

## Electronic Supplementary Information (ESI)

# Orthogonal non-covalent binding forces in solid state supramolecular herringbone-shaped “interlocked dimers”. Pseudopolymorphism in [(ppy)Pd( $\mu$ -pz)]<sub>2</sub> (ppy = 2-phenylpyridine, pz = pyrazol-1-yl) complex.

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|   | TRANS |  |  |  | CIS                    |  |                        |  |
|---|-------|--|--|--|------------------------|--|------------------------|--|
| 1 |       |  |  |  | wR2= 0.0946 R1= 0.0472 |  | wR2= 0.0920 R1= 0.0471 |  |
|   |       |  |  |  |                        |  |                        |  |
| 2 |       |  |  |  | wR2= 0.0885 R1= 0.0464 |  | wR2= 0.0927 R1= 0.0473 |  |
|   |       |  |  |  |                        |  |                        |  |
| 3 |       |  |  |  | wR2=0.0977 R1= 0.0479  |  | wR2= 0.0945 R1= 0.0478 |  |
|   |       |  |  |  |                        |  |                        |  |
| 4 |       |  |  |  | wR2=0.0913 R1= 0.0471  |  | wR2= 0.0945 R1= 0.0473 |  |
|   |       |  |  |  |                        |  |                        |  |

**Table S1.** Conformational features in complexes containing the  $\{Pd(\mu\text{-pz})\}_2$  core (pz = pyrazol-1-yl or related ligands).

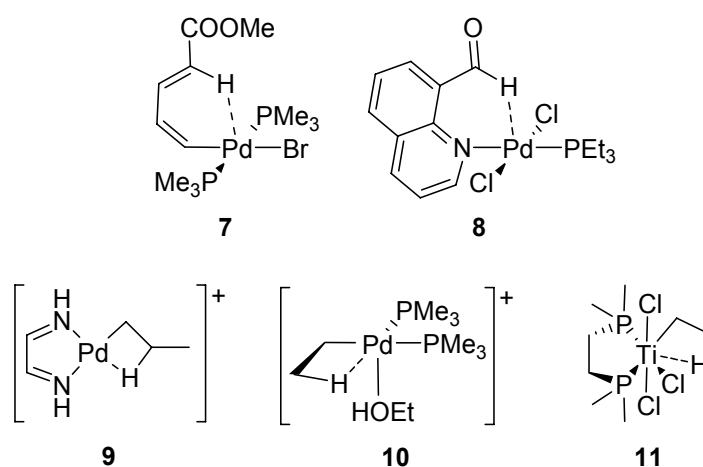
| REFCODE  | Bridging ligand                           | $d_{Pd\cdots Pd}$<br>(Å) | $d_{pz^*-pz^*}$<br>(Å) | $\beta$ (°)    |
|----------|-------------------------------------------|--------------------------|------------------------|----------------|
| DOYJIK   | 3-Phenyl-5-(6-methyl-2-pyridyl)pyrazolate | 3.097                    | 4.079                  | 87.5           |
| FEPLS    | Pyrazolate                                | 3.375                    | 4.119                  | 88.9           |
| FEPLIW   | 3,5-Dimethylpyrazolate                    | 3.191                    | 4.143                  | 87.6           |
| FEPLOC   | 3-t-Butyl-5-methylpyrazolate              | 3.046                    | 4.086                  | 86.9           |
| FEPLUI   | 3,5-Di-t-butylpyrazolate                  | 2.834                    | 4.251                  | 98.2           |
| HENFOW   | 3,5-Dimethylpyrazolate                    | 3.468                    | 4.273                  | 106.5          |
| HENGAI   | 3,5-Dimethylpyrazolate                    | 3.344                    | 4.424                  | 119.9          |
| HENGEN   | 3,5-Dimethylpyrazolate                    | 3.323                    | 4.199                  | 103.3          |
| IHONEY   | 3-t-Butylpyrazolyl                        | 3.176                    | 3.940                  | 79.1           |
| IHONIC   | 3-t-Butylpyrazolyl                        | 3.38                     | 4.398                  | 111.3          |
| IMOXOX   | 3,5-bis(4-(n-Dodecyloxy)phenyl)pyrazolate | 3.287                    | 5.160                  | 133.4          |
| MECJAG   | 3,5-Dimethylpyrazolate                    | 3.269                    | 4.341                  | 111.6          |
| MECJEK   | 3,5-Dimethylpyrazolate                    | 3.272                    | 4.381                  | 115.1          |
| MANWIH   | Pyrazolate                                | 3.493                    | 4.645                  | 125.2          |
| MAQFEQ   | 3,5-Diphenylpyrazolate                    | 3.029                    | 4.333                  | 109.6          |
| MAQFIU   | 3,5-Diphenylpyrazolate                    | 3.097                    | 4.289                  | 109.0          |
| MUZXIO   | 3,5-bis(Trifluoromethyl)pyrazole          | 3.217                    | 4.427                  | 101.8          |
| OFUKEF   | Pyrazolate                                | 3.423                    | 4.308                  | 98.2           |
| OHUQOX   | Pyrazolate                                | 3.454                    | 4.243                  | 103.0          |
| PEJROM   | Pyrazolate                                | 3.423                    | 4.507                  | 126.5          |
| PEJRUS   | Pyrazolate                                | 3.434                    | 4.373                  | 112.6          |
| PEJSAZ   | Pyrazolate                                | 3.363<br>3.362           | 4.340<br>4.333         | 112.8<br>111.2 |
| PEJSED   | 3-t-Butylpyrazolyl                        | 3.228                    | 4.227                  | 102.2          |
| PEMSEG   | 3-t-Butylpyrazolyl                        | 3.267                    | 4.374                  | 111.4          |
| PEYBOL   | 3,5-Diphenylpyrazolate                    | 3.041                    | 4.313                  | 107.2          |
| PZALPD10 | 3,5-Dimethylpyrazolate                    | 3.343                    | 4.390                  | 105.0          |
| RETGAZ   | 3,5-Dimethylpyrazolate                    | 3.397                    | 4.061                  | 89.7           |
| UKAVEH   | 3,5-Dimethylpyrazolate                    | 3.513                    | 4.247                  | 79.1           |

|           |                                    |       |       |       |
|-----------|------------------------------------|-------|-------|-------|
| UKAVAD    | 3,5-Dimethylpyrazolate             | 3.402 | 4.157 | 85.2  |
| VERRUG    | 3,5-Dimethylpyrazolate             | 3.149 | 3.910 | 80.7  |
| VIDJAU    | 5-Phenyl-3-p-tolylpyrazolate       | 3.030 | 4.066 | 89.5  |
| WEFCIU    | 3,5-bis(trifluoromethyl)pyrazolate | 3.267 | 4.350 | 97.0  |
| YAFSAZ    | 3,5-dimethylpyrazolate             | 3.115 | 4.227 | 98.1  |
| XAXCUU    |                                    | 3.486 | 4.339 | 105.7 |
| CIHRER    | 3,5-Diphenylpyrazolate             | 3.030 | 4.062 | 91.8  |
| EDUSIG    | 4-benzyl-3,5-diphenylpyrazolate    | 2.999 | 4.275 | 105.4 |
| Complex 1 | Pyrazolate                         | 3.543 | 3.869 | 116.4 |
|           |                                    | 3.461 | 4.457 | 116.4 |
| Complex 2 | Pyrazolate                         | 3.305 | 4.277 | 97.0  |
|           |                                    | 3.327 | 4.154 | 97.9  |
| Complex 3 | Pyrazolate                         | 3.252 | 4.288 | 98.1  |
|           |                                    | 3.259 | 4.261 | 98.2  |

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## Study on model agostic and anagostic reference compounds.

The TSI component in all studied dimeric compounds includes the interaction of an aromatic H atom with the Pd atom of the outer unit. For comparative purposes, already reported reference compounds or simplified models **7-11** have been calculated at the working level of theory. Compounds **7**<sup>1</sup> and **8**<sup>2</sup> are early examples displaying well established anagostic Pd···H interactions, whereas the Pd···H bonding in **9**<sup>3</sup> and **10**<sup>4</sup> has prototypical agostic nature. Compound **11** was the first structurally characterized example of  $\beta$ -agostic M···H bond.<sup>5</sup>



Anagostic M–H–C bonds are best described as a “hydrogen bond” involving a 3-centre-4-electron orbital interaction with an electrostatic contribution in which the metal serves as a hydrogen bond acceptor. They are characterized by relatively long M···H distances ( $\approx 2.3$ – $3.2$  Å) and large M–H–C angles ( $\approx 110$ – $170^\circ$ ) as those exhibited by

<sup>1</sup> Roe, D. M.; Bailey, P. M.; Moseley, K.; Maitlis, P. M. *J. Chem. Soc., Chem. Commun.*, **1972**, 1273-1274.

<sup>2</sup> Pd-Analog of the reported Pt counterpart: Albinati, A.; Anklin, C. G.; Pregosin, P. S. *Inorg. Chim. Acta*, **1984**, *90*, L37-L38.

<sup>3</sup> Siegbahn, E. M.; Strömberg, S.; Zetterberg, K. *Organometallics*, **1996**, *15*, 5542-5550.

<sup>4</sup> Raharintsalama, R.; Munakata, H.; Koyama, M.; Kubo, M.; Miyamoto, A. *Applied Surface Science*, **2005**, *244*, 631-635.

<sup>5</sup> (a) Dawoodi, Z.; Green, M. L. H.; Mtetwa, V. S. B.; Prout, K. *J. Chem. Soc., Chem. Commun.*, **1982**, 802-803. (b) Dawoodi, Z.; Green, M. L. H.; Mtetwa, V. S. B.; Prout, K.; Schultz, A. J.; Williams, J. M.; Koetzle, T. F. *J. Chem. Soc., Dalton Trans.*, **1986**, 1629-1637.

model compounds **7** and **8**<sup>6</sup> (Table S2). On the contrary, agostic M–H–C interactions involve donation of the electron density associated with the C–H bond to a metal centre that has a ≤16-electron configuration, by virtue of the formation of a 3-centre-2-electron covalent bond, and feature short M–H distances ( $\approx 1.8$ – $2.3$  Å) together with acute M–H–C angles ( $\approx 90$ – $140^\circ$ ).

**Table S2:** Relevant calculated parameters related to the agostic/anagostic character of the C–H $\cdots$ M interaction in model compounds **7** - **11**.

|                                                | <b>7</b> | <b>8</b> | <b>9</b> | <b>10</b> | <b>11</b> |
|------------------------------------------------|----------|----------|----------|-----------|-----------|
| Angle C–H $\cdots$ Pd ( $^\circ$ )             | 132.0    | 99.0     | 99.8     | 97.6      | 97.7      |
| d <sub>H<math>\cdots</math>Pd</sub> (Å)        | 2.562    | 2.480    | 1.738    | 1.877     | 2.081     |
| WBI <sub>H<math>\cdots</math>Pd</sub>          | 0.012    | 0.007    | 0.205    | 0.097     | 0.091     |
| $\rho(r_c)_{H\cdots Pd}$ <sup>a)</sup>         | 1.609    | 2.226    | 8.903    | 6.544     | 3.538     |
| $\nabla^2\rho(r_c)_{H\cdots Pd}$ <sup>b)</sup> | 4.395    | 7.395    | 22.802   | 21.821    | 11.913    |
| d <sub>C<math>\cdots</math>H</sub> (Å)         | 1.096    | 1.116    | 1.251    | 1.888     | 1.134     |
| WBI <sub>C<math>\cdots</math>H</sub>           | 0.884    | 0.871    | 0.668    | 0.764     | 0.791     |
| $\rho(r_c)_{C\cdots H}$ <sup>d)</sup>          | 0.276    | 0.273    | 0.180    | 0.210     | 0.247     |
| $\nabla^2\rho(r_c)_{C\cdots H}$ <sup>e)</sup>  | -0.957   | -0.953   | -0.309   | -0.479    | -0.704    |
| $q_N(H)$ <sup>f)</sup>                         | 0.250    | 0.192    | 0.210    | 0.225     | 0.265     |

<sup>a)</sup> in  $e/a_0^3 \times 10^2$ ; <sup>b)</sup> in  $e/a_0^5 \times 10^2$ ; <sup>c)</sup> BCP not found; <sup>d)</sup> in  $e/a_0^3$ ; <sup>e)</sup> in  $e/a_0^5$ ; <sup>f)</sup> natural charge on H, in au.

<sup>6</sup> Slight deviation for the normal range of M–H–C angles in compound **8** is due to internal strain.

**Calculated structures:** cartesian coordinates (in Å) and energies computed for compounds studied.-

**Compound 1<sub>I</sub><sup>t-bt</sup>:**

**E = -1664.26184486 au**

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | N  | -0.25325880 | -2.12895604 | -0.14038253 |
| N  | 2.05003099  | 0.00000000  | 0.00000000  | N  | -0.84086812 | -2.75546479 | 0.91215332  |
| C  | 2.63378834  | 1.24460985  | 0.00000000  | C  | -0.04977246 | -3.05329117 | -1.11168836 |
| C  | 4.03507004  | 1.35499417  | -0.02045225 | C  | -0.51209225 | -4.30425091 | -0.67908792 |
| C  | 4.82812992  | 0.20790497  | -0.02505540 | C  | -1.01106505 | -4.06550296 | 0.60802250  |
| C  | 4.21268096  | -1.05044856 | -0.00250822 | H  | 0.40507337  | -2.75821937 | -2.05488365 |
| C  | 2.81891807  | -1.11022705 | 0.00991070  | H  | -0.49950966 | -5.24453144 | -1.22193404 |
| C  | 1.67694031  | 2.34726761  | 0.05185067  | H  | -1.47740104 | -4.73651673 | 1.32496921  |
| C  | 0.30310887  | 1.96586676  | 0.10651853  | Pd | -1.48508265 | -1.58069343 | 2.44583437  |
| C  | -0.65751699 | 2.98389911  | 0.22022879  | N  | -2.06173157 | -0.46154566 | 4.06373775  |
| C  | -0.27683282 | 4.33430912  | 0.25387487  | C  | -1.54648116 | -0.87137401 | 5.27054513  |
| C  | 1.07578702  | 4.69817974  | 0.17896854  | C  | -1.89652513 | -0.18326186 | 6.44534907  |
| C  | 2.05192580  | 3.70479338  | 0.08230056  | C  | -2.74945219 | 0.91835357  | 6.38421278  |
| H  | 2.27411921  | -2.05531626 | 0.02788146  | C  | -3.24549660 | 1.33244181  | 5.14114791  |
| H  | 4.79330167  | -1.97348752 | 0.00540141  | C  | -2.87628096 | 0.61399733  | 4.00368581  |
| H  | 5.91684254  | 0.29373083  | -0.03998242 | C  | -0.63445020 | -2.00807381 | 5.16948137  |
| H  | 4.49464850  | 2.34409910  | -0.02635880 | C  | -0.41307705 | -2.50205427 | 3.84931274  |
| H  | -1.71644431 | 2.72406393  | 0.28382020  | C  | 0.50263823  | -3.55419967 | 3.68628671  |
| H  | -1.04351156 | 5.10981554  | 0.33861690  | C  | 1.15932262  | -4.11664794 | 4.79176274  |
| H  | 1.36685581  | 5.75066010  | 0.20076981  | C  | 0.91837359  | -3.63611849 | 6.08738160  |
| H  | 3.10661362  | 3.99046429  | 0.03307181  | C  | 0.02519931  | -2.57971418 | 6.27515191  |
| N  | -2.03293323 | 0.11993198  | 0.00874552  | H  | -3.22479367 | 0.88054724  | 3.00478021  |
| N  | -2.68686954 | -0.55695727 | 0.98844849  | H  | -3.90647894 | 2.19443990  | 5.04499413  |
| C  | -4.01528203 | -0.48709065 | 0.72448626  | H  | -3.02062058 | 1.45351586  | 7.29687541  |
| C  | -4.22674561 | 0.25207845  | -0.44798771 | H  | -1.49049081 | -0.51486686 | 7.40177474  |
| C  | -2.94025449 | 0.61151163  | -0.87033361 | H  | 0.70884004  | -3.94207556 | 2.68632752  |
| H  | -4.72651823 | -0.97691079 | 1.38614232  | H  | 1.86522179  | -4.93832115 | 4.64027939  |
| H  | -5.17201970 | 0.48390755  | -0.92931905 | H  | 1.42827267  | -4.08020173 | 6.94511365  |
| H  | -2.60957701 | 1.17948226  | -1.73624532 | H  | -0.15437065 | -2.20066530 | 7.28533720  |

**Compound 1<sub>I</sub><sup>c-bt</sup>:**

**E = -1664.26044617 au**

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | H | -1.71336920 | 2.71849429  | 0.34834048  |
| N  | 2.04857723  | 0.00000000  | 0.00000000  | H | -1.03897207 | 5.10221626  | 0.44231214  |
| C  | 2.63263057  | 1.24525676  | 0.00000000  | H | 1.36916029  | 5.74666124  | 0.28828108  |
| C  | 4.03401095  | 1.35449752  | -0.04158575 | H | 3.10820603  | 3.99014243  | 0.07360216  |
| C  | 4.82641261  | 0.20742641  | -0.06984890 | N | -2.03334234 | 0.13815419  | -0.03875712 |
| C  | 4.21095408  | -1.05119246 | -0.04991743 | N | -2.74133778 | -0.46214227 | 0.95272364  |
| C  | 2.81763169  | -1.11008217 | -0.01440151 | C | -4.06160483 | -0.34045697 | 0.67196940  |
| C  | 1.67750990  | 2.34704654  | 0.07256070  | C | -4.21435226 | 0.35954110  | -0.53188175 |
| C  | 0.30420388  | 1.96504678  | 0.12975707  | C | -2.90583020 | 0.63950330  | -0.94658383 |
| C  | -0.65561733 | 2.97974479  | 0.27404615  | H | -4.80103680 | -0.75847621 | 1.34985598  |
| C  | -0.27362537 | 4.32888488  | 0.33100832  | H | -5.14012173 | 0.61852810  | -1.03614931 |
| C  | 1.07826771  | 4.69468418  | 0.24829499  | H | -2.53485065 | 1.16298178  | -1.82372372 |
| C  | 2.05366264  | 3.70397311  | 0.12434159  | N | -0.26406802 | -2.12302770 | -0.14538608 |
| H  | 2.27217166  | -2.05507598 | 0.00110961  | N | -0.97281516 | -2.72396149 | 0.84714736  |
| H  | 4.79142182  | -1.97434151 | -0.06353562 | C | -0.03027044 | -3.04050585 | -1.11736077 |
| H  | 5.91473377  | 0.29331038  | -0.10298258 | C | -0.59185046 | -4.27060145 | -0.74847028 |
| H  | 4.49348982  | 2.34366772  | -0.04791911 | C | -1.18305812 | -4.01793354 | 0.49700951  |

|    |             |             |             |   |             |             |            |
|----|-------------|-------------|-------------|---|-------------|-------------|------------|
| H  | 0.50998060  | -2.75642867 | -2.01841242 | C | -3.18370558 | 0.83622478  | 3.81439500 |
| H  | -0.58398558 | -5.20207741 | -1.30682042 | C | -3.58764715 | 1.51898613  | 4.97198287 |
| H  | -1.75309558 | -4.67524977 | 1.15081206  | C | -3.20198281 | 1.06553767  | 6.24238165 |
| Pd | -1.71990216 | -1.45827373 | 2.40856055  | C | -2.39450677 | -0.06754878 | 6.35358280 |
| N  | -0.78467023 | -2.40225895 | 3.96769551  | H | 0.26523114  | -3.75672432 | 2.81164029 |
| C  | -1.09184861 | -1.91266134 | 5.21578137  | H | 1.32893543  | -4.91012070 | 4.78534958 |
| C  | -0.53406822 | -2.51869366 | 6.35557774  | H | 0.76680100  | -4.07152811 | 7.10621112 |
| C  | 0.33474523  | -3.60097661 | 6.22030710  | H | -0.78493369 | -2.13181150 | 7.34401456 |
| C  | 0.64891302  | -4.07138224 | 4.93838470  | H | -3.48967004 | 1.21240114  | 2.83588206 |
| C  | 0.06698991  | -3.44230128 | 3.83761256  | H | -4.20868910 | 2.41467089  | 4.88120151 |
| C  | -1.98036805 | -0.75440160 | 5.19507334  | H | -3.52350110 | 1.59826270  | 7.13999132 |
| C  | -2.38776331 | -0.31742320 | 3.89960290  | H | -2.08356248 | -0.41186359 | 7.34418367 |

