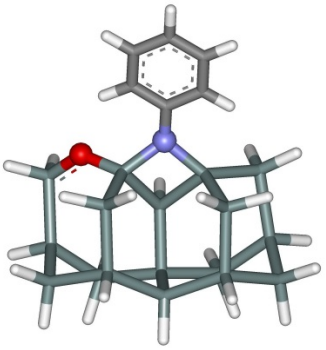


E (RB+HF-LYP) = -5296.84599298

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | 2.902364 | 2.255756 | -0.895069 |
| 2 | 14 | 0 | 0.260495 | 4.551281 | 0.875455 |
| 3 | 14 | 0 | 1.182618 | 3.851083 | -1.185250 |
| 4 | 14 | 0 | -0.498479 | 2.790409 | -2.452917 |
| 5 | 1 | 0 | 2.385099 | 2.125715 | 3.143638 |
| 6 | 14 | 0 | -0.540686 | 2.674506 | 2.073070 |
| 7 | 14 | 0 | 1.329707 | 1.287380 | 2.505078 |
| 8 | 14 | 0 | 2.197569 | 0.424837 | 0.481387 |
| 9 | 1 | 0 | 0.988883 | 0.183037 | 3.438270 |
| 10 | 1 | 0 | 1.295524 | 5.255102 | 1.684505 |
| 11 | 1 | 0 | -0.846834 | 5.512322 | 0.610682 |
| 12 | 1 | 0 | 1.722886 | 5.030387 | -1.924988 |
| 13 | 1 | 0 | 4.091657 | 2.875665 | -0.240592 |
| 14 | 1 | 0 | 3.339414 | 1.770187 | -2.235959 |
| 15 | 1 | 0 | -1.627616 | 3.725054 | -2.721962 |
| 16 | 1 | 0 | 0.048330 | 2.343242 | -3.765133 |
| 17 | 14 | 0 | 0.351683 | -0.665607 | -0.756028 |
| 18 | 14 | 0 | -2.236375 | 1.601216 | 0.807512 |
| 19 | 14 | 0 | -1.345747 | 0.917747 | -1.281697 |
| 20 | 14 | 0 | -3.029287 | -0.095882 | -2.602950 |
| 21 | 14 | 0 | -4.876810 | -1.244474 | 0.515003 |
| 22 | 14 | 0 | -3.898994 | -1.989255 | -1.506452 |
| 23 | 14 | 0 | -2.087762 | -3.505434 | -1.129302 |
| 24 | 1 | 0 | -5.948549 | -0.260928 | 0.191414 |
| 25 | 1 | 0 | -0.759172 | -1.517693 | 3.536971 |
| 26 | 14 | 0 | -3.247434 | -0.237259 | 1.910722 |
| 27 | 14 | 0 | -1.682093 | -1.929499 | 2.445737 |
| 28 | 14 | 0 | -0.533261 | -2.478825 | 0.442499 |
| 29 | 1 | 0 | -2.419233 | -3.144585 | 2.889863 |
| 30 | 1 | 0 | -5.505305 | -2.383400 | 1.241867 |
| 31 | 1 | 0 | -3.304675 | 2.613342 | 0.547909 |
| 32 | 1 | 0 | 0.993804 | -1.169007 | -2.005712 |
| 33 | 1 | 0 | -4.110689 | 0.909390 | -2.806862 |
| 34 | 1 | 0 | -2.470569 | -0.452519 | -3.937185 |
| 35 | 1 | 0 | -1.375314 | -3.760587 | -2.402747 |
| 36 | 1 | 0 | -2.595922 | -4.755987 | -0.521466 |
| 37 | 1 | 0 | -4.933801 | -2.651182 | -2.361470 |
| 38 | 1 | 0 | -3.906236 | 0.253029 | 3.157910 |
| 39 | 1 | 0 | -1.116971 | 3.128224 | 3.373925 |
| 40 | 7 | 0 | 3.220048 | -0.879690 | 0.795282 |
| 41 | 8 | 0 | 0.007857 | -3.957064 | 0.186044 |
| 42 | 6 | 0 | 4.285080 | -1.502203 | 0.281406 |
| 43 | 6 | 0 | 5.104594 | -0.987717 | -0.774964 |
| 44 | 6 | 0 | 4.649309 | -2.775018 | 0.827363 |
| 45 | 6 | 0 | 6.193112 | -1.698332 | -1.241245 |
| 46 | 1 | 0 | 4.862331 | -0.022893 | -1.203597 |
| 47 | 6 | 0 | 5.738659 | -3.475584 | 0.347432 |
| 48 | 1 | 0 | 4.027138 | -3.171555 | 1.620042 |
| 49 | 6 | 0 | 6.518214 | -2.945122 | -0.688045 |
| 50 | 1 | 0 | 6.801469 | -1.289859 | -2.040534 |
| 51 | 1 | 0 | 5.989176 | -4.441508 | 0.771070 |
| 52 | 1 | 0 | 7.373063 | -3.496491 | -1.062052 |

Phenylnitrene adduct, Structure C (relaxed subsurface)

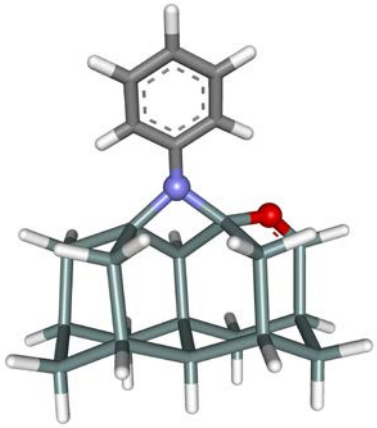


E (RB+HF-LYP) = -5297.0010554

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | 1.811588 | 4.181325 | 1.008871 |
| 2 | 14 | 0 | -0.961309 | 3.276805 | -1.811510 |
| 3 | 14 | 0 | 1.333213 | 3.797830 | -1.282601 |
| 4 | 14 | 0 | 2.993914 | 2.181473 | -1.843003 |
| 5 | 1 | 0 | 1.432976 | 2.571806 | 3.747390 |
| 6 | 1 | 0 | -1.665653 | 3.557063 | 1.933436 |
| 7 | 14 | 0 | -1.314687 | 1.403970 | -0.421634 |
| 8 | 14 | 0 | -1.109581 | 2.177790 | 1.816827 |
| 9 | 14 | 0 | 1.199828 | 2.293251 | 2.298641 |
| 10 | 1 | 0 | -1.861699 | 1.305603 | 2.754486 |
| 11 | 1 | 0 | -1.795744 | 4.488740 | -1.568394 |
| 12 | 1 | 0 | -1.043670 | 2.932024 | -3.257163 |
| 13 | 1 | 0 | 1.662696 | 5.052279 | -2.026039 |
| 14 | 1 | 0 | 1.063821 | 5.356188 | 1.539550 |
| 15 | 1 | 0 | 3.268224 | 4.482380 | 1.108026 |
| 16 | 1 | 0 | 2.956597 | 1.820942 | -3.288246 |
| 17 | 1 | 0 | 4.325312 | 2.788376 | -1.558012 |
| 18 | 14 | 0 | 2.376103 | 0.299429 | 1.719829 |
| 19 | 14 | 0 | 0.360302 | -0.021978 | -1.214779 |
| 20 | 14 | 0 | 2.588347 | 0.180689 | -0.635759 |
| 21 | 14 | 0 | 3.357996 | -1.844158 | -1.591946 |
| 22 | 14 | 0 | -0.277420 | -3.867534 | -1.732945 |
| 23 | 14 | 0 | 1.957243 | -3.631358 | -0.876949 |
| 24 | 14 | 0 | 2.232671 | -3.636094 | 1.478850 |
| 25 | 1 | 0 | -0.234128 | -3.704740 | -3.209438 |
| 26 | 1 | 0 | 1.541979 | -1.789258 | 3.966550 |
| 27 | 1 | 0 | -1.841004 | -1.091266 | 2.913427 |
| 28 | 14 | 0 | -1.260705 | -1.389555 | -0.281719 |
| 29 | 14 | 0 | -0.995279 | -1.922799 | 2.019912 |
| 30 | 14 | 0 | 1.318530 | -1.700571 | 2.492321 |
| 31 | 1 | 0 | -1.336122 | -3.355691 | 2.253226 |
| 32 | 1 | 0 | -0.706391 | -5.251217 | -1.409425 |
| 33 | 1 | 0 | 0.169659 | -0.057003 | -2.697287 |
| 34 | 1 | 0 | 3.718311 | 0.362160 | 2.371048 |
| 35 | 1 | 0 | 3.311176 | -1.669486 | -3.071210 |
| 36 | 1 | 0 | 4.759515 | -2.186357 | -1.217470 |
| 37 | 1 | 0 | 3.698706 | -3.729391 | 1.734041 |
| 38 | 1 | 0 | 1.585230 | -4.830856 | 2.090755 |
| 39 | 1 | 0 | 2.599557 | -4.887248 | -1.380455 |
| 40 | 6 | 0 | -6.590883 | -0.133839 | 0.083592 |
| 41 | 6 | 0 | -5.873358 | -1.314635 | -0.103503 |
| 42 | 6 | 0 | -4.499066 | -1.286082 | -0.318386 |
| 43 | 6 | 0 | -3.802787 | -0.065016 | -0.338428 |
| 44 | 6 | 0 | -4.535567 | 1.118990 | -0.159349 |
| 45 | 6 | 0 | -5.911219 | 1.082289 | 0.048634 |
| 46 | 1 | 0 | -7.661790 | -0.160601 | 0.245620 |
| 47 | 1 | 0 | -6.387144 | -2.269635 | -0.091880 |
| 48 | 1 | 0 | -3.964727 | -2.213460 | -0.496470 |
| 49 | 1 | 0 | -4.026327 | 2.077772 | -0.186998 |
| 50 | 1 | 0 | -6.452310 | 2.012198 | 0.184725 |
| 51 | 7 | 0 | -2.408527 | -0.038427 | -0.543059 |
| 52 | 8 | 0 | -1.441329 | -2.831474 | -1.106426 |

