

Supporting Information

Mechanistic study of Pd(OAc)₂-catalyzed intramolecular C–H functionalization reaction involving CO/isonitrile insertion

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Complete Reference for Ref (20):

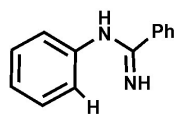
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, Jr., J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revision C.01*, Gaussian, Inc., Wallingford, CT, 2010.

Calculated imaginary frequencies of all transition states species

| | |
|--------------------------------|----------|
| TSI | -983.98 |
| TSII_{CO} | -356.84 |
| TSIII_{CO} | -214.96 |
| TSIV_{CO} | -713.05 |
| TSV | -1019.75 |
| TSVI | -1004.58 |
| TSVI'_{CO} | -175.78 |
| TSVII_{CO} | -215.48 |
| TSVIII_{CO} | -456.04 |
| TSI_{t-BuNC} | -1155.38 |
| TSII_{t-BuNC} | -366.60 |
| TSIII_{t-BuNC} | -347.10 |
| TSIV_{t-BuNC} | -882.27 |
| TSV_{t-BuNC} | -569.62 |
| TSVI_{t-BuNC} | -395.46 |
| TSVI'_{t-BuNC} | -258.62 |
| TSVII_{t-BuNC} | -381.15 |
| TSVII'_{t-BuNC} | -258.11 |

Cartesian coordinates and electronic energies

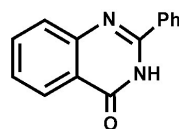
Sub



E= -612.0977065au

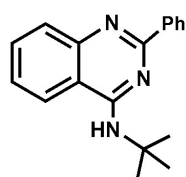
| | | | |
|---|-----------|-----------|-----------|
| H | -2.603798 | 1.916557 | 1.089123 |
| C | -2.883191 | 0.985101 | 0.604295 |
| C | -1.897953 | 0.230124 | -0.049397 |
| C | -4.201872 | 0.535991 | 0.656300 |
| C | -0.490736 | 0.749030 | -0.114561 |
| C | -2.262392 | -0.982976 | -0.653792 |
| C | -4.556405 | -0.671690 | 0.049608 |
| H | -4.951934 | 1.125487 | 1.176422 |
| N | 0.461207 | -0.230456 | 0.106539 |
| N | -0.173693 | 1.973828 | -0.351168 |
| C | -3.584461 | -1.427967 | -0.607737 |
| H | -1.515631 | -1.564156 | -1.188522 |
| H | -5.584777 | -1.020216 | 0.088349 |
| C | 1.866557 | -0.165811 | 0.077659 |
| H | 0.091383 | -1.111153 | 0.433770 |
| H | -3.855631 | -2.362048 | -1.092227 |
| C | 2.563193 | -1.342603 | 0.408623 |
| C | 2.592218 | 0.985337 | -0.270392 |
| C | 3.953894 | -1.372989 | 0.390009 |
| H | 2.006260 | -2.238236 | 0.679826 |
| C | 3.987268 | 0.935729 | -0.286710 |
| H | 2.055950 | 1.892456 | -0.510888 |
| C | 4.678943 | -0.231189 | 0.039831 |
| H | 4.470562 | -2.293299 | 0.649768 |
| H | 4.537781 | 1.833172 | -0.557727 |
| H | 5.764900 | -0.252325 | 0.024773 |
| H | -1.018041 | 2.513641 | -0.542677 |

P_{CO}



E= -724.2663726au

| | | | |
|---|-----------|-----------|-----------|
| H | 2.478213 | 1.967741 | -0.647237 |
| C | 2.878391 | 1.003232 | -0.345531 |
| C | 2.022529 | -0.058379 | -0.011041 |
| C | 4.261672 | 0.824603 | -0.343530 |
| C | 0.545920 | 0.085734 | 0.004222 |
| C | 2.581241 | -1.306099 | 0.311454 |
| C | 4.807715 | -0.415077 | -0.008129 |
| H | 4.910435 | 1.653449 | -0.612208 |
| N | -0.208713 | -0.969729 | -0.076212 |
| N | 0.026377 | 1.360478 | 0.109853 |
| C | 3.962031 | -1.480150 | 0.315622 |
| H | 1.911917 | -2.123114 | 0.556384 |
| H | 5.885479 | -0.552438 | -0.004022 |
| C | -1.582547 | -0.791483 | -0.062431 |
| H | 4.381071 | -2.448637 | 0.574240 |
| C | -2.410817 | -1.929785 | -0.145616 |
| C | -2.192055 | 0.484791 | 0.023377 |
| C | -3.790381 | -1.791978 | -0.142071 |
| H | -1.935920 | -2.903408 | -0.213332 |
| C | -3.589442 | 0.611376 | 0.026784 |
| C | -4.386873 | -0.520241 | -0.056418 |
| H | -4.418319 | -2.676700 | -0.207005 |
| H | -4.015809 | 1.607096 | 0.096637 |
| H | -5.469033 | -0.427342 | -0.055837 |
| H | 0.640108 | 2.155407 | 0.240364 |
| C | -1.340955 | 1.673040 | 0.127896 |
| O | -1.711297 | 2.834402 | 0.233625 |

P_t-BuNC

E= -861.6383137au

| | | | |
|---|-----------|-----------|-----------|
| H | 2.154691 | -1.818704 | -0.000380 |
| C | 2.872961 | -1.007104 | -0.000190 |
| C | 2.403969 | 0.315472 | -0.000047 |
| C | 4.241638 | -1.273710 | -0.000098 |
| C | 0.945371 | 0.615098 | -0.000142 |
| C | 3.337221 | 1.365379 | 0.000186 |
| C | 5.162263 | -0.223736 | 0.000142 |
| H | 4.589844 | -2.303499 | -0.000224 |
| N | 0.585666 | 1.886209 | -0.000219 |
| N | 0.107711 | -0.458048 | -0.000208 |
| C | 4.703797 | 1.096825 | 0.000284 |
| H | 2.968076 | 2.384775 | 0.000287 |
| H | 6.229160 | -0.432038 | 0.000213 |
| C | -0.753849 | 2.146223 | -0.000156 |
| H | 5.414380 | 1.919440 | 0.000479 |
| C | -1.183034 | 3.498464 | -0.000129 |
| C | -1.732939 | 1.112839 | -0.000102 |
| C | -2.526194 | 3.809493 | 0.000041 |
| H | -0.416371 | 4.266765 | -0.000214 |
| C | -3.103657 | 1.459044 | 0.000139 |
| C | -3.496934 | 2.783863 | 0.000212 |
| H | -2.843519 | 4.848930 | 0.000074 |
| H | -3.874582 | 0.692154 | 0.000315 |
| H | -4.553388 | 3.036353 | 0.000400 |
| C | -1.201380 | -0.239062 | -0.000308 |
| H | -3.036751 | -1.078549 | -0.000554 |
| N | -2.053675 | -1.299078 | -0.000602 |
| C | -1.732153 | -2.746377 | 0.000063 |
| C | -3.088979 | -3.472102 | 0.000076 |
| H | -2.936585 | -4.555642 | 0.000449 |
| H | -3.676131 | -3.216474 | 0.891132 |
| H | -3.675813 | -3.217070 | -0.891361 |
| C | -0.947226 | -3.127264 | -1.269552 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.525185 | -2.880103 | -2.167298 |
| H | 0.003296 | -2.592645 | -1.311210 |
| H | -0.747161 | -4.205079 | -1.276652 |
| C | -0.947710 | -3.126322 | 1.270248 |
| H | -1.525895 | -2.878268 | 2.167603 |
| H | -0.747896 | -4.204179 | 1.278360 |
| H | 0.002916 | -2.591876 | 1.311786 |

CO

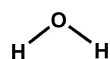
E= -113.3069138au

| | | | |
|---|----------|----------|-----------|
| O | 0.000000 | 0.000000 | 0.487597 |
| C | 0.000000 | 0.000000 | -0.650130 |

t-BuNC

E= -250.6606398au

| | | | |
|---|-----------|-----------|-----------|
| C | 2.365635 | 0.000046 | 0.000533 |
| N | 1.187596 | 0.000046 | 0.000430 |
| C | -0.256163 | -0.000029 | -0.000062 |
| C | -0.735420 | 1.120753 | -0.941447 |
| H | -1.830225 | 1.145681 | -0.961003 |
| H | -0.370741 | 2.094929 | -0.601100 |
| H | -0.372541 | 0.952423 | -1.960186 |
| C | -0.735506 | -1.375611 | -0.500114 |
| H | -0.371567 | -1.567623 | -1.514279 |
| H | -0.372024 | -2.173829 | 0.154568 |
| H | -1.830300 | -1.405263 | -0.511075 |
| C | -0.736515 | 0.254814 | 1.440942 |
| H | -0.373256 | 1.220849 | 1.805237 |
| H | -1.831333 | 0.260176 | 1.471014 |
| H | -0.373366 | -0.527499 | 2.114697 |

H₂O

E= -76.4070235au

| | | | |
|---|----------|----------|----------|
| O | 0.000000 | 0.000000 | 0.119426 |
|---|----------|----------|----------|

| | | | |
|---|----------|-----------|-----------|
| H | 0.000000 | 0.762617 | -0.477705 |
| H | 0.000000 | -0.762617 | -0.477705 |

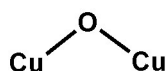
CuO



$$E = -271.2741752\text{au}$$

| | | | |
|----|----------|----------|-----------|
| Cu | 0.000000 | 0.000000 | 0.380416 |
| O | 0.000000 | 0.000000 | -1.379008 |

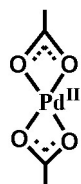
Cu₂O



$$E = -467.4913696\text{au}$$

| | | | |
|----|----------|-----------|-----------|
| O | 0.000000 | 0.000000 | 1.027329 |
| Cu | 0.000000 | 1.347609 | -0.141701 |
| Cu | 0.000000 | -1.347609 | -0.141701 |

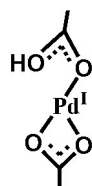
PdOAc₂



$$E = -583.7324381\text{au}$$

| | | | |
|----|-----------|-----------|-----------|
| O | 1.762003 | -1.087590 | -0.009654 |
| O | -1.761791 | 1.087474 | -0.009776 |
| C | 2.435346 | 0.000106 | -0.004694 |
| O | 1.761746 | 1.087663 | -0.009705 |
| C | -2.435329 | -0.000151 | -0.004744 |
| O | -1.761910 | -1.087759 | -0.009783 |
| C | -3.931103 | 0.000187 | 0.035866 |
| H | -4.261126 | 0.017682 | 1.081365 |
| H | -4.319492 | 0.891686 | -0.462214 |
| H | -4.319529 | -0.906424 | -0.433829 |
| C | 3.931126 | 0.000249 | 0.035785 |
| H | 4.319384 | 0.900172 | -0.446864 |
| H | 4.261284 | -0.001414 | 1.081377 |
| H | 4.319547 | -0.898141 | -0.449614 |
| Pd | -0.000015 | -0.000092 | -0.009395 |

PdOAc·AcOH



$$E = -584.3344236\text{au}$$

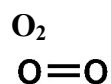
| | | | |
|----|-----------|-----------|-----------|
| O | 1.084992 | 1.240827 | 0.001199 |
| O | -1.675234 | 1.615126 | -0.002623 |
| C | 2.211552 | 0.641659 | -0.003267 |
| O | 2.288552 | -0.627129 | -0.006594 |
| C | -2.409602 | 0.520283 | 0.001060 |
| O | -1.959569 | -0.634463 | 0.004663 |
| C | 3.477130 | 1.465695 | 0.002629 |
| H | 3.461739 | 2.169573 | -0.835627 |
| H | 3.522087 | 2.056443 | 0.923984 |
| H | 4.356633 | 0.823183 | -0.064648 |
| C | -3.888133 | 0.791003 | -0.001465 |
| H | -4.152486 | 1.396902 | 0.871296 |
| H | -4.153324 | 1.369834 | -0.892355 |
| H | -4.439723 | -0.148867 | 0.012395 |
| H | -0.696177 | 1.425869 | -0.001936 |
| Pd | 0.170557 | -0.920862 | 0.000434 |

AcOH



$$E = -229.0776099\text{au}$$

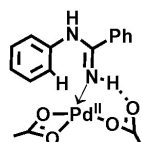
| | | | |
|---|-----------|-----------|-----------|
| O | 0.778567 | -1.046702 | 0.000042 |
| C | 0.092509 | 0.125642 | -0.000010 |
| O | 0.645826 | 1.201966 | -0.000035 |
| C | -1.397605 | -0.109742 | -0.000013 |
| H | -1.917514 | 0.848481 | -0.000330 |
| H | -1.685324 | -0.691726 | -0.881879 |
| H | -1.685388 | -0.691143 | 0.882221 |
| H | 1.723657 | -0.803127 | 0.000066 |



E= -150.316605au

| | | | |
|---|----------|----------|-----------|
| O | 0.000000 | 0.000000 | 0.607108 |
| O | 0.000000 | 0.000000 | -0.607108 |

I

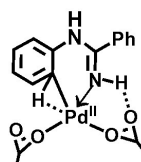


E=-1195.8645233au

| | | | |
|---|-----------|-----------|-----------|
| C | -0.877799 | -1.597260 | -1.734112 |
| C | -0.335402 | -2.263626 | -0.626931 |
| C | -1.005680 | -3.361887 | -0.077029 |
| C | -2.213335 | -3.790336 | -0.626171 |
| C | -2.767566 | -3.119212 | -1.717734 |
| C | -2.094625 | -2.024247 | -2.265074 |
| C | 1.510710 | -0.676518 | 0.031712 |
| H | -0.586180 | -3.869487 | 0.788172 |
| H | -2.723959 | -4.645649 | -0.192205 |
| H | -3.712213 | -3.447991 | -2.141170 |
| H | -2.511607 | -1.498726 | -3.119471 |
| N | 0.851659 | 0.436890 | -0.025567 |
| N | 0.931893 | -1.911237 | -0.092903 |
| C | 2.986210 | -0.683173 | 0.247387 |
| C | 3.573368 | 0.294548 | 1.066162 |
| C | 3.801296 | -1.652595 | -0.358701 |
| C | 4.950605 | 0.297647 | 1.276164 |
| H | 2.946458 | 1.040135 | 1.545472 |
| C | 5.179366 | -1.645241 | -0.145911 |
| H | 3.360550 | -2.390494 | -1.023086 |
| C | 5.755673 | -0.672272 | 0.673415 |
| H | 5.394542 | 1.054899 | 1.915722 |
| H | 5.803070 | -2.392535 | -0.628255 |
| H | 6.829372 | -0.667801 | 0.839347 |
| H | -0.351396 | -0.760169 | -2.177482 |
| O | -3.068228 | 1.218780 | 0.940394 |
| C | -2.938072 | 0.176115 | 1.660050 |

| | | | |
|----|-----------|-----------|-----------|
| O | -1.811538 | -0.434619 | 1.639604 |
| C | -4.067111 | -0.339004 | 2.506829 |
| H | -4.922897 | 0.336186 | 2.449345 |
| H | -4.358225 | -1.335572 | 2.157737 |
| H | -3.735059 | -0.436399 | 3.545500 |
| H | 1.387702 | 1.313338 | -0.086944 |
| H | 1.464002 | -2.672977 | 0.304215 |
| O | -0.883675 | 2.517730 | -0.998679 |
| C | 0.163398 | 3.294580 | -1.034055 |
| O | 1.248129 | 3.102035 | -0.470582 |
| C | -0.072465 | 4.547314 | -1.870000 |
| H | 0.869175 | 5.080071 | -2.016088 |
| H | -0.514372 | 4.284884 | -2.835925 |
| H | -0.784101 | 5.200172 | -1.352276 |
| Pd | -1.076275 | 0.960611 | 0.259451 |

II

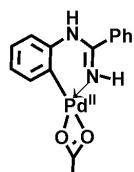


E= -1195.848611au

| | | | |
|---|-----------|-----------|-----------|
| C | -1.008245 | 1.899344 | 0.552288 |
| C | 0.133509 | 2.449228 | -0.072083 |
| C | 1.800870 | 0.614227 | 0.068463 |
| H | -3.119841 | 2.063241 | 0.837083 |
| C | -2.267810 | 2.478467 | 0.313328 |
| C | 0.001135 | 3.561331 | -0.908487 |
| C | -1.257805 | 4.119817 | -1.132445 |
| C | -2.397198 | 3.576435 | -0.532495 |
| H | 0.879876 | 3.975421 | -1.395812 |
| H | -1.346920 | 4.980594 | -1.789595 |
| H | -3.372675 | 4.017452 | -0.712165 |
| N | 1.426523 | 1.930744 | 0.171724 |
| N | 0.945933 | -0.320693 | -0.175943 |
| C | 3.254176 | 0.325160 | 0.239922 |
| C | 3.646762 | -0.871428 | 0.860261 |
| C | 4.238361 | 1.214475 | -0.219875 |
| C | 4.999279 | -1.161484 | 1.028366 |

| | | | |
|----|-----------|-----------|-----------|
| H | 2.893259 | -1.570662 | 1.208643 |
| C | 5.590385 | 0.918370 | -0.051548 |
| H | 3.957875 | 2.121212 | -0.750472 |
| C | 5.973272 | -0.267661 | 0.577775 |
| H | 5.290976 | -2.088020 | 1.513917 |
| H | 6.342808 | 1.608746 | -0.421841 |
| H | 7.026773 | -0.497392 | 0.709984 |
| H | 2.172728 | 2.603273 | 0.271322 |
| Pd | -1.076598 | -0.411653 | -0.182809 |
| O | -3.078839 | -0.635787 | -0.228385 |
| C | -3.641983 | -0.517843 | 0.941758 |
| C | -5.105026 | -0.940282 | 0.954609 |
| O | -3.070895 | -0.106287 | 1.958814 |
| H | -5.165520 | -2.031507 | 0.873613 |
| H | -5.577034 | -0.622749 | 1.886793 |
| H | -5.637835 | -0.520811 | 0.095691 |
| H | -0.912262 | 1.211081 | 1.399417 |
| O | -1.093608 | -2.361023 | -0.792353 |
| C | -0.117360 | -3.215048 | -0.733875 |
| O | 1.055269 | -3.004448 | -0.388546 |
| C | -0.556614 | -4.613796 | -1.158655 |
| H | -1.330127 | -4.980657 | -0.476036 |
| H | -0.995401 | -4.579462 | -2.160750 |
| H | 0.299985 | -5.290485 | -1.147187 |
| H | 1.299985 | -1.289132 | -0.263980 |