Compound **1<sub>1</sub><sup>t<sup>ch</sup></sup>**:

E = -1664.20814126 au

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | N  | -0.16979154 | -1.95926017 | 0.97464363  |
| N  | 2.06845243  | 0.00000000  | 0.00000000  | N  | -0.73434884 | -3.00081872 | 0.26903156  |
| C  | 2.61821219  | 1.26084789  | 0.00000000  | C  | 0.87080614  | -2.46934990 | 1.67634514  |
| C  | 4.00083420  | 1.42382780  | 0.19837822  | C  | 1.03806250  | -3.83306969 | 1.39089831  |
| C  | 4.82986254  | 0.30600904  | 0.28264898  | C  | 0.00630055  | -4.11550695 | 0.48864518  |
| C  | 4.26907407  | -0.96829984 | 0.13034069  | H  | 1.47200196  | -1.80965267 | 2.29922296  |
| C  | 2.88408397  | -1.07767200 | -0.00235862 | H  | 1.79253884  | -4.51259621 | 1.77710087  |
| C  | 1.67470011  | 2.30054201  | -0.39502751 | H  | -0.28045852 | -5.05420319 | 0.02273885  |
| C  | 0.37404148  | 1.82673383  | -0.75133276 | Pd | -2.79094301 | -2.88847508 | 0.09330996  |
| C  | -0.42469644 | 2.68853919  | -1.52248208 | N  | -4.85939544 | -2.88847509 | 0.09330996  |
| C  | -0.01949947 | 4.00429736  | -1.79952990 | C  | -5.40915520 | -4.14932298 | 0.09330996  |
| C  | 1.20087357  | 4.49702146  | -1.31784179 | C  | -6.79177721 | -4.31230289 | -0.10506826 |
| C  | 2.06117339  | 3.63322045  | -0.63926440 | C  | -7.62080555 | -3.19448413 | -0.18933902 |
| H  | 2.39521811  | -2.04580060 | -0.10030203 | C  | -7.06001708 | -1.92017525 | -0.03703073 |
| H  | 4.88278824  | -1.86963685 | 0.12317048  | C  | -5.67502698 | -1.81080309 | 0.09566858  |
| H  | 5.90531264  | 0.42823085  | 0.42864330  | C  | -4.46564312 | -5.18901710 | 0.48833747  |
| H  | 4.42039802  | 2.42942577  | 0.24482058  | C  | -3.16498448 | -4.71520891 | 0.84464272  |
| H  | -1.37494963 | 2.33935877  | -1.92611319 | C  | -2.36624657 | -5.57701427 | 1.61579204  |
| H  | -0.66881466 | 4.64942390  | -2.39813150 | C  | -2.77144354 | -6.89277244 | 1.89283987  |
| H  | 1.49723549  | 5.53054823  | -1.50931305 | C  | -3.99181657 | -7.38549654 | 1.41115175  |
| H  | 3.04846667  | 3.98729488  | -0.32966439 | C  | -4.85211639 | -6.52169553 | 0.73257437  |
| N  | -2.05659417 | 0.11234364  | -0.17572160 | H  | -5.18616113 | -0.84267449 | 0.19361199  |
| N  | -2.62115147 | -0.92921491 | -0.88133367 | H  | -7.67373125 | -1.01883824 | -0.02986052 |
| C  | -3.66174915 | -0.41912518 | -1.58303518 | H  | -8.69625565 | -3.31670595 | -0.33533334 |
| C  | -3.82900551 | 0.94459461  | -1.29758835 | H  | -7.21134102 | -5.31790086 | -0.15151062 |
| C  | -2.79724356 | 1.22703187  | -0.39533522 | H  | -1.41599338 | -5.22783385 | 2.01942315  |
| H  | -4.26294497 | -1.07882241 | -2.20591300 | H  | -2.12212834 | -7.53789897 | 2.49144146  |
| H  | -4.58348185 | 1.62412112  | -1.68379091 | H  | -4.28817849 | -8.41902331 | 1.60262301  |
| H  | -2.51048449 | 2.16572811  | 0.07057111  | H  | -5.83940967 | -6.87576997 | 0.42297436  |

Compound **1<sub>2</sub><sup>t<sup>bt-nn</sup></sup>**:

E = -3329.42708164 au (B3LYP/aug6-31G\*\*/SDDecp)

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | C | -0.24219161 | 4.34253192  | 0.30734152  |
| N  | 2.07153478  | 0.00000000  | 0.00000000  | C | 1.10926387  | 4.69414371  | 0.24083394  |
| C  | 2.64514816  | 1.23912084  | 0.00000000  | C | 2.07266501  | 3.69611085  | 0.12700979  |
| C  | 4.04147243  | 1.35696197  | -0.04095595 | H | 2.30280312  | -2.04519533 | 0.00550915  |
| C  | 4.83455677  | 0.21523593  | -0.06609756 | H | 4.80846959  | -1.95686118 | -0.05401954 |
| C  | 4.22726609  | -1.04173528 | -0.04476765 | H | 5.91636793  | 0.30490796  | -0.09716217 |
| C  | 2.83861259  | -1.10320513 | -0.01232080 | H | 4.49794929  | 2.33962562  | -0.04843211 |
| C  | 1.68690487  | 2.34662686  | 0.07333722  | H | -1.68648290 | 2.74997808  | 0.30821943  |
| C  | 0.31575795  | 1.97486135  | 0.12468268  | H | -0.99789598 | 5.11878656  | 0.40061612  |
| C  | -0.63187745 | 2.99907155  | 0.25243781  | H | 1.40844687  | 5.73706819  | 0.28233849  |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H  | 3.12213757  | 3.97464845  | 0.08371293  | C  | -1.82831600 | -3.14962484 | 10.20362356 |
| N  | -2.03934511 | 0.12572329  | -0.00543937 | C  | -3.17977148 | -3.50123663 | 10.27013115 |
| N  | -2.74656187 | -0.58451010 | 0.90543833  | C  | -4.14317262 | -2.50320376 | 10.38395529 |
| C  | -4.04855458 | -0.50946939 | 0.56456226  | H  | -4.37331071 | 3.23810241  | 10.50545594 |
| C  | -4.19552390 | 0.26672001  | -0.58875503 | H  | -6.87897718 | 3.14976827  | 10.56498462 |
| C  | -2.89114364 | 0.64091393  | -0.91599170 | H  | -7.98687553 | 0.88799914  | 10.60812725 |
| H  | -4.79547830 | -1.01745030 | 1.15981576  | H  | -6.56845690 | -1.14671853 | 10.55939719 |
| H  | -5.10638617 | 0.51290980  | -1.11377440 | H  | -0.38402471 | -1.55707101 | 10.20274566 |
| H  | -2.51937027 | 1.23642944  | -1.73767342 | H  | -1.07261164 | -3.92587949 | 10.11034897 |
| N  | -0.24481600 | -2.13090699 | -0.16554321 | H  | -3.47895449 | -4.54416111 | 10.22862660 |
| N  | -0.90807620 | -2.81259622 | 0.79901191  | H  | -5.19264518 | -2.78174137 | 10.42725216 |
| C  | -0.01141595 | -2.98050077 | -1.18732809 | N  | -0.03116249 | 1.06718379  | 10.51640445 |
| C  | -0.52713224 | -4.24254011 | -0.88218947 | N  | 0.67605427  | 1.77741718  | 9.60552676  |
| C  | -1.09150840 | -4.08239571 | 0.38534184  | C  | 1.97804698  | 1.70237646  | 9.94640282  |
| H  | 0.50113371  | -2.63536938 | -2.07542649 | C  | 2.12501631  | 0.92618706  | 11.09972012 |
| H  | -0.50539767 | -5.13494909 | -1.48968363 | C  | 0.82063604  | 0.55199315  | 11.42695679 |
| H  | -1.61158557 | -4.79139097 | 1.01361883  | H  | 2.72497071  | 2.21035738  | 9.35114932  |
| Pd | -1.71674389 | -1.78467976 | 2.37728757  | H  | 3.03587858  | 0.67999727  | 11.62473949 |
| N  | -2.47250428 | -0.82204968 | 4.04647476  | H  | 0.44886267  | -0.04352237 | 12.24863850 |
| C  | -2.08978715 | -1.35846132 | 5.24175898  | N  | -1.82569160 | 3.32381407  | 10.67650830 |
| C  | -2.52701385 | -0.77671512 | 6.43918348  | N  | -1.16243139 | 4.00550330  | 9.71195317  |
| C  | -3.33349269 | 0.35612171  | 6.40473214  | C  | -0.97899920 | 5.27530279  | 10.12562324 |
| C  | -3.70597940 | 0.89496517  | 5.17145796  | C  | -1.54337536 | 5.43544718  | 11.39315456 |
| C  | -3.25217626 | 0.27237600  | 4.01457803  | C  | -2.05909165 | 4.17340784  | 11.69829317 |
| C  | -1.18480813 | -2.50675477 | 5.12277603  | H  | -0.45892203 | 5.98429805  | 9.49734626  |
| C  | -0.81703303 | -2.86995400 | 3.79958116  | H  | -1.56510993 | 6.32785616  | 12.00064871 |
| C  | 0.10307772  | -3.91292804 | 3.63954705  | H  | -2.57164131 | 3.82827646  | 12.58639158 |
| C  | 0.62412637  | -4.59218941 | 4.74693392  | Pd | -0.35376371 | 2.97758684  | 8.13367752  |
| C  | 0.23574721  | -4.24018547 | 6.04194285  | N  | 0.40199668  | 2.01495676  | 6.46449033  |
| C  | -0.66576895 | -3.19506296 | 6.23101632  | C  | 0.01927955  | 2.55136839  | 5.26920610  |
| H  | -3.49563415 | 0.64578615  | 3.02692631  | C  | 0.45650625  | 1.96962219  | 4.07178160  |
| H  | -4.31742807 | 1.78716825  | 5.10087390  | C  | 1.26298509  | 0.83678537  | 4.10623295  |
| H  | -3.64503430 | 0.82398929  | 7.33321017  | C  | 1.63547180  | 0.29794191  | 5.33950712  |
| H  | -2.22121669 | -1.19291538 | 7.39150591  | C  | 1.18166866  | 0.92053108  | 6.49638706  |
| H  | 0.41975766  | -4.20336238 | 2.64317137  | C  | -0.88569947 | 3.69966184  | 5.38818906  |
| H  | 1.33334350  | -5.40277022 | 4.59601770  | C  | -1.25347457 | 4.06286108  | 6.71138392  |
| H  | 0.63515128  | -4.77439885 | 6.89928192  | C  | -2.17358532 | 5.10583511  | 6.87141804  |
| H  | -0.96203670 | -2.92249044 | 7.24019208  | C  | -2.69463397 | 5.78509649  | 5.76403116  |
| Pd | -2.07050760 | 1.19290708  | 10.51096508 | C  | -2.30625480 | 5.43309254  | 4.46902224  |
| N  | -4.14204238 | 1.19290708  | 10.51096508 | C  | -1.40473865 | 4.38797003  | 4.27994876  |
| C  | -4.71565577 | -0.04621376 | 10.51096508 | H  | 1.42512655  | 0.54712093  | 7.48403878  |
| C  | -6.11198004 | -0.16405488 | 10.55192104 | H  | 2.24692047  | -0.59426118 | 5.41009118  |
| C  | -6.90506437 | 0.97767117  | 10.57706265 | H  | 1.57452670  | 0.36891778  | 3.17775492  |
| C  | -6.29777368 | 2.23464237  | 10.55573273 | H  | 0.15070910  | 2.38582246  | 3.11945917  |
| C  | -4.90912019 | 2.29611222  | 10.52328588 | H  | -2.49026526 | 5.39626946  | 7.86779372  |
| C  | -3.75741248 | -1.15371978 | 10.43762787 | H  | -3.40385110 | 6.59567730  | 5.91494738  |
| C  | -2.38626555 | -0.78195428 | 10.38628241 | H  | -2.70565888 | 5.96730592  | 3.61168316  |
| C  | -1.43863016 | -1.80616448 | 10.25852727 | H  | -1.10847090 | 4.11539751  | 3.27077300  |

Compound  $1_2^{t-bt-nn}$ .

E = -3328.54752336 au (mPW1B95/aug6-31G\*\*/SDDecp)

BSSE = 0.01448 au

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | C | -0.27710334 | 4.34107246  | -0.16229263 |
| N  | 2.05064037  | 0.00000000  | 0.00000000  | C | 1.07850130  | 4.70215235  | -0.12383594 |
| C  | 2.63656343  | 1.24391026  | 0.00000000  | C | 2.05582724  | 3.70648910  | -0.06801269 |
| C  | 4.03704010  | 1.35208070  | 0.06034981  | H | 2.26802134  | -2.05611200 | 0.05782384  |
| C  | 4.82676044  | 0.20340121  | 0.11098675  | H | 4.78783294  | -1.97818154 | 0.14149408  |
| C  | 4.20910323  | -1.05457759 | 0.10360513  | H | 5.91454637  | 0.28790135  | 0.15785538  |
| C  | 2.81622469  | -1.11232889 | 0.05127376  | H | 4.49828090  | 2.34035136  | 0.06982025  |
| C  | 1.67993195  | 2.34842121  | -0.05238589 | H | -1.72075241 | 2.73364246  | -0.13856726 |
| C  | 0.30368801  | 1.96840377  | -0.07683789 | H | -1.04450765 | 5.11903648  | -0.21115755 |
| C  | -0.65929026 | 2.99049578  | -0.12958676 | H | 1.37059929  | 5.75416977  | -0.13729834 |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H  | 3.11144149  | 3.99080217  | -0.03963646 | C  | 0.68114484  | -2.58475562 | 10.26866424 |
| N  | -2.02878039 | 0.12320581  | 0.06679420  | C  | -0.67445981 | -2.94583550 | 10.23020755 |
| N  | -2.62498247 | -0.37743564 | 1.17993132  | C  | -1.65178574 | -1.95017225 | 10.17438429 |
| C  | -3.96625616 | -0.32215533 | 0.98921172  | H  | -1.86397984 | 3.81242885  | 10.04854777 |
| C  | -4.24428154 | 0.22835139  | -0.26996959 | H  | -4.38379143 | 3.73449839  | 9.96487753  |
| C  | -2.98387140 | 0.49052401  | -0.82240061 | H  | -5.51050486 | 1.46841550  | 9.94851623  |
| H  | -4.63933617 | -0.68695691 | 1.76201114  | H  | -4.09423940 | -0.58403451 | 10.03655136 |
| H  | -5.21572783 | 0.40081869  | -0.72328741 | H  | 2.12479391  | -0.97732563 | 10.24493887 |
| H  | -2.70428148 | 0.90809621  | -1.78646240 | H  | 1.44854914  | -3.36271964 | 10.31752916 |
| N  | -0.26450358 | -2.12418020 | 0.10766602  | H  | -0.96655780 | -3.99785292 | 10.24366995 |
| N  | -0.81449983 | -2.61008541 | 1.25138396  | H  | -2.70740000 | -2.23448533 | 10.14600807 |
| C  | -0.12959152 | -3.15680909 | -0.76156063 | N  | 2.43282190  | 1.63311103  | 10.03957741 |
| C  | -0.59730597 | -4.33736001 | -0.16773452 | N  | 3.02902397  | 2.13375248  | 8.92644029  |
| C  | -1.02751095 | -3.94067461 | 1.10538683  | C  | 4.37029766  | 2.07847218  | 9.11715989  |
| H  | 0.28168105  | -2.98242841 | -1.75363942 | C  | 4.64832304  | 1.52796545  | 10.37634119 |
| H  | -0.63287605 | -5.33276289 | -0.60000039 | C  | 3.38791290  | 1.26579284  | 10.92877221 |
| H  | -1.47167760 | -4.51433385 | 1.91492570  | H  | 5.04337767  | 2.44327375  | 8.34436046  |
| Pd | -1.35232774 | -1.25458498 | 2.67966810  | H  | 5.61976934  | 1.35549815  | 10.82965901 |
| N  | -1.80481739 | 0.06052501  | 4.18972054  | H  | 3.10832299  | 0.84822063  | 11.89283400 |
| C  | -1.22252339 | -0.22367364 | 5.40153118  | N  | 0.66854509  | 3.88049704  | 9.99870559  |
| C  | -1.40147451 | 0.64930157  | 6.48710540  | N  | 1.21854133  | 4.36640225  | 8.85498765  |
| C  | -2.19870539 | 1.78545944  | 6.34253448  | C  | 1.43155245  | 5.69699145  | 9.00098478  |
| C  | -2.79915719 | 2.04921580  | 5.10491502  | C  | 1.00134748  | 6.09367686  | 10.27410613 |
| C  | -2.56432451 | 1.16896764  | 4.04789324  | C  | 0.53363302  | 4.91312593  | 10.86793224 |
| C  | -0.39955732 | -1.43109134 | 5.39440145  | H  | 1.87571911  | 6.27065069  | 8.19144591  |
| C  | -0.24918003 | -2.06766329 | 4.12716405  | H  | 1.03691756  | 7.08907974  | 10.70637200 |
| C  | 0.61086582  | -3.17462406 | 4.04577672  | H  | 0.12236045  | 4.73874525  | 11.86001102 |
| C  | 1.26743664  | -3.66255746 | 5.18853106  | Pd | 1.75636925  | 3.01090182  | 7.42670351  |
| C  | 1.07124484  | -3.05707120 | 6.43803502  | N  | 2.20885889  | 1.69579183  | 5.91665107  |
| C  | 0.24009770  | -1.93803289 | 6.54173709  | C  | 1.62656490  | 1.97999048  | 4.70484043  |
| H  | -2.97230433 | 1.33218781  | 3.04931244  | C  | 1.80551601  | 1.10701527  | 3.61926621  |
| H  | -3.40651322 | 2.93960849  | 4.94067327  | C  | 2.60274689  | -0.02914260 | 3.76383713  |
| H  | -2.31702119 | 2.47550430  | 7.18029986  | C  | 3.20319870  | -0.29289896 | 5.00145659  |
| H  | -0.88540890 | 0.45312159  | 7.42851206  | C  | 2.96836601  | 0.58734921  | 6.05847836  |
| H  | 0.76874249  | -3.67073820 | 3.08523022  | C  | 0.80359882  | 3.18740818  | 4.71197016  |
| H  | 1.92519967  | -4.53276401 | 5.10214652  | C  | 0.65322154  | 3.82398013  | 5.97920756  |
| H  | 1.56118234  | -3.45133990 | 7.33128764  | C  | -0.20682431 | 4.93094090  | 6.06059489  |
| H  | 0.08800242  | -1.46636465 | 7.51612131  | C  | -0.86339514 | 5.41887431  | 4.91784055  |
| Pd | 0.40404150  | 1.75631684  | 10.10637161 | C  | -0.66720334 | 4.81338804  | 3.66833659  |
| N  | -1.64659887 | 1.75631685  | 10.10637161 | C  | 0.16394381  | 3.69434974  | 3.56463452  |
| C  | -2.23252193 | 0.51240659  | 10.10637161 | H  | 3.37634583  | 0.42412903  | 7.05705917  |
| C  | -3.63299860 | 0.40423616  | 10.04602180 | H  | 3.81055473  | -1.18329165 | 5.16569834  |
| C  | -4.42271893 | 1.55291565  | 9.99538486  | H  | 2.72106269  | -0.71918745 | 2.92607175  |
| C  | -3.80506172 | 2.81089444  | 10.00276648 | H  | 1.28945040  | 1.30319525  | 2.67785955  |
| C  | -2.41218318 | 2.86864574  | 10.05509785 | H  | -0.36470099 | 5.42705504  | 7.02114139  |
| C  | -1.27589045 | -0.59210436 | 10.15875750 | H  | -1.52115817 | 6.28908086  | 5.00422509  |
| C  | 0.10035349  | -0.21208693 | 10.18320950 | H  | -1.15714084 | 5.20765674  | 2.77508397  |
| C  | 1.06333176  | -1.23417894 | 10.23595837 | H  | 0.31603908  | 3.22268150  | 2.59025030  |