Phenylnitrene adduct, (fixed subsurface)

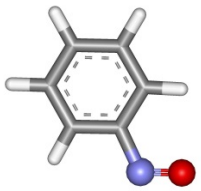


E (RB+HF-LYP) = -5296.94661517

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | 1.181107 | 3.475402 | -1.656976 |
| 2 | 14 | 0 | -1.259557 | 4.356737 | 1.391139 |
| 3 | 14 | 0 | -1.134576 | 4.264235 | -0.968516 |
| 4 | 14 | 0 | -2.617516 | 2.583068 | -1.707646 |
| 5 | 1 | 0 | 2.412208 | 3.175084 | 1.767798 |
| 6 | 14 | 0 | -0.572685 | 2.286980 | 2.312008 |
| 7 | 14 | 0 | 1.655235 | 1.895998 | 1.647794 |
| 8 | 14 | 0 | 1.657395 | 1.234400 | -0.624968 |
| 9 | 1 | 0 | 2.306804 | 0.896885 | 2.532014 |
| 10 | 1 | 0 | -0.386221 | 5.446500 | 1.915201 |
| 11 | 1 | 0 | -2.660843 | 4.666735 | 1.796274 |
| 12 | 1 | 0 | -1.530537 | 5.584486 | -1.545821 |
| 13 | 1 | 0 | 2.165250 | 4.542478 | -1.308868 |
| 14 | 1 | 0 | 1.158272 | 3.366493 | -3.144398 |
| 15 | 1 | 0 | -4.013661 | 2.905416 | -1.293010 |
| 16 | 1 | 0 | -2.601315 | 2.496567 | -3.196709 |
| 17 | 14 | 0 | -0.010626 | 0.029865 | -1.633443 |
| 18 | 14 | 0 | -2.023000 | 0.561870 | 1.568862 |
| 19 | 14 | 0 | -2.011290 | 0.479105 | -0.806031 |
| 20 | 14 | 0 | -3.531820 | -1.162087 | -1.581635 |
| 21 | 14 | 0 | -3.094895 | -3.161143 | 1.644089 |
| 22 | 14 | 0 | -2.977925 | -3.286458 | -0.714461 |
| 23 | 14 | 0 | -0.728115 | -3.949115 | -1.539491 |
| 24 | 1 | 0 | -4.475132 | -2.764923 | 2.046323 |
| 25 | 1 | 0 | 1.629544 | -1.384862 | 2.747525 |
| 26 | 14 | 0 | -1.518229 | -1.586141 | 2.442324 |
| 27 | 14 | 0 | 0.722285 | -2.103913 | 1.816588 |
| 28 | 14 | 0 | 1.087557 | -1.586045 | -0.487281 |
| 29 | 1 | 0 | 0.957526 | -3.566629 | 1.976103 |
| 30 | 1 | 0 | -2.813206 | -4.494872 | 2.249692 |
| 31 | 1 | 0 | -3.404462 | 0.914340 | 2.021029 |
| 32 | 1 | 0 | 0.136251 | -0.013375 | -3.112407 |
| 33 | 1 | 0 | -4.913031 | -0.778566 | -1.169057 |
| 34 | 1 | 0 | -3.500684 | -1.187414 | -3.072756 |
| 35 | 1 | 0 | -0.839512 | -3.931819 | -3.022723 |
| 36 | 1 | 0 | -0.500096 | -5.344971 | -1.087243 |
| 37 | 1 | 0 | -3.946049 | -4.309892 | -1.212911 |
| 38 | 1 | 0 | -1.570053 | -1.539336 | 3.934964 |
| 39 | 1 | 0 | -0.617112 | 2.364083 | 3.803628 |
| 40 | 7 | 0 | 2.516547 | -0.431794 | -0.726398 |
| 41 | 8 | 0 | 0.675237 | -3.094315 | -1.132046 |
| 42 | 6 | 0 | 3.865734 | -0.692265 | -0.440702 |
| 43 | 6 | 0 | 4.797311 | 0.349690 | -0.302333 |
| 44 | 6 | 0 | 4.324150 | -2.012868 | -0.287691 |
| 45 | 6 | 0 | 6.124461 | 0.083206 | 0.015756 |
| 46 | 1 | 0 | 4.478016 | 1.376749 | -0.457986 |
| 47 | 6 | 0 | 5.651528 | -2.271834 | 0.034842 |
| 48 | 1 | 0 | 3.639483 | -2.842105 | -0.442100 |
| 49 | 6 | 0 | 6.561505 | -1.228042 | 0.192947 |
| 50 | 1 | 0 | 6.821448 | 0.907424 | 0.119211 |
| 51 | 1 | 0 | 5.977545 | -3.299432 | 0.151394 |
| 52 | 1 | 0 | 7.596917 | -1.433901 | 0.436076 |

Nitrosobenzene (gas phase)

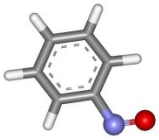


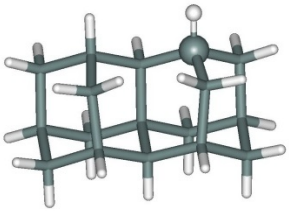
E (RB+HF-LYP) = -361.63922801

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.275634 | 1.334795 | 0.000058 |
| 2 | 6 | 0 | 0.091100 | 1.101548 | 0.000394 |
| 3 | 6 | 0 | 0.553711 | -0.220453 | 0.000149 |
| 4 | 6 | 0 | -0.334774 | -1.297455 | -0.000009 |
| 5 | 6 | 0 | -1.705710 | -1.055235 | -0.000174 |
| 6 | 6 | 0 | -2.172410 | 0.258410 | -0.000245 |
| 7 | 1 | 0 | -1.653953 | 2.350684 | 0.000094 |
| 8 | 1 | 0 | 0.810643 | 1.911293 | 0.000946 |
| 9 | 1 | 0 | 0.068620 | -2.303681 | -0.000162 |
| 10 | 1 | 0 | -2.405860 | -1.882239 | -0.000119 |
| 11 | 1 | 0 | -3.239564 | 0.450757 | -0.000577 |
| 12 | 7 | 0 | 1.949072 | -0.579553 | 0.000862 |
| 13 | 8 | 0 | 2.729864 | 0.350051 | -0.000905 |

Nitrosobenzene adsorption, Structure D (relaxed subsurface)



