SUPPORTING INFORMATION

Role of Backbones of Nucleic Acids on the Stability of Hg$^{2+}$ Mediated Canonical Base Pairs and Thymine-Thymine Mispair: A DFT Study

Surjit Bhai a,b, and Bishwajit Ganguly a,b,*

aComputation and Simulation Unit (Analytical and Environmental Science Division and Centralized Instrument Facility), CSIR-Central Salt and Marine Chemicals Research Institute, Bhavnagar, Gujarat, India-364 002.
bAcademy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, Uttar Pradesh, India

*Corresponding Author. Fax: (+91)-278-2567562, E-mail: gang_12@rediffmail.com; ganguly@csmcri.res.in
# Table of Content

| Figure S1 | Page No-3 |
|-----------|-----------|
| The optimized structure of canonical base pairs $\text{D}_{\text{AT}}$, $\text{D}_{\text{GC}}$, and mispair $\text{D}_{\text{TT}}$ mediated with Hg$^{2+}$ in DNA. |

| Figure S2 | Page no-4-5 |
|-----------|-------------|
| The optimized structure of canonical base pairs $\text{P}_{\text{AT}}$, $\text{P}_{\text{GC}}$, and mispair $\text{P}_{\text{TT}}$ mediated with Hg$^{2+}$ in DNA. |

| Table S1 | Page no-4-5 |
|----------|-------------|
| Binding energies ($\Delta E$) and free energies ($\Delta G$) of canonical and mispair AT, GC, and TT base pairs optimized at B3LYP-D3/6-31G* level of theory in the gaseous phase. |

| Table S2 | Page no-6 |
|----------|-----------|
| The calculated free energies ($\Delta G$) of canonical and mispair optimized at B3LYP-D3/6-31G* level of theory in the aqueous phase. |

| TABLE S3 | Page no-7 |
|----------|-----------|
| The electronic, free energies, and enthalpy calculated with explicit water molecules for mispair dimer systems at B3LYP-D3/6-31G* level of theory in aqueous phase. |

| Figure S3 | Page no-6 |
|-----------|-----------|
| The comparison between the Hg$^{2+}$ mediated DNA-DNA, DNA-PNA, and PNA-PNA duplexes in the mispair duplexes. |

| Helix Parameter | Page no-7 |
|----------------|-----------|

| Scheme S1 | Page no-8 |
|-----------|-----------|
| The schematic view, helix parameters, and conformation of TTTT dimer systems a) $\text{TTTT}_{\text{D}}$, b) $\text{TTTT}_{\text{P}}$, and c) $\text{TTTT}_{\text{P}}$ with Hg$^{2+}$ ion. |

| Figure S4 | Page no-9 |
|-----------|-----------|
| Stacking in DNA-DNA, DNA-PNA, and PNA-PNA duplexes |

| Cartesian Coordinates | Page no 10-39 |
|-----------------------|--------------|

| Reference | Page No -39 |
|-----------|-------------|
**Figure S1:** The optimized structure of canonical base pairs $\text{dAT}_D$, $\text{dGC}_D$, and mispair $\text{dT}_D\text{dT}_D$ mediated with Hg$^{2+}$ in DNA using B3LYP-D3/6-31G* level of theory in the gaseous phase. The distances are given in Angstrom (Å). Dark grey: Carbon, Red: Oxygen, White: Hydrogen, Blue: Nitrogen, Cyan: Mercury, Violet: Sodium.

**Figure S2:** The optimized structure of canonical base pairs $\text{pAT}_P$, $\text{pGC}_P$, and mispair $\text{pTT}_P$ mediated with Hg$^{2+}$ in DNA using B3LYP-D3/6-31G* level of theory in the gaseous phase. The distances are given in Angstrom (Å). Dark grey: Carbon, Red: Oxygen, White: Hydrogen, Blue: Nitrogen, Cyan: Mercury, Violet: Sodium.
Table S1: Binding energies (ΔE) and free energies (ΔG) of canonical and mispair AT, GC, and TT base pairs optimized at B3LYP-D3/6-31G* level of theory in the gaseous phase. Values are given in kcal/mol.

| Hg$^{2+}$ mediated systems | B3LYP-D3/6-31G* ΔE | B3LYP-D3/6-31G* ΔG | BSSE corrected ΔG |
|---------------------------|---------------------|---------------------|-------------------|
| D AT_D                    | -49.8               | -41.2               | -42.8             |
| D GC_D                    | -59.4               | -49.4               | -51.5             |
| D TT_D                    | -145.7              | -134.2              | -136.8            |
| P AT_P                    | -17.6               | -9.7                | -10.9             |
| P GC_P                    | -44.5               | -35.1               | -37.0             |
| P TT_P                    | -125.2              | -108.4              | -116.3            |

Table S2: The calculated free energies (ΔG) of canonical and mispair optimized at B3LYP-D3/6-31G* level of theory in the aqueous phase. Values are given in kcal/mol.

| Hg$^{2+}$ mediated systems | B3LYP-D3/6-31G* ΔG |
|---------------------------|-------------------|
| D AT_D                    | -42.9             |
| D GC_D                    | -38.7             |
| D TT_D                    | -59.5             |
| P AT_P                    | -40.2             |
| P GC_P                    | -36.8             |
| P TT_P                    | -64.9             |
| D ATGC_D                  | -106.2            |
| D TTTT_D                  | -138.2            |
| D TTTTP                   | -140.6            |
| P TTTTP                   | -142.5            |
**Table S3.** The electronic, free energies, and enthalpy calculated with explicit water molecules for mispair dimer systems at B3LYP-D3/6-31G* level of theory in aqueous phase.

| Explicit solvent model Hg$^{2+}$ mediated systems | B3LYP-D3/6-31G* $\Delta$E (kcal/mol) | B3LYP-D3/6-31G* $\Delta$G (kcal/mol) | B3LYP-D3/6-31G* $\Delta$H (kcal/mol) |
|--------------------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|
| $\text{dTTTT}_D$                                | -190.4                               | -146.3                               | -173.3                               |
| $\text{pTTTT}_P$                                | -181.1                               | -136.0                               | -167.7                               |
| $\text{pTTTP}_P$                                | -193.3                               | -148.2                               | -178.7                               |

The energies for the complexation of explicit water molecules calculated using equation B:

$$\Delta E = E_{\text{mispair Complex}} - (E_{\text{DNA/PNA}} + E_{\text{Hg}^{2+}} + 2xE_{\text{explicit Water molecule}}) \quad \text{-------------------(B)}$$

Where $E_{\text{mispair Complex}}$ refers to the energy of dimer mispair ($\text{dTTTT}_D, \text{dTTTT}_P,$ and $\text{pTTTT}_P$), $E_{\text{DNA/PNA}}$ is the energy of parent dimer thymine mispair, $E_{\text{Hg}^{2+}}$ is the energy of the mercury ion and $E_{\text{explicit Water molecules}}$ is the energy of two explicit water molecules.
Figure S3. The comparison between the Hg$^{2+}$ mediated DNA-DNA, DNA-PNA, and PNA-PNA duplexes in the mispair duplexes. a) $D$TTTT$D$ consecutive mispair from top view a’) side view b) $D$TTTT$P$ consecutive mispair from top view b’) side view c) $P$TTTT$P$ consecutive mispair from top view c’) side view.
Helix Parameters