III

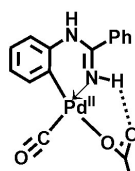


E= -966.78257au

| | | | |
|---|-----------|----------|-----------|
| C | 1.057259 | 1.402937 | -0.040255 |
| C | -0.180674 | 2.063367 | -0.098349 |
| C | -1.648626 | 0.048490 | -0.013802 |
| H | 3.182992 | 1.696382 | -0.002881 |
| C | 2.218249 | 2.192718 | -0.046159 |
| C | -0.248784 | 3.466352 | -0.167197 |

| | | | |
|----|-----------|-----------|-----------|
| C | 0.915043 | 4.224710 | -0.173787 |
| C | 2.156416 | 3.584825 | -0.111490 |
| H | -1.220347 | 3.957227 | -0.213502 |
| H | 0.852203 | 5.308032 | -0.226395 |
| H | 3.073541 | 4.167951 | -0.115729 |
| N | -1.419575 | 1.378639 | -0.096763 |
| N | -0.674730 | -0.813998 | 0.049462 |
| C | -3.076350 | -0.376404 | -0.000986 |
| C | -3.479959 | -1.491432 | -0.751415 |
| C | -4.026770 | 0.318714 | 0.763004 |
| C | -4.812234 | -1.901434 | -0.738175 |
| H | -2.753809 | -2.017981 | -1.364368 |
| C | -5.358110 | -0.096744 | 0.775252 |
| H | -3.717811 | 1.162331 | 1.374439 |
| C | -5.753564 | -1.205606 | 0.024229 |
| H | -5.116499 | -2.759474 | -1.330520 |
| H | -6.083577 | 0.440273 | 1.379509 |
| H | -6.791073 | -1.527155 | 0.033675 |
| H | -2.235907 | 1.953202 | -0.252724 |
| O | 3.415024 | -0.677902 | 0.033914 |
| C | 3.398128 | -1.961532 | 0.086941 |
| O | 2.293071 | -2.576899 | 0.111376 |
| C | 4.711934 | -2.703752 | 0.125657 |
| H | 5.337773 | -2.394707 | -0.717831 |
| H | 5.250871 | -2.446869 | 1.044341 |
| H | 4.542559 | -3.781556 | 0.090401 |
| H | -0.981028 | -1.771515 | 0.188866 |
| Pd | 1.313559 | -0.549815 | 0.032189 |

IV_{CO}

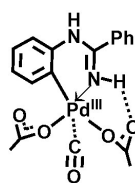


E= -1080.1129417au

| | | | |
|----|-----------|----------|-----------|
| Pd | 1.378020 | 0.558994 | -0.045172 |
| H | -2.808681 | 1.448318 | 0.801963 |
| C | -3.436939 | 0.623195 | 0.481154 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.850486 | -0.566415 | 0.019696 |
| C | -4.824401 | 0.747183 | 0.520101 |
| C | -1.365199 | -0.688777 | -0.010877 |
| C | -3.675731 | -1.615491 | -0.416147 |
| C | -5.640336 | -0.305251 | 0.098395 |
| H | -5.267883 | 1.670093 | 0.882153 |
| N | -0.849721 | -1.927504 | 0.187481 |
| N | -0.598271 | 0.333144 | -0.209832 |
| C | -5.063218 | -1.484957 | -0.375213 |
| H | -3.239237 | -2.521711 | -0.828370 |
| H | -6.721510 | -0.203397 | 0.130331 |
| C | 0.497374 | -2.340374 | 0.102676 |
| H | -1.511715 | -2.650063 | 0.430753 |
| H | -5.691047 | -2.299660 | -0.724649 |
| C | 0.690514 | -3.734512 | 0.154390 |
| C | 1.591729 | -1.458394 | -0.028534 |
| C | 1.959721 | -4.284625 | 0.059891 |
| H | -0.175773 | -4.386385 | 0.258512 |
| C | 2.862896 | -2.058144 | -0.139851 |
| C | 3.057435 | -3.437310 | -0.097145 |
| H | 2.088319 | -5.362404 | 0.101172 |
| H | 3.741188 | -1.433873 | -0.262579 |
| H | 4.061525 | -3.843842 | -0.180880 |
| H | -1.020013 | 1.270398 | -0.353062 |
| C | 3.255401 | 0.946280 | 0.177364 |
| O | 4.334844 | 1.279314 | 0.337649 |
| C | 0.144489 | 3.415417 | -0.139378 |
| O | -1.020684 | 2.997770 | -0.284918 |
| C | 0.398285 | 4.918794 | -0.061219 |
| H | 1.051962 | 5.226632 | -0.884701 |
| H | -0.544179 | 5.467332 | -0.115930 |
| H | 0.917390 | 5.162207 | 0.872027 |
| O | 1.218027 | 2.703346 | -0.048255 |

V_{CO}

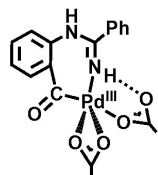


E= -1308.5420304au

| | | | |
|----|-----------|-----------|-----------|
| Pd | -1.063505 | -0.231144 | 0.119757 |
| H | 2.850945 | -1.686003 | -0.936873 |
| C | 3.616172 | -0.964516 | -0.667937 |
| C | 3.248425 | 0.288655 | -0.151969 |
| C | 4.963446 | -1.283098 | -0.827459 |
| C | 1.804433 | 0.621358 | 0.005163 |
| C | 4.248089 | 1.203489 | 0.215880 |
| C | 5.953851 | -0.364474 | -0.472029 |
| H | 5.238367 | -2.252960 | -1.231513 |
| N | 1.450403 | 1.918948 | -0.179601 |
| N | 0.929637 | -0.282437 | 0.308445 |
| C | 5.593969 | 0.877452 | 0.055047 |
| H | 3.980596 | 2.156289 | 0.665621 |
| H | 7.002722 | -0.618383 | -0.597475 |
| C | 0.185634 | 2.510658 | 0.035552 |
| H | 6.359544 | 1.588520 | 0.352106 |
| C | 0.159594 | 3.916271 | 0.079708 |
| C | -0.998625 | 1.775799 | 0.205434 |
| C | -1.031372 | 4.594611 | 0.304196 |
| H | 1.086846 | 4.471576 | -0.052824 |
| C | -2.187732 | 2.477604 | 0.441065 |
| C | -2.211032 | 3.872464 | 0.495244 |
| H | -1.035114 | 5.680430 | 0.336596 |
| H | -3.111010 | 1.922938 | 0.567050 |
| H | -3.148717 | 4.390070 | 0.678437 |
| H | 1.210750 | -1.281365 | 0.402245 |
| C | -1.576389 | -0.913785 | 2.739353 |
| C | -0.246392 | -3.227314 | 0.131099 |
| O | -1.214591 | -2.377655 | 0.116880 |
| C | -0.687199 | -4.676855 | -0.050935 |
| H | -1.461119 | -4.927845 | 0.681752 |
| H | -1.130255 | -4.802468 | -1.045349 |
| H | 0.163836 | -5.352269 | 0.057934 |

| | | | |
|---|-----------|-----------|-----------|
| O | 0.968282 | -2.971729 | 0.277595 |
| O | -1.939934 | -1.673739 | 3.501423 |
| O | -1.786983 | -0.250229 | -2.061922 |
| C | -4.139696 | -0.509520 | -2.524977 |
| H | -4.418478 | -1.569481 | -2.526584 |
| H | -4.997291 | 0.065408 | -2.165379 |
| H | -3.878778 | -0.211672 | -3.542629 |
| C | -2.967434 | -0.319801 | -1.599311 |
| O | -3.151668 | -0.252871 | -0.338489 |
| H | 2.180792 | 2.540072 | -0.496458 |

VI_{CO}

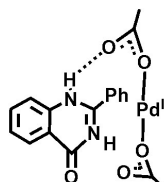


E= -1308.5496348au

| | | | |
|----|-----------|-----------|-----------|
| Pd | -1.218699 | -0.317258 | -0.086085 |
| H | 2.673384 | -1.948299 | -1.303266 |
| C | 3.492261 | -1.350694 | -0.915576 |
| C | 3.225530 | -0.114987 | -0.304702 |
| C | 4.804173 | -1.805316 | -1.027413 |
| C | 1.815526 | 0.354085 | -0.186542 |
| C | 4.290496 | 0.649026 | 0.199709 |
| C | 5.860733 | -1.037185 | -0.531484 |
| H | 5.000831 | -2.760522 | -1.505050 |
| N | 1.646559 | 1.719074 | -0.263357 |
| N | 0.835349 | -0.465596 | -0.036949 |
| C | 5.601538 | 0.188002 | 0.085758 |
| H | 4.094273 | 1.583289 | 0.718967 |
| H | 6.882411 | -1.395647 | -0.620065 |
| C | 0.536615 | 2.552202 | -0.031275 |
| H | 6.417440 | 0.780043 | 0.490300 |
| C | 0.625502 | 3.843788 | -0.583736 |
| C | -0.582436 | 2.251322 | 0.783238 |
| C | -0.348514 | 4.805513 | -0.351926 |
| H | 1.482900 | 4.087586 | -1.207224 |
| C | -1.554671 | 3.244378 | 1.016122 |
| C | -1.450057 | 4.509674 | 0.456332 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.245491 | 5.787707 | -0.803656 |
| H | -2.401688 | 2.988313 | 1.644365 |
| H | -2.214595 | 5.255846 | 0.647415 |
| H | 1.031231 | -1.474621 | 0.143252 |
| C | -0.891905 | 0.926793 | 1.401540 |
| C | -0.571108 | -3.167386 | 0.964685 |
| O | -1.468935 | -2.239896 | 0.989796 |
| C | -1.076683 | -4.501249 | 1.513760 |
| H | -1.682317 | -4.345756 | 2.410532 |
| H | -1.713514 | -4.977438 | 0.759495 |
| H | -0.229383 | -5.154914 | 1.731747 |
| O | 0.596874 | -3.079040 | 0.541357 |
| O | -1.099826 | 0.685900 | 2.549472 |
| O | -2.366658 | -1.262972 | -1.947582 |
| C | -4.778873 | -1.081838 | -1.922649 |
| H | -5.244165 | -1.872923 | -1.323124 |
| H | -5.404925 | -0.189138 | -1.836681 |
| H | -4.724049 | -1.411261 | -2.962315 |
| C | -3.392473 | -0.810880 | -1.385303 |
| O | -3.299966 | -0.112604 | -0.301075 |
| H | 2.438598 | 2.204654 | -0.661611 |

VII_{CO}

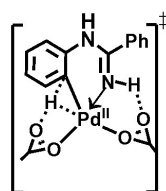


E= -1308.6097052au

| | | | |
|---|-----------|-----------|-----------|
| C | -2.622840 | -1.776678 | 0.338334 |
| C | -2.590098 | -0.414372 | 0.681751 |
| C | -0.239531 | -0.520850 | 1.099750 |
| H | -3.830871 | -3.420592 | -0.305962 |
| C | -3.836311 | -2.369374 | -0.037620 |
| C | -3.759169 | 0.361436 | 0.636601 |
| C | -4.951405 | -0.244770 | 0.262256 |
| C | -4.997402 | -1.609672 | -0.069015 |
| H | -3.708544 | 1.417379 | 0.880968 |
| H | -5.859869 | 0.349573 | 0.225274 |
| H | -5.939660 | -2.065698 | -0.357001 |

| | | | |
|----|-----------|-----------|-----------|
| N | -1.386347 | 0.163998 | 1.090600 |
| N | -0.225634 | -1.808372 | 0.705823 |
| C | 1.007092 | 0.082198 | 1.627330 |
| C | 1.169861 | 1.481284 | 1.734736 |
| C | 2.033455 | -0.762982 | 2.097316 |
| C | 2.345890 | 2.007813 | 2.266135 |
| H | 0.384535 | 2.158351 | 1.417677 |
| C | 3.197153 | -0.222625 | 2.634040 |
| H | 1.923680 | -1.838131 | 2.050458 |
| C | 3.362262 | 1.162228 | 2.712689 |
| H | 2.460137 | 3.085521 | 2.333777 |
| H | 3.975545 | -0.888273 | 2.994499 |
| H | 4.274364 | 1.579137 | 3.130457 |
| Pd | 0.980546 | 0.745729 | -1.256601 |
| C | -1.368812 | -2.543633 | 0.304463 |
| O | -1.485723 | 2.737778 | 0.528905 |
| C | -1.129501 | 3.032933 | -0.646498 |
| C | -1.710677 | 4.287759 | -1.284472 |
| O | -0.309972 | 2.388498 | -1.379067 |
| H | -2.203063 | 4.027821 | -2.227388 |
| H | -2.423023 | 4.770389 | -0.612933 |
| H | -0.900999 | 4.984587 | -1.526581 |
| H | 0.711791 | -2.181354 | 0.358573 |
| O | 2.095357 | -2.467899 | -0.381889 |
| C | 3.861868 | -2.501027 | -1.991002 |
| H | 3.590040 | -2.721451 | -3.029482 |
| H | 4.716736 | -1.818168 | -2.017167 |
| H | 4.133884 | -3.429188 | -1.485107 |
| C | 2.681027 | -1.838786 | -1.291635 |
| O | 2.400176 | -0.667342 | -1.734290 |
| H | -1.355762 | 1.226147 | 1.058620 |
| O | -1.260753 | -3.702814 | -0.047527 |

TSI

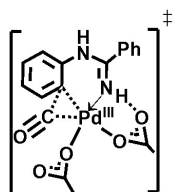


E= -1195.839426au

| | | | |
|----|-----------|-----------|-----------|
| C | 1.332535 | -1.536138 | -0.147310 |
| C | 0.181372 | -2.358518 | -0.077081 |
| C | -1.620269 | -0.662840 | 0.019601 |
| H | 3.372403 | -1.477321 | -0.828550 |
| C | 2.484645 | -2.097848 | -0.752593 |
| C | 0.230342 | -3.701098 | -0.479733 |
| C | 1.396755 | -4.226264 | -1.025625 |
| C | 2.526104 | -3.415506 | -1.188625 |
| H | -0.661881 | -4.319115 | -0.405607 |
| H | 1.417415 | -5.265023 | -1.343854 |
| H | 3.430088 | -3.818856 | -1.635300 |
| N | -1.061635 | -1.866525 | 0.372620 |
| N | -0.912902 | 0.276814 | -0.515598 |
| C | -3.080700 | -0.504814 | 0.271910 |
| C | -3.583656 | 0.758110 | 0.625223 |
| C | -3.966199 | -1.587715 | 0.149168 |
| C | -4.946453 | 0.923716 | 0.864587 |
| H | -2.909886 | 1.605771 | 0.703304 |
| C | -5.328802 | -1.415112 | 0.388103 |
| H | -3.604963 | -2.560745 | -0.174687 |
| C | -5.820499 | -0.159967 | 0.751778 |
| H | -5.324808 | 1.903535 | 1.140716 |
| H | -6.005819 | -2.257542 | 0.278989 |
| H | -6.882220 | -0.025642 | 0.938912 |
| H | -1.701109 | -2.550736 | 0.751499 |
| Pd | 1.048407 | 0.577364 | -0.297368 |
| O | 3.035591 | 0.945459 | 0.224247 |
| C | 3.357873 | 0.406811 | 1.334843 |
| C | 4.627156 | 0.900733 | 1.997718 |
| O | 2.681189 | -0.494747 | 1.916627 |
| H | 4.366433 | 1.719399 | 2.678808 |
| H | 5.087096 | 0.102274 | 2.583880 |

| | | | |
|---|-----------|-----------|-----------|
| H | 5.323459 | 1.287969 | 1.251241 |
| H | 1.753901 | -0.932063 | 0.930346 |
| O | 0.893071 | 2.606045 | -0.601081 |
| C | -0.168744 | 3.319843 | -0.783355 |
| O | -1.347096 | 2.918743 | -0.826148 |
| C | 0.134449 | 4.803816 | -0.967458 |
| H | 0.717314 | 5.175906 | -0.118719 |
| H | 0.744603 | 4.944611 | -1.866215 |
| H | -0.794444 | 5.369822 | -1.061319 |
| H | -1.370067 | 1.179739 | -0.739708 |