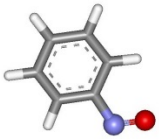


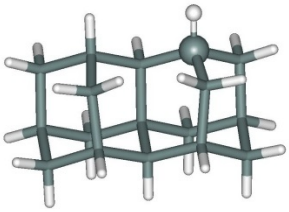
E (RB+HF-LYP) = -5298.04675605

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | 0.232356 | 3.845903 | -1.148892 |
| 2 | 14 | 0 | -3.045249 | 3.989087 | 0.978245 |
| 3 | 14 | 0 | -2.128607 | 3.972494 | -1.202424 |
| 4 | 14 | 0 | -2.926781 | 2.050183 | -2.315317 |
| 5 | 1 | 0 | 2.401534 | 1.890328 | 0.127927 |
| 6 | 1 | 0 | 0.428879 | 3.526719 | 2.765794 |
| 7 | 14 | 0 | -2.323840 | 2.073285 | 2.166557 |
| 8 | 14 | 0 | 0.036820 | 2.183344 | 2.249729 |
| 9 | 14 | 0 | 0.910256 | 1.930900 | 0.067032 |
| 10 | 1 | 0 | 0.593157 | 1.164954 | 3.179545 |
| 11 | 1 | 0 | -2.617425 | 5.216679 | 1.707927 |
| 12 | 1 | 0 | -4.532419 | 4.011800 | 0.883120 |
| 13 | 1 | 0 | -2.550229 | 5.204704 | -1.933244 |
| 14 | 1 | 0 | 0.800945 | 5.067028 | -0.509217 |
| 15 | 1 | 0 | 0.750638 | 3.784862 | -2.545289 |
| 16 | 1 | 0 | -4.414642 | 2.083628 | -2.403310 |
| 17 | 1 | 0 | -2.392529 | 2.001705 | -3.706372 |
| 18 | 14 | 0 | 0.103924 | -0.025997 | -1.006106 |
| 19 | 14 | 0 | -3.086513 | 0.117957 | 1.060769 |
| 20 | 14 | 0 | -2.262386 | 0.091134 | -1.165384 |
| 21 | 14 | 0 | -3.110624 | -1.787677 | -2.329354 |
| 22 | 14 | 0 | -3.398789 | -3.735692 | 0.944576 |
| 23 | 14 | 0 | -2.486154 | -3.784180 | -1.236989 |
| 24 | 14 | 0 | -0.122967 | -3.878634 | -1.192638 |
| 25 | 1 | 0 | -4.882081 | -3.620050 | 0.855001 |
| 26 | 1 | 0 | 2.226654 | -2.142306 | 0.101146 |
| 27 | 1 | 0 | 0.484347 | -1.271095 | 3.158287 |
| 28 | 14 | 0 | -2.499980 | -1.906773 | 2.148580 |
| 29 | 14 | 0 | -0.159119 | -2.233339 | 2.224287 |
| 30 | 14 | 0 | 0.740925 | -2.055424 | 0.045183 |
| 31 | 1 | 0 | 0.104392 | -3.607434 | 2.739820 |
| 32 | 1 | 0 | -3.084677 | -5.002802 | 1.664320 |
| 33 | 1 | 0 | -4.578801 | 0.187458 | 1.011897 |
| 34 | 1 | 0 | 0.665453 | -0.033829 | -2.390912 |
| 35 | 1 | 0 | -4.595301 | -1.677628 | -2.408738 |
| 36 | 1 | 0 | -2.581458 | -1.772998 | -3.723142 |
| 37 | 1 | 0 | 0.386930 | -3.846398 | -2.592618 |
| 38 | 1 | 0 | 0.325100 | -5.157992 | -0.572875 |
| 39 | 1 | 0 | -3.026975 | -4.962153 | -1.978881 |
| 40 | 1 | 0 | -3.056590 | -1.899873 | 3.534483 |
| 41 | 1 | 0 | -2.877156 | 2.109462 | 3.553146 |
| 42 | 6 | 0 | 8.859710 | -0.435430 | -0.095309 |
| 43 | 6 | 0 | 7.663915 | -1.135181 | -0.043350 |
| 44 | 6 | 0 | 6.458952 | -0.421007 | -0.064302 |
| 45 | 6 | 0 | 6.445306 | 0.973577 | -0.136276 |
| 46 | 6 | 0 | 7.650213 | 1.668579 | -0.188118 |
| 47 | 6 | 0 | 8.852964 | 0.963619 | -0.167611 |
| 48 | 1 | 0 | 9.802925 | -0.969472 | -0.080309 |
| 49 | 1 | 0 | 7.634699 | -2.216445 | 0.012537 |
| 50 | 1 | 0 | 5.489185 | 1.484238 | -0.149978 |
| 51 | 1 | 0 | 7.654119 | 2.750673 | -0.243977 |
| 52 | 1 | 0 | 9.793135 | 1.502266 | -0.208088 |
| 53 | 7 | 0 | 5.161683 | -1.042767 | -0.015084 |
| 54 | 8 | 0 | 5.163031 | -2.255449 | 0.049679 |

Nitrosobenzene adsorption, (fixed subsurface)



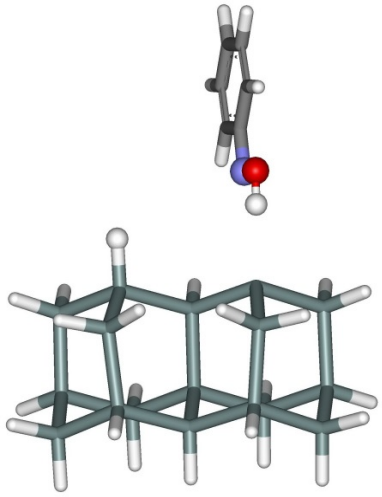


E (RB+HF-LYP) = -5298.04675605

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | 0.369574 | 3.797011 | -1.192219 |
| 2 | 14 | 0 | -2.844258 | 4.074314 | 1.014339 |
| 3 | 14 | 0 | -1.984796 | 4.020182 | -1.188875 |
| 4 | 14 | 0 | -2.888871 | 2.132227 | -2.279346 |
| 5 | 1 | 0 | 2.488628 | 1.753807 | 0.029379 |
| 6 | 1 | 0 | 0.653030 | 3.467415 | 2.716550 |
| 7 | 14 | 0 | -2.171776 | 2.130620 | 2.185878 |
| 8 | 14 | 0 | 0.192510 | 2.142193 | 2.210295 |
| 9 | 14 | 0 | 0.999246 | 1.854808 | 0.006258 |
| 10 | 1 | 0 | 0.728678 | 1.100512 | 3.126086 |
| 11 | 1 | 0 | -2.348171 | 5.283438 | 1.731538 |
| 12 | 1 | 0 | -4.331202 | 4.157859 | 0.957063 |
| 13 | 1 | 0 | -2.373894 | 5.268656 | -1.910092 |
| 14 | 1 | 0 | 1.001661 | 4.992847 | -0.564343 |
| 15 | 1 | 0 | 0.852683 | 3.718317 | -2.600290 |
| 16 | 1 | 0 | -4.375866 | 2.226417 | -2.330124 |
| 17 | 1 | 0 | -2.392135 | 2.061923 | -3.683326 |
| 18 | 14 | 0 | 0.086447 | -0.067406 | -1.043789 |
| 19 | 14 | 0 | -3.042273 | 0.208496 | 1.101703 |
| 20 | 14 | 0 | -2.276410 | 0.147631 | -1.144514 |
| 21 | 14 | 0 | -3.230862 | -1.694336 | -2.284790 |
| 22 | 14 | 0 | -3.515953 | -3.629150 | 0.997366 |
| 23 | 14 | 0 | -2.661894 | -3.714981 | -1.206668 |
| 24 | 14 | 0 | -0.304207 | -3.906581 | -1.222442 |
| 25 | 1 | 0 | -4.995066 | -3.452896 | 0.945267 |
| 26 | 1 | 0 | 2.147659 | -2.270017 | 0.011463 |
| 27 | 1 | 0 | 0.521577 | -1.334420 | 3.113052 |
| 28 | 14 | 0 | -2.512511 | -1.838754 | 2.176365 |
| 29 | 14 | 0 | -0.186581 | -2.264911 | 2.193733 |
| 30 | 14 | 0 | 0.665799 | -2.121708 | -0.007243 |
| 31 | 1 | 0 | 0.029332 | -3.650728 | 2.700002 |
| 32 | 1 | 0 | -3.235816 | -4.908183 | 1.710034 |
| 33 | 1 | 0 | -4.531175 | 0.339625 | 1.090275 |
| 34 | 1 | 0 | 0.612600 | -0.098402 | -2.442147 |
| 35 | 1 | 0 | -4.711252 | -1.522939 | -2.326613 |
| 36 | 1 | 0 | -2.737152 | -1.701597 | -3.691602 |
| 37 | 1 | 0 | 0.170940 | -3.893686 | -2.634902 |
| 38 | 1 | 0 | 0.106778 | -5.203875 | -0.614331 |
| 39 | 1 | 0 | -3.269118 | -4.869762 | -1.933493 |
| 40 | 1 | 0 | -3.033299 | -1.809077 | 3.575830 |
| 41 | 1 | 0 | -2.687940 | 2.189355 | 3.585963 |
| 42 | 6 | 0 | 8.800499 | -0.539306 | -0.102355 |
| 43 | 6 | 0 | 7.609135 | -1.248139 | -0.079716 |
| 44 | 6 | 0 | 6.399578 | -0.541454 | -0.081068 |
| 45 | 6 | 0 | 6.377092 | 0.854667 | -0.104675 |
| 46 | 6 | 0 | 7.577603 | 1.558798 | -0.127253 |
| 47 | 6 | 0 | 8.784878 | 0.861326 | -0.126042 |
| 48 | 1 | 0 | 9.747135 | -1.067475 | -0.101832 |
| 49 | 1 | 0 | 7.586862 | -2.330854 | -0.061206 |
| 50 | 1 | 0 | 5.417699 | 1.359355 | -0.104746 |
| 51 | 1 | 0 | 7.574580 | 2.642182 | -0.145605 |
| 52 | 1 | 0 | 9.721647 | 1.407090 | -0.143682 |
| 53 | 7 | 0 | 5.106158 | -1.172802 | -0.058560 |
| 54 | 8 | 0 | 5.115026 | -2.386973 | -0.036539 |