The helixes i.e., DNA-DNA, DNA-PNA, and PNA-PNA have different duplexes forms. The DNA duplexes have their standard helix that is well known as $B$-form. The triplex formation of PNA$_2$/DNA is known to form a unique $P$-form helix, which is different from the well-known $A$- and $B$-form of duplexes.\textsuperscript{1} Currently, there are four high-resolution structures of PNA-RNA; PNA-DNA and PNA-PNA duplexes are available determined by the NMR methods and X-ray crystallography.\textsuperscript{2–9} From these structures, they have concluded that when PNA strands hybridized to the other nucleotides (RNA, DNA, and PNA) and they adopt their $P$-form duplexes.\textsuperscript{1} The helix parameters such as X-displacement, tilt, rise, twist angles are different in DNA-DNA ($\delta$TTTT$_D$), DNA-PNA ($\delta$TTTT$_P$), and PNA-PNA ($\rho$TTTT$_P$) duplexes (Scheme S1). The helix parameters of the standard DNA-DNA duplexes have negligible X-displacement from the helix axis, whereas, in the case of DNA-PNA and PNA-PNA duplexes, the X-displacement varies (Scheme S1). The fluctuations arise in the X-displacement from the helix axis leads to the wider and more unwound helix than the standard $B$-form of DNA duplexes. The other helix parameters i.e., “rise” and “tilt” in the case of $B$-form of DNA and $P$-form of PNA duplexes have negligible changes in the duplexes, whereas A-form of duplexes that arise in RNA duplexes (Figure S3). The flexibility of the PNA backbone does not perturb the helix and maintain its Watson-Crick base pairing. Due to the large base-pair displacement and other helix parameters that arise by the PNA-duplexes, the study of Hg$^{2+}$ mediated PNA-PNA duplexes causes the shift of the base pairs, which can adopt $P$-form of duplexes. The stability of the PNA-PNA duplexes as compared to PNA-DNA and DNA-DNA is caused by the base pair shifting which leads to the $P$-helix in PNA-PNA duplexes. The interactions of the thymine nucleobases to the mercury ion could be the cause of better stability in the case of PNA-PNA duplexes (Table 1). The twist angle in the case of PNA-PNA duplex is less as compared to DNA-DNA and hybrid DNA-PNA duplexes. The stacking of the nucleobases in the PNA and DNA systems varies which can lead to the difference in their helicity (Figure S4).
Scheme S1. The schematic view, helix parameters, and conformation of TTTT dimer systems a) $d_{TTTT_D}$, b) $d_{TTTT_P}$ and c) $p_{TTTT_P}$ with Hg$^{2+}$ ion. BB depicts DNA/PNA backbone here.
Figure S4. Stacking in DNA-DNA, DNA-PNA, and PNA-PNA duplexes. Duplexes are truncated by Discovery Studio software and images were captured from the PDB ID: 1BNA, 1NR8, and 1UNN. Dotted Blue color depicts the hydrogen bond interaction between the nucleobases and the red color depicts the stacking interaction between the nucleobases.
Cartesian Coordinates of optimized geometries of canonical base pairs and dimer model using B3LYP-D3/6-31G* level of theory in the aqueous phase:

| AT |    |    |    |
|----|----|----|----|
| P  | 8.71435900 | -2.62888000 | -0.37420700 |
| O  | 10.09696300 | -3.24783500 | -0.35460700 |
| O  | 7.62358900  | -3.18156000 | 0.41483000  |
| O  | 8.73270100  | -2.07845000 | 0.18605800  |
| C  | 9.48633800  | -4.05452000 | -0.49010000 |
| C  | 9.60537000  | 1.28883000  | 0.06841700  |
| O  | 7.59886000  | 1.44015500  | 0.38871300  |
| C  | 9.50850000  | 1.54760700  | 1.45474200  |
| O  | 9.06951800  | 2.93861300  | 1.74686300  |
| C  | 7.53972000  | 1.12938600  | 1.85161500  |
| C  | 6.72151900  | 1.53262600  | 0.61729200  |
| N  | 5.54423900  | 0.70512700  | 0.38871300  |
| C  | 4.24744500  | -1.11668000 | 0.08629500  |
| C  | 3.49149800  | 0.03224100  | -0.05087500 |
| C  | 2.11010300  | 0.21956000  | -0.29767700 |
| N  | 1.27763200  | -0.81741600 | -0.45656700 |
| N  | 1.67999000  | 1.50555000  | -0.37278000 |
| C  | 2.55668400  | 2.52995200  | -0.19584200 |
| N  | 3.85342400  | 2.45072100  | 0.05681300  |
| C  | 4.27543900  | 1.17231400  | 0.12281000  |
| O  | -8.22706400 | -2.79064100 | 0.43712400  |
| O  | -9.62230200 | -3.31776000 | 0.67967300  |
| O  | -7.49225600 | -3.25828800 | -0.80035800 |
| O  | -8.21634800 | -1.14622500 | 0.36360200  |
| C  | -8.73315900 | -0.38723500 | 1.46658600  |
| C  | -8.27601000 | 1.05757600  | 1.33952500  |
| O  | -6.84829400 | 1.13453300  | 1.50106900  |
| C  | -8.59697200 | 1.73020800  | -0.00728900 |
| O  | -8.87431600 | 3.10143000  | 0.28186700  |
| C  | -7.28898200 | 1.56308300  | -0.78246700 |
| C  | -6.23786200 | 1.67912500  | 0.32917800  |
| N  | -4.99450700 | 0.95465900  | 0.06874200  |
| C  | -3.78670400 | 1.66017300  | -0.05158500 |
| C  | -3.75869200 | 2.89658300  | 0.02872000  |
| N  | -2.66548800 | 0.90862500  | -0.27092400 |
| C  | -2.64385100 | -0.46146000 | -0.38319700 |
| O  | -1.57571900 | -1.07840400 | -0.58919100 |
| C  | -3.92016900 | -1.16350500 | -0.26082300 |
| C  | -3.95359800 | -2.66305200 | -0.38334600 |
| C  | -5.02680900 | -0.41907200 | -0.03967100 |
| H  | 9.36808020  | -0.18154600 | -1.57454000 |
| H  | 10.55056800 | -0.16235500 | -0.23795700 |
| H  | 9.56628500  | 2.05217900  | -0.57306900 |
| H  | 9.72488900  | 0.96494900  | 1.97054900  |
| H  | 9.94633400  | 3.23526300  | 1.45355600  |
| H  | 7.50263300  | 0.05030600  | 2.00499800  |
| H  | 7.19962800  | 1.63774900  | 2.75602800  |
| H  | 6.34477700  | 2.55609600  | 0.70051700  |
| H  | 6.32549900  | -1.30797600 | 0.49682200  |
| H  | 0.25474200  | -0.75055200 | -0.51378600 |
| H  | 2.12165000  | 3.52206600  | -0.27168500 |
| H  | -9.82894400 | -0.43157100 | 1.46986800  |
| H  | -8.35863800 | -0.79826600 | 2.41056000  |
| H  | -8.75024000 | 1.63125500  | 2.14517400  |
| H  | -9.44808400 | 1.25279400  | -0.50961000 |
| H  | -8.99340700 | 3.56257200  | -0.56422800 |
| H  | -7.15252100 | 2.32066200  | -1.55911100 |
| Atom | X (Å)  | Y (Å)  | Z (Å)  |
|------|--------|--------|--------|
| H    | -7.25363800 | 0.57296300 | -1.24339500 |
| H    | -5.95057400 | 2.71626900 | 0.50247400  |
| H    | -3.45511200 | -2.98592200 | -1.30489200 |
| H    | -4.98428800 | -3.03323300 | -0.40282200 |
| H    | -3.41772000 | -3.14217800 | 0.44595600  |
| H    | -6.01056200 | -0.85518800 | 0.07392900  |
| H    | 1.67130200  | -1.74129700 | -0.33873300 |
| O    | 8.22773100  | -2.41955000 | -1.93211200 |
| H    | 8.96108200  | -2.64351300 | -2.52946000 |
| O    | -7.35391000 | -3.09965200 | 1.79567100  |
| H    | -6.40557700 | -2.95781100 | 1.63338400  |
| Na   | -9.43102200 | -3.63024900 | -1.32055000 |
| Na   | 9.21667300  | -5.00716600 | 1.05951100  |
| Hg   | -0.68075600 | 2.07506600  | -0.63304200 |
| O    | -8.42458700 | 1.20397700  | -0.18773900 |
| C    | -7.50063200 | 1.60948100  | -1.20266200 |
| C    | -6.69375500 | 2.77718200  | -0.64885100 |
| O    | -5.99399100 | 2.41514500  | 0.56161100  |
| C    | -5.58784300 | 3.25912200  | -1.60269900 |
| O    | -5.19607400 | 4.59732400  | -1.31685900 |
| C    | -4.41619900 | 2.53443300  | -1.21913200 |
| C    | -4.66589200 | 2.05442300  | 0.27512500  |
| N    | -4.45955700 | 0.60288000  | 0.59194400  |
| C    | -3.13756300 | 1.42620000  | 0.54636300  |
| O    | -2.23367800 | 0.95175400  | 0.29399300  |
| N    | -2.92002700 | -1.19225500 | 0.77100400  |
| C    | -3.93577200 | -2.02917600 | 1.04271700  |
| N    | -3.66457800 | -3.32739500 | 1.24698000  |
| C    | -5.28207800 | -1.56579500 | 1.10025200  |
| C    | -5.49357900 | -0.23273200 | 0.86984900  |
| P    | 8.09178200  | -0.22729700 | -2.03112000 |
| O    | 8.89038400  | 0.23579200  | -3.23629700 |
| O    | 7.96452100  | -1.72618800 | -1.85819000 |
| O    | 8.76555800  | 0.33937500  | -0.63132500 |
| C    | 9.01250900  | 1.74547500  | -0.49601400 |
| C    | 8.10678300  | 2.33567400  | 0.57213900  |
| O    | 6.72504200  | 2.15292400  | 0.19417600  |
| C    | 8.24605300  | 1.69334100  | 1.95665500  |
| O    | 9.29380500  | 2.35316200  | 2.64636700  |
| C    | 6.84685600  | 1.90120800  | 2.55309900  |
| C    | 5.91113500  | 1.82478000  | 1.33862800  |
| N    | 5.29024700  | 0.53087900  | 1.12687200  |
| C    | 5.90318600  | -0.70341100 | 0.93297200  |
| N    | 5.04928200  | -1.67314700 | 0.72074400  |
| C    | 3.80150700  | -1.06330600 | 0.77585700  |
| C    | 2.47662600  | -1.58478500 | 0.60543600  |
| O    | 2.16043400  | -2.77185800 | 0.35327400  |
| N    | 1.48337700  | -0.62299700 | 0.74137200  |
| C    | 1.73733800  | 0.68511400  | 0.99847400  |
| N    | 0.65341100  | 1.50094900  | 1.16917200  |
| N    | 2.95650600  | 1.22554600  | 1.14345500  |
| C    | 3.92942300  | 0.30531000  | 1.02099800  |
| H    | -8.03945300 | 1.92302000  | -2.10371600 |
| H    | -6.83795800 | 0.77700900  | -1.47553000 |
| H    | -7.37873900 | 3.58482900  | -0.37410500 |
| H    | -5.87441300 | 3.14485500  | -2.65655000 |
| H    | -5.94067900 | 5.18253200  | -1.53170900 |
| H    | -4.43390700 | 1.42755700  | -1.80035700 |
| H    | -3.45769600 | 2.84472600  | -1.38474700 |
| H    | -3.99240900 | 2.60531700  | 0.93366300  |
| H    | -2.71283200 | -3.66238200 | 1.29206400  |
| H    | -6.11241100 | -2.21846500 | 1.30639600  |
| H    | -6.47832400 | 0.21299000  | 0.89677800  |
H    10.05181600  1.88485500  -0.17981800
H     8.87375500  2.26196800  -1.45150200
H     8.31732000  3.41010700   0.66531600
H     8.46914400  0.62542500   1.84342100
H     9.51002100  1.83045500   3.43444700
H     6.57680400  1.17901800   3.32629700
H     6.80764300  2.90777300   2.98136100
H     5.08645000  2.53694900   1.39627900
H     6.97890300  -0.80039800   0.91964400
H     0.84179400  2.49269800   1.11872000
H    -0.24915800  1.20090800   0.81103400
H    -4.39764300   3.96253000  1.51210000
P     -3.94758700 -0.13587300  -0.44408900
O    -0.72832900 -0.24070200  -1.90669800
O    -8.31599400 -1.36034600  -0.04967200
O   -10.45228400  0.19001300   0.58268000
N    9.26340500  -2.04930700  -3.82385100
H   -7.91917800  -1.73447400  -0.85395000
Hg   -0.52116700  -1.77010100   0.36213200