TSII_{CO}

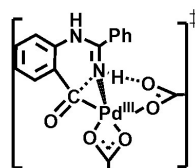


E=-1308.5147031au

| | | | |
|----|-----------|-----------|-----------|
| Pd | -1.201397 | -0.320055 | 0.293639 |
| H | 2.894465 | -1.709206 | -1.449459 |
| C | 3.670966 | -1.085031 | -1.017985 |
| C | 3.314500 | 0.059272 | -0.288082 |
| C | 5.013746 | -1.410477 | -1.195971 |
| C | 1.869304 | 0.380411 | -0.101918 |
| C | 4.321500 | 0.862231 | 0.270513 |
| C | 6.012599 | -0.604278 | -0.643986 |
| H | 5.279815 | -2.294495 | -1.767967 |
| N | 1.565373 | 1.731227 | -0.068393 |
| N | 0.962407 | -0.512311 | 0.018147 |
| C | 5.664293 | 0.529104 | 0.092950 |
| H | 4.059497 | 1.723865 | 0.879167 |
| H | 7.058739 | -0.862237 | -0.782612 |
| C | 0.318849 | 2.378518 | -0.022886 |
| H | 6.436232 | 1.149019 | 0.539933 |
| C | 0.311523 | 3.727708 | -0.424064 |
| C | -0.901778 | 1.802321 | 0.404824 |
| C | -0.855666 | 4.480946 | -0.406313 |
| H | 1.239900 | 4.182440 | -0.764564 |
| C | -2.075125 | 2.578417 | 0.412427 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.062284 | 3.907832 | 0.007784 |
| H | -0.821678 | 5.519538 | -0.722782 |
| H | -3.001920 | 2.109219 | 0.724608 |
| H | -2.978382 | 4.490151 | 0.014938 |
| H | 1.171030 | -1.523769 | 0.090429 |
| C | -0.822359 | 0.606493 | 1.907862 |
| C | -0.646415 | -3.293371 | 0.601487 |
| O | -1.544393 | -2.364836 | 0.689358 |
| C | -1.222277 | -4.693783 | 0.803791 |
| H | -1.826181 | -4.728068 | 1.715761 |
| H | -1.883869 | -4.938683 | -0.034698 |
| H | -0.415648 | -5.427774 | 0.857298 |
| O | 0.567360 | -3.155219 | 0.372685 |
| O | -0.549495 | 0.874097 | 3.000153 |
| O | -1.936719 | -0.677427 | -1.751734 |
| C | -4.242572 | -0.815744 | -2.433283 |
| H | -4.556481 | -1.862326 | -2.342896 |
| H | -5.113529 | -0.183631 | -2.241831 |
| H | -3.866835 | -0.654776 | -3.446592 |
| C | -3.157998 | -0.544710 | -1.416291 |
| O | -3.473237 | -0.217046 | -0.230169 |
| H | 2.321651 | 2.329118 | -0.371898 |

TSIII_{CO}

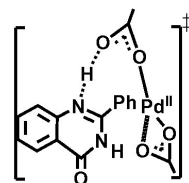


E= -1308.5398004au

| | | | |
|----|-----------|-----------|-----------|
| Pd | 1.147963 | 0.491968 | -0.088687 |
| H | -2.611581 | 1.783557 | -0.421034 |
| C | -3.387378 | 1.031300 | -0.524350 |
| C | -3.088637 | -0.324316 | -0.300970 |
| C | -4.684219 | 1.406186 | -0.867912 |
| C | -1.701334 | -0.715798 | 0.035717 |
| C | -4.109631 | -1.286011 | -0.405377 |
| C | -5.691022 | 0.445093 | -0.986320 |
| H | -4.906705 | 2.454190 | -1.044188 |

| | | | |
|---|-----------|-----------|-----------|
| N | -1.298207 | -1.971131 | -0.298585 |
| N | -0.853077 | 0.073933 | 0.642887 |
| C | -5.403512 | -0.901062 | -0.747902 |
| H | -3.910354 | -2.329741 | -0.176277 |
| H | -6.700311 | 0.744586 | -1.254211 |
| C | -0.098055 | -2.588614 | 0.075665 |
| H | -6.188078 | -1.648928 | -0.816068 |
| C | 0.160042 | -3.870169 | -0.439930 |
| C | 0.814740 | -2.012302 | 0.990532 |
| C | 1.292199 | -4.573100 | -0.054471 |
| H | -0.542635 | -4.311021 | -1.143348 |
| C | 1.945050 | -2.755800 | 1.386045 |
| C | 2.189534 | -4.018143 | 0.868310 |
| H | 1.475341 | -5.559259 | -0.470408 |
| H | 2.629680 | -2.302514 | 2.095175 |
| H | 3.072869 | -4.569559 | 1.174137 |
| H | -1.143376 | 1.036522 | 0.974308 |
| C | 0.693526 | -0.644976 | 1.555399 |
| C | 0.061502 | 3.129347 | 1.131976 |
| O | 1.114562 | 2.528908 | 0.720344 |
| C | 0.292277 | 4.565325 | 1.593062 |
| H | 1.085818 | 5.040518 | 1.011761 |
| H | -0.636728 | 5.135436 | 1.517238 |
| H | 0.604580 | 4.549503 | 2.644067 |
| O | -1.096779 | 2.650598 | 1.216153 |
| O | 0.861872 | -0.262207 | 2.675762 |
| O | 1.924023 | 1.153326 | -2.336122 |
| C | 4.320243 | 1.355065 | -2.581709 |
| H | 4.693897 | 2.323028 | -2.227848 |
| H | 5.099387 | 0.611276 | -2.391444 |
| H | 4.113020 | 1.425194 | -3.651593 |
| C | 3.055175 | 1.009440 | -1.821794 |
| O | 3.203115 | 0.586219 | -0.609657 |
| H | -1.899488 | -2.496449 | -0.918435 |

TSIV_{CO}

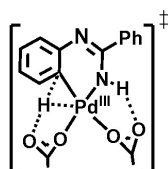


E= -1308.6109479au

| | | | |
|----|-----------|-----------|-----------|
| C | -2.421751 | -0.674025 | 1.467323 |
| C | -1.426353 | 0.305643 | 1.661008 |
| C | 0.291063 | -1.221367 | 1.152816 |
| H | -4.515912 | -1.121141 | 1.480181 |
| C | -3.774094 | -0.345617 | 1.640007 |
| C | -1.793290 | 1.610389 | 2.032882 |
| C | -3.136507 | 1.916970 | 2.203002 |
| C | -4.131181 | 0.943474 | 2.007714 |
| H | -1.019803 | 2.356397 | 2.180477 |
| H | -3.419273 | 2.925771 | 2.490076 |
| H | -5.176845 | 1.202076 | 2.143589 |
| N | -0.077445 | -0.000313 | 1.470852 |
| N | -0.630297 | -2.210125 | 1.050457 |
| C | 1.712225 | -1.567433 | 0.950535 |
| C | 2.690759 | -1.053174 | 1.815463 |
| C | 2.079486 | -2.429545 | -0.096326 |
| C | 4.024624 | -1.418310 | 1.644813 |
| H | 2.406001 | -0.377833 | 2.614995 |
| C | 3.417226 | -2.782432 | -0.260915 |
| H | 1.328634 | -2.743058 | -0.815017 |
| C | 4.388513 | -2.285783 | 0.611997 |
| H | 4.779323 | -1.027001 | 2.320755 |
| H | 3.702992 | -3.434068 | -1.081456 |
| H | 5.429913 | -2.566894 | 0.481603 |
| Pd | 0.035360 | 1.294624 | -1.732767 |
| C | -2.028745 | -2.032756 | 1.082977 |
| O | 1.483425 | 1.933426 | 1.504106 |
| C | 1.802424 | 2.654010 | 0.491676 |
| C | 2.818695 | 3.747553 | 0.763631 |
| O | 1.372937 | 2.532715 | -0.680721 |
| H | 2.552743 | 4.289908 | 1.675726 |
| H | 3.799860 | 3.288054 | 0.931474 |
| H | 2.885242 | 4.433321 | -0.082287 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.323035 | -3.129414 | 0.753681 |
| O | -0.328670 | -1.289164 | -1.668627 |
| C | -1.943138 | -2.035333 | -3.289131 |
| H | -2.498495 | -2.613669 | -2.542862 |
| H | -2.635850 | -1.594393 | -4.008413 |
| H | -1.273289 | -2.729866 | -3.808614 |
| C | -1.121129 | -0.967992 | -2.590378 |
| O | -1.269691 | 0.245515 | -2.971504 |
| H | 0.712326 | 0.944840 | 1.405706 |
| O | -2.770485 | -2.968533 | 0.839742 |

TSV

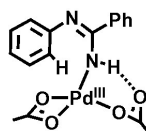


E= -1195.1894272au

| | | | |
|---|-----------|-----------|-----------|
| C | 1.306803 | -1.527382 | -0.154789 |
| C | 0.137197 | -2.362454 | -0.294337 |
| C | -1.607793 | -0.735146 | -0.146318 |
| H | 3.417885 | -1.424077 | -0.543859 |
| C | 2.529787 | -2.042935 | -0.630523 |
| C | 0.298724 | -3.709738 | -0.747079 |
| C | 1.522315 | -4.175200 | -1.188876 |
| C | 2.645677 | -3.330856 | -1.153873 |
| H | -0.592327 | -4.327257 | -0.789940 |
| H | 1.614220 | -5.189479 | -1.566713 |
| H | 3.608981 | -3.689430 | -1.505139 |
| N | -1.147182 | -2.007495 | -0.084790 |
| N | -0.886748 | 0.264258 | -0.613425 |
| C | -3.035631 | -0.537765 | 0.232247 |
| C | -3.545865 | 0.749613 | 0.475035 |
| C | -3.882804 | -1.649487 | 0.373304 |
| C | -4.880615 | 0.914573 | 0.840152 |
| H | -2.908094 | 1.623911 | 0.386939 |
| C | -5.215352 | -1.476861 | 0.740329 |
| H | -3.482686 | -2.639334 | 0.188171 |
| C | -5.718829 | -0.194882 | 0.973152 |
| H | -5.263622 | 1.913857 | 1.026437 |

| | | | |
|----|-----------|-----------|-----------|
| H | -5.862142 | -2.343985 | 0.842313 |
| H | -6.758507 | -0.060994 | 1.259768 |
| Pd | 1.040764 | 0.570120 | -0.311566 |
| O | 2.926263 | 0.965644 | 0.485221 |
| C | 3.112615 | 0.400300 | 1.616312 |
| C | 4.277680 | 0.897751 | 2.445596 |
| O | 2.382543 | -0.524697 | 2.082626 |
| H | 3.943698 | 1.767281 | 3.023756 |
| H | 4.610772 | 0.125019 | 3.140732 |
| H | 5.095673 | 1.220304 | 1.797779 |
| H | 1.590761 | -0.956362 | 0.984082 |
| O | 0.935045 | 2.584433 | -0.692996 |
| C | -0.117577 | 3.309417 | -0.906268 |
| O | -1.298113 | 2.920280 | -0.923281 |
| C | 0.209485 | 4.775038 | -1.164635 |
| H | 0.823911 | 5.172680 | -0.350738 |
| H | 0.794946 | 4.862314 | -2.086441 |
| H | -0.711214 | 5.354033 | -1.258593 |
| H | -1.340663 | 1.179435 | -0.798166 |

VIII

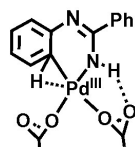


E= -1195.221434au

| | | | |
|---|-----------|-----------|-----------|
| C | 0.405064 | -1.742213 | 1.642010 |
| C | 0.100201 | -2.295944 | 0.354077 |
| C | 0.781847 | -3.489318 | -0.047950 |
| C | 1.724656 | -4.074521 | 0.775197 |
| C | 2.013118 | -3.510859 | 2.030345 |
| C | 1.344049 | -2.350646 | 2.455656 |
| C | -1.421009 | -0.580942 | -0.358237 |
| H | 0.539171 | -3.899732 | -1.022462 |
| H | 2.242444 | -4.973860 | 0.454258 |
| H | 2.749856 | -3.977683 | 2.677785 |
| H | 1.563545 | -1.928660 | 3.432236 |
| N | -0.751819 | 0.531137 | -0.314863 |
| N | -0.818730 | -1.806373 | -0.488696 |
| C | -2.912573 | -0.588233 | -0.389427 |

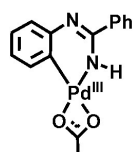
| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | -3.646162 | 0.508519 | 0.095680 | C | -1.984544 | 2.460010 | 0.635888 |
| C | -3.595847 | -1.709444 | -0.887714 | C | -0.065509 | 3.424533 | -1.176490 |
| C | -5.038801 | 0.479785 | 0.070625 | C | -1.342403 | 3.961700 | -1.158821 |
| H | -3.137274 | 1.379642 | 0.497953 | C | -2.310422 | 3.480003 | -0.261124 |
| C | -4.989032 | -1.727985 | -0.913252 | H | 0.694949 | 3.787686 | -1.859641 |
| H | -3.024861 | -2.550751 | -1.263982 | H | -1.593935 | 4.769414 | -1.840401 |
| C | -5.713807 | -0.634798 | -0.434163 | H | -3.301808 | 3.921975 | -0.243074 |
| H | -5.597471 | 1.330954 | 0.449204 | N | 1.538114 | 1.865920 | -0.409000 |
| H | -5.508177 | -2.595969 | -1.310121 | N | 0.938754 | -0.371446 | -0.202624 |
| H | -6.800190 | -0.650742 | -0.452603 | C | 3.272146 | 0.273471 | 0.176666 |
| H | -0.121049 | -0.854963 | 1.975337 | C | 3.652651 | -0.980368 | 0.684757 |
| O | 3.293371 | 1.167147 | -0.555385 | C | 4.253837 | 1.254990 | -0.037535 |
| C | 3.294444 | 0.050291 | -1.167980 | C | 4.992193 | -1.244573 | 0.962216 |
| O | 2.177464 | -0.565545 | -1.294947 | H | 2.911613 | -1.751110 | 0.872917 |
| C | 4.554277 | -0.517362 | -1.755490 | C | 5.591370 | 0.983753 | 0.241558 |
| H | 5.421868 | -0.174941 | -1.186590 | H | 3.955472 | 2.220206 | -0.430333 |
| H | 4.507312 | -1.608941 | -1.769425 | C | 5.964473 | -0.266099 | 0.741104 |
| H | 4.658507 | -0.164662 | -2.788490 | H | 5.274882 | -2.216768 | 1.355351 |
| H | -1.277424 | 1.419329 | -0.308590 | H | 6.343098 | 1.748488 | 0.067240 |
| O | 0.851792 | 2.706984 | 0.709302 | H | 7.007807 | -0.476511 | 0.959895 |
| C | -0.238692 | 3.415293 | 0.737220 | Pd | -1.059824 | -0.339714 | -0.211377 |
| O | -1.330928 | 3.121378 | 0.229497 | O | -3.064533 | -0.450944 | -0.159825 |
| C | -0.057787 | 4.733258 | 1.480441 | C | -3.594086 | -0.393479 | 1.033892 |
| H | -1.025130 | 5.221336 | 1.613947 | C | -5.078415 | -0.728016 | 1.050278 |
| H | 0.418325 | 4.561231 | 2.450447 | O | -2.972910 | -0.102759 | 2.060892 |
| H | 0.604592 | 5.387811 | 0.903251 | H | -5.206472 | -1.804392 | 0.889439 |
| Pd | 1.200490 | 0.995179 | -0.294722 | H | -5.511175 | -0.455340 | 2.015047 |

IX



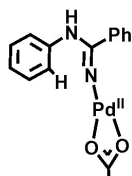
E= -1195.2026657au

| | | | | | | | |
|---|-----------|----------|-----------|---|----------|-----------|-----------|
| C | -0.718068 | 1.856262 | 0.606402 | H | 0.034119 | -5.285557 | -1.141358 |
| C | 0.277837 | 2.341572 | -0.319372 | H | 1.239004 | -1.364364 | -0.194511 |
| C | 1.845604 | 0.578730 | -0.113872 | | | | |
| H | -2.694468 | 2.111590 | 1.377240 | | | | |

X

E= -966.1382495au

| | | | |
|----|-----------|-----------|-----------|
| C | 1.016635 | 1.405648 | -0.046179 |
| C | -0.276547 | 2.033204 | -0.045524 |
| C | -1.642566 | 0.085312 | 0.047362 |
| H | 3.135104 | 1.741518 | -0.093698 |
| C | 2.155940 | 2.211002 | -0.094155 |
| C | -0.342403 | 3.469339 | -0.087552 |
| C | 0.797474 | 4.238341 | -0.135370 |
| C | 2.057345 | 3.606110 | -0.140641 |
| H | -1.333077 | 3.912909 | -0.085786 |
| H | 0.729806 | 5.321817 | -0.169596 |
| H | 2.963499 | 4.205575 | -0.179037 |
| N | -1.483133 | 1.429153 | -0.011931 |
| N | -0.653130 | -0.772802 | 0.159461 |
| C | -3.054487 | -0.393500 | 0.000869 |
| C | -3.374984 | -1.682468 | -0.456445 |
| C | -4.091299 | 0.458065 | 0.414319 |
| C | -4.698982 | -2.117142 | -0.478188 |
| H | -2.596924 | -2.340708 | -0.834915 |
| C | -5.413143 | 0.018128 | 0.398959 |
| H | -3.840664 | 1.459413 | 0.744646 |
| C | -5.721409 | -1.270197 | -0.044453 |
| H | -4.932385 | -3.112746 | -0.844783 |
| H | -6.205074 | 0.683565 | 0.731418 |
| H | -6.753445 | -1.609573 | -0.061525 |
| O | 3.408221 | -0.636297 | -0.058868 |
| C | 3.410059 | -1.920839 | 0.027689 |
| O | 2.313560 | -2.542331 | 0.129925 |
| C | 4.730541 | -2.647910 | 0.012316 |
| H | 5.304816 | -2.354836 | -0.872505 |
| H | 5.316545 | -2.360356 | 0.892272 |
| H | 4.571811 | -3.727733 | 0.015071 |
| H | -0.942883 | -1.739113 | 0.292939 |
| Pd | 1.314118 | -0.526168 | 0.057093 |