Nitrosobenzene adsorption TS (relaxed subsurface)

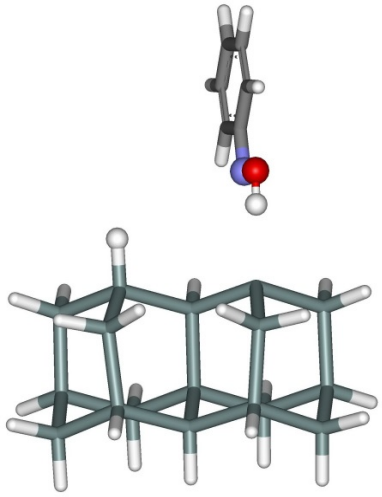


E (RB+HF-LYP) = -5297.99010745

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | -0.718282 | -4.095775 | 0.487825 |
| 2 | 14 | 0 | -4.357597 | -2.963966 | -0.386458 |
| 3 | 14 | 0 | -2.837820 | -3.493147 | 1.347279 |
| 4 | 14 | 0 | -2.548392 | -1.569176 | 2.683564 |
| 5 | 1 | 0 | 1.439449 | -2.779001 | -1.452372 |
| 6 | 1 | 0 | -1.705914 | -3.389280 | -3.255528 |
| 7 | 14 | 0 | -3.466028 | -1.236190 | -1.735945 |
| 8 | 14 | 0 | -1.437685 | -2.063083 | -2.627590 |
| 9 | 14 | 0 | 0.126450 | -2.357638 | -0.878712 |
| 10 | 1 | 0 | -0.905872 | -1.164818 | -3.686918 |
| 11 | 1 | 0 | -4.618518 | -4.168306 | -1.225740 |
| 12 | 1 | 0 | -5.654378 | -2.539469 | 0.213361 |
| 13 | 1 | 0 | -3.384392 | -4.614466 | 2.168726 |
| 14 | 1 | 0 | -0.823278 | -5.351786 | -0.308927 |
| 15 | 1 | 0 | 0.209771 | -4.359437 | 1.624508 |
| 16 | 1 | 0 | -3.847934 | -1.153545 | 3.285814 |
| 17 | 1 | 0 | -1.605402 | -1.856696 | 3.802206 |
| 18 | 14 | 0 | 0.412906 | -0.384738 | 0.407852 |
| 19 | 14 | 0 | -3.141266 | 0.709589 | -0.417943 |
| 20 | 14 | 0 | -1.679400 | 0.211699 | 1.382141 |
| 21 | 14 | 0 | -1.413705 | 2.106221 | 2.775349 |
| 22 | 14 | 0 | -2.109617 | 4.429282 | -0.177242 |
| 23 | 14 | 0 | -0.567755 | 3.934104 | 1.544936 |
| 24 | 14 | 0 | 1.537552 | 3.283016 | 0.661889 |
| 25 | 1 | 0 | -3.430313 | 4.763962 | 0.428548 |
| 26 | 1 | 0 | 3.495155 | 0.856056 | -1.480765 |
| 27 | 1 | 0 | -0.225247 | 1.178022 | -3.623464 |
| 28 | 14 | 0 | -2.322074 | 2.574692 | -1.632305 |
| 29 | 14 | 0 | -0.155297 | 2.158784 | -2.506623 |
| 30 | 14 | 0 | 1.298721 | 1.443937 | -0.796100 |
| 31 | 1 | 0 | 0.364631 | 3.437983 | -3.071287 |
| 32 | 1 | 0 | -1.654852 | 5.619209 | -0.952061 |
| 33 | 1 | 0 | -4.472405 | 1.088277 | 0.147489 |
| 34 | 1 | 0 | 1.353464 | -0.714263 | 1.520447 |
| 35 | 1 | 0 | -2.733450 | 2.452285 | 3.377634 |
| 36 | 1 | 0 | -0.488424 | 1.759462 | 3.892180 |
| 37 | 1 | 0 | 2.440483 | 2.944410 | 1.797999 |
| 38 | 1 | 0 | 2.145186 | 4.431770 | -0.070070 |
| 39 | 1 | 0 | -0.419458 | 5.124900 | 2.437728 |
| 40 | 1 | 0 | -3.284036 | 2.904600 | -2.728761 |
| 41 | 1 | 0 | -4.417061 | -0.934325 | -2.847262 |
| 42 | 6 | 0 | 8.097582 | -1.085680 | -0.666152 |
| 43 | 6 | 0 | 6.895068 | -0.492934 | -0.997071 |
| 44 | 6 | 0 | 5.827030 | -0.504654 | -0.053538 |
| 45 | 6 | 0 | 6.026113 | -1.105713 | 1.221633 |
| 46 | 6 | 0 | 7.244442 | -1.675343 | 1.534800 |
| 47 | 6 | 0 | 8.282758 | -1.674183 | 0.594071 |
| 48 | 1 | 0 | 8.911871 | -1.084969 | -1.381634 |
| 49 | 1 | 0 | 6.748627 | -0.016409 | -1.956602 |
| 50 | 1 | 0 | 5.201696 | -1.098420 | 1.923960 |
| 51 | 1 | 0 | 7.395740 | -2.129028 | 2.507090 |
| 52 | 1 | 0 | 9.237115 | -2.123333 | 0.842873 |
| 53 | 7 | 0 | 4.602478 | 0.021925 | -0.254063 |
| 54 | 8 | 0 | 4.447812 | 0.545954 | -1.475003 |

Nitrosobenzene adsorption TS (fixed subsurface)