P     -9.10080300  -0.89339000  0.24210500
O    -10.5681200  -0.53714200  0.19065600
O     -8.56654300  -1.87180900  -0.78065600
O     -8.16681600   0.45346800  0.09095700
C    -3.84170500  1.54491400  1.00394900
C    -7.26157200  2.58368300  0.74400800
O    -5.97223300  2.05049600  1.09572900
C    -7.15283100  3.05819400  -0.72531700
O    -6.89634200  4.45744400  -0.82445800
C    -6.01103000  2.19401800  -1.26990100
C    -5.10549000  2.00722800  -0.04368500
N    -4.35250200   0.75708100  -0.02833000
C    -2.94612500   0.79262700  0.03380700
O    -2.33980900  1.87339700  0.03384700
N    -2.31267600  -0.41671700  0.07607700
C    -2.94627800  -1.64393200  0.07530900
O    -2.28258600  -2.69568800  0.10459300
C    -4.41080200  -1.64036200  0.03875300
C    -5.14945600  -2.94926200  0.05391500
C    -5.03580400  -0.44230500  -0.00541700
P     9.01138600  -1.31287400  -0.19791300
O   10.49580700  -1.00772300  -0.16374700
O    8.35515400  -2.20629600   0.81447900
O    8.18176900   0.11781000  -0.12932000
C    8.35096000  1.09810600  -1.15760900
C    7.31112700   2.19291100  -0.97522000
O     5.99701800  1.66739900  -1.22948800
C    7.26544800  2.81235300  0.43221000
O     6.93132500  4.19073800  0.25860000
C    6.13700400  2.02810900  1.10471800
C    5.17443000  1.77654800  -0.06340000
N     4.36560700  0.56686600  0.05633600
C     2.96174800  0.66465300  0.04449200
O     2.40380300  1.77057900   0.00322900
N     2.27244900  -0.51451900  -0.09029200
C     2.85139700  -1.76860000  0.14153800
C    2.14214900  -2.79073900   0.17522700
C     4.31442700  -1.82965000   0.15288200
C     4.99281800  -3.16952500  0.21026200
|   |   |   |   
|---|---|---|---|
| H | -8.25911400 | 1.18342900 | -1.26764100 |
| H | -9.33144500 | 1.96685000 | 0.86435600 |
| H | -7.46895900 | 3.44941100 | 1.38550000 |
| H | -8.08739700 | 2.89508000 | -0.36369200 |
| H | -6.06385800 | 4.65376800 | -1.60315900 |
| H | -5.49051700 | 1.23071700 | -0.03234700 |
| H | -5.26675000 | 2.79581900 | -0.07638300 |
| H | -6.08739700 | 2.89508000 | -0.36369200 |
| H | -4.35504200 | 2.79581900 | -0.03234700 |
| H | -6.22607500 | -2.79593300 | -0.07638300 |
| H | -4.98029000 | -3.48956900 | 0.99433000 |
| H | -4.79264500 | -3.60455600 | -0.74983700 |
| H | -6.11446400 | -0.35000800 | -0.01854600 |

---

\( p_{\text{ATP}} \)

|   |   |   |   |   |
|---|---|---|---|---|
| P | -9.10080300 | -0.89339000 | 0.24210500 |
| O | -10.56881200 | -0.53714200 | 0.19065600 |
| O | -8.56654300 | -1.87180900 | -0.78065600 |
| C | -8.16681600 | 0.45346800 | 0.09095700 |
| C | -8.34170500 | 1.54491400 | 0.00394900 |
| C | -7.26157200 | 2.58368300 | 0.74400800 |
| O | -5.97223300 | 2.05049600 | 1.09572900 |
| C | -7.15283100 | 3.05819400 | -0.72531700 |
| O | -6.89634200 | 4.45744400 | -0.82445800 |
| C | -6.01110300 | 2.19401800 | -1.26990100 |
| N | -5.32509000 | 0.75070100 | -0.02383300 |
| C | -2.94612500 | 0.79262700 | 0.03380700 |
| O | -2.33980900 | 1.87339700 | 0.03387400 |
| N | -2.32126700 | -0.41671700 | 0.07607700 |
| C | -2.94612500 | -1.64393200 | 0.07530900 |
| C | -2.28586000 | -2.69566800 | 0.10459300 |
| C | -4.41080200 | 1.64036200 | 0.03875300 |
| C | -5.14945600 | 0.29426200 | 0.05391500 |
| C | -5.03580400 | -0.44230500 | -0.00541700 |
| P | -10.01386000 | -1.31287400 | -0.19791300 |
| O | -10.49580700 | -1.00772300 | -0.16374700 |
| O | -8.35515400 | -2.80429600 | 0.81447900 |
| O | -8.18176900 | 0.11787100 | -0.19932900 |
| C | Collection: 1.15760000 | -0.97592200 | 1.66739900 | -1.22988000 |
| Atoms | x         | y         | z         |
|-------|-----------|-----------|-----------|
| C     | 7.26544800| 2.81235300| 0.43221000|
| O     | 6.93132500| 4.19073800| 0.25860000|
| C     | 6.13700400| 2.02810900| 1.10471800|
| C     | 5.17443000| 1.77654800| -0.06340000|
| N     | 4.36560700| 0.56686600| 0.05633600|
| C     | 2.96174800| 0.66465300| 0.04449200|
| O     | 2.40380300| 1.77057900| 0.00322900|
| N     | 2.27244900|-0.51451900| 0.09092900|
| C     | 2.85139700|-1.76860000| 0.14153800|
| O     | 2.14214900|-2.79073900| 0.17526200|
| H     | -8.25911400|1.18342900| 2.03527600|
| H     | -9.33144500|1.99685000| 0.86435600|
| H     | -7.46895900|3.44941100| 1.38550000|
| H     | -8.07397000|2.89850800|-1.26764100|
| H     | -6.06385800|4.65376800|-0.36369200|
| H     | -6.40402000|1.23071700|-1.60315900|
| H     | -4.35504200|2.79581900| 0.02324700|
| H     | -6.22670500|-2.79593300|-0.07638300|
| H     | -4.98092900|-3.48956900| 0.99433000|
| H     | -4.79264500|-3.60456000|-0.74983700|
| H     | -6.11446400|-0.35000000|-0.01854600|
| H     | 9.35561700| 1.53880600|-1.11011400|
| H     | 8.21953000| 0.63525200|-2.14188100|
| H     | 7.51858100| 2.98329500|-1.70789800|
| H     | 8.22403200| 2.70259500| 0.95664500|
| H     | 6.80033400| 4.57569600| 1.14024400|
| H     | 5.65972100| 2.81137000| 1.91864900|
| H     | 6.52467000| 1.84928000| 1.49610500|
| H     | 4.46781300| 2.59782300|-0.18218800|
| H     | 6.43302900|-3.74827800| 1.06993900|
| H     | 6.07840000|-3.05629800| 0.29540600|
| H     | 4.76496500|-3.76646600|-0.68235400|
| H     | 6.07633700|-0.62177700| 0.08117800|
| O     | -8.78065800|-1.39642900| 1.77338400|
| O     | 8.70424300|-1.82809500|-1.73138200|
| H     | -7.90572300|-1.81906100| 1.81592400|
| H     | 7.81282000|-2.21365200|-1.77459700|
| Hg    | -0.01666000|-0.48083600| 0.08642500|
| Na    | -10.80763800|-1.92573100|-1.75238500|
| Na    | 11.27611600| 0.54639600| 1.19758500|