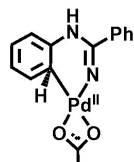
XI

E= -966.7254719au

| | | | |
|---|-----------|-----------|-----------|
| H | 1.204776 | 1.318310 | 1.713185 |
| C | 0.985476 | 2.090819 | 0.984186 |
| C | -0.070954 | 1.909201 | 0.081212 |
| C | 1.742384 | 3.260982 | 0.947132 |
| C | -0.897451 | 0.657651 | 0.123712 |
| C | -0.352850 | 2.908693 | -0.863333 |
| C | 1.457337 | 4.254678 | 0.008120 |
| H | 2.556175 | 3.395787 | 1.653815 |
| N | -2.261298 | 0.891370 | 0.091323 |
| N | -0.372908 | -0.510262 | 0.172957 |
| C | 0.410906 | 4.075374 | -0.899124 |
| H | -1.153353 | 2.760711 | -1.583346 |
| H | 2.051051 | 5.164273 | -0.019384 |
| C | -3.346237 | -0.002332 | 0.041100 |
| H | -2.513324 | 1.862720 | 0.209980 |
| H | 0.192012 | 4.840036 | -1.639359 |
| C | -4.636161 | 0.557279 | 0.079002 |
| C | -3.205532 | -1.394595 | -0.058352 |
| C | -5.761826 | -0.257322 | 0.014010 |
| H | -4.751853 | 1.636889 | 0.156968 |
| C | -4.345290 | -2.197969 | -0.125693 |
| H | -2.217438 | -1.833765 | -0.077189 |
| C | -5.624910 | -1.643988 | -0.090470 |
| H | -6.749218 | 0.195511 | 0.044765 |
| H | -4.221859 | -3.274964 | -0.203429 |
| H | -6.503083 | -2.280991 | -0.140892 |
| O | 3.168231 | -2.432608 | -0.087568 |
| C | 3.800246 | -1.338276 | -0.181698 |
| O | 3.131621 | -0.244488 | -0.132541 |
| C | 5.291218 | -1.295400 | -0.375862 |
| H | 5.738483 | -2.241171 | -0.062840 |
| H | 5.511483 | -1.134982 | -1.437767 |

| | | | |
|----|----------|-----------|----------|
| H | 5.722655 | -0.462259 | 0.185440 |
| Pd | 1.315130 | -1.319693 | 0.065376 |

XII

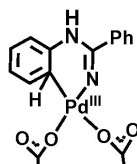


E= -966.73264au

| | | | |
|---|-----------|-----------|-----------|
| O | 1.863747 | -2.466253 | -0.304469 |
| C | 3.066795 | -2.047695 | -0.309650 |
| O | 3.307492 | -0.829487 | -0.014913 |
| C | 4.189578 | -2.978177 | -0.691487 |
| H | 4.254069 | -3.034130 | -1.784704 |
| H | 5.141101 | -2.606308 | -0.304739 |
| H | 3.989635 | -3.984941 | -0.315362 |
| H | -2.699342 | -2.315345 | -0.055546 |
| C | -3.460028 | -1.541831 | -0.051022 |
| C | -3.049088 | -0.199479 | -0.008346 |
| C | -4.814198 | -1.861599 | -0.085168 |
| C | -1.589099 | 0.110570 | 0.030565 |
| C | -4.022445 | 0.811834 | 0.003143 |
| C | -5.779266 | -0.849054 | -0.079228 |
| H | -5.119893 | -2.903784 | -0.121751 |
| N | -1.248019 | 1.412774 | -0.434610 |
| N | -0.745594 | -0.756848 | 0.440520 |
| C | -5.379869 | 0.486897 | -0.032628 |
| H | -3.720697 | 1.853296 | 0.068914 |
| H | -6.835796 | -1.101687 | -0.109552 |
| C | 0.017218 | 1.930238 | -0.231638 |
| H | -1.762629 | 1.752744 | -1.238051 |
| H | -6.123466 | 1.279327 | -0.016827 |
| C | 0.592311 | 2.826991 | -1.153042 |
| C | 0.738862 | 1.595783 | 0.958318 |
| C | 1.852612 | 3.357587 | -0.912942 |
| H | 0.050801 | 3.085606 | -2.059376 |
| C | 2.021351 | 2.167879 | 1.169744 |
| C | 2.587612 | 3.020283 | 0.237337 |
| H | 2.284853 | 4.034853 | -1.644868 |

| | | | |
|----|----------|-----------|----------|
| H | 2.549344 | 1.925126 | 2.087016 |
| H | 3.579017 | 3.432200 | 0.393435 |
| H | 0.185563 | 1.209693 | 1.812723 |
| Pd | 1.195190 | -0.474643 | 0.276927 |

XIII



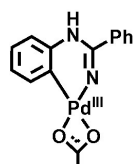
E= -1195.1768083au

| | | | |
|---|-----------|-----------|-----------|
| O | 3.051970 | -0.290339 | 1.970602 |
| C | 3.612202 | -0.710628 | 0.952865 |
| O | 3.051235 | -0.784809 | -0.224185 |
| C | 5.055118 | -1.196404 | 0.965355 |
| H | 5.071972 | -2.283647 | 0.830033 |
| H | 5.617712 | -0.757416 | 0.135460 |
| H | 5.525618 | -0.943944 | 1.917802 |
| H | -3.133221 | -1.530920 | -0.695091 |
| C | -3.761878 | -0.777674 | -0.235354 |
| C | -3.185935 | 0.431548 | 0.186464 |
| C | -5.120598 | -1.004053 | -0.030436 |
| C | -1.741456 | 0.686865 | -0.049211 |
| C | -3.981887 | 1.394398 | 0.829063 |
| C | -5.914195 | -0.038446 | 0.595294 |
| H | -5.561544 | -1.940724 | -0.359321 |
| N | -1.353085 | 2.036926 | -0.097102 |
| N | -0.875691 | -0.226717 | -0.262110 |
| C | -5.341329 | 1.158235 | 1.029788 |
| H | -3.534224 | 2.311343 | 1.200860 |
| H | -6.973715 | -0.221885 | 0.751667 |
| C | -0.019571 | 2.442433 | -0.246198 |
| H | -2.043413 | 2.648827 | -0.517931 |
| H | -5.948570 | 1.904869 | 1.533723 |
| C | 0.288143 | 3.488075 | -1.124716 |
| C | 1.016854 | 1.842686 | 0.518833 |
| C | 1.603048 | 3.933916 | -1.247354 |
| H | -0.500144 | 3.940966 | -1.721033 |
| C | 2.335467 | 2.323395 | 0.384261 |

| | | | |
|----|-----------|-----------|-----------|
| C | 2.634764 | 3.349661 | -0.504719 |
| H | 1.823343 | 4.742571 | -1.939074 |
| H | 3.094788 | 1.877832 | 1.015509 |
| H | 3.654322 | 3.706753 | -0.608684 |
| H | 0.775740 | 1.244628 | 1.400397 |
| Pd | 1.062708 | -0.469383 | -0.196649 |
| O | -1.276290 | -2.645885 | -0.065715 |
| C | -0.202601 | -3.081470 | -0.502056 |
| O | 0.907458 | -2.434944 | -0.671494 |
| C | -0.089042 | -4.548359 | -0.918411 |
| H | -1.015568 | -5.076849 | -0.688169 |
| H | 0.114215 | -4.604573 | -1.992901 |
| H | 0.751946 | -5.014941 | -0.397409 |

| | | | |
|----|-----------|-----------|-----------|
| H | -3.593826 | 1.193617 | 1.418597 |
| C | -5.655312 | -1.217961 | 0.193196 |
| H | -5.078566 | -2.740896 | -1.222399 |
| H | -5.927249 | 0.396450 | 1.598987 |
| H | -6.677033 | -1.575833 | 0.284456 |
| H | -2.190014 | 2.126553 | -0.139443 |
| O | 3.314862 | -0.773641 | 0.174827 |
| C | 3.262279 | -2.054625 | 0.233443 |
| O | 2.140578 | -2.633517 | 0.143519 |
| C | 4.537521 | -2.836991 | 0.417270 |
| H | 5.259839 | -2.555400 | -0.355725 |
| H | 4.981803 | -2.587708 | 1.387247 |
| H | 4.338358 | -3.909222 | 0.370939 |
| Pd | 1.209144 | -0.601406 | -0.088455 |

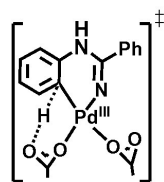
XIV



E= -966.1183409au

| | | | |
|---|-----------|-----------|-----------|
| C | 1.069009 | 1.389545 | -0.068507 |
| C | -0.123871 | 2.133379 | -0.055607 |
| C | -1.619910 | 0.175957 | -0.178565 |
| H | 3.211985 | 1.531919 | -0.101685 |
| C | 2.282353 | 2.091603 | -0.090455 |
| C | -0.096349 | 3.540440 | -0.048868 |
| C | 1.117721 | 4.213401 | -0.051062 |
| C | 2.312676 | 3.486965 | -0.071651 |
| H | -1.031981 | 4.097329 | -0.046036 |
| H | 1.132061 | 5.299574 | -0.042133 |
| H | 3.267643 | 4.005461 | -0.069409 |
| N | -1.387471 | 1.517419 | -0.037880 |
| N | -0.669701 | -0.652561 | -0.451587 |
| C | -3.024166 | -0.293955 | -0.045774 |
| C | -3.445969 | -1.418114 | -0.772836 |
| C | -3.925440 | 0.353987 | 0.813600 |
| C | -4.756454 | -1.874175 | -0.652359 |
| H | -2.740217 | -1.914224 | -1.430781 |
| C | -5.236883 | -0.106070 | 0.927476 |

TSVI

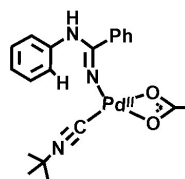


E= -1195.1610315au

| | | | |
|---|-----------|-----------|-----------|
| O | 2.189342 | 0.324493 | 1.951304 |
| C | 2.940910 | -0.480163 | 1.326107 |
| O | 2.835745 | -0.742573 | 0.077664 |
| C | 4.025888 | -1.209473 | 2.083103 |
| H | 3.637587 | -2.207119 | 2.319111 |
| H | 4.913068 | -1.332063 | 1.457251 |
| H | 4.270479 | -0.690498 | 3.011387 |
| H | -3.312380 | -0.837667 | -1.758459 |
| C | -3.795539 | -0.574969 | -0.823191 |
| C | -3.108383 | 0.228980 | 0.100325 |
| C | -5.085529 | -1.013584 | -0.536210 |
| C | -1.730797 | 0.684120 | -0.212227 |
| C | -3.719687 | 0.571814 | 1.317049 |
| C | -5.697252 | -0.660236 | 0.669935 |
| H | -5.615857 | -1.630334 | -1.255901 |
| N | -1.334881 | 1.902112 | 0.303568 |
| N | -0.961547 | -0.013080 | -0.980250 |
| C | -5.011660 | 0.128689 | 1.596300 |

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -3.173297 | 1.148265 | 2.058237 | H | -0.670277 | -0.214371 | 2.302860 |
| H | -6.703573 | -1.005022 | 0.890405 | C | -0.273101 | -1.224803 | 2.296833 |
| C | -0.090168 | 2.495350 | 0.026467 | C | 0.757541 | -1.552484 | 1.405153 |
| H | -2.091275 | 2.535334 | 0.535232 | C | -0.779331 | -2.183105 | 3.174576 |
| H | -5.476670 | 0.389325 | 2.542633 | C | 1.317041 | -0.520819 | 0.457475 |
| C | -0.062874 | 3.877682 | -0.206138 | C | 1.274935 | -2.856258 | 1.410942 |
| C | 1.092984 | 1.716321 | -0.040852 | C | -0.267020 | -3.483050 | 3.167051 |
| C | 1.126512 | 4.496061 | -0.577701 | H | -1.572770 | -1.914551 | 3.867103 |
| H | -0.980754 | 4.457842 | -0.139777 | N | 2.697506 | -0.367519 | 0.636782 |
| C | 2.269702 | 2.380535 | -0.466203 | N | 0.671584 | 0.143503 | -0.426169 |
| C | 2.297182 | 3.743954 | -0.732226 | C | 0.758959 | -3.817783 | 2.281621 |
| H | 1.134937 | 5.566072 | -0.766329 | H | 2.064435 | -3.120534 | 0.712810 |
| H | 3.184316 | 1.798777 | -0.533187 | H | -0.666522 | -4.230464 | 3.847298 |
| H | 3.220502 | 4.226343 | -1.038867 | C | 3.623629 | 0.430013 | -0.048935 |
| H | 1.425824 | 0.962366 | 0.962549 | H | 3.067855 | -0.853254 | 1.441294 |
| Pd | 0.907106 | -0.384369 | -0.611189 | H | 1.155982 | -4.829283 | 2.263711 |
| O | 0.857335 | -2.307292 | -1.271483 | C | 4.945512 | 0.444715 | 0.436896 |
| C | 0.858392 | -3.195796 | -0.307574 | C | 3.307730 | 1.193223 | -1.186319 |
| O | 0.818417 | -2.948276 | 0.895665 | C | 5.927360 | 1.198816 | -0.197424 |
| C | 0.930451 | -4.625752 | -0.838356 | H | 5.199330 | -0.143746 | 1.317273 |
| H | 1.904158 | -4.792676 | -1.312368 | C | 4.305993 | 1.942713 | -1.810847 |
| H | 0.799918 | -5.331779 | -0.015648 | H | 2.290937 | 1.186516 | -1.555133 |
| H | 0.163658 | -4.791444 | -1.601636 | C | 5.615689 | 1.956487 | -1.329568 |

II_t-BuNC

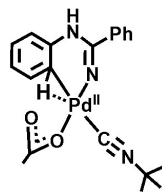


E= -1217.4385921au

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|----------|-----------|
| O | -0.911010 | -2.313502 | -1.762110 | H | -0.805811 | 3.755444 | 2.190046 |
| C | -2.149498 | -2.370337 | -2.069045 | H | -0.498533 | 4.434244 | 0.578479 |
| O | -2.919308 | -1.409587 | -1.742648 | C | -3.114038 | 4.391129 | -0.356496 |
| C | -2.680017 | -3.561577 | -2.825086 | H | -2.379834 | 4.511420 | -1.158849 |
| H | -2.355801 | -4.485309 | -2.335881 | H | -3.987091 | 3.867584 | -0.757885 |
| H | -3.769775 | -3.526686 | -2.881498 | H | -3.427232 | 5.384227 | -0.018418 |
| H | -2.263107 | -3.562254 | -3.838530 | C | -3.548596 | 3.410129 | 1.943686 |
| Pd | -1.194031 | -0.401342 | -0.849136 | H | -3.123964 | 2.835145 | 2.772467 |

| | | | |
|---|-----------|----------|----------|
| H | -3.869533 | 4.384605 | 2.325554 |
| H | -4.426428 | 2.878414 | 1.563830 |

III_{t-BuNC}

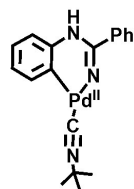


E= -1217.4231685au

| | | | |
|----|-----------|-----------|-----------|
| C | -0.364896 | -2.431064 | 0.441575 |
| C | -1.232315 | -2.310540 | -0.680763 |
| C | -2.156688 | -0.119582 | -0.004337 |
| H | 1.247091 | -3.522516 | 1.337957 |
| C | 0.603318 | -3.459599 | 0.467672 |
| C | -1.089544 | -3.216712 | -1.749811 |
| C | -0.119970 | -4.209945 | -1.698616 |
| C | 0.741011 | -4.336588 | -0.597198 |
| H | -1.740349 | -3.128957 | -2.616545 |
| H | -0.023899 | -4.893386 | -2.538726 |
| H | 1.498687 | -5.113455 | -0.580819 |
| N | -2.233994 | -1.359493 | -0.702415 |
| N | -1.096474 | 0.434040 | 0.433192 |
| C | -3.491260 | 0.537483 | 0.187722 |
| C | -3.546104 | 1.924097 | 0.401859 |
| C | -4.690721 | -0.191368 | 0.172225 |
| C | -4.767858 | 2.564478 | 0.586896 |
| H | -2.612087 | 2.475251 | 0.424489 |
| C | -5.915929 | 0.452572 | 0.358925 |
| H | -4.665682 | -1.269435 | 0.043064 |
| C | -5.959262 | 1.831750 | 0.562992 |
| H | -4.794510 | 3.639141 | 0.748271 |
| H | -6.835039 | -0.127634 | 0.352062 |
| H | -6.912767 | 2.333333 | 0.705941 |
| H | -2.896670 | -1.408551 | -1.465841 |
| Pd | 0.727748 | -0.387486 | 0.151742 |
| O | 2.687020 | -1.087983 | -0.119592 |
| C | 3.189488 | -1.529436 | 0.995212 |
| C | 4.636047 | -2.004299 | 0.874289 |

| | | | |
|---|-----------|-----------|-----------|
| O | 2.578325 | -1.602773 | 2.068746 |
| H | 5.039077 | -2.239096 | 1.861770 |
| H | 4.677852 | -2.900354 | 0.243852 |
| H | 5.252336 | -1.240559 | 0.389041 |
| H | -0.629901 | -1.938438 | 1.378472 |
| C | 1.417526 | 1.416021 | -0.176017 |
| N | 1.848554 | 2.485492 | -0.347215 |
| C | 2.404104 | 3.807813 | -0.534107 |
| C | 1.559375 | 4.794038 | 0.293039 |
| H | 1.962576 | 5.805029 | 0.174528 |
| H | 0.517903 | 4.791608 | -0.042643 |
| H | 1.582988 | 4.530738 | 1.354765 |
| C | 3.862496 | 3.776871 | -0.040922 |
| H | 3.908765 | 3.510404 | 1.019315 |
| H | 4.449254 | 3.048327 | -0.608526 |
| H | 4.311694 | 4.766736 | -0.172246 |
| C | 2.334158 | 4.141147 | -2.035629 |
| H | 1.298521 | 4.129928 | -2.389132 |
| H | 2.749457 | 5.139830 | -2.205560 |
| H | 2.911092 | 3.419363 | -2.621823 |