Compound  $\mathbf{1_2^{t-bt-nn}}$ :

E = -3329.17684060 au (mPW1B95/aug6-311G\*\*/SDDecp)

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | C | 2.05909798  | 3.70049137  | -0.05638235 |
| N  | 2.05401576  | 0.00000000  | 0.00000000  | H | 2.28009394  | -2.05239834 | 0.03948651  |
| C  | 2.63791902  | 1.24165470  | 0.00000000  | H | 4.79029166  | -1.96905406 | 0.10304931  |
| C  | 4.03577753  | 1.35181798  | 0.00485263  | H | 5.91219165  | 0.29332428  | 0.12381420  |
| C  | 4.82619428  | 0.20784965  | 0.08624802  | H | 4.49417712  | 2.33899032  | 0.05723239  |
| C  | 4.21157100  | -1.04759124 | 0.07674878  | H | -1.70924571 | 2.73763850  | -0.14333166 |
| C  | 2.82213994  | -1.10767962 | 0.03659653  | H | -1.03088028 | 5.11436058  | -0.20706497 |
| C  | 1.68280244  | 2.34528935  | -0.04515164 | H | 1.37893860  | 5.74535179  | -0.12107989 |
| C  | 0.30930550  | 1.96931382  | -0.07372021 | H | 3.11264178  | 3.98345470  | -0.02356665 |
| C  | -0.64948357 | 2.99062368  | -0.12774874 | N | -2.03059978 | 0.12817425  | 0.05433379  |
| C  | -0.26602880 | 4.33697262  | -0.15660312 | N | -2.64483124 | -0.37822708 | 1.15246257  |
| C  | 1.08638409  | 4.69563688  | -0.11234426 | C | -3.98009875 | -0.29336469 | 0.95304415  |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C  | -4.23590849 | 0.28263509  | -0.29637301 | C  | -1.88053494 | -2.03556452 | 10.26320527 |
| C  | -2.96919463 | 0.52930772  | -0.83371708 | H  | -2.10153090 | 3.71732519  | 10.16733641 |
| H  | -4.66680325 | -0.65770349 | 1.71044291  | H  | -4.61172861 | 3.63398092  | 10.10377362 |
| H  | -5.19806498 | 0.48024572  | -0.75393354 | H  | -5.73362861 | 1.37160258  | 10.08300873 |
| H  | -2.67654805 | 0.95886855  | -1.78569370 | H  | -4.31561408 | -0.67406346 | 10.14959053 |
| N  | -0.26609391 | -2.12493979 | 0.11114432  | H  | 1.88780874  | -1.07271165 | 10.35015459 |
| N  | -0.83972557 | -2.61735043 | 1.23839885  | H  | 1.20944331  | -3.44943373 | 10.41388789 |
| C  | -0.09252503 | -3.15419393 | -0.75058412 | H  | -1.20037557 | -4.08042493 | 10.32790281 |
| C  | -0.55740921 | -4.33841410 | -0.16869401 | H  | -2.93407874 | -2.31852784 | 10.23038958 |
| C  | -1.02693485 | -3.94847869 | 1.08926169  | N  | 2.20916282  | 1.53675260  | 10.15248914 |
| H  | 0.33909496  | -2.97750595 | -1.73088607 | N  | 2.82339428  | 2.04315393  | 9.05436035  |
| H  | -0.56764717 | -5.33235485 | -0.60012689 | C  | 4.15866179  | 1.95829155  | 9.25377877  |
| H  | -1.48061851 | -4.52879019 | 1.88528758  | C  | 4.41447153  | 1.38229176  | 10.50319593 |
| Pd | -1.41220849 | -1.27804295 | 2.67219701  | C  | 3.14775767  | 1.13561913  | 11.04054000 |
| N  | -1.88849774 | 0.03018269  | 4.18192010  | H  | 4.84536629  | 2.32263035  | 8.49638002  |
| C  | -1.35051850 | -0.27132524 | 5.40683642  | H  | 5.37662802  | 1.18468113  | 10.96075646 |
| C  | -1.56387885 | 0.58531323  | 6.49501666  | H  | 2.85511109  | 0.70605830  | 11.99251663 |
| C  | -2.34343842 | 1.72707940  | 6.33687908  | N  | 0.44465695  | 3.78986664  | 10.09567860 |
| C  | -2.89421619 | 2.01135715  | 5.08534126  | N  | 1.01828861  | 4.28227728  | 8.96842408  |
| C  | -2.63394938 | 1.14305367  | 4.02967381  | C  | 1.20549789  | 5.61340554  | 9.11756124  |
| C  | -0.53378529 | -1.48098930 | 5.41038481  | C  | 0.73597225  | 6.00334095  | 10.37551694 |
| C  | -0.35211712 | -2.10703506 | 4.14533561  | C  | 0.27108807  | 4.81912078  | 10.95740704 |
| C  | 0.49922551  | -3.21731922 | 4.07809162  | H  | 1.65918155  | 6.19371704  | 8.32153534  |
| C  | 1.11982369  | -3.71754086 | 5.23116220  | H  | 0.74621021  | 6.99728170  | 10.80694982 |
| C  | 0.89630737  | -3.12124699 | 6.47680966  | H  | -0.16053192 | 4.64243280  | 11.93770899 |
| C  | 0.07217325  | -2.00034929 | 6.56668106  | Pd | 1.59077153  | 2.94296980  | 7.53462592  |
| H  | -3.01067667 | 1.32167494  | 3.02410588  | N  | 2.06706078  | 1.63474416  | 6.02490282  |
| H  | -3.48334639 | 2.90939229  | 4.91040579  | C  | 1.52908154  | 1.93625209  | 4.79998650  |
| H  | -2.48927950 | 2.40671054  | 7.17554456  | C  | 1.74244189  | 1.07961362  | 3.71180626  |
| H  | -1.09458398 | 0.36714004  | 7.45325604  | C  | 2.52200146  | -0.06215255 | 3.86994385  |
| H  | 0.67882340  | -3.70694991 | 3.12092502  | C  | 3.07277923  | -0.34643030 | 5.12148167  |
| H  | 1.77294795  | -4.58953858 | 5.15517782  | C  | 2.81251242  | 0.52187318  | 6.17714911  |
| H  | 1.36234154  | -3.52398667 | 7.37630220  | C  | 0.71234833  | 3.14591615  | 4.79643812  |
| H  | -0.09779861 | -1.53534946 | 7.53910254  | C  | 0.53068016  | 3.77196191  | 6.06148732  |
| Pd | 0.17856304  | 1.66492685  | 10.20682292 | C  | -0.32066247 | 4.88224607  | 6.12873130  |
| N  | -1.87545272 | 1.66492685  | 10.20682292 | C  | -0.94126066 | 5.38246771  | 4.97566072  |
| C  | -2.45935598 | 0.42327215  | 10.20682292 | C  | -0.71774434 | 4.78617384  | 3.73001327  |
| C  | -3.85721450 | 0.31310887  | 10.15830029 | C  | 0.10638979  | 3.66527614  | 3.64014187  |
| C  | -4.64763124 | 1.45707721  | 10.12057490 | H  | 3.18923971  | 0.34325191  | 7.18271704  |
| C  | -4.03300796 | 2.71251810  | 10.13007415 | H  | 3.66190943  | -1.24446543 | 5.29641714  |
| C  | -2.64357690 | 2.77260648  | 10.17022639 | H  | 2.66784254  | -0.74178369 | 3.03127837  |
| C  | -1.50423941 | -0.68036249 | 10.25197457 | H  | 1.27314702  | 1.29778681  | 2.75356689  |
| C  | -0.13074247 | -0.30438697 | 10.28054313 | H  | -0.50026036 | 5.37187676  | 7.08589791  |
| C  | 0.82804660  | -1.32569683 | 10.33457167 | H  | -1.59438491 | 6.25446543  | 5.05164510  |
| C  | 0.44459183  | -2.67204577 | 10.36342605 | H  | -1.18377850 | 5.18891352  | 2.83052072  |
| C  | -0.90782106 | -3.03071003 | 10.31916719 | H  | 0.27636165  | 3.20027631  | 2.66772039  |

Compound  $\mathbf{1}_2^{t\text{-}bt\text{-}nn}$ : E = -22488.9202649 au (mPW1B95/aug6-31G\*\*/3-21G\*)

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | H | 4.85290961  | -1.94839526 | 0.03194134  |
| N  | 2.09209022  | 0.00000000  | 0.00000000  | H | 5.95167497  | 0.32878915  | 0.05940561  |
| C  | 2.66120719  | 1.24816199  | 0.00000000  | H | 4.51510873  | 2.36533229  | 0.03626104  |
| C  | 4.06179089  | 1.37354153  | 0.02615807  | H | -1.70970187 | 2.73832405  | -0.08492273 |
| C  | 4.86396179  | 0.23256651  | 0.03917010  | H | -1.03206154 | 5.12514566  | -0.14324035 |
| C  | 4.26151620  | -1.03217330 | 0.02567988  | H | 1.38519957  | 5.75462718  | -0.07363172 |
| C  | 2.86769941  | -1.10361872 | 0.00910177  | H | 3.12064492  | 3.99120409  | -0.00955264 |
| C  | 1.69261298  | 2.34601964  | -0.02564973 | N | -2.06454115 | 0.15040179  | 0.02398986  |
| C  | 0.31497725  | 1.97837816  | -0.03433199 | N | -2.65797959 | -0.35632895 | 1.12997619  |
| C  | -0.64864754 | 2.99552421  | -0.07758361 | C | -3.99944444 | -0.28736345 | 0.94609148  |
| C  | -0.26559880 | 4.34600724  | -0.10218034 | C | -4.27870055 | 0.28052060  | -0.30583209 |
| C  | 1.09013464  | 4.70343084  | -0.06865231 | C | -3.01716773 | 0.53819772  | -0.85902426 |
| C  | 2.06543800  | 3.70555300  | -0.03009185 | H | -4.67151426 | -0.65717436 | 1.71789632  |
| H  | 2.32807340  | -2.05327769 | 0.01257793  | H | -5.25023836 | 0.46488261  | -0.75443507 |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H  | -2.73406550 | 0.96532874  | -1.81824021 | H  | -4.11836711 | 3.66769176  | 9.89800771  |
| N  | -0.24872908 | -2.16734457 | 0.03243122  | H  | -5.21713248 | 1.39050735  | 9.87054344  |
| N  | -0.80998279 | -2.65843654 | 1.16334251  | H  | -3.78056624 | -0.64603579 | 9.89368802  |
| C  | -0.11824713 | -3.19189541 | -0.84698272 | H  | 2.44424437  | -1.01902756 | 10.01487179 |
| C  | -0.60089951 | -4.37477640 | -0.26886224 | H  | 1.76660404  | -3.40584916 | 10.07318941 |
| C  | -1.03467331 | -3.98542321 | 1.00588586  | H  | -0.65065708 | -4.03533068 | 10.00358077 |
| H  | 0.29952310  | -3.00951875 | -1.83528430 | H  | -2.38610242 | -2.27190759 | 9.93950170  |
| H  | -0.64553004 | -5.36495212 | -0.71233073 | N  | 2.79908365  | 1.56889470  | 9.90595919  |
| H  | -1.48858795 | -4.56113303 | 1.80904155  | N  | 3.39252209  | 2.07562545  | 8.79997287  |
| Pd | -1.30638830 | -1.24702762 | 2.60709884  | C  | 4.73398694  | 2.00665995  | 8.98385758  |
| N  | -1.70559729 | 0.11454691  | 4.14428745  | C  | 5.01324305  | 1.43877590  | 10.23578115 |
| C  | -1.06817436 | -0.16114503 | 5.32686838  | C  | 3.75171023  | 1.18109878  | 10.78897331 |
| C  | -1.19626089 | 0.72099612  | 6.41359503  | H  | 5.40605676  | 2.37647086  | 8.21205273  |
| C  | -1.99622215 | 1.85837905  | 6.28971555  | H  | 5.98478085  | 1.25441389  | 10.68438413 |
| C  | -2.66374370 | 2.10509895  | 5.08417817  | H  | 3.46860800  | 0.75396776  | 11.74818926 |
| C  | -2.47817724 | 1.21305466  | 4.02706708  | N  | 0.98327158  | 3.88664107  | 9.89751784  |
| C  | -0.25496312 | -1.37707091 | 5.29326866  | N  | 1.54452529  | 4.37773304  | 8.76660655  |
| C  | -0.15774143 | -2.04584904 | 4.03957715  | C  | 1.76921581  | 5.70471971  | 8.92406320  |
| C  | 0.67514171  | -3.16710661 | 3.94131458  | C  | 1.33544200  | 6.09407290  | 10.19881130 |
| C  | 1.37540067  | -3.63931597 | 5.06440312  | C  | 0.85278963  | 4.91119191  | 10.77693178 |
| C  | 1.24906422  | -2.99753072 | 6.30361978  | H  | 2.22313045  | 6.28042953  | 8.12090751  |
| C  | 0.43606160  | -1.86667795 | 6.41820914  | H  | 1.38007254  | 7.08424862  | 10.64227980 |
| H  | -2.93614445 | 1.36240340  | 3.04744531  | H  | 0.43501940  | 4.72881525  | 11.76523336 |
| H  | -3.27993967 | 2.99333919  | 4.94343002  | Pd | 2.04093080  | 2.96632411  | 7.32285022  |
| H  | -2.06734185 | 2.56530447  | 7.11791656  | N  | 2.44013979  | 1.60474959  | 5.78566161  |
| H  | -0.63105149 | 0.54551303  | 7.33102793  | C  | 1.80271686  | 1.88044153  | 4.60308067  |
| H  | 0.77982053  | -3.68679730 | 2.98641889  | C  | 1.93080339  | 0.99830038  | 3.51635403  |
| H  | 2.01547613  | -4.52138784 | 4.96924749  | C  | 2.73076465  | -0.13908255 | 3.64023351  |
| H  | 1.77827455  | -3.37237911 | 7.18239044  | C  | 3.39828620  | -0.38580246 | 4.84577088  |
| H  | 0.34980255  | -1.36148654 | 7.38346660  | C  | 3.21271974  | 0.50624184  | 5.90288198  |
| Pd | 0.73454250  | 1.71929650  | 9.92994906  | C  | 0.98950562  | 3.09636741  | 4.63668039  |
| N  | -1.35754772 | 1.71929650  | 9.92994906  | C  | 0.89228393  | 3.76514553  | 5.89037190  |
| C  | -1.92666469 | 0.47113451  | 9.92994906  | C  | 0.05940079  | 4.88640310  | 5.98863448  |
| C  | -3.32724840 | 0.34575497  | 9.90379099  | C  | -0.64085817 | 5.35861247  | 4.86554594  |
| C  | -4.12941929 | 1.48673000  | 9.89077895  | C  | -0.51452172 | 4.71682722  | 3.62632928  |
| C  | -3.52697370 | 2.75146980  | 9.90426918  | C  | 0.29848090  | 3.58597445  | 3.51173992  |
| C  | -2.13315691 | 2.82291522  | 9.92084728  | H  | 3.67068695  | 0.35689310  | 6.88250375  |
| C  | -0.95807048 | -0.62672314 | 9.95559879  | H  | 4.01448216  | -1.27404269 | 4.98651904  |
| C  | 0.41956525  | -0.25908166 | 9.96428105  | H  | 2.80188435  | -0.84600797 | 2.81203250  |
| C  | 1.38319004  | -1.27622771 | 10.00753266 | H  | 1.36559399  | 1.17378347  | 2.59892113  |
| C  | 1.00014130  | -2.62671074 | 10.03212940 | H  | -0.04527803 | 5.40609380  | 6.94353017  |
| C  | -0.35559214 | -2.98413434 | 9.99860137  | H  | -1.28093363 | 6.24068434  | 4.96070157  |
| C  | -1.33089550 | -1.98625650 | 9.96004090  | H  | -1.04373205 | 5.09167561  | 2.74755862  |
| H  | -1.59353090 | 3.77257419  | 9.91737113  | H  | 0.38473995  | 3.08078304  | 2.54648246  |

Compound  $\text{I}_2^{t\text{-}bt\text{-}nn}$  (2<sup>nd</sup> minimum): E = -3328.54453494 au