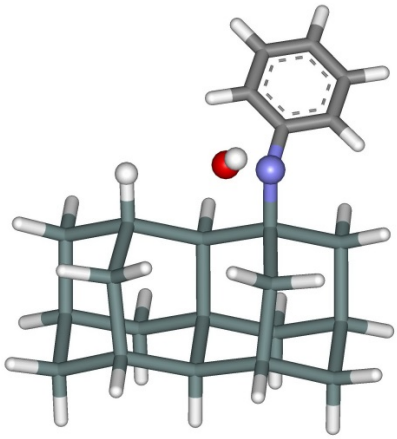


E (RB+HF-LYP) = -5297.589958625

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | 3.135048 | -3.448824 | -1.414278 |
| 2 | 14 | 0 | 5.319303 | -1.437597 | 1.128737 |
| 3 | 14 | 0 | 4.856440 | -1.847292 | -1.154642 |
| 4 | 14 | 0 | 4.113483 | 0.172730 | -2.123176 |
| 5 | 1 | 0 | 0.125191 | -3.771055 | -0.414478 |
| 6 | 1 | 0 | 2.438949 | -3.781993 | 2.439528 |
| 7 | 14 | 0 | 3.344059 | -0.749510 | 2.236826 |
| 8 | 14 | 0 | 1.788329 | -2.514345 | 1.998163 |
| 9 | 14 | 0 | 1.186291 | -2.728306 | -0.278826 |
| 10 | 1 | 0 | 0.593915 | -2.301518 | 2.858600 |
| 11 | 1 | 0 | 5.848623 | -2.671374 | 1.776774 |
| 12 | 1 | 0 | 6.367657 | -0.383457 | 1.233458 |
| 13 | 1 | 0 | 6.094788 | -2.323817 | -1.839980 |
| 14 | 1 | 0 | 3.569122 | -4.766031 | -0.866840 |
| 15 | 1 | 0 | 2.853944 | -3.632533 | -2.866593 |
| 16 | 1 | 0 | 5.169441 | 1.219310 | -2.012071 |
| 17 | 1 | 0 | 3.825422 | -0.026700 | -3.572351 |
| 18 | 14 | 0 | 0.412604 | -0.684306 | -1.201625 |
| 19 | 14 | 0 | 2.552998 | 1.267631 | 1.271161 |
| 20 | 14 | 0 | 2.149764 | 0.935808 | -1.044653 |
| 21 | 14 | 0 | 1.477727 | 2.967094 | -2.057556 |
| 22 | 14 | 0 | 0.002438 | 4.175912 | 1.252916 |
| 23 | 14 | 0 | -0.480410 | 3.791221 | -1.030361 |
| 24 | 14 | 0 | -2.179225 | 2.151392 | -1.294520 |
| 25 | 1 | 0 | 1.114680 | 5.162179 | 1.361172 |
| 26 | 1 | 0 | -3.368102 | -1.416390 | -0.353257 |
| 27 | 1 | 0 | -1.096900 | -0.519883 | 2.896524 |
| 28 | 14 | 0 | 0.600978 | 2.138997 | 2.299542 |
| 29 | 14 | 0 | -1.262507 | 0.689566 | 2.045323 |
| 30 | 14 | 0 | -1.574167 | 0.139878 | -0.224856 |
| 31 | 1 | 0 | -2.471781 | 1.413875 | 2.531991 |
| 32 | 1 | 0 | -1.186197 | 4.754339 | 1.941969 |
| 33 | 1 | 0 | 3.635211 | 2.287723 | 1.421290 |
| 34 | 1 | 0 | 0.147490 | -0.931633 | -2.651553 |
| 35 | 1 | 0 | 2.586510 | 3.956684 | -1.938989 |
| 36 | 1 | 0 | 1.239037 | 2.728267 | -3.509814 |
| 37 | 1 | 0 | -2.394029 | 1.932838 | -2.753844 |
| 38 | 1 | 0 | -3.454401 | 2.670838 | -0.723658 |
| 39 | 1 | 0 | -0.895133 | 5.072413 | -1.676314 |
| 40 | 1 | 0 | 0.874852 | 2.383683 | 3.747144 |
| 41 | 1 | 0 | 3.636594 | -0.527625 | 3.684357 |
| 42 | 6 | 0 | -8.267160 | -2.676457 | -0.184889 |
| 43 | 6 | 0 | -6.902662 | -2.465542 | -0.208157 |
| 44 | 6 | 0 | -6.398844 | -1.135920 | -0.111078 |
| 45 | 6 | 0 | -7.309455 | -0.051220 | 0.034136 |
| 46 | 6 | 0 | -8.668865 | -0.290822 | 0.073492 |
| 47 | 6 | 0 | -9.155291 | -1.599790 | -0.041259 |
| 48 | 1 | 0 | -8.656475 | -3.684931 | -0.264822 |
| 49 | 1 | 0 | -6.208009 | -3.289616 | -0.295574 |
| 50 | 1 | 0 | -6.903358 | 0.949860 | 0.110943 |
| 51 | 1 | 0 | -9.360708 | 0.535384 | 0.186703 |
| 52 | 1 | 0 | -10.222936 | -1.783378 | -0.011816 |
| 53 | 7 | 0 | -5.096092 | -0.791436 | -0.141798 |
| 54 | 8 | 0 | -4.277653 | -1.834700 | -0.316730 |

N-Si bond formation, Structure E (relaxed subsurface)

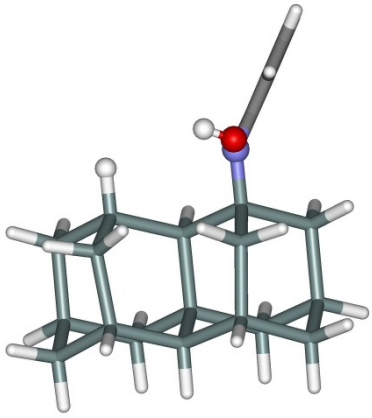


E (RB+HF-LYP) = -5298.09181084

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | -2.567774 | -3.487286 | 0.897487 |
| 2 | 14 | 0 | -5.091027 | -0.817963 | -0.442102 |
| 3 | 14 | 0 | -4.140200 | -1.819599 | 1.478398 |
| 4 | 14 | 0 | -2.992743 | -0.149012 | 2.687342 |
| 5 | 1 | 0 | 0.068672 | -3.653833 | -0.872620 |
| 6 | 1 | 0 | -2.841957 | -2.832075 | -2.978220 |
| 7 | 14 | 0 | -3.376626 | 0.063679 | -1.816491 |
| 8 | 14 | 0 | -1.982203 | -1.750075 | -2.417286 |
| 9 | 14 | 0 | -0.883573 | -2.571850 | -0.493110 |
| 10 | 1 | 0 | -1.013286 | -1.352930 | -3.473304 |
| 11 | 1 | 0 | -5.875722 | -1.824774 | -1.212113 |
| 12 | 1 | 0 | -6.026882 | 0.263676 | -0.022917 |
| 13 | 1 | 0 | -5.221531 | -2.408286 | 2.323629 |
| 14 | 1 | 0 | -3.246857 | -4.605954 | 0.183026 |
| 15 | 1 | 0 | -1.968889 | -4.043726 | 2.143891 |
| 16 | 1 | 0 | -3.932798 | 0.927467 | 3.112048 |
| 17 | 1 | 0 | -2.381319 | -0.726588 | 3.918057 |
| 18 | 14 | 0 | 0.270443 | -0.847571 | 0.656197 |
| 19 | 14 | 0 | -2.208340 | 1.741925 | -0.615073 |
| 20 | 14 | 0 | -1.281833 | 0.808364 | 1.358553 |
| 21 | 14 | 0 | -0.190876 | 2.480905 | 2.625264 |
| 22 | 14 | 0 | 0.531410 | 4.489063 | -0.552242 |
| 23 | 14 | 0 | 1.519515 | 3.482253 | 1.344427 |
| 24 | 14 | 0 | 3.086733 | 1.805080 | 0.756104 |
| 25 | 1 | 0 | -0.462583 | 5.506119 | -0.107585 |
| 26 | 1 | 0 | 2.876553 | -1.938248 | -2.858068 |
| 27 | 1 | 0 | 0.752177 | 0.386808 | -3.554568 |
| 28 | 14 | 0 | -0.507402 | 2.819753 | -1.866346 |
| 29 | 14 | 0 | 1.216783 | 1.330295 | -2.503360 |
| 30 | 14 | 0 | 2.024590 | 0.174376 | -0.602333 |
| 31 | 1 | 0 | 2.341127 | 2.125382 | -3.077562 |
| 32 | 1 | 0 | 1.567479 | 5.185813 | -1.366360 |
| 33 | 1 | 0 | -3.202171 | 2.788285 | -0.225885 |
| 34 | 1 | 0 | 0.890717 | -1.447967 | 1.876094 |
| 35 | 1 | 0 | -1.187122 | 3.507537 | 3.043941 |
| 36 | 1 | 0 | 0.378659 | 1.868567 | 3.858976 |
| 37 | 1 | 0 | 3.629271 | 1.203535 | 2.004283 |
| 38 | 1 | 0 | 4.221003 | 2.417391 | 0.007413 |
| 39 | 1 | 0 | 2.228751 | 4.520378 | 2.150485 |
| 40 | 1 | 0 | -1.101200 | 3.435544 | -3.090227 |
| 41 | 1 | 0 | -3.978121 | 0.666221 | -3.043477 |
| 42 | 6 | 0 | 5.054066 | -3.633823 | 0.774333 |
| 43 | 6 | 0 | 4.071344 | -3.048920 | -0.020223 |
| 44 | 6 | 0 | 4.176734 | -1.699050 | -0.380725 |
| 45 | 6 | 0 | 5.285119 | -0.958513 | 0.050970 |
| 46 | 6 | 0 | 6.248501 | -1.548035 | 0.864786 |
| 47 | 6 | 0 | 6.140635 | -2.888788 | 1.230516 |
| 48 | 1 | 0 | 4.963026 | -4.680171 | 1.044852 |
| 49 | 1 | 0 | 3.228664 | -3.628365 | -0.372155 |
| 50 | 1 | 0 | 5.399632 | 0.068798 | -0.273300 |
| 51 | 1 | 0 | 7.099176 | -0.960954 | 1.192740 |
| 52 | 1 | 0 | 6.899134 | -3.349823 | 1.852212 |
| 53 | 7 | 0 | 3.202973 | -1.048955 | -1.187827 |
| 54 | 8 | 0 | 2.455117 | -1.993135 | -1.990311 |