IV_{t-BuNC}

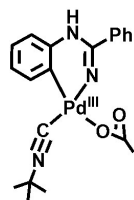


E= -988.3423999au

| | | | |
|---|-----------|-----------|----------|
| C | 0.271748 | 1.371464 | 0.063589 |
| C | -1.001379 | 1.982441 | 0.074532 |
| C | -2.355434 | -0.104467 | 0.007403 |
| H | 2.388813 | 1.763115 | 0.093783 |
| C | 1.399882 | 2.207272 | 0.102378 |
| C | -1.100934 | 3.390312 | 0.131434 |
| C | 0.031579 | 4.189523 | 0.175817 |
| C | 1.296192 | 3.596947 | 0.159756 |
| H | -2.087842 | 3.850473 | 0.136588 |
| H | -0.073709 | 5.270341 | 0.220248 |
| H | 2.194392 | 4.207981 | 0.193447 |
| N | -2.204594 | 1.278687 | 0.028538 |

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| N | -1.390143 | -0.936347 | 0.003981 | C | 2.546938 | 0.259893 | -0.219509 |
| C | -3.777420 | -0.578482 | -0.020138 | H | -1.880144 | 2.736316 | -0.472502 |
| C | -4.096501 | -1.804596 | 0.582511 | C | -0.860652 | 3.007249 | -0.222713 |
| C | -4.795972 | 0.150813 | -0.652370 | C | 1.721456 | 3.784334 | 0.403270 |
| C | -5.405571 | -2.279839 | 0.568560 | C | 0.722454 | 4.745391 | 0.336934 |
| H | -3.301025 | -2.369782 | 1.056835 | C | -0.577672 | 4.353183 | 0.014199 |
| C | -6.107356 | -0.328536 | -0.668014 | H | 2.745124 | 4.078587 | 0.630763 |
| H | -4.562857 | 1.078657 | -1.168620 | H | 0.959541 | 5.788551 | 0.525476 |
| C | -6.417304 | -1.542199 | -0.053556 | H | -1.373445 | 5.090667 | -0.049375 |
| H | -5.639145 | -3.227813 | 1.046236 | N | 2.524891 | 1.543212 | 0.249797 |
| H | -6.883251 | 0.243867 | -1.169669 | N | 1.523547 | -0.251546 | -0.812128 |
| H | -7.438327 | -1.914348 | -0.063602 | C | 3.802950 | -0.518264 | -0.054545 |
| H | -3.042174 | 1.822260 | 0.181748 | C | 4.133299 | -1.498132 | -1.003889 |
| Pd | 0.498346 | -0.633510 | -0.001315 | C | 4.645572 | -0.305996 | 1.047769 |
| C | 2.501344 | -0.757232 | -0.033839 | C | 5.302799 | -2.240577 | -0.858621 |
| N | 3.667656 | -0.872838 | -0.054695 | H | 3.472080 | -1.657769 | -1.849218 |
| C | 5.105152 | -1.014278 | -0.081218 | C | 5.815779 | -1.051632 | 1.185533 |
| C | 5.719478 | 0.394172 | -0.187408 | H | 4.370707 | 0.415127 | 1.812788 |
| H | 6.811222 | 0.314899 | -0.210714 | C | 6.147653 | -2.016868 | 0.232044 |
| H | 5.387235 | 0.895493 | -1.101699 | H | 5.557024 | -2.993148 | -1.599419 |
| H | 5.434156 | 1.009185 | 0.671763 | H | 6.461197 | -0.886755 | 2.043570 |
| C | 5.539171 | -1.706467 | 1.224588 | H | 7.058979 | -2.597914 | 0.342251 |
| H | 5.248501 | -1.111130 | 2.095570 | H | 3.428747 | 1.971336 | 0.407347 |
| H | 5.081040 | -2.696565 | 1.310966 | Pd | -0.378187 | 0.043199 | -0.457792 |
| H | 6.627622 | -1.825090 | 1.230873 | C | -2.337723 | 0.251482 | -0.118708 |
| C | 5.476424 | -1.869366 | -1.307416 | N | -3.479016 | 0.106811 | 0.063034 |
| H | 5.140704 | -1.389918 | -2.232046 | C | -4.838208 | -0.387829 | 0.219963 |
| H | 6.563693 | -1.990527 | -1.352321 | C | -5.794125 | 0.814854 | 0.183873 |
| H | 5.018023 | -2.861054 | -1.243301 | H | -6.823139 | 0.458949 | 0.295062 |

V_{t-BuNC}

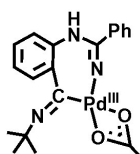


E= -1216.7904936au

| | | | | | | | |
|---|----------|----------|-----------|---|-----------|-----------|----------|
| C | 0.117544 | 1.998621 | -0.139722 | H | -5.916340 | -1.502306 | 1.723556 |
| C | 1.427559 | 2.429587 | 0.163963 | H | -4.204724 | -1.967587 | 1.569833 |

| | | | |
|---|-----------|-----------|-----------|
| O | -1.097793 | -1.928571 | -0.773845 |
| C | -1.448620 | -2.738249 | 0.190190 |
| O | -2.527566 | -3.338262 | 0.209476 |
| C | -0.441071 | -2.938377 | 1.325113 |
| H | 0.557051 | -3.135301 | 0.920039 |
| H | -0.371267 | -2.023858 | 1.928334 |
| H | -0.752770 | -3.763440 | 1.969755 |

VI_{t-BuNC}

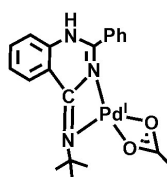


E=-1216.8026447au

| | | | |
|---|-----------|-----------|-----------|
| C | -0.870713 | 1.208371 | -1.048209 |
| C | 0.343754 | 1.139655 | -1.777704 |
| C | 1.822069 | -0.284077 | -0.271401 |
| H | -2.972913 | 1.648679 | -1.127622 |
| C | -2.045420 | 1.652970 | -1.691810 |
| C | 0.345175 | 1.603434 | -3.107379 |
| C | -0.812739 | 2.074100 | -3.712141 |
| C | -2.023398 | 2.089940 | -3.008241 |
| H | 1.274535 | 1.572160 | -3.671641 |
| H | -0.774853 | 2.413009 | -4.743439 |
| H | -2.935083 | 2.438224 | -3.483216 |
| N | 1.558284 | 0.710414 | -1.241506 |
| N | 0.987390 | -0.992219 | 0.374914 |
| C | 3.289733 | -0.473243 | -0.015412 |
| C | 3.761473 | -1.749517 | 0.327177 |
| C | 4.196790 | 0.595201 | -0.088233 |
| C | 5.116347 | -1.953266 | 0.577538 |
| H | 3.051989 | -2.567909 | 0.390625 |
| C | 5.554012 | 0.386733 | 0.164766 |
| H | 3.840833 | 1.597736 | -0.310723 |
| C | 6.017440 | -0.887548 | 0.494211 |
| H | 5.471527 | -2.947367 | 0.834882 |
| H | 6.245652 | 1.223330 | 0.112623 |
| H | 7.074091 | -1.049719 | 0.689002 |
| H | 2.352059 | 0.887222 | -1.843921 |

| | | | |
|----|-----------|-----------|-----------|
| Pd | -0.968460 | -1.178013 | 0.232760 |
| C | -0.964238 | 0.792797 | 0.364085 |
| N | -1.126775 | 1.288165 | 1.479608 |
| C | -1.199766 | 2.667408 | 2.003405 |
| C | -0.378740 | 2.673913 | 3.305105 |
| H | -0.435635 | 3.658218 | 3.783107 |
| H | -0.760044 | 1.921267 | 4.001648 |
| H | 0.673163 | 2.447481 | 3.101359 |
| C | -0.638677 | 3.703835 | 1.014661 |
| H | 0.395703 | 3.466165 | 0.742996 |
| H | -1.232262 | 3.757691 | 0.097714 |
| H | -0.647627 | 4.695055 | 1.482299 |
| C | -2.682226 | 2.947059 | 2.310470 |
| H | -3.087191 | 2.184260 | 2.982334 |
| H | -2.785508 | 3.926660 | 2.790538 |
| H | -3.279741 | 2.948606 | 1.392486 |
| O | -1.582173 | -3.411013 | -0.025538 |
| C | -2.774576 | -3.014505 | 0.080836 |
| C | -3.924984 | -3.997323 | 0.059526 |
| O | -3.042406 | -1.767454 | 0.236038 |
| H | -4.760789 | -3.590424 | -0.516969 |
| H | -3.604095 | -4.953845 | -0.358297 |
| H | -4.278206 | -4.160272 | 1.084673 |

VII_{t-BuNC}

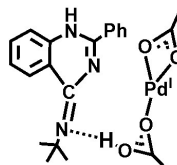


E= -1216.8698312au

| | | | |
|---|-----------|----------|-----------|
| H | 2.033481 | 1.541550 | 0.410683 |
| C | 1.720103 | 2.570751 | 0.272389 |
| C | 0.361682 | 2.882377 | 0.096169 |
| C | 2.674653 | 3.586129 | 0.263292 |
| C | -0.655873 | 1.807293 | 0.106904 |
| C | -0.013940 | 4.224374 | -0.100835 |
| C | 2.293317 | 4.916858 | 0.079848 |
| H | 3.720315 | 3.326853 | 0.398427 |
| N | -1.933499 | 2.150341 | 0.484378 |

| | | | |
|----|-----------|-----------|-----------|
| N | -0.368817 | 0.582975 | -0.230406 |
| C | 0.945798 | 5.233857 | -0.107433 |
| H | -1.049981 | 4.486365 | -0.301604 |
| H | 3.042367 | 5.704009 | 0.073170 |
| C | -3.010582 | 1.318423 | 0.205536 |
| H | 0.642806 | 6.263904 | -0.272856 |
| C | -4.323414 | 1.806930 | 0.267018 |
| C | -2.741691 | -0.012567 | -0.192504 |
| C | -5.375720 | 0.998257 | -0.140251 |
| H | -4.503966 | 2.825058 | 0.603074 |
| C | -3.823614 | -0.779852 | -0.657491 |
| C | -5.123415 | -0.288353 | -0.633084 |
| H | -6.391868 | 1.379819 | -0.102237 |
| H | -3.637941 | -1.768272 | -1.054084 |
| H | -5.940264 | -0.904333 | -0.995914 |
| C | -1.328680 | -0.448091 | -0.120510 |
| H | -2.109618 | 3.085768 | 0.822350 |
| N | -0.746768 | -1.597656 | 0.014259 |
| Pd | 1.386639 | -0.948827 | -0.161240 |
| C | -1.261342 | -2.952849 | 0.307315 |
| C | -2.434215 | -2.975007 | 1.309984 |
| H | -2.619858 | -4.009236 | 1.619988 |
| H | -2.173493 | -2.400134 | 2.205754 |
| H | -3.370343 | -2.579467 | 0.914673 |
| C | -1.602923 | -3.669043 | -1.016819 |
| H | -2.436579 | -3.203487 | -1.551573 |
| H | -0.732858 | -3.659600 | -1.681037 |
| H | -1.872136 | -4.712396 | -0.817435 |
| C | -0.084069 | -3.707723 | 0.964823 |
| H | 0.194816 | -3.233329 | 1.911518 |
| H | -0.373091 | -4.745332 | 1.168931 |
| H | 0.798757 | -3.704574 | 0.320209 |
| O | 3.154534 | -2.423021 | -0.016892 |
| C | 3.941372 | -1.437326 | -0.109892 |
| C | 5.442147 | -1.664256 | -0.100888 |
| O | 3.507064 | -0.244031 | -0.228944 |
| H | 5.921586 | -0.974356 | 0.600999 |
| H | 5.677935 | -2.695936 | 0.168426 |
| H | 5.847766 | -1.451144 | -1.096774 |

VIII_{t-BuNC}

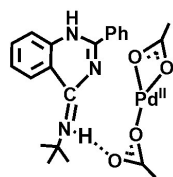


E= -1445.9534219au

| | | | |
|----|-----------|-----------|-----------|
| H | 2.652103 | 3.991263 | -0.123375 |
| C | 3.194084 | 3.048571 | -0.125914 |
| C | 2.499658 | 1.830548 | -0.214657 |
| C | 4.587834 | 3.065137 | -0.094827 |
| C | 1.018681 | 1.791185 | -0.239600 |
| C | 3.223194 | 0.629078 | -0.278575 |
| C | 5.301170 | 1.865948 | -0.146957 |
| H | 5.114873 | 4.013458 | -0.038358 |
| N | 0.353645 | 2.778773 | 0.444064 |
| N | 0.387624 | 0.853487 | -0.875519 |
| C | 4.615757 | 0.651691 | -0.239949 |
| H | 2.685448 | -0.310946 | -0.338351 |
| H | 6.387267 | 1.878144 | -0.116949 |
| C | -0.995796 | 2.995607 | 0.220618 |
| H | 5.166674 | -0.283886 | -0.274258 |
| C | -1.602312 | 4.178900 | 0.668981 |
| C | -1.720337 | 2.025923 | -0.516398 |
| C | -2.916516 | 4.451400 | 0.322142 |
| H | -1.024820 | 4.885760 | 1.259591 |
| C | -3.030656 | 2.368191 | -0.896353 |
| C | -3.623993 | 3.556857 | -0.490924 |
| H | -3.383520 | 5.371625 | 0.660940 |
| H | -3.593312 | 1.695047 | -1.524200 |
| H | -4.639097 | 3.784852 | -0.800795 |
| C | -1.007559 | 0.754656 | -0.820760 |
| H | 0.870040 | 3.410708 | 1.039828 |
| N | -1.433550 | -0.461571 | -1.034484 |
| Pd | 0.170628 | -1.650882 | 0.643534 |
| C | -2.797325 | -1.051935 | -0.988157 |
| C | -3.628619 | -0.612739 | 0.235786 |
| H | -4.522071 | -1.244131 | 0.304378 |
| H | -3.039053 | -0.748355 | 1.148630 |

| | | | | | | | |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -3.965034 | 0.423779 | 0.196441 | N | -0.289911 | 2.721557 | 0.230181 |
| C | -3.518391 | -0.827529 | -2.337869 | N | 0.169532 | 0.777776 | -0.970969 |
| H | -3.714379 | 0.222381 | -2.567201 | C | 4.337562 | 1.512676 | -0.431239 |
| H | -2.914855 | -1.232760 | -3.157398 | H | 2.667787 | 0.159108 | -0.572668 |
| H | -4.480646 | -1.351971 | -2.333820 | H | 5.809126 | 3.080283 | -0.251483 |
| C | -2.583780 | -2.579510 | -0.859726 | C | -1.648670 | 2.637539 | -0.008490 |
| H | -2.069754 | -2.820185 | 0.078094 | H | 5.071677 | 0.716661 | -0.512422 |
| H | -3.550935 | -3.094662 | -0.867606 | C | -2.510220 | 3.670113 | 0.393887 |
| H | -1.984688 | -2.965095 | -1.690756 | C | -2.131960 | 1.521960 | -0.734016 |
| O | -0.877003 | -0.988722 | 2.446915 | C | -3.838217 | 3.640862 | 0.000659 |
| C | -0.135869 | -1.685886 | 3.226597 | H | -2.120168 | 4.498627 | 0.979049 |
| C | -0.443583 | -1.655232 | 4.712752 | C | -3.469775 | 1.560140 | -1.171925 |
| O | 0.813162 | -2.387456 | 2.786571 | C | -4.312727 | 2.600819 | -0.814611 |
| H | 0.317950 | -2.197026 | 5.277307 | H | -4.503937 | 4.445133 | 0.299389 |
| H | -0.501464 | -0.618973 | 5.062025 | H | -3.838311 | 0.771235 | -1.811656 |
| H | -1.422817 | -2.113706 | 4.892373 | H | -5.340052 | 2.608725 | -1.164512 |
| C | 1.237735 | -2.438244 | -2.181639 | C | -1.161345 | 0.456993 | -1.002938 |
| O | 1.458557 | -2.510326 | -0.967996 | H | 0.066411 | 3.459401 | 0.822978 |
| C | 2.140129 | -3.104046 | -3.190609 | N | -1.399105 | -0.808728 | -1.311995 |
| H | 1.547130 | -3.722229 | -3.871828 | Pd | 0.862973 | -1.378654 | 0.835371 |
| H | 2.638524 | -2.338069 | -3.795180 | C | -2.558933 | -1.738447 | -1.099332 |
| H | 2.885916 | -3.713940 | -2.679915 | C | -3.405219 | -1.354581 | 0.127754 |
| O | 0.228164 | -1.791447 | -2.722127 | H | -4.046006 | -2.206620 | 0.378766 |
| H | -0.326491 | -1.303145 | -2.011280 | H | -2.752877 | -1.147216 | 0.983022 |