\[ \text{G} \text{G}_{\text{Cp}} \]
| Atoms | x         | y         | z         |
|-------|-----------|-----------|-----------|
| C     | -5.75548200| -0.41680900| 0.67459400|
| C     | -5.68750900| 0.37539200|-0.64082300|
| O     | -5.99247300| -0.20942900| -1.68271600|
| C     | -5.10093500| 2.34936300|-1.90554800|
| C     | -3.68447200| 2.35013800|-2.49866500|
| O     | -3.44805000| 3.01815400|-3.50393000|
| N     | -5.23002400| 1.66077200|-0.62810800|
| N     | -4.91359000| 2.45129900| 0.56715900|
| N     | -6.14057300| 3.18068100| 1.12781600|
| N     | -7.15209500| 2.22602500| 1.59550100|
| N     | -4.87403000| -1.57071000| 0.57300800|
| C     | -5.21160800| -2.91005000| 0.50477400|
| N     | -4.17102200| -3.70318600| 0.39632100|
| C     | -3.08211300| -2.84078000| 0.38049600|
| C     | -1.66991000| -3.06815100| 0.27051400|
| N     | -1.11679200| -4.19822800| 0.15730000|
| N     | -0.89955400| -1.92129600| 0.30479000|
| C     | -1.43833900| -0.67946100| 0.37619500|
| N     | -0.57254000| 0.38746600| 0.40274000|
N  -2.74753600  -0.39803800   0.46254300
C  -3.50456700  -1.51742400   0.48092500
H  -5.49570800   3.39260800  -1.80098900
H  -6.77940400   0.15107300  -1.56337700
H  -5.41217300    3.39260800   1.54943900
H  -5.75938700    1.87614800   2.63579200
H  -4.44614500    1.81348600   1.31986600
H  -5.79171200    0.39260800  -0.10087000
C  -3.50456700  -1.51742400   0.48092500
H  -5.49570800   3.39260800  -1.80098900
H  -6.77940400   0.15107300   1.54943900
H  -5.41217300    3.39260800   1.54943900
H  -5.75938700    1.87614800   2.63579200
H  -4.44614500    1.81348600   1.31986600
H  -5.79171200    0.39260800  -0.10087000
C  -0.88747800   2.82934700  -2.00758300
N  -3.99799600  -0.33682400   0.44586400
C  -2.65380300  -0.71140600   0.48379300
O  -1.79080300   0.15173500   0.76607500
N  -2.34476400  -1.99354700   0.18915000
C  -3.27285000  -2.95122900  -0.18152000
O  -2.90968900  -4.10345800  -0.47048300
C  -4.67676100  -2.53305600  -0.27463000
C  -4.96493300  -1.24325000  0.06630600
|  |         X         |         Y         |         Z         |
|---|----------------|----------------|----------------|
| P | 7.61672100 | 5.87341000 | 0.53571900 |
| O | 8.67332520 | 6.87036300 | 0.10370400 |
| O | 6.27773600 | 5.92759800 | -0.16689000 |
| O | 8.12887800 | 4.32743600 | 0.35544600 |
| C | 9.19963100 | 3.79800600 | 1.14289500 |
| C | 9.04412800 | 2.28474700 | 1.23648300 |
| O | 7.79210400 | 1.97420900 | 1.87524700 |
| C | 9.03207800 | 1.53670700 | -0.11340300 |
| O | 9.64769400 | 0.24894300 | 0.13399400 |
| C | 7.54091600 | 1.47245200 | -0.41748600 |
| C | 6.95399700 | 1.24579600 | 0.97391700 |
| N | 5.57298300 | 1.63656000 | 1.10578500 |
| C | 4.98878300 | 2.88674200 | 0.84235400 |
| N | 3.67422000 | 2.85458800 | 0.91241100 |
| C | 3.37112200 | 1.53187300 | 1.21876000 |
| C | 2.11776900 | 0.85525200 | 1.38062000 |
| O | 0.99314100 | 1.40349900 | 1.31228400 |
| N | 2.24622000 | -0.51473700 | 1.62089200 |
| C | 3.45628800 | -1.13228500 | 1.70383300 |
| N | 3.47540300 | -2.49145000 | 1.96494300 |
| N | 4.64466600 | -0.53658900 | 1.59480200 |
| C | 4.53504600 | 0.77825700 | 1.34163800 |
| P | 9.29096900 | -1.13632600 | -0.66294900 |
| O | 10.43617400 | -2.09444000 | 0.42025800 |
| O | 8.87314700 | -0.88339900 | -2.09826200 |
| O | 7.93034900 | -1.66081100 | 0.09235600 |
| C | 7.96547400 | -2.49990400 | 1.25371400 |
| C | 7.37005200 | -3.86666340 | 0.93648700 |
| O | 5.96612000 | -3.75746700 | 0.62816900 |
| C | 7.99440900 | -4.58222100 | -0.27902000 |
| O | 7.86419700 | -5.99961400 | -1.17432800 |
| C | 7.09947400 | -1.01045700 | -1.43516000 |
| C | 5.72009000 | -1.13432600 | 0.66294900 |
| O | 9.57310000 | -2.81693100 | -1.28797200 |
| C | 5.38857200 | -1.55297500 | 1.66343300 |
| O | 4.40391900 | -0.71662100 | -1.90693800 |
| C | 3.25961900 | -1.45755900 | 1.67009300 |
| C | 1.88728600 | -1.11537000 | 1.71698000 |
| N | 1.46209000 | 0.11858000 | -2.01875900 |
| N | 1.00304000 | -2.11667600 | -1.45489100 |
| C | 1.45198000 | -3.33967400 | -1.08615400 |
| N | 2.71004200 | -3.73750900 | -0.96361000 |
| C | 3.58016300 | -2.75886700 | -1.28465200 |
| P | -6.77234200 | 5.37385400 | -0.38850300 |
| O | -7.93632300 | 6.14050900 | 0.14424800 |
| O | -5.55271100 | 5.18293700 | 0.49446600 |
| O | -7.23077800 | 3.80413800 | -0.76733100 |
| C | -8.24889600 | 3.56743400 | -1.74793200 |
| C | -8.34501500 | 2.06733500 | -1.98402800 |
| O | -7.12816800 | 1.59680900 | -2.59320400 |
| C | -8.54257500 | 1.25143300 | -0.69203900 |
| O | -9.43956300 | 0.16020300 | -0.98612700 |
| C | -7.13525700 | 0.75512200 | -0.38374000 |
| C | -6.50047800 | 0.61519400 | -1.76965000 |
| N | -5.05130900 | 0.82784000 | -1.76081000 |
| C | -4.19566300 | -0.26418700 | -1.98561000 |
| O | -6.44751100 | -1.37405700 | -2.29726900 |
| N | -2.85763100 | -0.02814400 | -1.81818700 |
| C | -2.30582300 | 1.20447500 | 1.55467400 |
| O | -1.06797800 | 1.35633600 | -1.48244000 |
| C | -3.22441900 | 2.32070000 | -1.33920900 |
| C | -2.66850200 | 3.67786800 | -1.01157400 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | -4.55054000 | 2.06999400 | -1.44210400 |
| P    | -10.08545800 | -0.69329200 | 0.26473500 |
| O    | -11.24729000 | -1.47706600 | -0.30097000 |
| O    | -10.34196900 | 0.19910100 | 1.45833500 |
| C    | -8.48663400 | -2.73318500 | -0.23222400 |
| C    | -7.28516200 | -3.48716800 | 2.51197400 |
| O    | -6.12691800 | -2.63490900 | 0.25116800 |
| C    | -7.40928600 | -3.99136800 | 1.76147200 |
| O    | -6.16584000 | 4.05118100 | 0.69013300 |
| N    | -4.41325500 | -1.79333000 | 1.59818700 |
| C    | -3.02748000 | -2.01841900 | 1.45495300 |
| O    | -2.58776200 | -3.15526200 | 1.25966000 |
| N    | -2.20240000 | 0.92783900 | 1.56540900 |
| C    | -2.67294000 | 0.32678800 | 1.70872200 |
| N    | -1.82111100 | 1.35127800 | 1.75197300 |
| C    | -4.08318500 | 0.55349200 | 1.83590500 |
| C    | -4.89688700 | -0.52718700 | 1.78509800 |
| H    | 9.16223350 | 4.21425600 | 2.15519400 |
| H    | 9.86259600 | 1.89080200 | 1.85455700 |
| H    | 9.60895000 | 2.05602400 | -0.88714200 |
| H    | 7.22537800 | 2.44502000 | -0.80029600 |
| H    | 7.26456500 | 0.69912700 | -1.13012200 |
| H    | 6.97699500 | 0.18607900 | 1.23118400 |
| H    | 5.58574500 | 3.75726700 | 0.60342300 |
| H    | 4.36726100 | -2.91381900 | 1.71268600 |
| H    | 7.35927600 | -2.01609800 | 2.02516100 |
| H    | 8.99063600 | -2.62427100 | 1.61589900 |
| H    | 7.45332900 | -4.48173500 | 1.83516200 |
| H    | 9.03945000 | 0.28423400 | 0.42290100 |
| H    | 8.42411800 | -6.29901700 | 0.56038800 |
| H    | 7.47211100 | -3.20309900 | -1.85869600 |
| H    | 7.06123600 | -4.89065400 | -2.22241600 |
| H    | 5.08423000 | -4.81434000 | -0.88825500 |
| H    | 6.43932800 | -1.32057800 | -1.74760000 |
| H    | 0.50286600 | 0.42840100 | -1.82667500 |
| H    | 0.67610400 | -0.06706900 | -0.86933900 |
| H    | -9.21370500 | 3.95125800 | -1.39368000 |
| H    | -7.98805600 | 4.07113400 | -2.68524900 |
| H    | -9.17858500 | 1.87742700 | -2.67003100 |
| H    | -8.96628300 | 1.85389900 | 0.11444700 |
| H    | -7.13351700 | -0.19363400 | 0.14688100 |
| H    | -6.60364100 | 1.50973800 | 0.20015500 |
| H    | -6.65202100 | -0.38045900 | -2.18716600 |
| H    | -1.90723400 | 3.59895000 | -0.22682800 |
| H    | -3.45872100 | 4.35391300 | -0.66900700 |
| H    | -2.16901600 | 4.12501200 | -1.88091800 |
| H    | -5.30294500 | 2.83189800 | -1.28452500 |
| H    | -9.32111800 | 3.42956300 | -0.37106400 |
| H    | -8.23367900 | -2.28974100 | -2.20994400 |
| H    | -7.11871800 | -4.36028800 | -0.34508800 |
| H    | -8.42374300 | -3.85217200 | 2.15177200 |
| H    | -7.14811800 | -5.71085600 | 2.65328500 |
| H    | -5.96984500 | 3.63301700 | 3.39227500 |
| H    | -6.83886400 | -2.18716900 | 2.81692800 |
| H    | -4.71264900 | 3.79331900 | 1.26966600 |
| H    | -0.81598700 | 1.26885800 | 1.55381700 |
| H    | -4.48134800 | 1.55126100 | 1.96653700 |
| H    | -5.96956100 | 0.44295700 | 1.87839400 |
| H    | 2.69903900 | -3.01558300 | 1.58155500 |
| H    | 2.16847300 | 0.84085100 | -2.07410200 |
| H    | -6.37327500 | 3.97287100 | -1.80432000 |
| H    | -5.51866000 | 5.61933900 | -2.15174200 |
| H    | -2.19323300 | 2.28822000 | 1.82013500 |
| Element | X (Angstroms) | Y (Angstroms) | Z (Angstroms) |
|---------|--------------|--------------|--------------|
| O       | 7.39796800   | 5.97849200   | 2.16289900   |
| H       | 8.04029800   | 6.60755800   | 2.53079400   |
| Na      | 7.09859900   | 7.03826000   | -1.54467100  |
| Na      | 10.50822500  | -2.54939400  | -2.79728600  |
| Na      | -6.64870000  | 6.52137600   | 2.16557300   |
| Na      | -12.63805100 | -0.50691600  | 1.44022100   |
| Hg      | 0.10978500   | -1.55015900  | 1.78448200   |
| Hg      | -1.46416100  | -1.87142800  | 1.77146400   |