N-Si bond formation, (fixed subsurface)

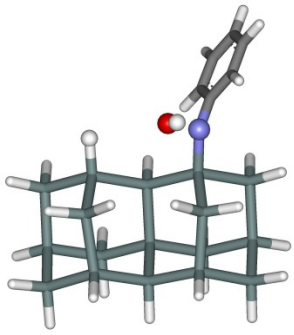


E (RB+HF-LYP) = -5298.09139547

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | 2.657986 | -3.510883 | -0.929244 |
| 2 | 14 | 0 | 5.105710 | -0.885742 | 0.628790 |
| 3 | 14 | 0 | 4.256168 | -1.822315 | -1.370403 |
| 4 | 14 | 0 | 3.177129 | -0.110101 | -2.584101 |
| 5 | 1 | 0 | -0.076586 | -3.708987 | 0.712325 |
| 6 | 1 | 0 | 2.754818 | -2.985604 | 2.963886 |
| 7 | 14 | 0 | 3.322463 | -0.042641 | 1.938226 |
| 8 | 14 | 0 | 1.916432 | -1.883038 | 2.411467 |
| 9 | 14 | 0 | 0.911933 | -2.631941 | 0.407466 |
| 10 | 1 | 0 | 0.895307 | -1.540337 | 3.437414 |
| 11 | 1 | 0 | 5.846848 | -1.919278 | 1.406510 |
| 12 | 1 | 0 | 6.064266 | 0.205558 | 0.294548 |
| 13 | 1 | 0 | 5.379721 | -2.387367 | -2.175753 |
| 14 | 1 | 0 | 3.294540 | -4.654619 | -0.216349 |
| 15 | 1 | 0 | 2.115449 | -4.021452 | -2.219678 |
| 16 | 1 | 0 | 4.140163 | 0.976204 | -2.923797 |
| 17 | 1 | 0 | 2.630723 | -0.646009 | -3.863294 |
| 18 | 14 | 0 | -0.176271 | -0.869732 | -0.745578 |
| 19 | 14 | 0 | 2.222240 | 1.677059 | 0.731185 |
| 20 | 14 | 0 | 1.399911 | 0.810139 | -1.317564 |
| 21 | 14 | 0 | 0.380354 | 2.525961 | -2.585870 |
| 22 | 14 | 0 | -0.505697 | 4.434059 | 0.611788 |
| 23 | 14 | 0 | -1.393735 | 3.491680 | -1.365757 |
| 24 | 14 | 0 | -2.983837 | 1.795631 | -0.911723 |
| 25 | 1 | 0 | 0.512155 | 5.461426 | 0.253123 |
| 26 | 1 | 0 | -3.015634 | -1.956142 | 2.683765 |
| 27 | 1 | 0 | -0.799766 | 0.202626 | 3.442441 |
| 28 | 14 | 0 | 0.459285 | 2.720131 | 1.924744 |
| 29 | 14 | 0 | -1.273001 | 1.184380 | 2.433163 |
| 30 | 14 | 0 | -1.991214 | 0.112722 | 0.446578 |
| 31 | 1 | 0 | -2.421301 | 1.937552 | 3.006841 |
| 32 | 1 | 0 | -1.582222 | 5.107959 | 1.391941 |
| 33 | 1 | 0 | 3.237044 | 2.731944 | 0.428815 |
| 34 | 1 | 0 | -0.716035 | -1.444244 | -2.015921 |
| 35 | 1 | 0 | 1.399096 | 3.562061 | -2.918178 |
| 36 | 1 | 0 | -0.124122 | 1.955262 | -3.866956 |
| 37 | 1 | 0 | -3.456075 | 1.246532 | -2.211923 |
| 38 | 1 | 0 | -4.157526 | 2.365775 | -0.192998 |
| 39 | 1 | 0 | -2.057559 | 4.557410 | -2.174462 |
| 40 | 1 | 0 | 0.988516 | 3.294512 | 3.197410 |
| 41 | 1 | 0 | 3.859194 | 0.518373 | 3.213974 |
| 42 | 6 | 0 | -6.528472 | -2.484299 | 0.066878 |
| 43 | 6 | 0 | -5.485680 | -1.967988 | 0.832414 |
| 44 | 6 | 0 | -4.261925 | -1.647221 | 0.226117 |
| 45 | 6 | 0 | -4.111914 | -1.862407 | -1.154486 |
| 46 | 6 | 0 | -5.167339 | -2.367121 | -1.906220 |
| 47 | 6 | 0 | -6.384244 | -2.684729 | -1.304107 |
| 48 | 1 | 0 | -7.467468 | -2.724893 | 0.553649 |
| 49 | 1 | 0 | -5.614055 | -1.800977 | 1.892294 |
| 50 | 1 | 0 | -3.164941 | -1.654833 | -1.637983 |
| 51 | 1 | 0 | -5.028552 | -2.525322 | -2.970061 |
| 52 | 1 | 0 | -7.201217 | -3.085304 | -1.892202 |
| 53 | 7 | 0 | -3.175348 | -1.133980 | 0.960867 |
| 54 | 8 | 0 | -3.396483 | -1.122815 | 2.373331 |

$H_2O$ formation TS (relaxed subsurface)

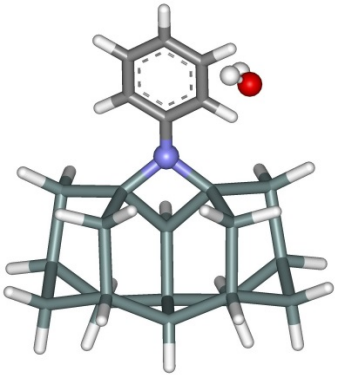


E (RB+HF-LYP) = -5298.08738593

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | -2.682238 | -3.476794 | 0.948100 |
| 2 | 14 | 0 | -5.130424 | -0.834217 | -0.570938 |
| 3 | 14 | 0 | -4.258518 | -1.777239 | 1.415590 |
| 4 | 14 | 0 | -3.140889 | -0.078412 | 2.613540 |
| 5 | 1 | 0 | 0.020111 | -3.721454 | -0.720946 |
| 6 | 1 | 0 | -2.810714 | -2.944871 | -2.957326 |
| 7 | 14 | 0 | -3.358079 | -0.010528 | -1.906793 |
| 8 | 14 | 0 | -1.960096 | -1.854368 | -2.399072 |
| 9 | 14 | 0 | -0.939979 | -2.624766 | -0.411306 |
| 10 | 1 | 0 | -0.950641 | -1.498551 | -3.431495 |
| 11 | 1 | 0 | -5.893968 | -1.862075 | -1.334336 |
| 12 | 1 | 0 | -6.073254 | 0.266353 | -0.222640 |
| 13 | 1 | 0 | -5.374293 | -2.330750 | 2.239717 |
| 14 | 1 | 0 | -3.346025 | -4.614616 | 0.249748 |
| 15 | 1 | 0 | -2.132767 | -3.993820 | 2.233741 |
| 16 | 1 | 0 | -4.085891 | 1.018169 | 2.970609 |
| 17 | 1 | 0 | -2.582358 | -0.623815 | 3.883603 |
| 18 | 14 | 0 | 0.182532 | -0.869612 | 0.720405 |
| 19 | 14 | 0 | -2.228358 | 1.699670 | -0.712766 |
| 20 | 14 | 0 | -1.374422 | 0.822691 | 1.318676 |
| 21 | 14 | 0 | -0.302089 | 2.520266 | 2.569359 |
| 22 | 14 | 0 | 0.529727 | 4.431009 | -0.631044 |
| 23 | 14 | 0 | 1.460268 | 3.475290 | 1.321484 |
| 24 | 14 | 0 | 3.033567 | 1.771933 | 0.832856 |
| 25 | 1 | 0 | -0.472984 | 5.462239 | -0.241319 |
| 26 | 1 | 0 | 2.996891 | -1.916227 | -2.730459 |
| 27 | 1 | 0 | 0.814721 | 0.230683 | -3.487379 |
| 28 | 14 | 0 | -0.478533 | 2.731821 | -1.931704 |
| 29 | 14 | 0 | 1.250269 | 1.204422 | -2.450280 |
| 30 | 14 | 0 | 1.998666 | 0.099335 | -0.492364 |
| 31 | 1 | 0 | 2.402828 | 1.967301 | -3.012757 |
| 32 | 1 | 0 | 1.589349 | 5.104271 | -1.434570 |
| 33 | 1 | 0 | -3.234083 | 2.756573 | -0.388041 |
| 34 | 1 | 0 | 0.740053 | -1.439818 | 1.986461 |
| 35 | 1 | 0 | -1.300912 | 3.566206 | 2.931062 |
| 36 | 1 | 0 | 0.219188 | 1.934473 | 3.837252 |
| 37 | 1 | 0 | 3.532578 | 1.210980 | 2.118746 |
| 38 | 1 | 0 | 4.195335 | 2.340218 | 0.093249 |
| 39 | 1 | 0 | 2.137735 | 4.537348 | 2.123641 |
| 40 | 1 | 0 | -1.023271 | 3.316182 | -3.193270 |
| 41 | 1 | 0 | -3.908679 | 0.557695 | -3.173396 |
| 42 | 6 | 0 | 5.271416 | -2.479768 | 1.790762 |
| 43 | 6 | 0 | 4.177875 | -1.989386 | 1.078551 |
| 44 | 6 | 0 | 4.326974 | -1.580963 | -0.250669 |
| 45 | 6 | 0 | 5.584029 | -1.685221 | -0.859426 |
| 46 | 6 | 0 | 6.669338 | -2.194399 | -0.154035 |
| 47 | 6 | 0 | 6.516632 | -2.588638 | 1.175964 |
| 48 | 1 | 0 | 5.145610 | -2.787221 | 2.822827 |
| 49 | 1 | 0 | 3.205028 | -1.930285 | 1.552266 |
| 50 | 1 | 0 | 5.699886 | -1.352232 | -1.884726 |
| 51 | 1 | 0 | 7.637805 | -2.269947 | -0.635646 |
| 52 | 1 | 0 | 7.364549 | -2.976135 | 1.729154 |
| 53 | 7 | 0 | 3.239534 | -1.058087 | -1.011701 |
| 54 | 8 | 0 | 2.639278 | -2.089629 | -1.850145 |