IX_{t-BuNC}

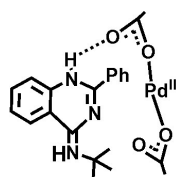


E= -1445.9581505au

| | | | | | | | |
|---|----------|----------|-----------|---|-----------|-----------|-----------|
| H | 1.717994 | 4.356628 | -0.169394 | H | -2.715980 | -3.862694 | -0.714993 |
| C | 2.442352 | 3.546405 | -0.205886 | H | -1.240746 | -3.418678 | -1.612412 |
| C | 2.021162 | 2.211278 | -0.345443 | O | -0.604657 | -0.569579 | 2.154146 |
| C | 3.799614 | 3.857006 | -0.174617 | C | -0.293315 | -1.210097 | 3.233616 |
| C | 0.585554 | 1.867478 | -0.377810 | C | -1.154718 | -0.938919 | 4.457925 |
| C | 2.981922 | 1.193080 | -0.470132 | O | 0.650603 | -2.022881 | 3.280909 |
| C | 4.750205 | 2.838650 | -0.280913 | H | -0.729425 | -1.419785 | 5.341092 |
| H | 4.113874 | 4.892240 | -0.078058 | H | -1.244982 | 0.139401 | 4.627053 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.166183 | -1.327152 | 4.289059 |
| C | 1.920582 | -2.421690 | -1.702251 |
| O | 2.304834 | -2.132611 | -0.515425 |
| C | 2.981510 | -3.033107 | -2.613145 |
| H | 2.586567 | -3.943475 | -3.075643 |
| H | 3.209387 | -2.332368 | -3.425058 |
| H | 3.896985 | -3.262314 | -2.064089 |
| O | 0.775338 | -2.237647 | -2.181845 |
| H | -0.511437 | -1.317872 | -1.578829 |

X_t-BuNC

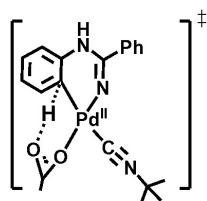


E= -1445.9864412au

| | | | |
|---|-----------|-----------|-----------|
| C | 1.520804 | -1.115723 | 1.610204 |
| C | 0.146907 | -0.834118 | 1.754912 |
| C | 0.474926 | 1.282699 | 0.742970 |
| H | 3.083679 | -2.551939 | 2.081393 |
| C | 2.023699 | -2.321314 | 2.140355 |
| C | -0.714967 | -1.746259 | 2.395350 |
| C | -0.194371 | -2.927775 | 2.890798 |
| C | 1.178783 | -3.216927 | 2.771634 |
| H | -1.764923 | -1.492195 | 2.491971 |
| H | -0.852324 | -3.635747 | 3.386113 |
| H | 1.576100 | -4.141427 | 3.179161 |
| N | -0.344316 | 0.365068 | 1.279741 |
| N | 1.783615 | 1.083257 | 0.599486 |
| C | -0.080839 | 2.577754 | 0.293332 |
| C | -1.398363 | 2.691757 | -0.178877 |
| C | 0.744718 | 3.714281 | 0.315472 |
| C | -1.877820 | 3.927185 | -0.611929 |
| H | -2.039742 | 1.820480 | -0.244944 |
| C | 0.253751 | 4.947747 | -0.102366 |
| H | 1.764982 | 3.618065 | 0.669778 |
| C | -1.059289 | 5.057154 | -0.568446 |
| H | -2.893288 | 4.001607 | -0.989923 |
| H | 0.896199 | 5.823250 | -0.068797 |

| | | | |
|----|-----------|-----------|-----------|
| H | -1.439801 | 6.018412 | -0.903151 |
| Pd | -2.181962 | -1.154724 | -1.216161 |
| C | 2.302677 | -0.111092 | 0.906636 |
| N | 3.578027 | -0.366683 | 0.577114 |
| C | 4.495748 | 0.445820 | -0.273957 |
| C | 5.729764 | -0.445229 | -0.498267 |
| H | 6.479517 | 0.097111 | -1.081416 |
| H | 6.191551 | -0.735962 | 0.453667 |
| H | 5.467391 | -1.353233 | -1.055455 |
| C | 3.838311 | 0.774771 | -1.627745 |
| H | 3.412756 | -0.125403 | -2.080793 |
| H | 3.028519 | 1.495293 | -1.507646 |
| H | 4.591560 | 1.195854 | -2.303532 |
| C | 4.908036 | 1.724436 | 0.475507 |
| H | 5.406210 | 1.480421 | 1.420617 |
| H | 5.604540 | 2.304878 | -0.139852 |
| H | 4.035679 | 2.345072 | 0.689205 |
| O | -2.974542 | 0.432000 | 1.722517 |
| C | -3.911001 | 0.222733 | 0.907163 |
| C | -5.339277 | 0.474653 | 1.374166 |
| O | -3.789910 | -0.201250 | -0.289603 |
| H | -5.733847 | -0.446130 | 1.821588 |
| H | -5.359452 | 1.256777 | 2.136970 |
| H | -5.982711 | 0.740202 | 0.532032 |
| O | 0.726987 | -1.071818 | -1.423515 |
| C | 1.320300 | -2.740749 | -3.055884 |
| H | 0.942053 | -3.737833 | -3.294801 |
| H | 1.471263 | -2.201249 | -3.999051 |
| H | 2.287787 | -2.814822 | -2.550849 |
| C | 0.328494 | -1.966702 | -2.192782 |
| O | -0.906520 | -2.294784 | -2.357729 |
| H | -1.394006 | 0.501977 | 1.366781 |
| H | 3.875216 | -1.321440 | 0.717125 |

TSI_t-BuNC

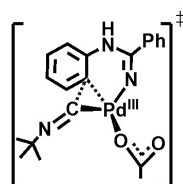


E= -1217.4036982au

| | | | |
|----|-----------|-----------|-----------|
| C | -1.101399 | -2.060184 | -0.316250 |
| C | -2.399428 | -1.492344 | -0.319482 |
| C | -1.762663 | 0.882814 | 0.018556 |
| H | 0.055818 | -3.733995 | -1.022385 |
| C | -0.937988 | -3.295629 | -0.999185 |
| C | -3.489483 | -2.209000 | -0.855471 |
| C | -3.288455 | -3.434154 | -1.473477 |
| C | -1.999355 | -3.978363 | -1.573497 |
| H | -4.486406 | -1.773228 | -0.824644 |
| H | -4.138759 | -3.963029 | -1.897019 |
| H | -1.840778 | -4.927434 | -2.077320 |
| N | -2.641433 | -0.217384 | 0.175442 |
| N | -0.530210 | 0.879515 | -0.303749 |
| C | -2.448347 | 2.202403 | 0.249002 |
| C | -2.037295 | 3.326084 | -0.483974 |
| C | -3.470533 | 2.353147 | 1.199254 |
| C | -2.646909 | 4.562380 | -0.286196 |
| H | -1.235789 | 3.203983 | -1.204742 |
| C | -4.074836 | 3.596250 | 1.402636 |
| H | -3.774582 | 1.506879 | 1.810197 |
| C | -3.670111 | 4.703184 | 0.656990 |
| H | -2.325874 | 5.420721 | -0.871118 |
| H | -4.857230 | 3.697376 | 2.150418 |
| H | -4.143635 | 5.669217 | 0.811016 |
| H | -3.618574 | 0.047550 | 0.171559 |
| Pd | 0.584821 | -0.765236 | -0.184887 |
| O | 1.862762 | -2.449122 | 0.353316 |
| C | 1.404531 | -3.054346 | 1.370531 |
| C | 2.305611 | -4.043957 | 2.084292 |
| O | 0.225915 | -2.905875 | 1.830663 |
| H | 2.350990 | -3.793570 | 3.148878 |
| H | 1.874462 | -5.047806 | 2.005476 |

| | | | |
|---|-----------|-----------|-----------|
| H | 3.308608 | -4.038596 | 1.654777 |
| H | -0.484603 | -2.266224 | 0.852777 |
| C | 2.172004 | 0.481090 | -0.241643 |
| N | 3.048133 | 1.249385 | -0.299679 |
| C | 4.097668 | 2.239983 | -0.378702 |
| C | 3.736900 | 3.383908 | 0.587079 |
| H | 4.512435 | 4.155555 | 0.542321 |
| H | 2.777326 | 3.833219 | 0.314710 |
| H | 3.668467 | 3.017204 | 1.615822 |
| C | 5.419595 | 1.565182 | 0.030361 |
| H | 5.359696 | 1.180113 | 1.052955 |
| H | 5.656959 | 0.734217 | -0.640998 |
| H | 6.232451 | 2.296977 | -0.019333 |
| C | 4.160553 | 2.743024 | -1.832927 |
| H | 3.208256 | 3.192995 | -2.129314 |
| H | 4.948046 | 3.498330 | -1.923259 |
| H | 4.385762 | 1.920921 | -2.519277 |

TSII_t-BuNC

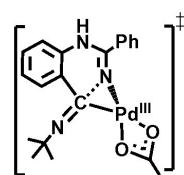


E= -1216.7637993au

| | | | |
|---|-----------|-----------|-----------|
| C | -1.272364 | -0.382783 | 1.094376 |
| C | -0.139540 | -1.021170 | 1.659379 |
| C | 1.726487 | -0.067929 | 0.227818 |
| H | -3.376681 | 0.010395 | 1.309519 |
| C | -2.514782 | -0.473884 | 1.758801 |
| C | -0.305080 | -1.743029 | 2.859535 |
| C | -1.539016 | -1.818639 | 3.492563 |
| C | -2.657010 | -1.173756 | 2.949941 |
| H | 0.559409 | -2.231957 | 3.304807 |
| H | -1.626880 | -2.380157 | 4.418610 |
| H | -3.621057 | -1.223528 | 3.446648 |
| N | 1.134589 | -1.016224 | 1.095022 |
| N | 1.160584 | 0.874400 | -0.406905 |
| C | 3.207938 | -0.268040 | 0.062267 |
| C | 4.036699 | 0.855725 | -0.071007 |

| | | | |
|----|-----------|-----------|-----------|
| C | 3.777050 | -1.549480 | 0.003390 |
| C | 5.410062 | 0.698555 | -0.244259 |
| H | 3.587726 | 1.842720 | -0.035238 |
| C | 5.153611 | -1.702619 | -0.172942 |
| H | 3.143700 | -2.431062 | 0.064234 |
| C | 5.973485 | -0.579848 | -0.293297 |
| H | 6.043582 | 1.576297 | -0.338541 |
| H | 5.581989 | -2.700081 | -0.224471 |
| H | 7.045012 | -0.699419 | -0.428382 |
| H | 1.818259 | -1.522385 | 1.643305 |
| Pd | -1.048350 | 1.295233 | -0.145675 |
| C | -1.443457 | -0.454809 | -0.735452 |
| N | -1.616087 | -1.348434 | -1.507177 |
| C | -1.815693 | -2.763448 | -1.787916 |
| C | -2.323098 | -3.477242 | -0.522075 |
| H | -2.475341 | -4.540433 | -0.737988 |
| H | -1.603076 | -3.389607 | 0.297072 |
| H | -3.275978 | -3.053905 | -0.189300 |
| C | -2.843485 | -2.871618 | -2.927684 |
| H | -3.805364 | -2.444676 | -2.625805 |
| H | -2.493255 | -2.338009 | -3.816377 |
| H | -2.997981 | -3.924011 | -3.188391 |
| C | -0.453805 | -3.329963 | -2.231765 |
| H | 0.286267 | -3.227957 | -1.431608 |
| H | -0.559961 | -4.391871 | -2.478184 |
| H | -0.083431 | -2.800567 | -3.114695 |
| O | -1.250514 | 3.077496 | -1.424955 |
| C | -1.005752 | 3.836812 | -0.429379 |
| C | -0.887270 | 5.328462 | -0.648912 |
| O | -0.832359 | 3.346320 | 0.728671 |
| H | 0.133086 | 5.559196 | -0.978094 |
| H | -1.575156 | 5.655075 | -1.433226 |
| H | -1.081254 | 5.868743 | 0.280586 |

TSIII_t-BuNC

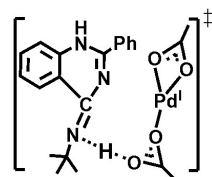


E= -1216.796688au

| | | | |
|----|-----------|-----------|-----------|
| Pd | -1.151483 | 0.682887 | 0.399140 |
| H | 2.529842 | 2.319315 | 0.354063 |
| C | 3.370963 | 1.634291 | 0.366309 |
| C | 3.112371 | 0.254798 | 0.366253 |
| C | 4.681706 | 2.104074 | 0.388866 |
| C | 1.690779 | -0.213695 | 0.343433 |
| C | 4.192152 | -0.642447 | 0.373177 |
| C | 5.752364 | 1.204944 | 0.404565 |
| H | 4.869796 | 3.174178 | 0.398786 |
| N | 1.483754 | -1.443794 | 0.965514 |
| N | 0.791267 | 0.497585 | -0.240741 |
| C | 5.504731 | -0.168501 | 0.392084 |
| H | 4.012785 | -1.713422 | 0.325193 |
| H | 6.774358 | 1.573767 | 0.422204 |
| C | 0.351432 | -2.237010 | 0.860194 |
| H | 6.332116 | -0.872936 | 0.386883 |
| C | 0.238932 | -3.372230 | 1.683529 |
| C | -0.659325 | -1.980717 | -0.097040 |
| C | -0.840452 | -4.235600 | 1.561083 |
| H | 1.015234 | -3.568778 | 2.419409 |
| C | -1.741899 | -2.876483 | -0.209478 |
| C | -1.839636 | -3.991907 | 0.608859 |
| H | -0.905452 | -5.103329 | 2.211341 |
| H | -2.503399 | -2.662652 | -0.952119 |
| H | -2.685860 | -4.665098 | 0.513690 |
| C | -0.633865 | -0.799049 | -0.973406 |
| O | -1.460818 | 2.218462 | 2.190678 |
| C | -3.736083 | 2.728457 | 2.835347 |
| H | -4.343228 | 1.983871 | 3.361619 |
| H | -3.264961 | 3.396951 | 3.558457 |
| H | -4.409534 | 3.297856 | 2.186114 |
| C | -2.689205 | 2.028930 | 1.997653 |
| O | -3.090162 | 1.226355 | 1.074732 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.201751 | -1.761732 | 1.601988 |
| N | -0.908030 | -0.718494 | -2.180978 |
| C | -0.915398 | 0.327165 | -3.205102 |
| C | 0.544217 | 0.641598 | -3.590120 |
| H | 0.561136 | 1.386586 | -4.393911 |
| H | 1.089021 | 1.031006 | -2.726324 |
| H | 1.051089 | -0.261163 | -3.948159 |
| C | -1.674504 | -0.251121 | -4.414488 |
| H | -1.193617 | -1.168343 | -4.769640 |
| H | -2.709612 | -0.488791 | -4.146153 |
| H | -1.688052 | 0.474324 | -5.235009 |
| C | -1.628519 | 1.601982 | -2.706720 |
| H | -1.068159 | 2.063294 | -1.886387 |
| H | -1.701797 | 2.328738 | -3.524386 |
| H | -2.640909 | 1.373070 | -2.357961 |

TSIV_{t-BuNC}

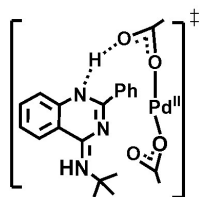


E= -1445.9511165au

| | | | |
|---|-----------|-----------|-----------|
| H | 2.602932 | 3.953890 | -0.080412 |
| C | 3.156271 | 3.020025 | -0.143392 |
| C | 2.478431 | 1.799400 | -0.303218 |
| C | 4.549462 | 3.055432 | -0.120043 |
| C | 0.998646 | 1.744666 | -0.324137 |
| C | 3.218496 | 0.615022 | -0.450778 |
| C | 5.279307 | 1.872522 | -0.253179 |
| H | 5.062901 | 4.006070 | -0.007126 |
| N | 0.324351 | 2.707730 | 0.380195 |
| N | 0.374444 | 0.813634 | -0.984000 |
| C | 4.610756 | 0.656965 | -0.420440 |
| H | 2.697217 | -0.328762 | -0.568370 |
| H | 6.365276 | 1.898858 | -0.229810 |
| C | -1.028207 | 2.914840 | 0.170785 |
| H | 5.174467 | -0.266022 | -0.520703 |
| C | -1.652345 | 4.076577 | 0.650216 |
| C | -1.739296 | 1.960649 | -0.595748 |

| | | | |
|----|-----------|-----------|-----------|
| C | -2.966523 | 4.341826 | 0.297721 |
| H | -1.089323 | 4.773456 | 1.265754 |
| C | -3.047343 | 2.297929 | -0.988031 |
| C | -3.656382 | 3.467181 | -0.553503 |
| H | -3.447993 | 5.245834 | 0.659011 |
| H | -3.586682 | 1.638024 | -1.651375 |
| H | -4.668248 | 3.698859 | -0.870836 |
| C | -1.012145 | 0.719670 | -0.946854 |
| H | 0.832820 | 3.317190 | 1.005846 |
| N | -1.456253 | -0.477096 | -1.238751 |
| Pd | 0.373018 | -1.565992 | 0.764267 |
| C | -2.794139 | -1.115744 | -1.090174 |
| C | -3.564597 | -0.654261 | 0.163300 |
| H | -4.408447 | -1.334482 | 0.323668 |
| H | -2.912678 | -0.701632 | 1.042556 |
| H | -3.972279 | 0.354449 | 0.090260 |
| C | -3.604041 | -0.958834 | -2.395717 |
| H | -3.871822 | 0.077305 | -2.619610 |
| H | -3.028768 | -1.343326 | -3.244589 |
| H | -4.534015 | -1.534151 | -2.324808 |
| C | -2.508666 | -2.627528 | -0.910981 |
| H | -1.909400 | -2.801444 | -0.009389 |
| H | -3.455402 | -3.168695 | -0.809324 |
| H | -1.967388 | -3.035504 | -1.768516 |
| O | -0.665019 | -0.680285 | 2.410123 |
| C | -0.270442 | -1.521368 | 3.302784 |
| C | -0.779217 | -1.321454 | 4.719293 |
| O | 0.501609 | -2.467808 | 3.023719 |
| H | -0.404413 | -2.107245 | 5.378048 |
| H | -0.456715 | -0.343665 | 5.094398 |
| H | -1.874665 | -1.325495 | 4.724124 |
| C | 1.159745 | -2.486135 | -2.048522 |
| O | 1.490305 | -2.486562 | -0.839461 |
| C | 2.039413 | -3.216575 | -3.044008 |
| H | 1.437947 | -3.935724 | -3.609429 |
| H | 2.448154 | -2.499492 | -3.764572 |
| H | 2.853512 | -3.731842 | -2.532163 |
| O | 0.123957 | -1.912811 | -2.554432 |
| H | -0.553498 | -1.245786 | -1.842860 |