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | H | 4.49809892  | 2.34017825  | 0.06361987  |
| N  | 2.04965442  | 0.00000000  | 0.00000000  | H | -1.72292348 | 2.73247085  | -0.06408289 |
| C  | 2.63504476  | 1.24472855  | 0.00000000  | H | -1.04804435 | 5.11946453  | -0.11260004 |
| C  | 4.03669546  | 1.35212982  | 0.04872905  | H | 1.36799299  | 5.75406671  | -0.09373990 |
| C  | 4.82700669  | 0.20341005  | 0.07779020  | H | 3.11020749  | 3.98979967  | -0.04127602 |
| C  | 4.20947008  | -1.05492261 | 0.06246491  | N | -2.03217266 | 0.12040133  | 0.03687197  |
| C  | 2.81599730  | -1.11279841 | 0.03154734  | N | -2.64129505 | -0.41822710 | 1.12461987  |
| C  | 1.67859781  | 2.34839832  | -0.04182265 | C | -3.97892504 | -0.38764982 | 0.90665710  |
| C  | 0.30267602  | 1.96870528  | -0.05070170 | C | -4.24168112 | 0.18506064  | -0.34635134 |
| C  | -0.66148601 | 2.99008412  | -0.06966937 | C | -2.97577865 | 0.48636504  | -0.86531784 |
| C  | -0.27972544 | 4.34120311  | -0.09189433 | H | -4.66054747 | -0.78405314 | 1.65616883  |
| C  | 1.07616059  | 4.70182630  | -0.08211669 | H | -5.20676207 | 0.34639147  | -0.81707871 |
| C  | 2.05415678  | 3.70602710  | -0.05352706 | H | -2.68444018 | 0.92973338  | -1.81422412 |
| H  | 2.26761742  | -2.05645119 | 0.03799619  | N | -0.26151186 | -2.13152067 | 0.09880897  |
| H  | 4.78934755  | -1.97861690 | 0.07786453  | N | -0.80024350 | -2.61037703 | 1.25123159  |
| H  | 5.91519892  | 0.28798281  | 0.11282017  | C | -0.12346756 | -3.17236754 | -0.75976461 |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C  | -0.57789212 | -4.35039209 | -0.15056507 | H  | -2.39111778 | -1.74529037 | 9.99522453  |
| C  | -1.00389450 | -3.94376461 | 1.12107709  | H  | 3.82990462  | -2.13758297 | 10.12292728 |
| H  | 0.27987461  | -3.00547509 | -1.75636983 | H  | 3.15502549  | -4.52457665 | 10.17144443 |
| H  | -0.60864842 | -5.35049572 | -0.57228812 | H  | 0.73898816  | -5.15917883 | 10.15258430 |
| H  | -1.44189040 | -4.51249657 | 1.93753691  | H  | -1.00322635 | -3.39491179 | 10.10012041 |
| Pd | -1.33345100 | -1.21302566 | 2.64017279  | N  | 4.13915380  | 0.47448655  | 10.02197242 |
| N  | -1.74632534 | 0.19025350  | 4.07706949  | N  | 4.74827619  | 1.01311498  | 8.93422452  |
| C  | -1.02409976 | 0.06294843  | 5.23781435  | C  | 6.08590618  | 0.98253770  | 9.15218729  |
| C  | -1.19120427 | 0.99803213  | 6.27317798  | C  | 6.34866226  | 0.40982724  | 10.40519573 |
| C  | -2.09757250 | 2.04646796  | 6.12244063  | C  | 5.08275980  | 0.10852284  | 10.92416223 |
| C  | -2.82525733 | 2.16024299  | 4.93048860  | H  | 6.76752861  | 1.37894102  | 8.40267556  |
| C  | -2.61221557 | 1.21556993  | 3.92690645  | H  | 7.31374321  | 0.24849640  | 10.87592310 |
| C  | -0.12900532 | -1.09007340 | 5.25554523  | H  | 4.79142132  | -0.33484551 | 11.87306851 |
| C  | -0.13507187 | -1.89589889 | 4.07959713  | N  | 2.36849301  | 2.72640855  | 9.96003542  |
| C  | 0.67790238  | -3.04095395 | 4.06324278  | N  | 2.90722464  | 3.20526491  | 8.80761280  |
| C  | 1.46513620  | -3.38058713 | 5.17621419  | C  | 3.11087564  | 4.53865249  | 8.93776730  |
| C  | 1.48804856  | -2.56128146 | 6.31550634  | C  | 2.68487326  | 4.94527997  | 10.20940946 |
| C  | 0.69571539  | -1.41110602 | 6.35116682  | C  | 2.23044870  | 3.76725542  | 10.81860900 |
| H  | -3.12996528 | 1.25568117  | 2.96733463  | H  | 3.54887155  | 5.10738445  | 8.12130748  |
| H  | -3.53817401 | 2.96949195  | 4.76741677  | H  | 2.71562956  | 5.94538360  | 10.63113251 |
| H  | -2.22475068 | 2.77562088  | 6.92541619  | H  | 1.82710654  | 3.60036297  | 11.81521423 |
| H  | -0.59108786 | 0.90497532  | 7.17938029  | Pd | 3.44043214  | 1.80791354  | 7.41867160  |
| H  | 0.70161740  | -3.67734955 | 3.17538614  | N  | 3.85330648  | 0.40463438  | 5.98177490  |
| H  | 2.07917509  | -4.28576532 | 5.14618549  | C  | 3.13108091  | 0.53193945  | 4.82103004  |
| H  | 2.11360764  | -2.81327318 | 7.17456231  | C  | 3.29818541  | -0.40314425 | 3.78566642  |
| H  | 0.74101279  | -0.75614259 | 7.22622696  | C  | 4.20455364  | -1.45158008 | 3.93640376  |
| Pd | 2.10698114  | 0.59488788  | 10.05884439 | C  | 4.93223847  | -1.56535511 | 5.12835579  |
| N  | 0.05732672  | 0.59488788  | 10.05884439 | C  | 4.71919672  | -0.62068205 | 6.13193795  |
| C  | -0.52806362 | -0.64984067 | 10.05884439 | C  | 2.23598646  | 1.68496128  | 4.80329916  |
| C  | -1.92971431 | -0.75724194 | 10.01011534 | C  | 2.24205302  | 2.49078677  | 5.97924726  |
| C  | -2.72002555 | 0.39147783  | 9.98105419  | C  | 1.42907877  | 3.63584183  | 5.99560161  |
| C  | -2.10248894 | 1.64981049  | 9.99637948  | C  | 0.64184494  | 3.97547501  | 4.88263020  |
| C  | -0.70901615 | 1.70768629  | 10.02729705 | C  | 0.61893258  | 3.15616935  | 3.74333805  |
| C  | 0.42838333  | -1.75351044 | 10.10066704 | C  | 1.41126575  | 2.00599390  | 3.70767757  |
| C  | 1.80430512  | -1.37381740 | 10.10954609 | H  | 5.23694643  | -0.66079329 | 7.09150976  |
| C  | 2.76846716  | -2.39519624 | 10.12851377 | H  | 5.64515515  | -2.37460407 | 5.29142762  |
| C  | 2.38670659  | -3.74631523 | 10.15073872 | H  | 4.33173182  | -2.18073300 | 3.13342820  |
| C  | 1.03082055  | -4.10693842 | 10.14096108 | H  | 2.69806901  | -0.31008744 | 2.87946410  |
| C  | 0.05282436  | -3.11113922 | 10.11237145 | H  | 1.40536374  | 4.27223743  | 6.88345825  |
| H  | -0.16063627 | 2.65133907  | 10.02084820 | H  | 0.02780605  | 4.88065321  | 4.91265891  |
| H  | -2.68236641 | 2.57350478  | 9.98097986  | H  | -0.00662649 | 3.40816106  | 2.88428208  |
| H  | -3.80821777 | 0.30690507  | 9.94602422  | H  | 1.36596835  | 1.35103047  | 2.83261743  |

Compound 1<sub>2</sub><sup>t-bt-nx</sup>:

E = -3328.54245674 au

BSSE = 0.01256194 au

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | H | 4.49891694  | 2.34055409  | 0.05214075  |
| N  | 2.05088031  | 0.00000000  | 0.00000000  | H | -1.72114108 | 2.73224801  | -0.14457120 |
| C  | 2.63649373  | 1.24408172  | 0.00000000  | H | -1.04712326 | 5.11892576  | -0.17804338 |
| C  | 4.03766513  | 1.35231313  | 0.04311605  | H | 1.36712524  | 5.75511021  | -0.07850630 |
| C  | 4.82828911  | 0.20365291  | 0.07439982  | H | 3.10891463  | 3.99217114  | 0.00718108  |
| C  | 4.21100058  | -1.05447662 | 0.06463161  | N | -2.02753419 | 0.12870716  | 0.01912824  |
| C  | 2.81754445  | -1.11227493 | 0.03106135  | N | -2.65353076 | -0.35470785 | 1.12260745  |
| C  | 1.67941742  | 2.34881988  | -0.04132106 | C | -3.98949199 | -0.30192527 | 0.89601424  |
| C  | 0.30378228  | 1.96831602  | -0.07970717 | C | -4.23286614 | 0.22970681  | -0.37836748 |
| C  | -0.66002989 | 2.98993537  | -0.12436292 | C | -2.95793419 | 0.48318626  | -0.90093606 |
| C  | -0.27908030 | 4.34124368  | -0.13551881 | H | -4.68321690 | -0.65387060 | 1.65635574  |
| C  | 1.07580571  | 4.70277575  | -0.08262669 | H | -5.19174476 | 0.39547041  | -0.85999207 |
| C  | 2.05393146  | 3.70726952  | -0.03467518 | H | -2.65192519 | 0.88628894  | -1.86307415 |
| H  | 2.26983501  | -2.05642246 | 0.03951914  | N | -0.27403313 | -2.12228624 | 0.15868064  |
| H  | 4.79050441  | -1.97809110 | 0.08687770  | N | -0.84756636 | -2.58103157 | 1.30319025  |
| H  | 5.91654906  | 0.28819039  | 0.10737831  | C | -0.13083047 | -3.17436884 | -0.68531579 |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C  | -0.61651651 | -4.33938974 | -0.07568046 | H  | 7.08966485  | 7.55673269  | 7.57166281  |
| C  | -1.06683272 | -3.91314227 | 1.18056914  | H  | 5.86832618  | 1.58926562  | 8.89370084  |
| H  | 0.29830863  | -3.02367542 | -1.67377965 | H  | 8.25566849  | 1.49756635  | 8.22927100  |
| H  | -0.65040828 | -5.34354306 | -0.48728820 | H  | 9.47629783  | 3.58261951  | 7.59508299  |
| H  | -1.53143138 | -4.46670934 | 1.99269366  | H  | 8.28830425  | 5.76098520  | 7.59923078  |
| Pd | -1.43268052 | -1.19237120 | 2.68186007  | N  | 3.42361597  | 2.12363892  | 9.71889702  |
| N  | -1.93915926 | 0.16667728  | 4.13155764  | N  | 2.40340844  | 1.49368597  | 9.08043299  |
| C  | -1.44257776 | -0.10011062 | 5.38475700  | C  | 2.22321008  | 0.29096995  | 9.68013441  |
| C  | -1.73540184 | 0.76656779  | 6.45006131  | C  | 3.14498134  | 0.13712372  | 10.72524110 |
| C  | -2.52303167 | 1.89833382  | 6.23308145  | C  | 3.88258862  | 1.32793543  | 10.71573397 |
| C  | -3.00929129 | 2.15928060  | 4.94721180  | H  | 1.44687657  | -0.38264187 | 9.32456884  |
| C  | -2.68964144 | 1.26957533  | 3.92053037  | H  | 3.25712783  | -0.70789776 | 11.39781472 |
| C  | -0.60807966 | -1.29922894 | 5.44414550  | H  | 4.69914778  | 1.66282226  | 11.35039766 |
| C  | -0.41047380 | -1.97718136 | 4.20427490  | N  | 1.77470221  | 4.47366669  | 9.76755481  |
| C  | 0.42557210  | -3.10556242 | 4.19804151  | N  | 0.79711919  | 3.87605234  | 9.03830067  |
| C  | 1.02097182  | -3.57064701 | 5.38219211  | C  | -0.40438613 | 4.16136362  | 9.59671234  |
| C  | 0.79602007  | -2.91347389 | 6.60045082  | C  | -0.20738947 | 4.97356115  | 10.72122090 |
| C  | -0.01540503 | -1.77583031 | 6.62933066  | C  | 1.18311255  | 5.13885048  | 10.79069991 |
| H  | -3.02730659 | 1.41719965  | 2.89392113  | H  | -1.31780124 | 3.76618480  | 9.15909492  |
| H  | -3.60838726 | 3.04367530  | 4.72947140  | H  | -0.96143058 | 5.37322562  | 11.39256798 |
| H  | -2.73445680 | 2.58256805  | 7.05713832  | H  | 1.79237791  | 5.68162603  | 11.51020332 |
| H  | -1.31896356 | 0.56855879  | 7.43840134  | Pd | 1.40173020  | 2.62524647  | 7.54458452  |
| H  | 0.61378709  | -3.63497905 | 3.26103032  | N  | 1.95013608  | 1.43874562  | 5.96460481  |
| H  | 1.65970318  | -4.45837451 | 5.35327878  | C  | 1.44748798  | 1.82217477  | 4.74490084  |
| H  | 1.25083896  | -3.28449483 | 7.52179522  | C  | 1.69282932  | 1.03493519  | 3.60855044  |
| H  | -0.18915414 | -1.25733442 | 7.57661405  | C  | 2.48450368  | -0.10931181 | 3.71465925  |
| Pd | 3.80106244  | 4.05343885  | 9.18858804  | C  | 3.03204585  | -0.45427658 | 4.95608420  |
| N  | 4.29477503  | 5.96109951  | 8.62663015  | C  | 2.73080418  | 0.34147535  | 6.06131368  |
| C  | 5.60410560  | 6.13921399  | 8.24716990  | C  | 0.68330008  | 3.06730718  | 4.78610280  |
| C  | 6.04860447  | 7.41724862  | 7.86570300  | C  | 0.53098854  | 3.65512462  | 6.07638321  |
| C  | 5.16178646  | 8.49375693  | 7.85720019  | C  | -0.18326613 | 4.86020031  | 6.17085552  |
| C  | 3.82629338  | 8.28453492  | 8.22526171  | C  | -0.73506298 | 5.46182945  | 5.02686775  |
| C  | 3.43326890  | 7.00061415  | 8.60350399  | C  | -0.56807632 | 4.87932300  | 3.76228516  |
| C  | 6.39567773  | 4.91144570  | 8.26262360  | C  | 0.14619858  | 3.68393663  | 3.63961240  |
| C  | 5.69179706  | 3.73288942  | 8.65233488  | H  | 3.10266800  | 0.11746454  | 7.06191469  |
| C  | 6.38505428  | 2.51205359  | 8.62105650  | H  | 3.65074654  | -1.34278092 | 5.08399253  |
| C  | 7.73546070  | 2.45965825  | 8.24271268  | H  | 2.65304996  | -0.73687550 | 2.83783587  |
| C  | 8.42367274  | 3.62800433  | 7.88303783  | H  | 1.23885654  | 1.30514258  | 2.65380798  |
| C  | 7.75267116  | 4.85226387  | 7.88885311  | H  | -0.30722509 | 5.34276881  | 7.14330960  |
| H  | 2.41024726  | 6.76600018  | 8.90130299  | H  | -1.28853251 | 6.40065290  | 5.12496291  |
| H  | 3.09621888  | 9.09456374  | 8.22210607  | H  | -0.98196359 | 5.35598095  | 2.87056771  |
| H  | 5.50724803  | 9.48641316  | 7.56020768  | H  | 0.29117903  | 3.24061524  | 2.65061977  |

Compound **1<sub>2</sub>**<sup>t-bt-xx</sup>:

E = -3328.53779359 au

BSSE = 0.01065 au

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | H | 4.49801693  | 2.33886304  | -0.02196985 |
| N  | 2.04885524  | 0.00000000  | 0.00000000  | H | -1.71717489 | 2.72073967  | 0.26177474  |
| C  | 2.63475731  | 1.24357843  | 0.00000000  | H | -1.04613202 | 5.10693077  | 0.32463508  |
| C  | 4.03652932  | 1.35055108  | -0.01621221 | H | 1.36433892  | 5.74965567  | 0.19995285  |
| C  | 4.82675359  | 0.20121483  | -0.01697468 | H | 3.10679000  | 3.99078780  | 0.03755343  |
| C  | 4.20833919  | -1.05582136 | 0.00536844  | N | -2.03374915 | 0.11896637  | 0.01707464  |
| C  | 2.81455854  | -1.11202793 | 0.01405111  | N | -2.67227899 | -0.52519308 | 1.02827563  |
| C  | 1.67832333  | 2.34686121  | 0.04682917  | C | -4.00429192 | -0.45772375 | 0.78467068  |
| C  | 0.30434954  | 1.96523628  | 0.09450594  | C | -4.23418882 | 0.24584340  | -0.40605737 |
| C  | -0.65821287 | 2.98158016  | 0.20378113  | C | -2.95396406 | 0.58769926  | -0.86092238 |
| C  | -0.27861875 | 4.33212494  | 0.24152427  | H | -4.70701585 | -0.91804701 | 1.47574920  |
| C  | 1.07421657  | 4.69701921  | 0.17416071  | H | -5.18702019 | 0.46780672  | -0.87703167 |
| C  | 2.05189780  | 3.70474003  | 0.08071130  | H | -2.63668491 | 1.12874808  | -1.74878798 |
| H  | 2.26734278  | -2.05569988 | 0.03308172  | N | -0.25864850 | -2.13308113 | -0.10344793 |
| H  | 4.78684552  | -1.98013910 | 0.01674371  | N | -0.83169723 | -2.72598063 | 0.97615558  |
| H  | 5.91569717  | 0.28445972  | -0.02856311 | C | -0.08312553 | -3.08262684 | -1.05540183 |

|    |              |             |             |    |             |             |             |
|----|--------------|-------------|-------------|----|-------------|-------------|-------------|
| C  | -0.54765896  | -4.31812857 | -0.58272109 | H  | -9.65768316 | -5.63349662 | 11.12320449 |
| C  | -1.01786659  | -4.04138802 | 0.70763441  | H  | -3.44249133 | -6.01537324 | 10.83945991 |
| H  | 0.35469285   | -2.81557651 | -2.01481171 | H  | -4.11353421 | -8.40156435 | 10.77659957 |
| H  | -0.55339913  | -5.27198318 | -1.10151680 | H  | -6.52400515 | -9.04428925 | 10.90128180 |
| H  | -1.47358332  | -4.69234886 | 1.44942949  | H  | -8.26645623 | -7.28542138 | 11.06368122 |
| Pd | -1.40882577  | -1.47882173 | 2.48507270  | N  | -3.12591709 | -3.41359995 | 11.08416001 |
| N  | -1.88074632  | -0.24854919 | 4.05631365  | N  | -2.48738724 | -2.76944050 | 10.07295902 |
| C  | -1.26788879  | -0.55689474 | 5.24646151  | C  | -1.15537431 | -2.83690983 | 10.31656397 |
| C  | -1.53802727  | 0.21203410  | 6.38980665  | C  | -0.92547742 | -3.54047698 | 11.50729202 |
| C  | -2.41524005  | 1.29462112  | 6.31060439  | C  | -2.20570217 | -3.88233284 | 11.96215702 |
| C  | -3.01239611  | 1.60582806  | 5.08435477  | H  | -0.45265039 | -2.37658657 | 9.62548545  |
| C  | -2.71921850  | 0.80651929  | 3.97872331  | H  | 0.02735395  | -3.76244030 | 11.97826632 |
| C  | -0.35827028  | -1.69882811 | 5.16263982  | H  | -2.52298132 | -4.42338166 | 12.85002262 |
| C  | -0.24856853  | -2.30798627 | 3.87777531  | N  | -4.90101773 | -1.16155245 | 11.20468258 |
| C  | 0.62911264   | -3.39531096 | 3.73687967  | N  | -4.32796900 | -0.56865295 | 10.12507907 |
| C  | 1.36718797   | -3.87449378 | 4.83152404  | C  | -4.14179964 | 0.74675444  | 10.39360023 |
| C  | 1.25107303   | -3.26850056 | 6.09098647  | C  | -4.61200727 | 1.02349498  | 11.68395573 |
| C  | 0.39206247   | -2.17819967 | 6.25403934  | C  | -5.07654070 | -0.21200674 | 12.15663647 |
| H  | -3.15359031  | 0.98855425  | 2.99501378  | H  | -3.68608291 | 1.39771528  | 9.65180516  |
| H  | -3.70969582  | 2.43731669  | 4.98020160  | H  | -4.60626710 | 1.97734959  | 12.20275144 |
| H  | -2.63685733  | 1.88428922  | 7.20237604  | H  | -5.51435909 | -0.47905707 | 13.11604636 |
| H  | -1.07510895  | -0.05354032 | 7.34100806  | Pd | -3.75084047 | -1.81581185 | 8.61616195  |
| H  | 0.74747242   | -3.87206621 | 2.76089211  | N  | -3.27891991 | -3.04608439 | 7.04492100  |
| H  | 2.04413510   | -4.72331488 | 4.69703516  | C  | -3.89177744 | -2.73773884 | 5.85477314  |
| H  | 1.83166955   | -3.63891530 | 6.93892390  | C  | -3.62163896 | -3.50666768 | 4.71142799  |
| H  | 0.30824783   | -1.69719429 | 7.23288609  | C  | -2.74442618 | -4.58925470 | 4.79063026  |
| Pd | -5.15966623  | -3.29463358 | 11.10123465 | C  | -2.14727012 | -4.90046164 | 6.01687987  |
| N  | -7.20852147  | -3.29463358 | 11.10123465 | C  | -2.44044773 | -4.10115287 | 7.12251134  |
| C  | -7.79442354  | -4.53821201 | 11.10123465 | C  | -4.80139595 | -1.59580547 | 5.93859483  |
| C  | -9.19619555  | -4.64518467 | 11.11744685 | C  | -4.91109770 | -0.98664731 | 7.22345934  |
| C  | -9.98641982  | -3.49584842 | 11.11820933 | C  | -5.78877887 | 0.10067738  | 7.36435497  |
| C  | -9.36800542  | -2.23881222 | 11.09586620 | C  | -6.52685420 | 0.57986020  | 6.26971061  |
| C  | -7.97422478  | -2.18260565 | 11.08718354 | C  | -6.41073926 | -0.02613302 | 5.01024818  |
| C  | -6.83798956  | -5.64149479 | 11.05440548 | C  | -5.55172870 | -1.11643391 | 4.84719530  |
| C  | -5.46401577  | -5.25986986 | 11.00672871 | H  | -2.00607592 | -4.28318783 | 8.10622087  |
| C  | -4.50145335  | -6.27621373 | 10.89745352 | H  | -1.44997041 | -5.73195027 | 6.12103304  |
| C  | -4.88104748  | -7.62675852 | 10.85971038 | H  | -2.52280890 | -5.17892280 | 3.89885861  |
| C  | -6.23388280  | -7.99165279 | 10.92707394 | H  | -4.08455728 | -3.24109326 | 3.76022659  |
| C  | -7.21156402  | -6.99937361 | 11.02052335 | H  | -5.90713865 | 0.57743263  | 8.34034254  |
| H  | -7.42700901  | -1.23893370 | 11.06815293 | H  | -7.20380133 | 1.42868130  | 6.40419948  |
| H  | -9.94651175  | -1.31449449 | 11.08449094 | H  | -6.99133578 | 0.34428172  | 4.16231075  |
| H  | -11.07536340 | -3.57909331 | 11.12979775 | H  | -5.46791406 | -1.59743929 | 3.86834856  |