Phenylnitrene adduct, Structure F (relaxed subsurface)

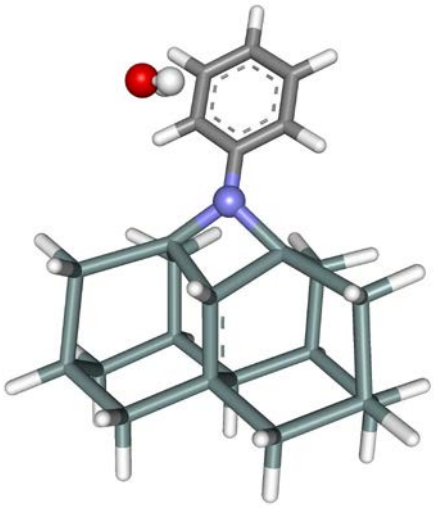


E (RB+HF-LYP) = -5298.12863032

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | 0.011859 | -3.435283 | -1.685290 |
| 2 | 14 | 0 | 3.159629 | -3.379631 | 0.879170 |
| 3 | 14 | 0 | 2.394785 | -3.216323 | -1.360504 |
| 4 | 14 | 0 | 3.457993 | -1.198340 | -2.068371 |
| 5 | 1 | 0 | -4.894808 | 0.937608 | -1.781912 |
| 6 | 1 | 0 | -0.210575 | -3.826581 | 2.120811 |
| 7 | 14 | 0 | 2.129021 | -1.726568 | 2.225348 |
| 8 | 14 | 0 | -0.139924 | -2.345315 | 1.958889 |
| 9 | 14 | 0 | -0.762654 | -1.729240 | -0.249541 |
| 10 | 1 | 0 | -1.048229 | -1.737461 | 2.963700 |
| 11 | 1 | 0 | 2.848472 | -4.711710 | 1.470854 |
| 12 | 1 | 0 | 4.642535 | -3.229885 | 0.843615 |
| 13 | 1 | 0 | 3.021276 | -4.337190 | -2.126879 |
| 14 | 1 | 0 | -0.384248 | -4.846609 | -1.406036 |
| 15 | 1 | 0 | -0.290529 | -3.146114 | -3.114665 |
| 16 | 1 | 0 | 4.928191 | -1.396776 | -1.920013 |
| 17 | 1 | 0 | 3.181667 | -0.897484 | -3.501303 |
| 18 | 14 | 0 | 0.379518 | 0.077511 | -1.151748 |
| 19 | 14 | 0 | 2.651176 | 0.506612 | 1.550686 |
| 20 | 14 | 0 | 2.595414 | 0.621446 | -0.812972 |
| 21 | 14 | 0 | 2.442797 | 2.747730 | -1.858388 |
| 22 | 14 | 0 | 1.238690 | 4.217204 | 1.273235 |
| 23 | 14 | 0 | 0.555184 | 3.919366 | -0.978743 |
| 24 | 14 | 0 | -1.658476 | 3.007218 | -1.354944 |
| 25 | 1 | 0 | 2.614979 | 4.790541 | 1.252065 |
| 26 | 1 | 0 | -4.700034 | 1.424836 | -3.221347 |
| 27 | 1 | 0 | -1.599822 | 0.555732 | 3.088119 |
| 28 | 14 | 0 | 1.161606 | 2.153487 | 2.431770 |
| 29 | 14 | 0 | -1.129427 | 1.627634 | 2.173743 |
| 30 | 14 | 0 | -1.462656 | 1.022418 | -0.102455 |
| 31 | 1 | 0 | -1.903792 | 2.862149 | 2.493722 |
| 32 | 1 | 0 | 0.357974 | 5.174171 | 2.001674 |
| 33 | 1 | 0 | 4.015497 | 0.813797 | 2.074268 |
| 34 | 1 | 0 | 0.057780 | 0.068539 | -2.612645 |
| 35 | 1 | 0 | 3.647983 | 3.603287 | -1.661577 |
| 36 | 1 | 0 | 2.308957 | 2.483083 | -3.318986 |
| 37 | 1 | 0 | -1.761126 | 2.752197 | -2.814489 |
| 38 | 1 | 0 | -2.656392 | 4.034530 | -0.951356 |
| 39 | 1 | 0 | 0.567001 | 5.273640 | -1.614588 |
| 40 | 1 | 0 | 1.499010 | 2.361291 | 3.872147 |
| 41 | 1 | 0 | 2.559303 | -1.897224 | 3.645773 |
| 42 | 6 | 0 | -5.291811 | -2.680857 | 0.137061 |
| 43 | 6 | 0 | -3.974984 | -2.322181 | -0.130519 |
| 44 | 6 | 0 | -3.540937 | -0.991963 | 0.017757 |
| 45 | 6 | 0 | -4.487767 | -0.038979 | 0.440159 |
| 46 | 6 | 0 | -5.806270 | -0.405500 | 0.702627 |
| 47 | 6 | 0 | -6.220949 | -1.727683 | 0.553343 |
| 48 | 1 | 0 | -5.593977 | -3.715117 | 0.013498 |
| 49 | 1 | 0 | -3.274034 | -3.078381 | -0.469786 |
| 50 | 1 | 0 | -4.186585 | 0.994809 | 0.579834 |
| 51 | 1 | 0 | -6.509362 | 0.351845 | 1.031753 |
| 52 | 1 | 0 | -7.246242 | -2.010174 | 0.759068 |
| 53 | 7 | 0 | -2.213249 | -0.632523 | -0.252750 |
| 54 | 8 | 0 | -4.613161 | 1.700040 | -2.303379 |

Phenylnitrene adduct, (fixed subsurface)



E (RB+HF-LYP) = -5298.06479827
(only selected bonds are shown in this structure)