The coordinates are in Angstroms.
O    -2.85653300  0.68051700  1.58370400
N    -2.35629300 -1.51509600  0.74736800
C    -2.71632100 -2.82462100  0.93400300
O    -1.85890900 -3.72374200  0.88287800
C    -4.14137900 -3.09511100  0.74736800
C    -4.58204400 -4.47970500  0.36774600
C    -5.00514100 -2.07498700  0.93768900
P    -8.70182500  3.27142900  0.63619300
O    -9.14788000  4.42670700  1.50484300
O    -1.85890900 -3.72374200  0.88287800
C    -6.36397600  4.45148000  0.36328500
C    -5.16287000  4.91462800 -2.02178500
O    -4.52041400  5.92872100 -2.39841800
O    -2.63651300  0.08301700 -3.15898500
H    8.33572100  0.08301700 -3.15898500
H    6.42577900  0.93414700 -1.96289800
H    5.31769500  0.93414700 -1.96289800
H    5.31769500  5.07464400 -0.45907300
H    3.63800700 -5.14412500 -0.45012800
H    3.46624800 -4.31372300  1.09984800
H    5.82272800  0.08301700 -3.15898500
H    0.70984750  3.73689800 -1.17539800
H    7.60294200  4.99404200 -0.01378800
H    5.22985200  5.07935600 -0.25092300
H    6.13597900  3.81262400  2.38290900
H    5.16749800  6.40938900  1.77659100
H    3.73354700  6.25167000  2.97212600
H    3.30241200  4.92931500  1.85666500
H    2.83573300  3.15235300  0.24364600
H    6.23283600 -0.45783300  3.24825300
H    5.74664300 -1.89483200  2.33849400
H    5.02392400 -1.57770500  3.92045500
H    5.37987500  1.49936600  2.05130600
H    9.64094600 -1.27020800  2.25604700
H    8.28980500  2.12685800  3.04956500
H    8.24881100  0.38518800  3.27446700
H    8.76364500  0.53360100  0.53548100
H    6.23249600  1.45895800 -0.06301700
H    6.66591100 -0.25807900 -0.23598200
H    5.06674700  1.06503800  1.97708300
H    4.29542200  5.21282200  1.13203100
H    4.09419900 -4.79047100 -0.56480000
H    5.66553800 -4.52115400  0.22156100
H    6.07597700 -2.20554800  0.86269900
H    6.72357600  5.46337500  0.58181200
H    6.06988400  3.97044100  1.30373000
H    4.46187700  5.26655300 -0.15221200
H    6.51904800  5.27284000 -2.12653700
H    4.74518100  6.17861100 -3.31412800
H    4.99748700  3.75727200 -3.83347500
D_TTTT_P