Compound 4<sub>1</sub><sup>t-bt</sup>:

E = -1049.83816344 au

Thermal correction to G = 0.196517 au

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | H  | -2.35331190 | 1.73434297  | -1.49177680 |
| N  | 2.04104477  | 0.00000000  | 0.00000000  | N  | -0.17828522 | -2.11891276 | -0.01351169 |
| C  | 2.58937358  | 1.19316848  | 0.00000000  | N  | -0.88323363 | -2.78477464 | 0.93809119  |
| C  | 1.67809208  | 2.30661786  | -0.01326411 | C  | 0.43636052  | -3.04083778 | -0.79436759 |
| C  | 0.35481138  | 1.94491396  | -0.00447558 | C  | 0.11936335  | -4.33024102 | -0.34675841 |
| C  | 2.66151928  | -0.81246121 | 0.04115320  | C  | -0.71480247 | -4.11824477 | 0.75664173  |
| H  | 3.68144057  | 1.30984778  | 0.01850905  | H  | 1.05037505  | -2.71811429 | -1.63250215 |
| H  | 2.04660914  | 3.33684630  | -0.01690840 | H  | 0.43731947  | -5.27971789 | -0.76623082 |
| H  | -0.43707893 | 2.70678492  | 0.01165716  | H  | -1.20970650 | -4.82592739 | 1.41690539  |
| N  | -2.01193124 | 0.25415247  | -0.01034255 | Pd | -1.97884663 | -1.76096248 | 2.30337819  |
| N  | -2.79990628 | -0.48144747 | 0.81661600  | N  | -2.98887494 | -0.89496224 | 3.85119929  |
| C  | -4.08739500 | -0.12467557 | 0.58736138  | C  | -2.75396752 | -1.43025300 | 5.02703849  |
| C  | -4.13816726 | 0.85582046  | -0.41236438 | C  | -1.84064260 | -2.54198601 | 5.04337031  |
| C  | -2.79866411 | 1.06828130  | -0.75712310 | C  | -1.33260946 | -2.86504769 | 3.81068534  |
| H  | -4.88991331 | -0.60573244 | 1.14250324  | H  | -3.60943488 | -0.08257280 | 3.80991783  |
| H  | -5.01647240 | 1.33463328  | -0.83412009 | H  | -3.23084368 | -1.03020397 | 5.93208923  |

H -1.58865171 -3.05102002 5.97855677 H -0.60524537 -3.68111733 3.69768212

Compound **4<sub>I</sub><sup>t-ch</sup>**:

E = -1049.82098622 au

Thermal correction to G = 0.197239 au

|               |             |             |                |             |             |
|---------------|-------------|-------------|----------------|-------------|-------------|
| Pd 0.00000000 | 0.00000000  | 0.00000000  | N -0.06228622  | -2.14223907 | -0.18591145 |
| N 2.04726335  | 0.00000000  | 0.00000000  | N -0.82999536  | -2.81429723 | -1.09866937 |
| C 2.60902721  | 1.18718885  | 0.00000000  | C 1.05270593   | -2.88897504 | 0.02890781  |
| C 1.70714407  | 2.30123239  | 0.04728640  | C 1.02840295   | -4.04554196 | -0.75676066 |
| C 0.38337040  | 1.94248331  | 0.04448738  | C -0.17955045  | -3.95359230 | -1.45182824 |
| H 2.66026850  | -0.81174441 | -0.10712205 | H 1.79028194   | -2.56143682 | 0.75859575  |
| H 3.70070514  | 1.29171384  | -0.05585702 | H 1.77190437   | -4.83473528 | -0.81333119 |
| H 2.07312451  | 3.33194040  | 0.05424256  | H -0.61640520  | -4.62938036 | -2.18127801 |
| H -0.39298962 | 2.71709566  | 0.01796864  | Pd -2.84549927 | -2.48275737 | -1.21370418 |
| N -2.01550376 | 0.33154307  | -0.11503037 | N -4.89276105  | -2.48275551 | -1.21369160 |
| N -2.78321359 | -0.34051760 | -1.02778465 | C -5.45452759  | -3.66994314 | -1.21369622 |
| C -3.89820821 | 0.40621708  | -1.24260087 | C -4.55264578  | -4.78398748 | -1.26100047 |
| C -3.87390408 | 1.56278505  | -0.45693365 | C -3.22887227  | -4.42523870 | -1.25820663 |
| C -2.66594861 | 1.47083824  | 0.23813022  | H -5.50576213  | -1.67100963 | -1.10655183 |
| H -4.63578537 | 0.07867780  | -1.97228756 | H -6.54620534  | -3.77446660 | -1.15782657 |
| H -4.61740837 | 2.35197574  | -0.40035999 | H -4.91862808  | -5.81469560 | -1.26796640 |
| H -2.22909163 | 2.14662831  | 0.96757577  | H -2.45251290  | -5.19985403 | -1.23170217 |

Compound **4<sub>I</sub><sup>t-TS</sup>**:

E = -1049.82036173 au

Thermal correction to G = 0.198741 au

$\nu = -48.78 \text{ cm}^{-1}$

|               |             |             |                |             |             |
|---------------|-------------|-------------|----------------|-------------|-------------|
| Pd 0.00000000 | 0.00000000  | 0.00000000  | N -0.08718376  | -2.14554627 | -0.31591649 |
| N 2.05468405  | 0.00000000  | 0.00000000  | N -1.11742318  | -2.82931555 | -0.90216915 |
| C 2.61786755  | 1.18715066  | 0.00000000  | C 1.03411195   | -2.89106392 | -0.51061440 |
| C 1.71718447  | 2.29993872  | -0.00619446 | C 0.74338835   | -4.05176527 | -1.23117019 |
| C 0.39441294  | 1.93842045  | 0.00351100  | C -0.63224864  | -3.96958456 | -1.45440508 |
| H 2.68822692  | -0.80103871 | -0.01757426 | H 1.98879190   | -2.57916049 | -0.09964302 |
| H 3.71109283  | 1.28852770  | -0.00930823 | H 1.42718026   | -4.83436000 | -1.54481806 |
| H 2.07914703  | 3.33127707  | -0.04189156 | H -1.30303679  | -4.65181302 | -1.96963177 |
| H -0.37986669 | 2.71092365  | -0.06849578 | Pd -3.06436357 | -2.48225720 | -0.43964432 |
| N -2.02056434 | 0.38651441  | 0.06605813  | N -5.02651921  | -2.43175401 | 0.14137184  |
| N -2.94725288 | -0.35409636 | -0.61644370 | C -5.53992186  | -3.59389456 | 0.47353064  |
| C -4.08765733 | 0.38095144  | -0.68403407 | C -4.66478149  | -4.72458279 | 0.33995564  |
| C -3.92018609 | 1.60394641  | -0.02807471 | C -3.40246671  | -4.40055969 | -0.08700999 |
| C -2.60204607 | 1.56001099  | 0.43196071  | H -5.60406714  | -1.59924862 | 0.28410372  |
| H -4.95094852 | -0.01601141 | -1.21501296 | H -6.57069325  | -3.66716869 | 0.84533410  |
| H -4.64069249 | 2.40702513  | 0.09373456  | H -4.99985850  | -5.73551903 | 0.58959405  |
| H -2.05021156 | 2.29295055  | 1.01142741  | H -2.63013419  | -5.17573141 | -0.17873720 |

Compound **4<sub>I</sub><sup>c-bt</sup>**:

E = -1049.83723985 au

|               |            |            |              |            |             |
|---------------|------------|------------|--------------|------------|-------------|
| Pd 0.00000000 | 0.00000000 | 0.00000000 | C 2.58828134 | 1.19335173 | 0.00000000  |
| N 2.03930168  | 0.00000000 | 0.00000000 | C 1.67881072 | 2.30747254 | -0.01292788 |

C 0.35507856 1.94622404 -0.00408173  
H 2.65951427 -0.81261153 0.03966477  
H 3.68059957 1.30817068 0.01779106  
H 2.04873890 3.33719355 -0.01585962  
H -0.43680257 2.70808170 0.01229836  
N -2.01650648 0.26561744 -0.02541720  
N -2.83330459 -0.35441992 0.86779989  
C -4.10881340 0.03044637 0.61765469  
C -4.12425426 0.91439149 -0.46721254  
C -2.77991149 1.03922543 -0.83557823  
H -4.92120391 -0.35880363 1.22575984  
H -4.98589306 1.38959762 -0.92526400  
H -2.31322689 1.62093060 -1.62621742  
N -0.18993160 -2.10862219 -0.00160908  
N -1.00545762 -2.72769389 0.89021690

C 0.44841253 -3.06021106 -0.72731849  
C 0.03684536 -4.33012730 -0.30266044  
C -0.87906353 -4.06790775 0.72435518  
H 1.14091303 -2.77261945 -1.51594970  
H 0.34552757 -5.29605202 -0.69089570  
H -1.46589521 -4.75146644 1.33474943  
Pd -2.10612327 -1.59877341 2.30317048  
N -1.53811790 -2.71564510 3.91212010  
C -2.03877819 -2.31908265 5.05996352  
C -2.91246672 -1.17779939 5.00790580  
C -3.07633935 -0.65859012 3.74837690  
H -0.88903027 -3.50633737 3.92020830  
H -1.78338219 -2.83957742 5.99297858  
H -3.37569493 -0.78053343 5.91607991  
H -3.70122739 0.23003319 3.58214016

Compound  $4_1^{c\text{-ch}}$ :

E = -1049.81984197 au

Pd 0.00000000 0.00000000 0.00000000  
N 2.03866188 0.00000000 0.00000000  
C 2.60756030 1.18355273 0.00000000  
C 1.70994357 2.30163353 -0.03542765  
C 0.38423659 1.94822431 -0.03548136  
H 2.64260378 -0.82044455 0.09157906  
H 3.70026955 1.28090942 0.04714702  
H 2.08078926 3.33065253 -0.02984965  
H -0.38458470 2.72980784 0.00825681  
N -0.03107443 -2.11329098 0.26256392  
N -0.79458600 -2.65058680 1.25850651  
C -0.17936641 -3.78143484 1.69446646  
C 0.99890324 -3.99797657 0.97097359  
C 1.04684460 -2.92061036 0.07898967  
H -0.60509822 -4.35188859 2.51817888  
H 1.70998053 -4.81196002 1.07696949  
H 1.77272461 -2.69374187 -0.69998151

N -2.03813373 0.30745403 0.03663561  
N -2.91322954 -0.34856263 0.86944180  
C -2.62795567 1.46903563 -0.34847532  
C -3.88597987 1.59384045 0.24281427  
C -4.01843585 0.43018628 1.00188535  
H -2.11108239 2.14008658 -1.02721583  
H -4.59669965 2.40741467 0.13687166  
H -4.83751851 0.10508006 1.63557738  
Pd -2.90676057 -2.38160354 1.21085370  
N -3.19744930 -4.38254108 1.47141325  
C -4.44021911 -4.79470063 1.37096341  
C -5.41414903 -3.77038700 1.12741117  
C -4.87825641 -2.51286252 1.00973213  
H -2.46659686 -5.09006056 1.57880373  
H -4.68555568 -5.86206067 1.45012900  
H -6.47629181 -4.00806529 1.01878579  
H -5.53016232 -1.66811306 0.75421495

Compound  $4_2^{t\text{-bt-nn}}$ :

E = -2099.69229474 au

BSSE = 0.00674 au

Pd 0.35621400 1.47243000 -4.42446400  
N 1.91707700 2.68203700 -4.93422000  
C 1.65784800 3.96839000 -4.88458400  
C 0.32173000 4.32726400 -4.48765400  
C -0.48524400 3.25361300 -4.20740100  
H -1.52036800 3.40410400 -3.86846900  
H 0.01715800 5.37566800 -4.41690500  
H 2.43287200 4.70775300 -5.12698800  
H 2.86577800 2.39157300 -5.18529700  
N -1.34100400 0.48955200 -3.90077100  
N -1.31208000 -0.62667600 -3.12466700  
C -2.58984200 -1.04821400 -2.96278100  
C -3.46562600 -0.20133200 -3.65514600  
C -2.63024700 0.76164900 -4.23001000  
H -2.79413800 -1.94067600 -2.37466000  
H -4.54529300 -0.27943000 -3.73791700  
H -2.86427600 1.61225900 -4.86511400

N 1.46513500 -0.30807800 -4.71664600  
N 1.59299600 -1.27133600 -3.76602400  
C 2.30852600 -0.61323900 -5.73436800  
C 2.98997500 -1.80238600 -5.44632800  
C 2.50822300 -2.17951700 -4.18777000  
H 2.35545400 0.02998100 -6.61094000  
H 3.71782000 -2.32140700 -6.06228400  
H 2.74636700 -3.04037700 -3.56824000  
Pd 0.42867500 -1.30473000 -2.10104900  
N -0.55187900 -1.47138500 -0.32136900  
C 0.20742800 -1.77006700 0.70454700  
C 1.60350700 -1.98246900 0.40898300  
C 1.92859200 -1.82641700 -0.91448400  
H -1.52726200 -1.22125900 -0.13099100  
H -0.20414900 -1.82308800 1.72307500  
H 2.31197100 -2.22335500 1.20870400  
H 2.96773100 -1.93130500 -1.25822900

|    |             |             |            |    |             |             |             |
|----|-------------|-------------|------------|----|-------------|-------------|-------------|
| Pd | -0.35621400 | -1.47243000 | 4.42446400 | N  | -1.46513500 | 0.30807800  | 4.71664600  |
| N  | -1.91707700 | -2.68203700 | 4.93422000 | N  | -1.59299600 | 1.27133600  | 3.76602400  |
| C  | -1.65784800 | -3.96839000 | 4.88458400 | C  | -2.50822300 | 2.17951700  | 4.18777000  |
| C  | -0.32173000 | -4.32726400 | 4.48765400 | C  | -2.98997500 | 1.80238600  | 5.44632800  |
| C  | 0.48524400  | -3.25361300 | 4.20740100 | C  | -2.30852600 | 0.61323900  | 5.73436800  |
| H  | -2.86577800 | -2.39157300 | 5.18529700 | H  | -2.74636700 | 3.04037700  | 3.56824000  |
| H  | -2.43287200 | -4.70775300 | 5.12698800 | H  | -3.71782000 | 2.32140700  | 6.06228400  |
| H  | -0.01715800 | -5.37566800 | 4.41690500 | H  | -2.35545400 | -0.02998100 | 6.61094000  |
| H  | 1.52036800  | -3.40410400 | 3.86846900 | Pd | -0.42867500 | 1.30473000  | 2.10104900  |
| N  | 1.34100400  | -0.48955200 | 3.90077100 | N  | 0.55187900  | 1.47138500  | 0.32136900  |
| N  | 1.31208000  | 0.62667600  | 3.12466700 | C  | -0.20742800 | 1.77006700  | -0.70454700 |
| C  | 2.58984200  | 1.04821400  | 2.96278100 | C  | -1.60350700 | 1.98246900  | -0.40898300 |
| C  | 3.46562600  | 0.20133200  | 3.65514600 | C  | -1.92859200 | 1.82641700  | 0.91448400  |
| C  | 2.63024700  | -0.76164900 | 4.23001000 | H  | 1.52726200  | 1.22125900  | 0.13099100  |
| H  | 2.79413800  | 1.94067600  | 2.37466000 | H  | 0.20414900  | 1.82308800  | -1.72307500 |
| H  | 4.54529300  | 0.27943000  | 3.73791700 | H  | -2.31197100 | 2.22335500  | -1.20870400 |
| H  | 2.86427600  | -1.61225900 | 4.86511400 | H  | -2.96773100 | 1.93130500  | 1.25822900  |

Compound  $4_2^{t\text{-bt-xx}}$ :

E = -2099.68408891 au

BSSE = 0.00645 au

|    |             |             |             |    |              |             |             |
|----|-------------|-------------|-------------|----|--------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | Pd | -7.31057733  | -6.28563721 | 5.60371142  |
| N  | 2.04097719  | 0.00000000  | 0.00000000  | N  | -9.35155452  | -6.28563721 | 5.60371142  |
| C  | 2.59013000  | 1.19279057  | 0.00000000  | C  | -9.90070733  | -7.47842778 | 5.60371142  |
| C  | 1.67892312  | 2.30611076  | -0.01803251 | C  | -8.98950045  | -8.59174798 | 5.62174392  |
| C  | 0.35543635  | 1.94477172  | -0.01214712 | C  | -7.66601368  | -8.23040893 | 5.61585854  |
| H  | -0.43541662 | 2.70764261  | 0.00449897  | H  | -9.97102574  | -5.47260421 | 5.55637628  |
| H  | 2.04725290  | 3.33637997  | -0.02124801 | H  | -10.99269919 | -7.59464690 | 5.58060734  |
| H  | 3.68212186  | 1.30900969  | 0.02310407  | H  | -9.35783023  | -9.62201718 | 5.62495943  |
| H  | 2.66044841  | -0.81303301 | 0.04733514  | H  | -6.87516071  | -8.99327982 | 5.59921245  |
| N  | -2.01148598 | 0.25299645  | -0.00696576 | N  | -5.29909135  | -6.53863366 | 5.61067718  |
| N  | -2.81014852 | -0.50333131 | 0.79164857  | N  | -4.50042881  | -5.78230590 | 4.81206285  |
| C  | -4.09158703 | -0.11333589 | 0.58032472  | C  | -3.21899030  | -6.17230132 | 5.02338670  |
| C  | -4.12804294 | 0.90548636  | -0.38102135 | C  | -3.18253439  | -7.19112358 | 5.98473276  |
| C  | -2.78592090 | 1.10808641  | -0.72052144 | C  | -4.52465643  | -7.39372362 | 6.32423286  |
| H  | -4.90099938 | -0.60940267 | 1.11244297  | H  | -2.40957795  | -5.67623455 | 4.49126845  |
| H  | -4.99867191 | 1.41544571  | -0.78197955 | H  | -2.31190542  | -7.70108293 | 6.38569097  |
| H  | -2.33101803 | 1.79411525  | -1.43054460 | H  | -4.97955930  | -8.07975246 | 7.03425602  |
| N  | -0.15224907 | -2.12192247 | 0.01802159  | N  | -7.15832826  | -4.16371474 | 5.58568983  |
| N  | -0.81261669 | -2.78383877 | 1.00355482  | N  | -6.49796064  | -3.50179845 | 4.60015660  |
| C  | 0.53208893  | -3.03617739 | -0.71244035 | C  | -6.76600616  | -2.17601082 | 4.71200231  |
| C  | 0.30777162  | -4.32048980 | -0.19835196 | C  | -7.61834895  | -1.96514741 | 5.80206337  |
| C  | -0.54457117 | -4.10962639 | 0.89170911  | C  | -7.84266626  | -3.24945982 | 6.31615177  |
| H  | 1.12843938  | -2.71305183 | -1.56322573 | H  | -6.33149172  | -1.47227791 | 4.00628609  |
| H  | 0.69961422  | -5.26461929 | -0.56443595 | H  | -8.01019155  | -1.02101791 | 6.16814736  |
| H  | -0.97908561 | -4.81335930 | 1.59742533  | H  | -8.43901671  | -3.57258539 | 7.16693714  |
| Pd | -2.04712572 | -1.81071232 | 2.29213985  | Pd | -5.26345161  | -4.47492490 | 3.31157157  |
| N  | -3.23572304 | -1.04038029 | 3.75966951  | N  | -4.07485429  | -5.24525692 | 1.84404191  |
| C  | -3.11059998 | -1.61560060 | 4.93270206  | C  | -4.19997735  | -4.67003662 | 0.67100936  |
| C  | -2.13706309 | -2.67216955 | 5.01049370  | C  | -5.17351424  | -3.61346766 | 0.59321772  |
| C  | -1.48489902 | -2.91966643 | 3.82913820  | C  | -5.82567831  | -3.36597079 | 1.77457322  |
| H  | -3.90436530 | -0.27059883 | 3.67228442  | H  | -3.40621203  | -6.01503838 | 1.93142700  |
| H  | -3.72416639 | -1.29827561 | 5.78555457  | H  | -3.58641094  | -4.98736160 | -0.18184315 |
| H  | -1.96604326 | -3.21279319 | 5.94589647  | H  | -5.34453407  | -3.07284402 | -0.34218506 |
| H  | -0.70136211 | -3.68944229 | 3.77003803  | H  | -6.60921522  | -2.59619493 | 1.83367339  |