TSV_{t-Bu}NC

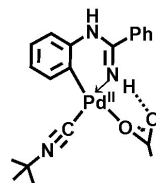


E= -1445.98079au

| | | | |
|----|-----------|-----------|-----------|
| C | -1.517856 | -1.268082 | -1.411879 |
| C | -0.172559 | -0.872167 | -1.614204 |
| C | -0.603417 | 1.187543 | -0.627338 |
| H | -2.956935 | -2.875939 | -1.716921 |
| C | -1.929547 | -2.546817 | -1.847853 |
| C | 0.726493 | -1.756131 | -2.256087 |
| C | 0.297174 | -3.001662 | -2.668515 |
| C | -1.037813 | -3.404170 | -2.463986 |
| H | 1.747876 | -1.433793 | -2.421946 |
| H | 0.994501 | -3.676348 | -3.156802 |
| H | -1.366677 | -4.384910 | -2.794009 |
| N | 0.268954 | 0.363242 | -1.202953 |
| N | -1.908819 | 0.920920 | -0.444292 |
| C | -0.131381 | 2.512204 | -0.150473 |
| C | 1.122950 | 2.657264 | 0.460764 |
| C | -0.965055 | 3.633920 | -0.278445 |
| C | 1.538117 | 3.906588 | 0.920901 |
| H | 1.753108 | 1.788289 | 0.614523 |
| C | -0.539648 | 4.883424 | 0.166988 |
| H | -1.940861 | 3.517407 | -0.738117 |
| C | 0.713716 | 5.023036 | 0.768712 |
| H | 2.504214 | 4.003963 | 1.408600 |
| H | -1.187840 | 5.747685 | 0.049369 |
| H | 1.041648 | 5.995918 | 1.125298 |
| Pd | 2.423811 | -1.180790 | 1.037995 |
| C | -2.373668 | -0.282154 | -0.774800 |
| N | -3.669446 | -0.574656 | -0.523671 |
| C | -4.681069 | 0.239372 | 0.202312 |
| C | -5.952553 | -0.626099 | 0.238279 |
| H | -6.753816 | -0.092917 | 0.758164 |
| H | -6.304402 | -0.857377 | -0.774714 |

| | | | |
|---|-----------|-----------|-----------|
| H | -5.777648 | -1.567947 | 0.773575 |
| C | -4.208704 | 0.533417 | 1.638421 |
| H | -4.037114 | -0.399662 | 2.187083 |
| H | -3.280088 | 1.106884 | 1.634119 |
| H | -4.976052 | 1.107247 | 2.170763 |
| C | -4.970749 | 1.542805 | -0.563596 |
| H | -5.300908 | 1.325666 | -1.585685 |
| H | -5.766705 | 2.099823 | -0.056428 |
| H | -4.079366 | 2.170142 | -0.608977 |
| O | 2.604307 | 0.943651 | -1.899376 |
| C | 3.659624 | 0.681115 | -1.204707 |
| C | 4.948605 | 1.231345 | -1.777950 |
| O | 3.699267 | 0.044521 | -0.129583 |
| H | 5.053270 | 0.918489 | -2.821638 |
| H | 4.907278 | 2.326242 | -1.771699 |
| H | 5.805468 | 0.892193 | -1.194379 |
| O | 0.027525 | -0.844148 | 1.642189 |
| C | -0.863738 | -2.509596 | 3.149119 |
| H | -0.895961 | -3.593505 | 3.002563 |
| H | -0.642930 | -2.328225 | 4.207375 |
| H | -1.832354 | -2.064979 | 2.909229 |
| C | 0.231120 | -1.895838 | 2.295987 |
| O | 1.370827 | -2.486377 | 2.292057 |
| H | 1.560612 | 0.669675 | -1.480085 |
| H | -3.954125 | -1.521324 | -0.722799 |

XI_{t-Bu}NC



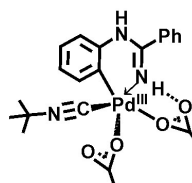
E= -1217.4786918au

| | | | |
|---|-----------|----------|-----------|
| C | -0.293115 | 1.863707 | 0.132337 |
| C | 0.968169 | 2.464781 | -0.081218 |
| C | 2.401685 | 0.423817 | -0.008375 |
| H | -2.361690 | 2.348968 | 0.496882 |
| C | -1.373458 | 2.752772 | 0.308216 |
| C | 1.108092 | 3.864300 | -0.154067 |

| | | | |
|----|-----------|-----------|-----------|
| C | 0.013783 | 4.701955 | 0.003184 |
| C | -1.239734 | 4.139185 | 0.246951 |
| H | 2.096145 | 4.290930 | -0.323689 |
| H | 0.141587 | 5.779382 | -0.054823 |
| H | -2.111287 | 4.774246 | 0.384373 |
| N | 2.174151 | 1.744714 | -0.233158 |
| N | 1.434398 | -0.383886 | 0.271648 |
| C | 3.816521 | -0.038769 | -0.110065 |
| C | 4.085440 | -1.345452 | -0.548967 |
| C | 4.886573 | 0.801200 | 0.237082 |
| C | 5.402028 | -1.790465 | -0.652032 |
| H | 3.265101 | -2.011327 | -0.798718 |
| C | 6.202030 | 0.350168 | 0.132250 |
| H | 4.696049 | 1.796809 | 0.629641 |
| C | 6.462825 | -0.945131 | -0.318007 |
| H | 5.598144 | -2.802286 | -0.995039 |
| H | 7.020421 | 1.006961 | 0.413758 |
| H | 7.487568 | -1.297086 | -0.399746 |
| H | 2.967835 | 2.286120 | -0.542431 |
| Pd | -0.551783 | -0.140840 | 0.177036 |
| C | -2.512282 | -0.079269 | 0.017902 |
| N | -3.669470 | -0.176340 | -0.103360 |
| O | 1.247085 | -3.084504 | 0.384616 |
| C | 0.010396 | -3.214909 | 0.275560 |
| C | -0.582676 | -4.624550 | 0.227574 |
| O | -0.869633 | -2.278417 | 0.205847 |
| H | -1.209343 | -4.739169 | -0.663573 |
| H | 0.211390 | -5.374275 | 0.221967 |
| H | -1.226869 | -4.783180 | 1.100078 |
| H | 1.639956 | -1.387458 | 0.426780 |
| C | -5.090319 | -0.384124 | -0.271084 |
| C | -5.609163 | -1.117975 | 0.979570 |
| H | -6.684515 | -1.296662 | 0.876552 |
| H | -5.103894 | -2.080656 | 1.101200 |
| H | -5.440240 | -0.519637 | 1.880200 |
| C | -5.759603 | 0.993844 | -0.421783 |
| H | -5.593420 | 1.607458 | 0.469245 |
| H | -5.363774 | 1.526690 | -1.291872 |
| H | -6.838139 | 0.862049 | -0.555461 |

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|---|-----------|-----------|-----------|
| C | -5.291100 | -1.239484 | -1.536116 |
| H | -4.781033 | -2.202250 | -1.436960 |
| H | -6.360256 | -1.422155 | -1.686079 |
| H | -4.897476 | -0.726490 | -2.419005 |

XII_{t-BuNC}

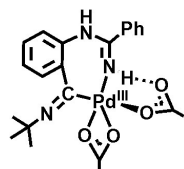


E=-1445.9079036au

| | | | |
|----|-----------|-----------|-----------|
| Pd | -0.974221 | -0.490491 | 0.362852 |
| H | 2.910505 | 1.923083 | -0.016177 |
| C | 3.707323 | 1.211154 | 0.174931 |
| C | 3.426759 | -0.163692 | 0.174884 |
| C | 5.003406 | 1.661712 | 0.417177 |
| C | 2.033232 | -0.632659 | -0.079448 |
| C | 4.461275 | -1.075035 | 0.438675 |
| C | 6.031459 | 0.749644 | 0.667767 |
| H | 5.209852 | 2.728088 | 0.410649 |
| N | 1.905815 | -1.813229 | -0.746504 |
| N | 1.005401 | 0.041835 | 0.305491 |
| C | 5.756402 | -0.618782 | 0.683207 |
| H | 4.249521 | -2.139453 | 0.495576 |
| H | 7.040430 | 1.104408 | 0.858588 |
| C | 0.722862 | -2.426023 | -1.222199 |
| H | 6.546307 | -1.333000 | 0.897780 |
| C | 0.910428 | -3.518557 | -2.089771 |
| C | -0.577629 | -2.012131 | -0.894806 |
| C | -0.175462 | -4.188076 | -2.638962 |
| H | 1.923658 | -3.835041 | -2.334352 |
| C | -1.660495 | -2.689529 | -1.464868 |
| C | -1.470360 | -3.769273 | -2.329520 |
| H | -0.008252 | -5.028190 | -3.307248 |
| H | -2.665929 | -2.374233 | -1.209370 |
| H | -2.330832 | -4.279770 | -2.753669 |
| H | 1.106370 | 0.931662 | 0.823757 |
| C | -1.468938 | 1.010481 | -1.180668 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.698551 | 2.086307 | 2.073161 |
| O | -1.439940 | 1.082762 | 1.776897 |
| C | -1.260755 | 2.976317 | 3.181788 |
| H | -2.340448 | 3.108814 | 3.065355 |
| H | -1.094348 | 2.485878 | 4.148414 |
| H | -0.753508 | 3.944109 | 3.189572 |
| O | 0.410696 | 2.379105 | 1.566968 |
| O | -1.269729 | -2.023225 | 2.142643 |
| C | -3.519954 | -2.664647 | 2.735868 |
| H | -4.300201 | -3.114423 | 2.115252 |
| H | -3.039991 | -3.425559 | 3.354899 |
| H | -3.996420 | -1.924552 | 3.389106 |
| C | -2.498031 | -1.965704 | 1.868907 |
| O | -2.913835 | -1.291523 | 0.858861 |
| H | 2.762571 | -2.198541 | -1.116496 |
| N | -1.485226 | 2.093514 | -1.615899 |
| C | -1.438774 | 3.497777 | -1.970726 |
| C | -2.561084 | 4.207248 | -1.190526 |
| H | -2.548557 | 5.275588 | -1.430216 |
| H | -3.540826 | 3.800264 | -1.459386 |
| H | -2.417139 | 4.087322 | -0.113094 |
| C | -0.053350 | 4.026406 | -1.551142 |
| H | 0.129236 | 3.828400 | -0.490406 |
| H | 0.735222 | 3.542398 | -2.137159 |
| H | -0.007074 | 5.105268 | -1.734330 |
| C | -1.655193 | 3.620669 | -3.488507 |
| H | -2.631745 | 3.220755 | -3.779292 |
| H | -1.612222 | 4.676102 | -3.776138 |
| H | -0.878864 | 3.079754 | -4.038686 |

XIII_{t-BuNC}



E= -1445.9132437au

| | | | |
|----|-----------|----------|-----------|
| Pd | 1.051364 | 0.721143 | -0.519154 |
| H | -3.057769 | 1.665416 | 0.795143 |
| C | -3.789005 | 1.061881 | 0.265760 |

| | | | |
|---|-----------|-----------|-----------|
| C | -3.364173 | -0.003894 | -0.544221 |
| C | -5.147433 | 1.353882 | 0.376349 |
| C | -1.904267 | -0.307515 | -0.647984 |
| C | -4.319242 | -0.751943 | -1.251636 |
| C | -6.093605 | 0.598079 | -0.319630 |
| H | -5.465470 | 2.177633 | 1.008719 |
| N | -1.593138 | -1.649965 | -0.741849 |
| N | -1.014958 | 0.622184 | -0.635271 |
| C | -5.676261 | -0.451454 | -1.139976 |
| H | -4.008863 | -1.544620 | -1.928550 |
| H | -7.150904 | 0.831827 | -0.231139 |
| C | -0.348350 | -2.264175 | -1.015608 |
| H | -6.403860 | -1.029688 | -1.702402 |
| C | -0.323425 | -3.312142 | -1.944679 |
| C | 0.844179 | -1.913771 | -0.339725 |
| C | 0.860456 | -3.986945 | -2.231195 |
| H | -1.243502 | -3.585118 | -2.455720 |
| C | 2.042433 | -2.574039 | -0.676115 |
| C | 2.052061 | -3.607727 | -1.605969 |
| H | 0.854913 | -4.793475 | -2.958408 |
| H | 2.960078 | -2.255519 | -0.192183 |
| H | 2.982717 | -4.113731 | -1.843743 |
| H | -1.329615 | 1.597047 | -0.464886 |
| C | 0.877370 | -0.845257 | 0.687326 |
| C | -0.034072 | 3.277355 | 0.905882 |
| O | 0.981615 | 2.492400 | 0.830511 |
| C | 0.230246 | 4.537456 | 1.732894 |
| H | 0.906425 | 4.326987 | 2.565333 |
| H | 0.709504 | 5.285032 | 1.089843 |
| H | -0.714716 | 4.946973 | 2.098123 |
| O | -1.153525 | 3.128490 | 0.372324 |
| O | 2.178929 | 2.103427 | -2.122763 |
| C | 4.583289 | 2.243224 | -1.911714 |
| H | 5.335806 | 1.450356 | -1.874339 |
| H | 4.558766 | 2.699828 | -2.903511 |
| H | 4.867265 | 3.007421 | -1.178602 |
| C | 3.218170 | 1.701178 | -1.549116 |
| O | 3.160431 | 0.825448 | -0.600032 |
| H | -2.393056 | -2.261740 | -0.813765 |

| | | | |
|---|-----------|-----------|----------|
| N | 0.901447 | -0.736539 | 1.914068 |
| C | 0.866957 | -1.738867 | 2.999901 |
| C | 2.306551 | -1.838461 | 3.538078 |
| H | 2.333787 | -2.490872 | 4.418280 |
| H | 2.979818 | -2.253689 | 2.780198 |
| H | 2.679423 | -0.849822 | 3.821681 |
| C | -0.059594 | -1.153497 | 4.080896 |
| H | 0.289072 | -0.162392 | 4.385214 |
| H | -1.082513 | -1.052987 | 3.701620 |
| H | -0.080349 | -1.808073 | 4.959574 |
| C | 0.353930 | -3.121054 | 2.560609 |
| H | 1.019756 | -3.595114 | 1.833955 |
| H | 0.285574 | -3.779948 | 3.433798 |
| H | -0.645369 | -3.046091 | 2.117132 |

TSVI_{t-BuNC}

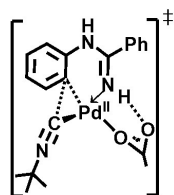


E=-1445.8782202au

| | | | |
|----|-----------|-----------|-----------|
| Pd | 1.065884 | 0.765518 | -0.110614 |
| H | -3.231204 | 1.494250 | 1.045567 |
| C | -3.911572 | 0.994117 | 0.361992 |
| C | -3.398086 | 0.156268 | -0.641376 |
| C | -5.287004 | 1.186849 | 0.474244 |
| C | -1.918780 | -0.025206 | -0.738659 |
| C | -4.282778 | -0.465272 | -1.536304 |
| C | -6.163514 | 0.556752 | -0.412980 |
| H | -5.674164 | 1.833076 | 1.256732 |
| N | -1.493568 | -1.286414 | -1.129086 |
| N | -1.081093 | 0.899160 | -0.462243 |
| C | -5.658468 | -0.264428 | -1.422477 |
| H | -3.902443 | -1.073129 | -2.353850 |
| H | -7.235062 | 0.712351 | -0.323622 |
| C | -0.198872 | -1.728264 | -1.466700 |
| H | -6.332586 | -0.740300 | -2.129145 |
| C | -0.113537 | -2.786103 | -2.387355 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.995835 | -1.219607 | -0.898779 |
| C | 1.116188 | -3.329951 | -2.746002 |
| H | -1.027195 | -3.172097 | -2.835488 |
| C | 2.231148 | -1.773022 | -1.284909 |
| C | 2.298038 | -2.817297 | -2.202355 |
| H | 1.149347 | -4.147107 | -3.461122 |
| H | 3.135575 | -1.347971 | -0.862173 |
| H | 3.261261 | -3.226055 | -2.493257 |
| H | -1.388124 | 1.805096 | -0.069135 |
| C | 0.853644 | -0.827935 | 0.937417 |
| C | 0.109483 | 3.215561 | 1.485585 |
| O | 1.113174 | 2.460799 | 1.199485 |
| C | 0.480194 | 4.413999 | 2.360889 |
| H | 1.218612 | 4.131591 | 3.116406 |
| H | 0.932938 | 5.187295 | 1.728708 |
| H | -0.413516 | 4.828018 | 2.833812 |
| O | -1.075352 | 3.085833 | 1.115440 |
| O | 1.908218 | 2.073577 | -1.727578 |
| C | 4.236611 | 2.620140 | -2.003021 |
| H | 5.149333 | 2.018283 | -2.005632 |
| H | 3.966632 | 2.911040 | -3.021201 |
| H | 4.433006 | 3.531023 | -1.425027 |
| C | 3.100653 | 1.863250 | -1.347516 |
| O | 3.360607 | 1.049033 | -0.403110 |
| H | -2.232911 | -1.931689 | -1.366253 |
| N | 0.738818 | -1.503430 | 1.906569 |
| C | 0.698179 | -2.756183 | 2.642236 |
| C | 1.834661 | -2.712875 | 3.680156 |
| H | 1.824143 | -3.633066 | 4.273772 |
| H | 2.808316 | -2.627105 | 3.187670 |
| H | 1.712307 | -1.859508 | 4.353724 |
| C | -0.671550 | -2.835009 | 3.340261 |
| H | -0.813805 | -1.983520 | 4.012423 |
| H | -1.483257 | -2.835973 | 2.605541 |
| H | -0.732506 | -3.758018 | 3.926210 |
| C | 0.888811 | -3.928493 | 1.662836 |
| H | 1.848350 | -3.852611 | 1.142552 |
| H | 0.866372 | -4.874455 | 2.214560 |
| H | 0.091944 | -3.946128 | 0.912803 |