P  -9.30694200  -2.60565100  0.92108600
O  -10.80797990  -2.53890000  1.11718500
O  -8.78051400  -3.43790300  -0.22490400
O  -8.66011500  -1.10802200  0.71234900
C  -8.93106800  -0.08751700  1.68314600
C  -7.87976100  1.00738800  1.57408100
O  -6.61624900  0.52632700  2.06362800
C  -7.63241800  1.51908900  0.13995200
O  -7.40448800  2.93162300  0.23047500
C  -6.39165200  0.72148000  -0.27880900
C  -5.62055700  0.56581500  1.03586800
N  -4.80789100  -0.64468600  1.10671900
C  -3.41668400  -0.54649100  1.30089400
O  -2.87551500  0.55070700  1.48426400
N  -2.71808700  -1.72030600  1.25828300
C  -3.28171200  -2.97525100  1.12288900
O  -2.56893100  -3.99522600  1.10570100
C  -4.74023700  -3.04057700  0.99948500
C  -5.40919200  -4.38022400  0.87505300
C  -5.42398500  -1.87435900  0.99662400
P  -6.94645200  3.78313600  -1.10089700
O  -7.47703100  5.19009000  -0.93606800
O  -7.28865800  3.04342200  -2.37397800
O  -5.30510900  3.77032200  -0.96601600
C  -4.72713400  4.50885400  0.12434800
C  -3.26048400  4.77093900  -0.15712100
O  -2.52733500  3.53024000  -0.08637600
C  -2.97706800  3.58129000  -1.54626000
O  -1.94857500  3.56521600  -1.36558300
C  -2.48507600  4.17209700  -2.34552700
C  -1.73758600  3.38193200  -1.26646800
N  -1.56100900  1.96160500  -1.53025100
C  -0.26195400  1.42349200  -1.54945900
O  0.72808200  2.14538400  -1.36058500
N  -0.16078800  0.08400800  -1.79923300
C  -1.22928400  -0.75314600  -2.05182000
O  -1.04537200  -1.96185700  -2.28591300
C  -2.56892300  -0.16296300  -1.99931500
C  -3.75087900  -1.05908600  -2.23119300
C  -2.66598000  1.15642200  -1.71944700
H  -9.92757600  0.33457700  1.50643400
H  -8.89623600  -0.50643300  2.69511700
H  -8.20055400  1.84564500  2.20352900
H  -8.48333000  1.32678600  -0.52034800
\[ p_{TTTT_T} \]

\[ \begin{align*}
\text{C} & \quad 8.17531100 \\
\text{C} & \quad 6.52540900 \\
\text{C} & \quad 6.40682200 \\
\text{N} & \quad 5.47863100 \\
\text{C} & \quad 4.11541100 \\
\text{O} & \quad 3.74030000 \\
\text{N} & \quad 3.26862100 \\
\text{C} & \quad 3.66264400 \\
\text{O} & \quad 2.82651900 \\
\text{C} & \quad 5.09670700 \\
\text{C} & \quad 5.51712600 \\
\text{C} & \quad 5.93044900 \\
\text{C} & \quad 6.68989200 \\
\text{C} & \quad 5.17069600 \\
\text{C} & \quad 4.04854000 \\
\text{C} & \quad 3.75345700 \\
\text{N} & \quad 3.08000500 \\
\text{C} & \quad 1.69694000 \\
\text{O} & \quad 1.04807800 \\
\text{N} & \quad 1.12563500 \\
\text{C} & \quad 1.82345100 \\
\text{O} & \quad 1.22580800 \\
\text{C} & \quad 3.27457500 \\
\text{C} & \quad 4.06655100 \\
\text{C} & \quad 3.82631500 \\
\text{H} & \quad 8.19372600 \\
\text{H} & \quad 6.05170100 \\
\text{H} & \quad 6.65409100 \\
\text{H} & \quad 5.07762500 \\
\text{H} & \quad 5.33317500 \\
\text{H} & \quad 7.00525700 \\
\text{H} & \quad 7.07285500 \\
\text{H} & \quad 6.87226800 \\
\text{H} & \quad 4.69270200
\end{align*} \]
Cartesian Coordinates of optimized geometries of mispair dimer model in explicit solvent model using B3LYP-D3/6-31G* level of theory in the aqueous phase:

\[ \text{dTTTT}_D \]