Compound **5<sub>1</sub><sup>t-bt</sup>**:

E = -1357.04944017 au

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | H  | -0.28236180 | -5.27728099 | -1.01230951 |
| N  | 2.04079482  | 0.00000000  | 0.00000000  | H  | -1.56776723 | -4.70231991 | 1.37806404  |
| C  | 2.58832339  | 1.19325617  | 0.00000000  | Pd | -1.68716769 | -1.51988216 | 2.42233179  |
| C  | 1.67645079  | 2.30656517  | -0.01730933 | N  | -2.36761406 | -0.37055298 | 3.98143976  |
| C  | 0.35338960  | 1.94381292  | -0.00788667 | C  | -1.96754584 | -0.78578383 | 5.22961518  |
| H  | 2.66164535  | -0.81169024 | 0.04282887  | C  | -2.40717225 | -0.08792112 | 6.36828497  |
| H  | 3.68034653  | 1.31054112  | 0.02029993  | C  | -3.22842747 | 1.03084026  | 6.23093396  |
| H  | 2.04478637  | 3.33692062  | -0.02655260 | C  | -3.60115729 | 1.45326698  | 4.94829819  |
| H  | -0.44006262 | 2.70405592  | -0.00021404 | C  | -3.14843092 | 0.72342003  | 3.84905112  |
| N  | -2.01908842 | 0.23196213  | -0.01372311 | C  | -1.06395099 | -1.93321075 | 5.21003643  |
| N  | -2.75620313 | -0.48111785 | 0.87741368  | C  | -0.73149651 | -2.43172585 | 3.91507725  |
| C  | -4.06434510 | -0.28160378 | 0.58376396  | C  | 0.20038720  | -3.47885586 | 3.83351389  |
| C  | -4.17811709 | 0.58088248  | -0.51625189 | C  | 0.76016366  | -4.03758769 | 4.99297877  |
| C  | -2.85489753 | 0.88094559  | -0.86187470 | C  | 0.40372896  | -3.55876572 | 6.26223861  |
| H  | 4.83413116  | -0.77297473 | 1.17495119  | C  | -0.50336777 | -2.50321282 | 6.37003163  |
| H  | -5.08558743 | 0.92630082  | -1.00210606 | H  | -3.40278658 | 0.99652641  | 2.82398136  |
| H  | -2.45281934 | 1.49876673  | -1.66086251 | H  | -4.23118120 | 2.32965049  | 4.79274882  |
| N  | -0.24534442 | -2.11875863 | -0.03999227 | H  | -3.56915258 | 1.57309785  | 7.11565944  |
| N  | -0.93991014 | -2.71985841 | 0.96033451  | H  | -2.09407691 | -0.42537180 | 7.35706999  |
| C  | 0.10156150  | -3.07274887 | -0.93801599 | H  | 0.49815895  | -3.86486347 | 2.85643640  |
| C  | -0.38195018 | -4.31794663 | -0.51380470 | H  | 1.48128475  | -4.85508490 | 4.90410259  |
| C  | -1.03810652 | -4.04498047 | 0.69331512  | H  | 0.83724346  | -4.00145302 | 7.16165821  |
| H  | 0.66207794  | -2.80155336 | -1.82977274 | H  | -0.76959367 | -2.12145001 | 7.35985032  |

Compound **5<sub>2</sub><sup>t-bt-nn-ii</sup>**:

E = -2714.11996456 au

BSSE = 0.01255 au

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | C  | -1.20651216 | -2.14858753 | 5.12959117  |
| N  | 2.04502575  | 0.00000000  | 0.00000000  | C  | -0.89065765 | -2.63035259 | 3.82520876  |
| C  | 2.59254645  | 1.19461324  | 0.00000000  | C  | -0.00017942 | -3.71139756 | 3.72136739  |
| C  | 1.68062331  | 2.30789901  | -0.00183927 | C  | 0.54008224  | -4.31477706 | 4.86919725  |
| C  | 0.35643642  | 1.94592380  | 0.00409567  | C  | 0.20833159  | -3.84296374 | 6.14733700  |
| H  | 2.67045394  | -0.80962703 | 0.00295654  | C  | -0.66154411 | -2.75660241 | 6.27788664  |
| H  | 3.68439088  | 1.31256999  | 0.00160495  | H  | -3.58358200 | 0.82900995  | 2.83758207  |
| H  | 2.04963604  | 3.33784791  | -0.00829367 | H  | -4.41332364 | 2.09323081  | 4.84558164  |
| H  | -0.43521133 | 2.70848283  | 0.00332859  | H  | -3.66817388 | 1.31397603  | 7.14366903  |
| N  | -2.01372425 | 0.24475966  | -0.02715306 | H  | -2.17811209 | -0.65971590 | 7.32109795  |
| N  | -2.78101009 | -0.49286911 | 0.81727782  | H  | 0.28162490  | -4.09135262 | 2.73687384  |
| C  | -4.07755845 | -0.27024737 | 0.49289146  | H  | 1.22409372  | -5.16194236 | 4.76213811  |
| C  | -4.15354643 | 0.63209705  | -0.57842846 | H  | 0.62799909  | -4.31661339 | 7.03803785  |
| C  | -2.81937792 | 0.93211101  | -0.87561998 | H  | -0.90839366 | -2.37515475 | 7.27308094  |
| H  | -4.86820457 | -0.77356485 | 1.04520540  | Pd | -1.42978763 | 0.13763243  | 10.01466266 |
| H  | -5.04403579 | 1.00302097  | -1.07666981 | N  | -3.47481338 | 0.13763243  | 10.01466266 |
| H  | -2.38970548 | 1.57393868  | -1.64071228 | C  | -4.02233408 | -1.05698080 | 10.01466266 |
| N  | -0.24798320 | -2.11167101 | -0.09231614 | C  | -3.11041094 | -2.17026658 | 10.01650193 |
| N  | -0.99423295 | -2.74932071 | 0.84699594  | C  | -1.78622404 | -1.80829136 | 10.01056699 |
| C  | 0.11501264  | -3.02390367 | -1.02829972 | H  | -4.10024156 | 0.94725946  | 10.01170612 |
| C  | -0.40951194 | -4.27821243 | -0.69122652 | H  | -5.11417850 | -1.17493756 | 10.01305771 |
| C  | -1.10761878 | -4.05474632 | 0.50295259  | H  | -3.47942367 | -3.20021548 | 10.02295633 |
| H  | 0.71342450  | -2.71745020 | -1.88337288 | H  | -0.99457629 | -2.57085040 | 10.01133407 |
| H  | -0.31009713 | -5.21141586 | -1.23706919 | N  | 0.58393663  | -0.10712723 | 10.04181572 |
| H  | -1.67668938 | -4.73635838 | 1.12998551  | N  | 1.35122246  | 0.63050154  | 9.19738484  |
| Pd | -1.78662466 | -1.62601658 | 2.34971233  | C  | 2.64777082  | 0.40787981  | 9.52177120  |
| N  | -2.51126521 | -0.55135878 | 3.94663907  | C  | 2.72375880  | -0.49446462 | 10.59309112 |
| C  | -2.10029778 | -0.99327801 | 5.18114005  | C  | 1.38959029  | -0.79447858 | 10.89028264 |
| C  | -2.52648980 | -0.32787529 | 6.34135267  | H  | 3.43841694  | 0.91119728  | 8.96945726  |
| C  | -3.36872387 | 0.77992577  | 6.23919961  | H  | 3.61424817  | -0.86538853 | 11.09133247 |
| C  | -3.78188145 | 1.21382805  | 4.97447094  | H  | 0.95991785  | -1.43630625 | 11.65537494 |
| C  | -3.32124427 | 0.52518016  | 3.85146174  | N  | -1.18180442 | 2.24930344  | 10.10697880 |

|    |             |             |             |   |             |             |            |
|----|-------------|-------------|-------------|---|-------------|-------------|------------|
| N  | -0.43555467 | 2.88695314  | 9.16766672  | C | -0.22327547 | 2.28621996  | 4.88507149 |
| C  | -0.32216885 | 4.19237875  | 9.51171007  | C | -0.53912998 | 2.76798502  | 6.18945390 |
| C  | -1.02027569 | 4.41584486  | 10.70588919 | C | -1.42960821 | 3.84903000  | 6.29329527 |
| C  | -1.54480027 | 3.16153610  | 11.04296238 | C | -1.96986987 | 4.45240950  | 5.14546541 |
| H  | 0.24690175  | 4.87399081  | 8.88467715  | C | -1.63811922 | 3.98059617  | 3.86732566 |
| H  | -1.11969050 | 5.34904830  | 11.25173185 | C | -0.76824351 | 2.89423484  | 3.73677602 |
| H  | -2.14321213 | 2.85508264  | 11.89803554 | H | 2.15379437  | -0.69137752 | 7.17708059 |
| Pd | 0.35683703  | 1.76364901  | 7.66495033  | H | 2.98353601  | -1.95559837 | 5.16908101 |
| N  | 1.08147758  | 0.68899121  | 6.06802359  | H | 2.23838625  | -1.17634359 | 2.87099363 |
| C  | 0.67051015  | 1.13091044  | 4.83352261  | H | 0.74832446  | 0.79734834  | 2.69356471 |
| C  | 1.09670218  | 0.46550772  | 3.67330999  | H | -1.71141252 | 4.22898506  | 7.27778882 |
| C  | 1.93893624  | -0.64229334 | 3.77546305  | H | -2.65388134 | 5.29957479  | 5.25252455 |
| C  | 2.35209383  | -1.07619562 | 5.04019172  | H | -2.05778672 | 4.45424582  | 2.97662481 |
| C  | 1.89145665  | -0.38754773 | 6.16320092  | H | -0.52139397 | 2.51278718  | 2.74158172 |

Compound  $S_2^{t\text{-}bt\text{-}nn\text{-}io}$ :

E = -2714.11925724 au

BSSE = 0.01396 au

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | H  | 1.64794458  | -3.09127565 | 7.11847995  |
| N  | 2.04344757  | 0.00000000  | 0.00000000  | H  | -0.15844250 | -1.41409413 | 7.32777363  |
| C  | 2.59076860  | 1.19445853  | 0.00000000  | Pd | 0.20806150  | 0.47385329  | 9.62634122  |
| C  | 1.67828745  | 2.30695600  | -0.01363408 | N  | -1.58982298 | 1.25955852  | 10.23968639 |
| C  | 0.35411384  | 1.94439497  | -0.01570686 | C  | -2.49566463 | 0.34482564  | 10.72294937 |
| H  | 2.66636439  | -0.81104274 | 0.02588022  | C  | -3.74855149 | 0.78506230  | 11.18668789 |
| H  | 3.68253407  | 1.31262201  | 0.01492143  | C  | -4.07970042 | 2.13859786  | 11.13456453 |
| H  | 2.04688898  | 3.33712637  | -0.01750762 | C  | -3.15442465 | 3.04975744  | 10.60819496 |
| H  | -0.43896149 | 2.70505942  | -0.01375872 | C  | -1.91935739 | 2.56909125  | 10.17288808 |
| N  | -2.02010875 | 0.22930399  | -0.01804093 | C  | -2.03485467 | -1.03882473 | 10.65220636 |
| N  | -2.74168825 | -0.43071567 | 0.92535733  | C  | -0.74938143 | -1.23176600 | 10.06121330 |
| C  | -4.05423834 | -0.24030370 | 0.64743691  | C  | -0.29972477 | -2.55211340 | 9.90093576  |
| C  | -4.18612665 | 0.56171498  | -0.49582943 | C  | -1.07303479 | -3.64125820 | 10.33134939 |
| C  | -2.86892588 | 0.83625441  | -0.88379851 | C  | -2.32236648 | -3.43582354 | 10.93389125 |
| H  | -4.81429268 | -0.69401067 | 1.27978128  | C  | -2.80497334 | -2.13555404 | 11.08842853 |
| H  | -5.10158220 | 0.88381470  | -0.98274707 | H  | -1.15185998 | 3.22624539  | 9.76222885  |
| H  | -2.48095846 | 1.40801360  | -1.72300960 | H  | -3.37418753 | 4.11561190  | 10.53769674 |
| N  | -0.24556370 | -2.11737524 | 0.01638339  | H  | -5.05311509 | 2.47939629  | 11.49384249 |
| N  | -0.90806947 | -2.65647942 | 1.07262907  | H  | -4.46073372 | 0.05711701  | 11.57693298 |
| C  | 0.09654109  | -3.12638329 | -0.82134363 | H  | 0.66385317  | -2.74316799 | 9.42421256  |
| C  | -0.35618207 | -4.34547893 | -0.29795657 | H  | -0.69701184 | -4.65850262 | 10.19193834 |
| C  | -0.98774272 | -3.99837381 | 0.90365716  | H  | -2.91930663 | -4.28521211 | 11.27254784 |
| H  | 0.62929117  | -2.91060980 | -1.74467443 | H  | -3.78415335 | -1.97698024 | 11.54892767 |
| H  | -0.25535484 | -5.33553675 | -0.73200417 | N  | 1.93748161  | -0.39472571 | 8.98280464  |
| H  | -1.48774894 | -4.61413076 | 1.64676545  | N  | 2.48691462  | 0.02184627  | 7.80936661  |
| Pd | -1.59061129 | -1.36003354 | 2.48422296  | C  | 3.67594762  | -0.60889774 | 7.66285066  |
| N  | -2.18521425 | -0.10367727 | 3.99910280  | C  | 3.91417221  | -1.44244172 | 8.76436622  |
| C  | -1.66629143 | -0.40112886 | 5.23523067  | C  | 2.78759044  | -1.27090412 | 9.57699595  |
| C  | -1.98533737 | 0.40320814  | 6.34366353  | H  | 4.28246407  | -0.41981400 | 6.77986680  |
| C  | -2.82168214 | 1.50732403  | 6.18151237  | H  | 4.78011553  | -2.06943809 | 8.95378042  |
| C  | -3.32571804 | 1.80680675  | 4.90847946  | H  | 2.53738238  | -1.70297887 | 10.54257347 |
| C  | -2.98099291 | 0.97728285  | 3.84170299  | N  | 1.14822970  | 2.36760571  | 9.34739033  |
| C  | -0.73142598 | -1.52352790 | 5.23101649  | N  | 1.47157601  | 2.79330724  | 8.09895191  |
| C  | -0.48170783 | -2.11467181 | 3.95816077  | C  | 1.93728755  | 4.06566785  | 8.17681164  |
| C  | 0.55222107  | -3.06115113 | 3.86213875  | C  | 1.91818265  | 4.48178457  | 9.51352935  |
| C  | 1.31117492  | -3.41618290 | 4.99326972  | C  | 1.41466833  | 3.37653167  | 10.21386457 |
| C  | 1.04059153  | -2.84071866 | 6.24458502  | H  | 2.26565899  | 4.58144249  | 7.27784549  |
| C  | 0.01451533  | -1.89818357 | 6.36362572  | H  | 2.23774785  | 5.43790492  | 9.91676226  |
| H  | -3.33448675 | 1.15698846  | 2.82534173  | H  | 1.22891839  | 3.24150552  | 11.27731487 |
| H  | -3.97254657 | 2.66769816  | 4.73438170  | Pd | 1.57043000  | 1.48378865  | 6.54552213  |
| H  | -3.06325042 | 2.13817062  | 7.04016212  | N  | 1.68546371  | 0.39769979  | 4.81995023  |
| H  | -1.55226898 | 0.17266128  | 7.32020823  | C  | 1.17647307  | 0.98188012  | 3.76271228  |
| H  | 0.78511805  | -3.51501148 | 2.89604100  | C  | 0.66494306  | 2.31570701  | 3.97065185  |
| H  | 2.12294673  | -4.14237025 | 4.89127557  | C  | 0.75233476  | 2.75321441  | 5.26576837  |

|   |            |             |            |   |            |            |            |
|---|------------|-------------|------------|---|------------|------------|------------|
| H | 1.96307269 | -0.58603679 | 4.73147601 | H | 0.23395638 | 2.88432457 | 3.14110998 |
| H | 1.11209789 | 0.45751656  | 2.79895275 | H | 0.36158469 | 3.73725730 | 5.56245628 |

Compound **5<sub>2</sub>**<sup>*t-bt-nn-oo*</sup>.