TSVI_{t-BuNC}

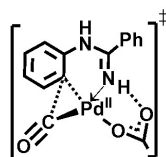


E=-1217.4117557au

| | | | |
|----|-----------|-----------|-----------|
| C | 1.188275 | -1.620281 | -0.635624 |
| C | 0.012355 | -2.341820 | -0.289411 |
| C | -1.892795 | -0.689295 | -0.201824 |
| H | 3.098803 | -1.747487 | -1.609809 |
| C | 2.210210 | -2.303432 | -1.327815 |
| C | -0.049277 | -3.716811 | -0.564107 |
| C | 1.006221 | -4.378492 | -1.185195 |
| C | 2.136625 | -3.665925 | -1.592527 |
| H | -0.958154 | -4.263991 | -0.322806 |
| H | 0.930518 | -5.445454 | -1.375766 |
| H | 2.953588 | -4.169014 | -2.101023 |
| N | -1.140078 | -1.759965 | 0.298867 |
| N | -1.471607 | 0.040979 | -1.174899 |
| C | -3.190204 | -0.476637 | 0.502643 |
| C | -4.293281 | 0.011983 | -0.214387 |
| C | -3.328013 | -0.736005 | 1.876046 |
| C | -5.510004 | 0.229685 | 0.428134 |
| H | -4.194309 | 0.208123 | -1.277529 |
| C | -4.546521 | -0.511680 | 2.516850 |
| H | -2.471010 | -1.075059 | 2.451246 |
| C | -5.640700 | -0.032733 | 1.794261 |
| H | -6.357641 | 0.603227 | -0.139200 |
| H | -4.636794 | -0.701478 | 3.582797 |
| H | -6.589858 | 0.140331 | 2.293844 |
| H | -1.711395 | -2.436411 | 0.789271 |
| Pd | 0.678392 | 0.404690 | -0.980403 |
| C | 1.969111 | -0.257392 | 0.209924 |
| N | 2.666290 | -0.340938 | 1.200030 |
| O | -1.520939 | 2.792694 | -1.389469 |
| C | -0.357885 | 3.206260 | -1.272306 |
| C | -0.076774 | 4.708260 | -1.353621 |

| | | | |
|---|-----------|-----------|-----------|
| O | 0.716011 | 2.501765 | -1.087656 |
| H | 0.557620 | 4.917517 | -2.222269 |
| H | -1.011518 | 5.265872 | -1.441400 |
| H | 0.472900 | 5.038232 | -0.465696 |
| H | -1.960398 | 0.932566 | -1.318131 |
| C | 3.395541 | 0.675327 | 1.987920 |
| C | 2.486844 | 1.055495 | 3.171136 |
| H | 3.004910 | 1.768654 | 3.822037 |
| H | 1.562500 | 1.519986 | 2.813191 |
| H | 2.227051 | 0.171455 | 3.762707 |
| C | 4.688363 | 0.016954 | 2.494559 |
| H | 4.464024 | -0.873327 | 3.091211 |
| H | 5.325956 | -0.283716 | 1.656270 |
| H | 5.250176 | 0.721780 | 3.117256 |
| C | 3.709794 | 1.910158 | 1.124072 |
| H | 2.796049 | 2.360720 | 0.723748 |
| H | 4.240011 | 2.657105 | 1.726345 |
| H | 4.350835 | 1.636705 | 0.278896 |

TSII_{CO}

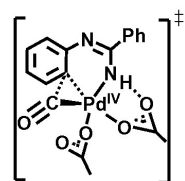


E= -1080.05262au

| | | | |
|----|-----------|-----------|-----------|
| Pd | 1.161759 | 1.004664 | -0.145233 |
| H | -2.905629 | 0.963069 | 0.022008 |
| C | -3.325383 | -0.038958 | 0.078551 |
| C | -2.487584 | -1.153474 | -0.093978 |
| C | -4.682395 | -0.226179 | 0.337452 |
| C | -1.038996 | -0.923641 | -0.366396 |
| C | -3.029394 | -2.445628 | -0.014446 |
| C | -5.217471 | -1.514481 | 0.416634 |
| H | -5.322844 | 0.639394 | 0.480922 |
| N | -0.168875 | -1.774854 | 0.313410 |
| N | -0.588695 | 0.014269 | -1.127644 |
| C | -4.389971 | -2.624261 | 0.235171 |
| H | -2.401559 | -3.317106 | -0.186921 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -6.276593 | -1.653590 | 0.615276 | C | -4.122607 | -1.238740 | -0.673374 |
| C | 1.220846 | -1.928103 | 0.064927 | C | -5.915575 | 0.353119 | -0.358756 |
| H | -0.613371 | -2.551639 | 0.782534 | H | -5.310568 | 2.333453 | 0.244639 |
| H | -4.803109 | -3.628050 | 0.280210 | N | -1.451411 | -1.912295 | -0.202962 |
| C | 1.667794 | -3.160882 | -0.427047 | N | -0.818728 | 0.343912 | -0.552258 |
| C | 2.169412 | -0.891388 | 0.276719 | C | -5.480787 | -0.934063 | -0.687382 |
| C | 3.013361 | -3.375080 | -0.719749 | H | -3.772796 | -2.235082 | -0.917385 |
| H | 0.940113 | -3.946145 | -0.614629 | H | -6.976144 | 0.590219 | -0.368364 |
| C | 3.515524 | -1.110516 | -0.079660 | C | -0.193217 | -2.415970 | -0.063272 |
| C | 3.940928 | -2.341649 | -0.565661 | H | -6.201720 | -1.702174 | -0.954236 |
| H | 3.331501 | -4.343909 | -1.094229 | C | -0.083886 | -3.834163 | -0.184031 |
| H | 4.232050 | -0.309507 | 0.075098 | C | 1.018036 | -1.723340 | 0.235512 |
| H | 4.986429 | -2.498027 | -0.812999 | C | 1.118978 | -4.490080 | -0.029910 |
| H | -1.307106 | 0.652104 | -1.463852 | H | -0.999874 | -4.370954 | -0.408951 |
| C | 2.021780 | 0.369460 | 1.366978 | C | 2.236749 | -2.395930 | 0.429418 |
| C | -0.526401 | 3.401981 | -0.318977 | C | 2.291015 | -3.773642 | 0.285632 |
| O | 0.672013 | 3.020073 | 0.007402 | H | 1.160094 | -5.570366 | -0.138913 |
| C | -0.727539 | 4.909374 | -0.167547 | H | 3.127520 | -1.829274 | 0.674813 |
| H | -1.736399 | 5.190281 | -0.476636 | H | 3.234008 | -4.294477 | 0.423527 |
| H | -0.564397 | 5.202820 | 0.875172 | H | -1.131230 | 1.323030 | -0.429571 |
| H | 0.009837 | 5.447061 | -0.772922 | C | 0.581911 | -0.315926 | 1.859410 |
| O | -1.454100 | 2.683135 | -0.716697 | C | 0.243926 | 3.288277 | 0.301047 |
| O | 2.225345 | 0.369713 | 2.525985 | O | 1.229712 | 2.448800 | 0.344926 |

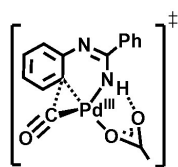
TSVII_{CO}



E= -1307.883348au

| | | | | | | | |
|----|-----------|-----------|-----------|---|----------|----------|-----------|
| Pd | 1.074750 | 0.345258 | 0.148818 | H | 4.594484 | 0.769554 | -2.748341 |
| H | -2.913698 | 1.815935 | 0.264476 | H | 4.826722 | 2.052838 | -1.538501 |
| C | -3.617487 | 1.037075 | -0.010598 | C | 3.299641 | 0.660336 | -1.046189 |
| C | -3.176683 | -0.255771 | -0.338387 | O | 3.233499 | 0.454941 | 0.222053 |
| C | -4.981376 | 1.331945 | -0.017965 | | | | |
| C | -1.724129 | -0.625827 | -0.331857 | | | | |

TSVIII_{CO}



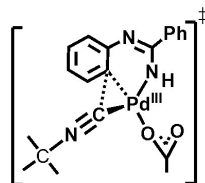
E= -1079.4082468au

| | | | |
|----|-----------|-----------|-----------|
| Pd | 1.179788 | 1.017019 | -0.082736 |
| H | -2.933596 | 0.931554 | 0.016538 |
| C | -3.306899 | -0.088130 | 0.052056 |
| C | -2.439026 | -1.177339 | -0.136577 |
| C | -4.658097 | -0.309581 | 0.316185 |
| C | -0.985954 | -0.959633 | -0.410307 |
| C | -2.947743 | -2.483293 | -0.049112 |
| C | -5.159940 | -1.610559 | 0.388949 |
| H | -5.318369 | 0.539647 | 0.467995 |
| N | -0.183728 | -2.013460 | -0.175474 |
| N | -0.551469 | 0.180564 | -0.940169 |
| C | -4.300339 | -2.696738 | 0.205661 |
| H | -2.270485 | -3.318106 | -0.187708 |
| H | -6.214793 | -1.777672 | 0.590024 |
| C | 1.168910 | -1.987463 | -0.172916 |
| H | -4.684201 | -3.711818 | 0.261575 |
| C | 1.804130 | -3.218524 | -0.515708 |
| C | 2.035400 | -0.871331 | 0.121153 |
| C | 3.173942 | -3.316489 | -0.660260 |
| H | 1.154646 | -4.066735 | -0.705559 |
| C | 3.432837 | -1.002539 | -0.021012 |
| C | 4.001478 | -2.201179 | -0.427260 |
| H | 3.616718 | -4.264756 | -0.951740 |
| H | 4.069329 | -0.156811 | 0.224463 |
| H | 5.078657 | -2.283110 | -0.535040 |
| H | -1.244218 | 0.934370 | -1.025144 |
| C | 1.754667 | 0.244500 | 1.549515 |
| C | -0.521019 | 3.465158 | -0.326293 |
| O | 0.670075 | 3.021555 | -0.049905 |
| C | -0.630148 | 4.983419 | -0.235246 |
| H | -1.634823 | 5.307383 | -0.512822 |
| H | -0.404470 | 5.310383 | 0.785580 |
| H | 0.108103 | 5.450815 | -0.895241 |

0 -1.507400 2.782815 -0.636552

0 1.714882 0.011953 2.687644

TSVII_{t-BuNC}

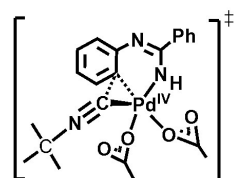


E= -1216.7754238au

| | | | |
|----|-----------|-----------|-----------|
| C | -1.098414 | -1.132043 | 0.898978 |
| C | 0.093740 | -1.152657 | 1.690751 |
| C | 1.262361 | 0.771935 | 0.914126 |
| H | -3.042608 | -1.992297 | 0.528861 |
| C | -2.163707 | -2.011523 | 1.167808 |
| C | 0.134619 | -2.103893 | 2.747959 |
| C | -0.935269 | -2.937050 | 3.024381 |
| C | -2.097939 | -2.898749 | 2.233865 |
| H | 1.040068 | -2.134371 | 3.346293 |
| H | -0.870136 | -3.634916 | 3.855079 |
| H | -2.930216 | -3.564219 | 2.443387 |
| N | 1.235882 | -0.426679 | 1.486792 |
| N | 0.180798 | 1.525171 | 0.686272 |
| C | 2.630872 | 1.308257 | 0.610727 |
| C | 2.842886 | 2.201989 | -0.450060 |
| C | 3.728616 | 0.906562 | 1.387399 |
| C | 4.121601 | 2.688211 | -0.724317 |
| H | 2.013905 | 2.500592 | -1.087055 |
| C | 5.002875 | 1.402704 | 1.120508 |
| H | 3.559755 | 0.206043 | 2.197592 |
| C | 5.204479 | 2.295373 | 0.063973 |
| H | 4.270279 | 3.371236 | -1.556301 |
| H | 5.841675 | 1.092768 | 1.738309 |
| H | 6.199328 | 2.679650 | -0.144857 |
| Pd | -1.587814 | 0.556276 | -0.193495 |
| C | -0.674821 | -0.939489 | -0.958220 |
| N | -0.038324 | -1.592725 | -1.714246 |
| C | 0.798162 | -2.727821 | -2.082831 |
| C | 2.258771 | -2.305039 | -1.833574 |
| H | 2.924461 | -3.136406 | -2.088850 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 2.524878 | -1.443576 | -2.453790 | H | 6.764827 | -0.252416 | -1.558177 |
| H | 2.412982 | -2.037321 | -0.783814 | C | 0.005942 | 2.518496 | -0.129157 |
| C | 0.411614 | -3.929134 | -1.200682 | H | 5.974814 | 2.093082 | -1.809662 |
| H | 0.563688 | -3.703227 | -0.141216 | C | -0.169245 | 3.914912 | 0.092885 |
| H | -0.637438 | -4.202910 | -1.351746 | C | -1.136471 | 1.695632 | 0.111226 |
| H | 1.034659 | -4.789834 | -1.466469 | C | -1.372238 | 4.440648 | 0.517636 |
| C | 0.558159 | -3.031076 | -3.570663 | H | 0.693798 | 4.547724 | -0.088872 |
| H | 0.802467 | -2.161909 | -4.189044 | C | -2.348205 | 2.231700 | 0.586289 |
| H | 1.191086 | -3.868823 | -3.880917 | C | -2.472121 | 3.597924 | 0.776799 |
| H | -0.487146 | -3.301823 | -3.751363 | H | -1.467117 | 5.512927 | 0.667299 |
| O | -2.211754 | 2.272285 | -1.384289 | H | -3.179727 | 1.563818 | 0.779868 |
| C | -3.021031 | 2.684683 | -0.476852 | H | -3.412956 | 4.013806 | 1.125886 |
| C | -3.806768 | 3.951333 | -0.735799 | C | -0.498292 | 0.023422 | 1.198730 |
| O | -3.154973 | 2.045887 | 0.603322 | C | -0.165884 | -3.034788 | -0.478655 |
| H | -3.117784 | 4.777751 | -0.940397 | O | -1.026821 | -2.303356 | -1.112800 |
| H | -4.431180 | 3.821179 | -1.626290 | C | -0.260819 | -4.520106 | -0.821000 |
| H | -4.434809 | 4.196664 | 0.122506 | H | -0.314613 | -4.659605 | -1.904779 |
| H | 0.392008 | 2.395875 | 0.201989 | H | 0.595754 | -5.059879 | -0.411878 |

TSVII[†]_{t-BuNC}



E= -1445.2611307au

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Pd | -1.159627 | -0.250944 | -0.584827 | O | 0.673230 | -2.625864 | 0.341751 |
| H | 2.745162 | -1.518562 | -0.710400 | O | -2.747906 | -0.177746 | -2.292001 |
| C | 3.441771 | -0.729409 | -0.984801 | C | -5.015160 | -0.814998 | -1.738650 |
| C | 2.991904 | 0.592587 | -1.132227 | H | -5.681429 | -0.465419 | -0.945260 |
| C | 4.797366 | -1.027054 | -1.132929 | H | -5.289928 | -0.366036 | -2.695636 |
| C | 1.545205 | 0.935827 | -0.968291 | H | -5.124363 | -1.903029 | -1.816689 |
| C | 3.917279 | 1.607362 | -1.418194 | C | -3.580029 | -0.494007 | -1.409576 |
| C | 5.711032 | -0.016271 | -1.436155 | O | -3.205245 | -0.579306 | -0.170734 |
| H | 5.138405 | -2.050865 | -1.005340 | N | -0.062704 | -0.124738 | 2.271112 |
| N | 1.268735 | 2.124482 | -0.474240 | C | 0.600746 | -0.706379 | 3.430966 |
| N | 0.634820 | 0.047663 | -1.412581 | C | -0.053258 | -2.077479 | 3.684396 |
| C | 5.267091 | 1.302014 | -1.576342 | H | 0.438215 | -2.553910 | 4.539385 |
| H | 3.559142 | 2.626650 | -1.513441 | H | -1.117861 | -1.966188 | 3.915111 |
| | | | | H | 0.060543 | -2.712312 | 2.801680 |
| | | | | C | 2.085581 | -0.866024 | 3.055444 |
| | | | | H | 2.184337 | -1.527568 | 2.191352 |
| | | | | H | 2.536637 | 0.102943 | 2.819492 |
| | | | | H | 2.621060 | -1.301397 | 3.905743 |
| | | | | C | 0.413135 | 0.247270 | 4.620876 |
| | | | | H | -0.648151 | 0.384350 | 4.851565 |

| | | | |
|---|----------|-----------|-----------|
| H | 0.906257 | -0.175137 | 5.502033 |
| H | 0.855285 | 1.226675 | 4.412704 |
| H | 1.024202 | -0.854751 | -1.670410 |