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 14 | 0 | 0.109600 | -3.649685 | -1.498134 |
| 2 | 14 | 0 | 3.112828 | -3.550164 | 1.161803 |
| 3 | 14 | 0 | 2.646750 | -3.550911 | -1.156901 |
| 4 | 14 | 0 | 3.266948 | -1.444552 | -2.022272 |
| 5 | 1 | 0 | -5.138226 | 0.147858 | -3.432988 |
| 6 | 1 | 0 | -0.763677 | -3.730244 | 2.019889 |
| 7 | 14 | 0 | 1.819574 | -1.885475 | 2.238476 |
| 8 | 14 | 0 | -0.487863 | -2.273516 | 1.862650 |
| 9 | 14 | 0 | -1.032632 | -1.673424 | -0.369195 |
| 10 | 1 | 0 | -1.300978 | -1.548392 | 2.871782 |
| 11 | 1 | 0 | 2.798058 | -4.882659 | 1.751692 |
| 12 | 1 | 0 | 4.566613 | -3.294734 | 1.369097 |
| 13 | 1 | 0 | 3.428603 | -4.632199 | -1.827648 |
| 14 | 1 | 0 | -0.372042 | -4.993244 | -1.058663 |
| 15 | 1 | 0 | -0.099201 | -3.577718 | -2.974273 |
| 16 | 1 | 0 | 4.722175 | -1.202077 | -1.807136 |
| 17 | 1 | 0 | 3.012818 | -1.394605 | -3.490614 |
| 18 | 14 | 0 | -0.064114 | 0.004597 | -1.552967 |
| 19 | 14 | 0 | 2.405844 | 0.245689 | 1.376837 |
| 20 | 14 | 0 | 2.035477 | 0.280223 | -0.967707 |
| 21 | 14 | 0 | 2.728571 | 2.353853 | -1.875296 |
| 22 | 14 | 0 | 2.017222 | 4.092922 | 1.451570 |
| 23 | 14 | 0 | 1.548891 | 4.131618 | -0.866515 |
| 24 | 14 | 0 | -0.920278 | 3.547771 | -1.227734 |
| 25 | 1 | 0 | 3.485649 | 4.243547 | 1.657879 |
| 26 | 1 | 0 | -5.330003 | 0.657711 | -2.008011 |
| 27 | 1 | 0 | -1.621447 | 0.784730 | 2.951640 |
| 28 | 14 | 0 | 1.255100 | 2.056923 | 2.387869 |
| 29 | 14 | 0 | -1.068373 | 1.797008 | 2.016273 |
| 30 | 14 | 0 | -1.452910 | 1.255063 | -0.264150 |
| 31 | 1 | 0 | -1.751629 | 3.092346 | 2.296281 |
| 32 | 1 | 0 | 1.343765 | 5.235413 | 2.132693 |
| 33 | 1 | 0 | 3.866003 | 0.445461 | 1.626562 |
| 34 | 1 | 0 | -0.395563 | 0.005610 | -3.001452 |
| 35 | 1 | 0 | 4.194639 | 2.512057 | -1.654928 |
| 36 | 1 | 0 | 2.491440 | 2.344942 | -3.347237 |
| 37 | 1 | 0 | -1.116011 | 3.531385 | -2.705770 |
| 38 | 1 | 0 | -1.748013 | 4.664306 | -0.683756 |
| 39 | 1 | 0 | 1.988558 | 5.435427 | -1.447083 |
| 40 | 1 | 0 | 1.526815 | 2.054291 | 3.856513 |
| 41 | 1 | 0 | 2.095799 | -1.916056 | 3.705982 |
| 42 | 6 | 0 | -5.600153 | -2.092886 | 0.552679 |
| 43 | 6 | 0 | -4.287959 | -1.887576 | 0.140594 |
| 44 | 6 | 0 | -3.750963 | -0.588859 | 0.047694 |
| 45 | 6 | 0 | -4.604109 | 0.493130 | 0.345451 |
| 46 | 6 | 0 | -5.917148 | 0.279356 | 0.756674 |
| 47 | 6 | 0 | -6.426414 | -1.014074 | 0.867552 |
| 48 | 1 | 0 | -5.982161 | -3.105782 | 0.618166 |
| 49 | 1 | 0 | -3.668884 | -2.740403 | -0.125293 |
| 50 | 1 | 0 | -4.230093 | 1.509470 | 0.253052 |
| 51 | 1 | 0 | -6.546170 | 1.133106 | 0.983326 |
| 52 | 1 | 0 | -7.450768 | -1.177225 | 1.179141 |
| 53 | 7 | 0 | -2.423560 | -0.381280 | -0.325044 |
| 54 | 8 | 0 | -5.301196 | 0.950114 | -2.927737 |

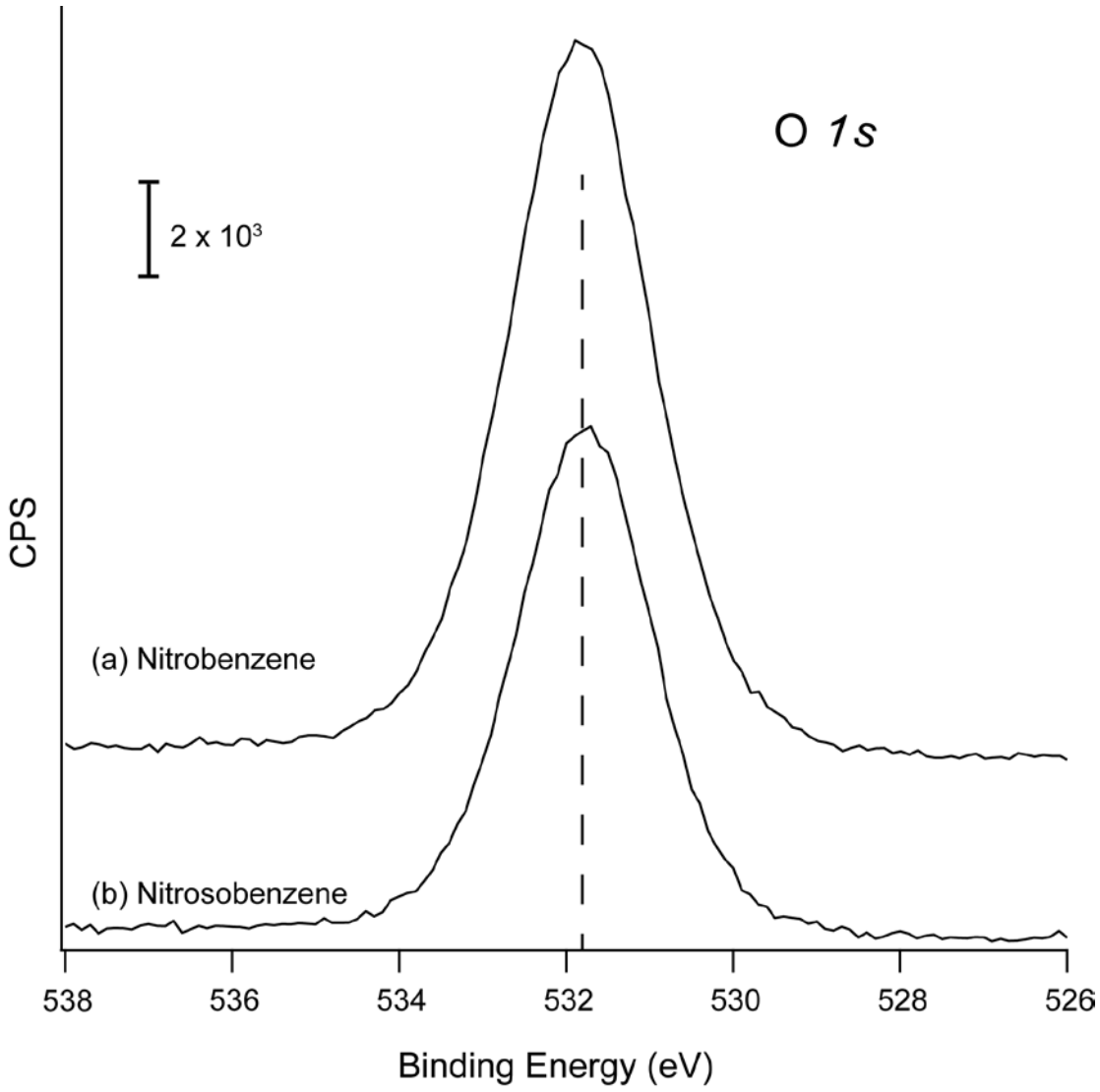



**Figure S1.** High resolution O 1s XPS spectrum of nitrobenzene (a) and nitrosobenzene (b) reacted with H-terminated Si(111) surface by wet-chemistry. The absolute position of the peak is calibrated by the position of the Si *2p* features.

**Complete reference 1:**
Chang, J. P.; Green, M. L.; Donnelly, V. M.; Opila, R. L.; Eng, J.; Sapjeta, J.; Silverman, P. J.; Weir, B.; Lu, H. C.; Gustafsson, T., Garfunkel, E. Profiling Nitrogen in Ultrathin Silicon Oxynitrides with Angle-resolved X-ray Photoelectron Spectroscopy. *J. Appl. Phys.* **2000,** *87*, 4449-4455.

**Complete reference 20:**
Gaussian 09, Revision A.1, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.