E = -2714.11437976 au

BSSE = 0.00815 au

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | Pd | 0.10121609  | 1.14408662  | 9.02313993  |
| N  | 2.05542217  | 0.00000000  | 0.00000000  | N  | -1.95420608 | 1.14408663  | 9.02313993  |
| C  | 2.63883349  | 1.24556117  | 0.00000000  | C  | -2.53761741 | -0.10147454 | 9.02313993  |
| C  | 4.04026685  | 1.35651537  | 0.03535702  | C  | -3.93905077 | -0.21242874 | 8.98778290  |
| C  | 4.83302847  | 0.20945752  | 0.07524909  | C  | -4.73181238 | 0.93462911  | 8.94789084  |
| C  | 4.21752591  | -1.04929095 | 0.08502918  | C  | -4.11630983 | 2.19337758  | 8.93811074  |
| C  | 2.82428147  | -1.10980926 | 0.04940154  | C  | -2.72306538 | 2.25389589  | 8.97373839  |
| C  | 1.68057882  | 2.34935668  | -0.01862497 | C  | -1.57936273 | -1.20527005 | 9.04176490  |
| C  | 0.30515076  | 1.96991968  | -0.03832701 | C  | -0.20393467 | -0.82583305 | 9.06146694  |
| C  | -0.65941235 | 2.99142916  | -0.04042393 | C  | 0.76062843  | -1.84734254 | 9.06356386  |
| C  | -0.27896777 | 4.34264632  | -0.02370693 | C  | 0.38018385  | -3.19855969 | 9.04684686  |
| C  | 1.07688044  | 4.70355789  | 0.00388963  | C  | -0.97566436 | -3.55947126 | 9.01925030  |
| C  | 2.05544839  | 3.70756841  | 0.00684236  | C  | -1.95423231 | -2.56348178 | 9.01629757  |
| H  | 2.28016925  | -2.05571761 | 0.06383434  | H  | -2.17895316 | 3.19980424  | 8.95930559  |
| H  | 4.79797184  | -1.97177962 | 0.12156674  | H  | -4.69675576 | 3.11586625  | 8.90157319  |
| H  | 5.92135371  | 0.29603036  | 0.10281812  | H  | -5.82013763 | 0.84805628  | 8.92032181  |
| H  | 4.49944655  | 2.34577928  | 0.03532801  | H  | -4.39823047 | -1.20169265 | 8.98781191  |
| H  | -1.72079259 | 2.73486925  | -0.04186369 | H  | 1.82200867  | -1.59078262 | 9.06500362  |
| H  | -1.04774744 | 5.12051141  | -0.02492986 | H  | 1.14896351  | -3.97642479 | 9.04806979  |
| H  | 1.36833684  | 5.75574562  | 0.02452755  | H  | -1.26712077 | -4.61165899 | 8.99861238  |
| H  | 3.11115077  | 3.99188787  | 0.03060573  | H  | -3.00993469 | -2.84780124 | 8.99253420  |
| N  | -2.02428082 | 0.13575863  | 0.10003631  | N  | 2.12549691  | 1.00832800  | 8.92310361  |
| N  | -2.58884475 | -0.30307081 | 1.25457387  | N  | 2.69006083  | 1.44715743  | 7.76856606  |
| C  | -3.93133175 | -0.15700199 | 1.14030138  | C  | 4.03254783  | 1.30108862  | 7.88283854  |
| C  | -4.24265352 | 0.38762903  | -0.11333372 | C  | 4.34386961  | 0.75645759  | 9.13647365  |
| C  | -3.00099421 | 0.55480619  | -0.74047454 | C  | 3.10221029  | 0.58928043  | 9.76361447  |
| H  | -4.58180677 | -0.46105990 | 1.95708304  | H  | 4.68302286  | 1.60514653  | 7.06605689  |
| H  | -5.22456707 | 0.61652687  | -0.51619172 | H  | 5.32578315  | 0.52755975  | 9.53933164  |
| H  | -2.74942313 | 0.94059519  | -1.72517318 | H  | 2.85063921  | 0.20349143  | 10.74831310 |
| N  | -0.25998166 | -2.12399176 | 0.11263519  | N  | 0.36119775  | 3.26807839  | 8.91050474  |
| N  | -0.74427876 | -2.60113601 | 1.28915325  | N  | 0.84549485  | 3.74522264  | 7.73398668  |
| C  | -0.02948053 | -3.18334280 | -0.70152227 | C  | 0.91334746  | 5.09741516  | 7.80097453  |
| C  | -0.36450359 | -4.37202445 | -0.03724243 | C  | 0.46571968  | 5.51611108  | 9.06038236  |
| C  | -0.81213137 | -3.95332854 | 1.22216540  | C  | 0.13069661  | 4.32742942  | 9.72466220  |
| H  | 0.34885823  | -3.02253081 | -1.70884580 | H  | 1.28625231  | 5.66921942  | 6.95490506  |
| H  | -0.30789768 | -5.38736818 | -0.41772946 | H  | 0.40911377  | 6.53145481  | 9.44086939  |
| H  | -1.18503622 | -4.52513279 | 2.06823487  | H  | -0.24764214 | 4.16661744  | 10.73198573 |
| Pd | -1.33313916 | -1.25882992 | 2.70552530  | Pd | 1.43435525  | 2.40291654  | 6.31761463  |
| N  | -1.74944614 | -0.02412459 | 4.27899025  | N  | 1.85066223  | 1.16821122  | 4.74414968  |
| C  | -1.16386981 | -0.35186760 | 5.40667459  | C  | 1.26508589  | 1.49595422  | 3.61646534  |
| C  | -0.37161730 | -1.55644444 | 5.37549735  | C  | 0.47283338  | 2.70053106  | 3.64764257  |
| C  | -0.28953229 | -2.13718060 | 4.13662993  | C  | 0.39074838  | 3.28126723  | 4.88651000  |
| H  | -2.24940791 | 0.86808981  | 4.25086299  | H  | 2.35062399  | 0.27599681  | 4.77227693  |
| H  | -1.24882727 | 0.28424960  | 6.29730228  | H  | 1.35004336  | 0.85983703  | 2.72583765  |
| H  | 0.11604274  | -1.92935690 | 6.28044262  | H  | -0.01482665 | 3.07344353  | 2.74269730  |
| H  | 0.30716599  | -3.04567047 | 3.97156178  | H  | -0.20594990 | 4.18975710  | 5.05157814  |

Compound **5<sub>2</sub>**<sup>*t-bt-nx-ii*</sup>.

E = -2714.11653156 au

BSSE = 0.01138338 au

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | Pd | 2.04646153  | 3.37122804  | 9.65407773  |
| N  | 2.04372721  | 0.00000000  | 0.00000000  | N  | 2.50324641  | 5.33318983  | 9.32607335  |
| C  | 2.59197445  | 1.19397885  | 0.00000000  | C  | 3.78144344  | 5.57543796  | 9.14969107  |
| C  | 1.68072383  | 2.30775670  | -0.00180379 | C  | 4.65752185  | 4.43675696  | 9.23342112  |
| C  | 0.35651808  | 1.94681627  | 0.00555415  | C  | 4.00894368  | 3.24998031  | 9.46390770  |
| H  | 2.66762487  | -0.81075118 | 0.00565882  | H  | 1.85160928  | 6.11689244  | 9.24084555  |
| H  | 3.68393101  | 1.31097224  | 0.00210995  | H  | 4.13719255  | 6.59401494  | 8.94319281  |
| H  | 2.04988230  | 3.33758270  | -0.00734384 | H  | 5.73903167  | 4.54681402  | 9.10832141  |
| H  | -0.43397930 | 2.71050768  | 0.00594825  | H  | 4.56596508  | 2.30500857  | 9.52859692  |
| N  | -2.01552794 | 0.23858284  | -0.03381863 | N  | 1.81942842  | 1.37634903  | 9.96989360  |
| N  | -2.79534042 | -0.52917586 | 0.77235021  | N  | 0.88453225  | 0.71407434  | 9.24028824  |
| C  | -4.08555810 | -0.31791445 | 0.41631109  | C  | 0.82038762  | -0.55529014 | 9.71061561  |
| C  | -4.14549074 | 0.60686007  | -0.63669545 | C  | 1.73257592  | -0.72084587 | 10.76275811 |
| C  | -2.80841529 | 0.93223052  | -0.88950267 | C  | 2.34454514  | 0.53191613  | 10.89173119 |
| H  | -4.88386344 | -0.84454966 | 0.93495128  | H  | 0.12684594  | -1.26458487 | 9.26446762  |
| H  | -5.02738791 | 0.97611705  | -1.15116387 | H  | 1.91521654  | -1.61292610 | 11.35410678 |
| H  | -2.36756094 | 1.59618997  | -1.62892966 | H  | 3.10572731  | 0.88181820  | 11.58445402 |
| N  | -0.23244518 | -2.11190716 | -0.09615864 | N  | -0.05879419 | 3.63782534  | 9.88841489  |
| N  | -0.97965530 | -2.76232715 | 0.83284438  | N  | -0.89387509 | 2.97738827  | 9.04576086  |
| C  | 0.16030016  | -3.01834123 | -1.02596330 | C  | -2.17347647 | 3.21966053  | 9.42020147  |
| C  | -0.34672925 | -4.28158923 | -0.69549985 | C  | -2.17444987 | 4.06657809  | 10.53588694 |
| C  | -1.06543155 | -4.06992684 | 0.48844695  | C  | -0.81722623 | 4.30250852  | 10.79381785 |
| H  | 0.76536100  | -2.70191309 | -1.87268409 | H  | -2.99745101 | 2.77625929  | 8.86697014  |
| H  | -0.22339401 | -5.21317499 | -1.23918111 | H  | -3.03314524 | 4.44538776  | 11.08171944 |
| H  | -1.63143757 | -4.76089923 | 1.10795541  | H  | -0.34084613 | 4.89376731  | 11.57250357 |
| Pd | -1.83566905 | -1.66889191 | 2.32040341  | Pd | -0.02622296 | 1.80249803  | 7.62514754  |
| N  | -2.65546022 | -0.65254377 | 3.91084866  | N  | 0.82607072  | 0.71238977  | 6.10521152  |
| C  | -2.26506969 | -1.09923442 | 5.15030815  | C  | 0.43877779  | 1.07867090  | 4.83890420  |
| C  | -2.74210007 | -0.45947217 | 6.30555304  | C  | 0.95093567  | 0.39642348  | 3.72415671  |
| C  | -3.62507703 | 0.61528571  | 6.19582301  | C  | 1.85739689  | -0.64867458 | 3.90444094  |
| C  | -4.01645172 | 1.05248398  | 4.92598642  | C  | 2.25886203  | -0.99339225 | 5.20012887  |
| C  | -3.49929468 | 0.39687694  | 3.80782498  | C  | 1.71980371  | -0.28566992 | 6.27533145  |
| C  | -1.33621746 | -2.22747034 | 5.10936887  | C  | -0.49112787 | 2.20575049  | 4.80607090  |
| C  | -0.95802859 | -2.67106242 | 3.80811316  | C  | -0.82478938 | 2.76920287  | 6.07225617  |
| C  | -0.02949197 | -3.72098642 | 3.71626215  | C  | -1.67096431 | 3.88980650  | 6.09108468  |
| C  | 0.48156152  | -4.33758509 | 4.86998988  | C  | -2.19382502 | 4.41919291  | 4.89932082  |
| C  | 0.07765514  | -3.91432979 | 6.14420371  | C  | -1.88004737 | 3.83920560  | 3.66154691  |
| C  | -0.82862879 | -2.85751623 | 6.26239055  | C  | -1.02443948 | 2.73481644  | 3.61351430  |
| H  | -3.74038704 | 0.70915412  | 2.79134719  | H  | 1.98830679  | -0.50594264 | 7.30922284  |
| H  | -4.67993255 | 1.90699197  | 4.79136094  | H  | 2.96210163  | -1.80514145 | 5.38792911  |
| H  | -3.98644751 | 1.11861175  | 7.09484091  | H  | 2.22896732  | -1.19794808 | 3.03650927  |
| H  | -2.40158889 | -0.79195711 | 7.28671839  | H  | 0.62672426  | 0.67203959  | 2.71876807  |
| H  | 0.30229180  | -4.06892202 | 2.73562400  | H  | -1.92391044 | 4.36401589  | 7.04194853  |
| H  | 1.19546478  | -5.16052219 | 4.77104025  | H  | -2.85072881 | 5.29314063  | 4.93982642  |
| H  | 0.46623044  | -4.40460273 | 7.03964207  | H  | -2.29515381 | 4.24887471  | 2.73751991  |
| H  | -1.14372012 | -2.52502198 | 7.25545413  | H  | -0.78437412 | 2.27343447  | 2.65045451  |

Compound **5<sub>2</sub>**<sup>t-bt-xx-ii</sup>.

E = -2714.11277967 au

BSSE = 0.0102904 au

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | C | -4.05559617 | -0.24680948 | 0.64389245  |
| N  | 2.04137133  | 0.00000000  | 0.00000000  | C | -4.18510532 | 0.57771866  | -0.48290955 |
| C  | 2.58810360  | 1.19358781  | 0.00000000  | C | -2.86652761 | 0.85666918  | -0.86261272 |
| C  | 1.67573298  | 2.30642236  | -0.02046010 | H | -4.81826287 | -0.70658988 | 1.26854698  |
| C  | 0.35297890  | 1.94326956  | -0.01200051 | H | -5.09926996 | 0.91407295  | -0.96249333 |
| H  | 2.66325962  | -0.81066860 | 0.04609043  | H | -2.47556675 | 1.44508254  | -1.68879006 |
| H  | 3.67996832  | 1.31154482  | 0.02311144  | N | -0.25936743 | -2.11975044 | -0.02662591 |
| H  | 2.04318554  | 3.33705353  | -0.03034719 | N | -0.94105733 | -2.69080203 | 0.99938766  |
| H  | -0.44176921 | 2.70191562  | -0.00544296 | C | 0.04546525  | -3.09281839 | -0.91915120 |
| N  | -2.01977211 | 0.23137069  | -0.00818858 | C | -0.45098953 | -4.32211943 | -0.46439823 |
| N  | -2.74380654 | -0.44566901 | 0.92081860  | C | -1.07028849 | -4.01727500 | 0.75450290  |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H  | 0.58826478  | -2.84587133 | -1.82864225 | C  | -1.96036414 | -3.05312005 | 10.18497544 |
| H  | -0.38159990 | -5.29060714 | -0.95019515 | C  | -1.83085498 | -3.87764819 | 11.31177745 |
| H  | -1.59337579 | -4.65537880 | 1.46224784  | C  | -3.14943270 | -4.15659871 | 11.69148062 |
| Pd | -1.61364068 | -1.43766675 | 2.45757467  | H  | -1.19769743 | -2.59333965 | 9.56032091  |
| N  | -2.19650851 | -0.21713141 | 4.00514987  | H  | -0.91669035 | -4.21400248 | 11.79136122 |
| C  | -1.68001527 | -0.54735973 | 5.23480837  | H  | -3.54039355 | -4.74501207 | 12.51765796 |
| C  | -2.04335483 | 0.19834299  | 6.36773924  | N  | -5.75659288 | -1.18017909 | 10.85549380 |
| C  | -2.91477946 | 1.28086626  | 6.24057093  | N  | -5.07490297 | -0.60912750 | 9.82948023  |
| C  | -3.41289296 | 1.61525276  | 4.97687037  | C  | -4.94567182 | 0.71734547  | 10.07436499 |
| C  | -3.02895593 | 0.83875194  | 3.88279546  | C  | -5.56497077 | 1.02218990  | 11.29326612 |
| C  | -0.76364357 | -1.68629780 | 5.20475014  | C  | -6.06142555 | -0.20711114 | 11.74801910 |
| C  | -0.55493913 | -2.27861810 | 3.92476593  | H  | -4.42258452 | 1.35544927  | 9.36662006  |
| C  | 0.34348810  | -3.35437036 | 3.83538317  | H  | -5.63436041 | 1.99067762  | 11.77906305 |
| C  | 1.00308131  | -3.84122674 | 4.97578658  | H  | -6.60422509 | -0.45405820 | 12.65751014 |
| C  | 0.78732126  | -3.25402715 | 6.23082505  | Pd | -4.40231963 | -1.86226278 | 8.37129322  |
| C  | -0.09110057 | -2.17299502 | 6.34292747  | N  | -3.81945180 | -3.08279812 | 6.82371803  |
| H  | -3.38512256 | 1.04233647  | 2.87229462  | C  | -4.33594504 | -2.75256980 | 5.59405952  |
| H  | -4.10167528 | 2.44793859  | 4.83316709  | C  | -3.97260548 | -3.49827252 | 4.46112865  |
| H  | -3.20942788 | 1.85149219  | 7.12363840  | C  | -3.10118085 | -4.58079579 | 4.58829696  |
| H  | -1.65855377 | -0.08598418 | 7.34779475  | C  | -2.60306735 | -4.91518229 | 5.85199753  |
| H  | 0.54244390  | -3.81571966 | 2.86548894  | C  | -2.98700438 | -4.13868147 | 6.94607243  |
| H  | 1.69837205  | -4.68032976 | 4.88041314  | C  | -5.25231674 | -1.61363173 | 5.62411775  |
| H  | 1.30833846  | -3.62953679 | 7.11447161  | C  | -5.46102118 | -1.02131143 | 6.90410197  |
| H  | -0.24748009 | -1.70195944 | 7.31766739  | C  | -6.35944841 | 0.05444083  | 6.99348472  |
| Pd | -6.01596031 | -3.29992953 | 10.82886789 | C  | -7.01904162 | 0.54129721  | 5.85308131  |
| N  | -8.05733164 | -3.29992953 | 10.82886789 | C  | -6.80328157 | -0.04590238 | 4.59804284  |
| C  | -8.60406391 | -4.49351734 | 10.82886789 | C  | -5.92485974 | -1.12693451 | 4.48594042  |
| C  | -7.69169329 | -5.60635189 | 10.84932800 | H  | -2.63083775 | -4.34226600 | 7.95657327  |
| C  | -6.36893921 | -5.24319909 | 10.84086840 | H  | -1.91428503 | -5.74786812 | 5.99570081  |
| H  | -8.67921993 | -2.48926093 | 10.78277747 | H  | -2.80653242 | -5.15142172 | 3.70522949  |
| H  | -9.69592863 | -4.61147435 | 10.80575646 | H  | -4.35740654 | -3.21394535 | 3.48107314  |
| H  | -8.05914585 | -6.63698306 | 10.85921508 | H  | -6.55840421 | 0.51579013  | 7.96337896  |
| H  | -5.57419110 | -6.00184515 | 10.83431085 | H  | -7.71433236 | 1.38040023  | 5.94845475  |
| N  | -3.99618820 | -3.53130022 | 10.83705648 | H  | -7.32429877 | 0.32960726  | 3.71439628  |
| N  | -3.27215376 | -2.85426052 | 9.90804929  | H  | -5.76848022 | -1.59797009 | 3.51120050  |

Compound **6<sub>1</sub>** :

E = -719.018233809 au

|    |             |             |            |   |             |             |             |
|----|-------------|-------------|------------|---|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000 | H | 4.86904906  | -1.92743898 | 0.00000000  |
| N  | 2.08502428  | 0.00000000  | 0.00000000 | H | 5.95118612  | 0.36070134  | 0.00000000  |
| C  | 2.64904208  | 1.25299293  | 0.00000000 | H | 4.49492018  | 2.38293170  | 0.00000000  |
| C  | 4.05006691  | 1.38711178  | 0.00000000 | H | -1.72340566 | 2.73505942  | 0.00000000  |
| C  | 4.86412417  | 0.25490091  | 0.00000000 | H | -1.05421862 | 5.11575484  | 0.00000000  |
| C  | 4.27167448  | -1.01493044 | 0.00000000 | H | 1.36204866  | 5.75470823  | 0.00000000  |
| C  | 2.87889728  | -1.09087370 | 0.00000000 | H | 3.10403618  | 3.99227073  | 0.00000000  |
| C  | 1.67649331  | 2.34642540  | 0.00000000 | N | -2.04298464 | 0.01638620  | 0.00000000  |
| C  | 0.30009707  | 1.96177428  | 0.00000000 | H | -2.35823245 | 0.56252491  | 0.81353772  |
| C  | -0.66021429 | 2.98840115  | 0.00000000 | H | -2.35823362 | 0.56252809  | -0.81353328 |
| C  | -0.28377162 | 4.33936494  | 0.00000000 | N | -0.49141659 | -2.18404684 | -0.00002054 |
| C  | 1.07112897  | 4.70196382  | 0.00000000 | H | -0.28526090 | -2.74408810 | -0.83170155 |
| C  | 2.04841024  | 3.70587709  | 0.00000000 | H | -0.28525900 | -2.74410430 | 0.83164945  |
| H  | 2.35660870  | -2.04988040 | 0.00000000 | H | -1.49841756 | -1.91282806 | -0.00001490 |

Compound **6<sub>2</sub><sup>π</sup>** :

E = -1438.04856169 au

BSSE = 0.0085147 au

C 0.00000000 0.00000000 0.00000000 H -4.91776979 -4.90726650 0.05194062

Compound **6<sub>2</sub><sup>T</sup>**:

E = -1438.04541361 au

BSSE = 0.0075519 au

|    |             |             |             |    |             |             |            |
|----|-------------|-------------|-------------|----|-------------|-------------|------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | Pd | 4.54686323  | 4.82778436  | 3.40488787 |
| N  | 2.08622886  | 0.00000000  | 0.00000000  | N  | 2.46063437  | 4.82778436  | 3.40488787 |
| C  | 2.64715491  | 1.25236447  | 0.00000000  | C  | 1.89970832  | 3.57541989  | 3.40488787 |
| C  | 4.04542705  | 1.39538266  | 0.03844873  | C  | 0.50143618  | 3.43240169  | 3.36643913 |
| C  | 4.86260383  | 0.26595925  | 0.05706781  | C  | -0.31574060 | 4.56182511  | 3.34782006 |
| C  | 4.27501410  | -1.00577878 | 0.04487423  | C  | 0.27184913  | 5.83356314  | 3.36001364 |
| C  | 2.88316284  | -1.08818303 | 0.02343277  | C  | 1.66370039  | 5.91596739  | 3.38145509 |
| C  | 1.67242504  | 2.34432949  | -0.05239447 | C  | 2.87443819  | 2.48345486  | 3.45728234 |
| C  | 0.29784582  | 1.95936923  | -0.09393147 | C  | 4.24901742  | 2.86841513  | 3.49881934 |
| C  | -0.66175071 | 2.98255400  | -0.19484187 | C  | 5.20861394  | 1.84523036  | 3.59972974 |
| C  | -0.28544918 | 4.33335729  | -0.23781955 | C  | 4.83231241  | 0.49442707  | 3.64270742 |
| C  | 1.06746942  | 4.69738637  | -0.16410230 | C  | 3.47939381  | 0.13039799  | 3.56899017 |
| C  | 2.04465091  | 3.70327954  | -0.07507338 | C  | 2.50221232  | 1.12450482  | 3.47996125 |
| H  | 2.36475206  | -2.04947570 | 0.02324454  | H  | 2.18211117  | 6.87726006  | 3.38164333 |
| H  | 4.87565183  | -1.91617553 | 0.05990671  | H  | -0.32878860 | 6.74395989  | 3.34498116 |
| H  | 5.94835933  | 0.37671218  | 0.09128516  | H  | -1.40149610 | 4.45107218  | 3.31360271 |
| H  | 4.48457529  | 2.39322663  | 0.06724685  | H  | 0.06228795  | 2.43455772  | 3.33764102 |
| H  | -1.72332300 | 2.72584251  | -0.24432982 | H  | 6.27018623  | 2.10194185  | 3.64921769 |
| H  | -1.05376541 | 5.10779290  | -0.32074180 | H  | 5.60062864  | -0.28000854 | 3.72562967 |
| H  | 1.35961351  | 5.75002348  | -0.18289890 | H  | 3.18724972  | -0.92223913 | 3.58778676 |
| H  | 3.09819077  | 3.99049372  | -0.01172379 | H  | 1.44867246  | 0.83729063  | 3.41661166 |
| N  | -2.04470269 | 0.01517954  | 0.01062764  | N  | 6.59156592  | 4.81260481  | 3.39426022 |
| H  | -2.36187362 | 0.62499572  | 0.77657592  | H  | 6.90873684  | 4.20278864  | 2.62831194 |
| H  | -2.36042485 | 0.49448519  | -0.84423654 | H  | 6.90728807  | 4.33329917  | 4.24912441 |
| N  | -0.48524385 | -2.18156207 | 0.10028000  | N  | 5.03210708  | 7.00934642  | 3.30460787 |
| H  | -0.28641116 | -2.77014809 | -0.71332209 | H  | 4.83327439  | 7.59793245  | 4.11820996 |
| H  | -0.26093557 | -2.70941689 | 0.94809063  | H  | 4.80779880  | 7.53720124  | 2.45679723 |
| H  | -1.49402702 | -1.91974845 | 0.10545299  | H  | 6.04089026  | 6.74753280  | 3.29943488 |

Compound **1<sub>1</sub><sup>t-bt</sup>**:

E = -2045.51896633 au

BSSE = 0.006176 au

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | H  | -1.04750729 | 5.09197849  | -0.48986015 |
| N  | 2.08639427  | 0.00000000  | 0.00000000  | H  | 1.36632827  | 5.73619198  | -0.42697674 |
| C  | 2.64599519  | 1.25504505  | 0.00000000  | H  | 3.10337835  | 3.98894534  | -0.17504933 |
| C  | 4.04431356  | 1.39478113  | 0.08925411  | N  | -2.04293195 | 0.01617973  | 0.02460785  |
| C  | 4.85865717  | 0.26495050  | 0.16371655  | H  | -2.35525155 | 0.61352153  | 0.80246081  |
| C  | 4.27180121  | -1.00835163 | 0.14641418  | H  | -2.36595631 | 0.50600455  | -0.82133912 |
| C  | 2.88150148  | -1.08860309 | 0.06558203  | N  | -0.49630550 | -2.18507429 | 0.09388486  |
| C  | 1.67492304  | 2.34486508  | -0.09613410 | H  | -0.30654184 | -2.76776295 | -0.72633456 |
| C  | 0.29935890  | 1.95865248  | -0.11892049 | H  | -0.28697833 | -2.72909794 | 0.93544642  |
| C  | -0.65974427 | 2.97688757  | -0.25519323 | H  | -1.50157936 | -1.90648990 | 0.09851828  |
| C  | -0.27954741 | 4.32154167  | -0.37605738 | Pd | 4.57497476  | 4.60079525  | 4.26757823  |
| C  | 1.07394731  | 4.68748172  | -0.34506655 | N  | 3.96544474  | 2.63075334  | 3.97516354  |
| C  | 2.04905892  | 3.70010212  | -0.19958640 | C  | 2.64257583  | 2.49243221  | 3.62847735  |
| H  | 2.36123989  | -2.04884705 | 0.05230626  | C  | 2.11740602  | 1.20966237  | 3.37848701  |
| H  | 4.87089437  | -1.91857472 | 0.19524284  | C  | 2.93613469  | 0.08779107  | 3.49623168  |
| H  | 5.94306272  | 0.37572545  | 0.23280076  | C  | 4.27808622  | 0.24462663  | 3.86881735  |
| H  | 4.48432152  | 2.39270818  | 0.10568903  | C  | 4.74853988  | 1.53786653  | 4.09235259  |
| H  | -1.72230011 | 2.72194458  | -0.27882020 | C  | 1.90770113  | 3.75564756  | 3.56837105  |

|   |             |             |            |   |             |            |            |
|---|-------------|-------------|------------|---|-------------|------------|------------|
| C | 2.66295762  | 4.93424923  | 3.85667622 | H | 0.11435529  | 7.20588099 | 3.51919637 |
| C | 1.98626325  | 6.16489502  | 3.82973401 | H | -1.17165042 | 5.13192121 | 2.99722192 |
| C | 0.61696361  | 6.23432588  | 3.53082794 | H | -0.03396927 | 2.92723640 | 3.02189120 |
| C | -0.10998957 | 5.07031758  | 3.24526663 | N | 5.16195212  | 6.53922975 | 4.54795188 |
| C | 0.53396736  | 3.83150165  | 3.26190637 | H | 4.57275519  | 6.94722459 | 5.28655584 |
| H | 5.78499019  | 1.73309350  | 4.37577463 | H | 4.92195723  | 7.07357311 | 3.70189788 |
| H | 4.94819344  | -0.60924128 | 3.97719886 | N | 6.75338204  | 4.38233719 | 4.76865991 |
| H | 2.53044174  | -0.90430575 | 3.29097436 | H | 7.41764572  | 4.07216929 | 4.05431072 |
| H | 1.07689544  | 1.09189918  | 3.06909995 | H | 7.01744532  | 3.96349389 | 5.66476415 |
| H | 2.52952455  | 7.08751526  | 4.04888575 | H | 6.78106229  | 5.42285642 | 4.84682959 |

# Compound 7:

E = -4005.10785525 au

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | H  | -2.34092235 | 2.55191273  | 0.71410504  |
| P  | 2.32902118  | 0.00000000  | 0.00000000  | C  | -3.09966189 | -0.34174973 | 1.55974071  |
| P  | -2.31823826 | 0.24506740  | 0.00000000  | H  | -4.17664964 | -0.11210328 | 1.56627365  |
| C  | 3.21824255  | -0.97606090 | -1.28532500 | H  | -2.95328956 | -1.42626541 | 1.66134919  |
| H  | 4.30688959  | -0.84285857 | -1.19072348 | H  | -2.59738811 | 0.16227120  | 2.39742475  |
| H  | 2.96980292  | -2.04152559 | -1.17793495 | Br | 0.08428709  | 1.49967426  | 2.07088981  |
| H  | 2.88722742  | -0.64884772 | -2.28060861 | C  | -0.02860471 | -1.29037959 | -1.51701266 |
| C  | 3.08792072  | -0.57327425 | 1.57525559  | H  | 0.11912857  | -2.33109236 | -1.18395583 |
| H  | 2.84640588  | -1.63338771 | 1.73600557  | C  | -0.16982097 | -1.10719420 | -2.86196571 |
| H  | 4.18112697  | -0.44285930 | 1.55201666  | H  | -0.14082190 | -2.00091106 | -3.50125696 |
| H  | 2.64921230  | 0.01530921  | 2.39305970  | C  | -0.39959867 | 0.13547036  | -3.57786502 |
| C  | 2.99826378  | 1.69968602  | -0.21511666 | H  | -0.58585435 | 0.03746336  | -4.65296462 |
| H  | 4.09739336  | 1.69896966  | -0.14681984 | C  | -0.43281302 | 1.39874978  | -3.06315400 |
| H  | 2.68764374  | 2.09354498  | -1.19302120 | H  | -0.23820276 | 1.58315086  | -2.00058028 |
| H  | 2.56580925  | 2.33363122  | 0.57161953  | C  | -0.75352263 | 2.60209830  | -3.83526807 |
| C  | -3.31304431 | -0.56809500 | -1.31806116 | O  | -0.89652808 | 3.72614191  | -3.34506229 |
| H  | -4.38170210 | -0.33751832 | -1.18866414 | O  | -0.89882476 | 2.37077097  | -5.18422640 |
| H  | -2.97028328 | -0.20376485 | -2.29646424 | C  | -1.23900205 | 3.54387549  | -5.95357053 |
| H  | -3.16095598 | -1.65556677 | -1.28246057 | H  | -2.19266472 | 3.96898356  | -5.60924487 |
| C  | -2.82926486 | 2.00832796  | -0.10661593 | H  | -0.45633396 | 4.30973280  | -5.85683582 |
| H  | -2.48991164 | 2.43791713  | -1.06015896 | H  | -1.31908193 | 3.19895500  | -6.99062476 |
| H  | -3.92421012 | 2.09677438  | -0.02715735 |    |             |             |             |

# Compound 8:

E = -2142.56461521 au

|    |             |             |            |   |             |             |             |
|----|-------------|-------------|------------|---|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000 | H | 2.09799419  | -0.88683957 | 2.54207406  |
| Cl | 2.34133006  | 0.00000000  | 0.00000000 | H | 1.92506983  | -2.51703414 | 1.93508788  |
| Cl | -2.35658677 | 0.16532250  | 0.00000000 | C | 1.43367949  | -2.29891353 | 4.06798730  |
| P  | -0.14736776 | -1.31232560 | 1.85087063 | H | 0.82835831  | -3.20834733 | 4.18502753  |
| C  | -1.16654950 | -0.50451216 | 3.17806193 | H | 2.45717438  | -2.53597372 | 4.39633293  |
| H  | -0.46553856 | 0.12983324  | 3.74698642 | H | 1.03919911  | -1.53703814 | 4.75702931  |
| H  | -1.84354496 | 0.16962384  | 2.63238972 | N | 0.09602493  | 1.13087233  | -1.82497802 |
| C  | -1.97289252 | -1.42434732 | 4.10413849 | C | -0.18487532 | 2.43352353  | -1.74748575 |
| H  | -1.33711095 | -2.10601380 | 4.68643774 | C | 0.22531163  | 3.36256620  | -2.72849157 |
| H  | -2.55085171 | -0.81583638 | 4.81630246 | C | 0.97891271  | 2.91253342  | -3.79673206 |
| H  | -2.69170976 | -2.02913949 | 3.53193209 | C | 1.26574608  | 1.52840836  | -3.92546858 |
| C  | -0.99520143 | -2.86352744 | 1.28326284 | C | 2.05524768  | 1.00196378  | -4.98518381 |
| H  | -2.04965795 | -2.57301868 | 1.14395842 | C | 2.31841165  | -0.35464464 | -5.05769333 |
| H  | -0.59364790 | -3.04178247 | 0.27143573 | C | 1.75412888  | -1.23815510 | -4.11013149 |
| C  | -0.84378087 | -4.13021778 | 2.13439373 | C | 0.95782899  | -0.77347895 | -3.06742817 |
| H  | -1.38536039 | -4.95918201 | 1.65400434 | C | 0.75216000  | 0.63516939  | -2.92612409 |
| H  | 0.20987312  | -4.43586937 | 2.21687781 | H | -0.74194420 | 2.74460931  | -0.86060074 |
| H  | -1.24772808 | -4.01132730 | 3.14964349 | H | -0.02897982 | 4.41641871  | -2.60932781 |
| C  | 1.46871995  | -1.78610804 | 2.62254783 | H | 1.36142608  | 3.60780919  | -4.54872145 |

|   |            |             |             |   |             |             |             |
|---|------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 2.45302918 | 1.69159555  | -5.73410802 | C | 0.20411189  | -1.77154197 | -2.25270447 |
| H | 2.93628490 | -0.75112368 | -5.86585501 | O | 0.56175179  | -2.94551004 | -2.11660092 |
| H | 1.90237595 | -2.31763696 | -4.19151100 | H | -0.78537157 | -1.42701300 | -1.86963343 |

### Compound 9:

E = -434.218221270 au

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | H | -0.26470994 | -2.43244365 | -0.95847174 |
| N  | 2.06613037  | 0.00000000  | 0.00000000  | H | -0.23453543 | -2.48265606 | 0.88369794  |
| C  | 2.66532243  | 1.15027371  | 0.00000000  | C | -1.89844371 | -1.31146103 | 0.02952967  |
| C  | 1.78791839  | 2.33577352  | 0.00430140  | H | -1.73603060 | -0.07238597 | -0.02036702 |
| N  | 0.51610525  | 2.08996713  | 0.00810170  | H | -2.45922843 | -1.39611972 | -0.91377057 |
| H  | 2.68113228  | -0.82192983 | -0.00347945 | C | -2.76505088 | -1.49261356 | 1.27741533  |
| H  | 3.75619042  | 1.25109171  | -0.00307108 | H | -3.59897415 | -0.77893313 | 1.30262627  |
| H  | 2.21398662  | 3.34543670  | 0.00398415  | H | -3.18685871 | -2.50792571 | 1.26286714  |
| H  | -0.08352116 | 2.92396542  | 0.01040225  | H | -2.17404985 | -1.37836688 | 2.19637421  |
| C  | -0.57664071 | -1.96148926 | -0.01905903 |   |             |             |             |

### Compound 10:

E = -1284.02652885 au

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Pd | 0.00000000  | 0.00000000  | 0.00000000  | H | -1.12667664 | 2.64576681  | 2.33281398  |
| P  | 2.27258624  | 0.00000000  | 0.00000000  | C | -2.28397141 | 2.63729954  | -0.52459912 |
| P  | -0.54838653 | 2.31064688  | 0.00000000  | H | -2.50426027 | 3.71526437  | -0.48989992 |
| C  | 2.99128872  | 0.38929685  | -1.64844495 | H | -2.44008690 | 2.27067411  | -1.54911768 |
| H  | 4.09045794  | 0.40173657  | -1.58906956 | H | -2.95924743 | 2.09998994  | 0.15533974  |
| H  | 2.67634262  | -0.37067932 | -2.37662552 | C | -0.17525025 | -2.06824256 | -0.03618940 |
| H  | 2.63452725  | 1.36944999  | -1.99236626 | H | 0.23966677  | -2.50989391 | -0.94887861 |
| C  | 3.10415262  | -1.57141063 | 0.47175652  | H | 0.20509221  | -2.53439141 | 0.87933885  |
| H  | 2.79848036  | -2.37482682 | -0.21243800 | C | -1.61856037 | -1.70366818 | -0.06152822 |
| H  | 4.19729988  | -1.45245041 | 0.42576597  | H | -1.80052279 | -0.53053574 | -0.01953350 |
| H  | 2.81429084  | -1.85338006 | 1.49362413  | H | -2.14411340 | -1.96853689 | -0.98817542 |
| C  | 3.05063556  | 1.22848885  | 1.12986926  | H | -2.18843342 | -2.00153545 | 0.82831826  |
| H  | 2.72806364  | 1.03987844  | 2.16332593  | O | -2.93449646 | 0.48283353  | 2.27675233  |
| H  | 4.14738998  | 1.15129429  | 1.07457624  | H | -3.82274126 | 0.63178301  | 2.65225139  |
| H  | 2.75035348  | 2.24719438  | 0.84829151  | C | -2.09770906 | -0.05682113 | 3.32503770  |
| C  | 0.42025603  | 3.42472292  | -1.10912015 | H | -1.89625165 | 0.71863290  | 4.08780487  |
| H  | 0.01782984  | 4.44850409  | -1.06960316 | H | -1.14007106 | -0.28115588 | 2.82282861  |
| H  | 1.47596748  | 3.45109742  | -0.80281674 | C | -2.68022013 | -1.30444162 | 3.97428738  |
| H  | 0.36492929  | 3.05965647  | -2.14463282 | H | -2.86324463 | -2.09470360 | 3.23083529  |
| C  | -0.44738114 | 3.15328798  | 1.63473974  | H | -1.99178888 | -1.69854068 | 4.73713322  |
| H  | 0.57635641  | 3.09611746  | 2.03008796  | H | -3.63434422 | -1.08219623 | 4.47773166  |
| H  | -0.74220567 | 4.20988038  | 1.54364620  |   |             |             |             |

### Compound 11:

E = -2439.36376626 au

|    |             |             |             |   |             |            |             |
|----|-------------|-------------|-------------|---|-------------|------------|-------------|
| Ti | 0.00000000  | 0.00000000  | 0.00000000  | H | 1.60519824  | 3.28680891 | 1.74836953  |
| Cl | 2.31248666  | 0.00000000  | 0.00000000  | C | -0.24775501 | 3.61982004 | 0.64029085  |
| Cl | -2.27399351 | 0.49099699  | 0.00000000  | H | -0.01493335 | 4.65960444 | 0.35559183  |
| Cl | -0.24036022 | -1.73127051 | 1.61208903  | H | -1.33725011 | 3.54984350 | 0.80387279  |
| P  | 0.14317728  | 2.45117763  | -0.76192253 | C | 1.79017085  | 3.04659945 | -1.34426243 |
| P  | 0.18546713  | 1.36316639  | 2.18388626  | H | 1.73501429  | 4.09340563 | -1.68060120 |
| C  | 0.51748807  | 3.17494362  | 1.89475105  | H | 2.52671512  | 2.94659470 | -0.53544112 |
| H  | 0.24011242  | 3.76728825  | 2.78219311  | H | 2.12640385  | 2.40612565 | -2.17209856 |

|   |             |            |             |   |             |             |             |
|---|-------------|------------|-------------|---|-------------|-------------|-------------|
| C | -0.98662239 | 3.03771586 | -2.09396281 | H | 1.50358946  | 1.48464766  | 4.25619748  |
| H | -2.00765826 | 2.70147495 | -1.86580893 | H | 1.28692300  | -0.20124902 | 3.65312287  |
| H | -0.95974512 | 4.13525943 | -2.17239135 | C | 0.00423495  | -0.09656545 | -2.14377996 |
| H | -0.67759512 | 2.60044372 | -3.05374669 | H | 0.89635799  | 0.29268727  | -2.64850892 |
| C | -1.35189783 | 1.35508413 | 3.19610048  | H | -0.92175214 | 0.27162828  | -2.59817045 |
| H | -1.19090776 | 1.85355222 | 4.16430507  | C | 0.02446554  | -1.59640619 | -1.92412362 |
| H | -2.15609991 | 1.85465192 | 2.63822724  | H | 0.00123507  | -1.90680515 | -0.83391797 |
| H | -1.64682460 | 0.30729337 | 3.34961102  | H | -0.86125423 | -2.10508207 | -2.33094480 |
| C | 1.49196201  | 0.83913111 | 3.36467015  | H | 0.94588410  | -2.07323433 | -2.28527821 |
| H | 2.46607789  | 0.86934373 | 2.85749340  |   |             |             |             |