|      |         |         |         |
|------|---------|---------|---------|
|      | 9.14884300 | -2.86495900 | -0.10568500 |
| O    | 10.22707300 | -1.80868900 | -0.00507000 |
| O    | 8.15017900  | -2.97621900 | 1.02594700  |
| O    | 8.27635900  | -2.66463900 | -1.48904200 |
| C    | 8.72032500  | -1.79429300 | -2.53535800 |
| C    | 7.70152500  | -0.69815900 | -2.78397500 |
| O    | 6.46628300  | -1.26734800 | -3.25811600 |
| C    | 7.30662020  | 0.15041000  | -1.57024700 |
| O    | 8.28576900  | 1.17647500  | -1.39624000 |
| C    | 5.92206300  | 0.65130400  | -1.98827600 |
| C    | 5.35650900  | -0.55643800 | -2.74161600 |
| N    | 4.54836200  | -1.45903400 | -1.87621300 |
| C    | 3.23376600  | -1.05579300 | -1.61848400 |
| O    | 2.84390800  | 0.05620500  | -2.01286800 |
| N    | 2.43605500  | -1.93479900 | -0.94668600 |
| C    | 2.83748200  | -3.17882200 | -0.52034700 |
| O    | 2.02332900  | -3.96625400 | 0.01340500  |
| C    | 4.23896000  | -3.53261200 | -0.72822100 |
C       4.74572800   -4.84741600   -0.20618200
C       5.02186500   -2.66490600   -1.41874400
P       8.48394500    1.93272700    0.04565000
O       9.75950900    2.72980200   -0.09772700
O       8.30022000    0.97581700    1.19989000
O       7.19098200    2.93908500    0.12762700
C       6.97378600    3.90954500   -0.90515800
C       5.67549100    4.64631300   -0.61336900
O       4.58214400    3.71130300   -0.57744200
C       5.64955700    5.41247700    0.73258200
O       5.01604400    6.68468300    0.61968100
C       4.90312900    4.44459800    1.65319500
C       3.92442700    3.75231800    0.69494000
N       3.54169400    2.40153600    1.08876200
C       2.18415200    2.08682800    1.25889600
O       1.30950300    2.94918700    1.06128600
N       1.89870400    0.81774200    1.65937400
C       2.83970300   -0.16469300    1.91745600
O       1.89579000   -0.16262000    2.74373700
C       1.30754800   -0.22537300    2.25912400
O       -6.80593700   -0.16262000    2.74373700
C       -8.15734800   -0.22537300    2.25912400
O       -8.82322400   -0.16469300    1.91745600
C       -6.86620300   -0.16469300    1.91745600
O       -5.91231400    0.27460400    1.75121100
N       -4.69724400   -0.53916000    1.74817000
C       -3.44789900    0.06538200    1.94588900
O       -3.35327200   -1.29128100    2.12827600
C       -2.36505600   -0.76164600    1.92457100
C       -2.41187400   -2.12879700    1.73311000
O       -1.36760800   -2.80987600    1.76285500
C       -3.72503900   -2.72103300    1.50173600
C       -3.82892900   -4.18781100    1.19897500
C       -4.79805000   -1.89981600    1.53197700
O       -8.94639300   -2.33721800   -0.66170000
N       -9.17130300    3.46966000   -0.42886300
O       -9.35006900   -1.28215700   -1.68118300
O       -7.48501100    2.89265300   -1.15359500
C       -6.80163300    3.83366000   -0.30747500
C       -5.36786400    3.97720000   -0.77662800
O       -4.67515200    2.73925700   -0.56218600
C       -5.19750200    4.33794000   -2.27381000
O       -4.25250000    5.40664000   -2.33134200
C       -4.64342800    3.04204100   -2.87672500
C       -3.83584900    2.49268500   -1.69890100
N       -3.48137700    1.08661100   -1.73492800
C       -2.18667600    0.70172700   -1.32092000
O       -1.35586000    1.56124800   -0.99312600
N       -1.90698400   -0.63218100   -1.32713000
C       -2.81486900   -1.61723200   -1.64722000
O       -2.49104700   -2.82297800   -1.64280300
C       -4.17181700   -1.19742200   -2.00656700
C       -5.20745600   -2.23720800   -2.32637100
C       -4.42722900    0.12872300   -2.03972400
H       8.84917900   -2.38889000   -3.44604900
H       9.67458400   -1.32961800   -2.27183700
H       8.10775200   -0.02278700   -3.55560800
H       7.24837000   -0.47026200   -0.67242600
H       5.28063600    0.97814900   -1.17315300
| Element | X    | Y    | Z    |
|---------|------|------|------|
| H       | 6.04377900  | 1.48291100  | -2.68966000  |
| H       | 4.69693300  | -0.25974600  | -3.55901500  |
| H       | 5.81263200  | -4.91934200  | 0.87857500   |
| H       | 6.06058400  | -2.86856000  | -1.64356300  |
| H       | 6.90457700  | 3.40914700   | -1.87586900  |
| H       | 7.80599900  | 4.62311900   | -0.93783800  |
| H       | 5.50648000  | 5.36104700   | -1.20426700  |
| H       | 5.32832700  | -1.22803400  | 2.87014000   |
| H       | 5.52640700  | 1.76311800   | 1.04089900   |
| H       | -9.73164600 | -1.68687000  | 2.05898900   |
| O       | 9.90116900  | -4.30481300  | -0.35435000  |
| H       | 9.27511600  | -5.03625200  | -0.21686200  |
| H       | 5.88548200  | 5.52759200   | -0.93438600  |
| H       | 6.41009700  | 5.38752100   | 0.47741700   |
| O       | 7.57276100  | 6.27130300   | 0.88357400   |
| O       | 5.88548200  | 5.52759200   | -0.93438600  |
O           -3.73661100  1.55286600  1.69784100
N           -2.61903800  -0.44679100  1.72294700
C           -2.56709800  -1.80852200  1.95164300
O           -1.51521800  -2.44553300  1.76099500
C           -3.79442200  -2.45076200  2.42056500
C           -3.80754800  -3.94470400  2.56785900
C           -4.85877000  0.41713000  -0.96557500
C           -8.31254400    2.73755700  -0.75390500
C           -6.80126000    2.95902200  -0.95651000
C           -5.73550500    1.12955000  -2.29377900
C           -5.48677000    0.41771300  -0.96557500
N           -4.89315800   -0.89509700  -1.12527300
C           -3.52983700  -0.96389800  -1.42497700
O           -2.90022600    0.08002200  -1.65558600
N           -2.96232400  -2.20852000  -1.42363700
C           -3.65612400  -3.36809900  -1.16537500
O           -3.07125700  -4.47690300  -1.12514100
C           -3.59150300  -3.26704900  -0.92583600
C           -3.87958500  -4.51873000  -0.66580300
C           -5.63852100  -2.02904700  -0.96557500
H           -8.72573800    3.21784000  -0.96557500
H           -5.62279700    1.56827300  -0.96557500
H           -4.78821700  -3.04770900  -0.96557500
H           -5.05395300  -2.27680700  -0.96557500
H           -3.76396800    1.85660700  -0.96557500
C           -5.40240600    0.63568700  -3.37541800
C           -6.42158400    0.29364000  -3.37541800
C           -6.54427500    3.11105400  -3.44859300
H           -6.79689600    2.40717000  -4.24528600
H           -7.37421700    3.80265900  -3.30350400
C           -5.30177400    3.93552800  -3.82369900
O           -5.27179000    5.15814300  -3.69292800
N           -4.26710200    3.19520800  -4.29178100
H           -3.37168300    3.64457800  -4.43211700
H           -4.12805000    2.18161800  -4.25705900
N           -6.99203000    1.34358000  -0.93797800
H           -8.73477000    1.02293500  -1.89942100
H           -6.24600000    2.55460600  -0.11065300
C           -9.33781800    0.48814800  -0.08657400
O           -9.85741000  -0.54586000  -0.50042000
C           -9.43807500    0.85913700  1.39933800
H           -9.87248400  -0.01681000  1.88761000
H           -10.14037300    1.09113700  1.50475400
N           -8.18161700    1.24712300  2.05525400
H           -7.24696500    2.69496700  3.25884900
C           -9.05462400    2.04969300  4.26668700
H           -9.02065600    2.98898700  4.81979900
H           -10.04982500    1.68996400  3.98037700
N           -8.39403100    0.99251800  5.04418700
H           -9.05469300    0.58706500  5.70387100
H           -7.65425500    1.40315400  5.61228000
O           -7.33759000  -0.75919200  1.44002200
H           -6.22070400  -0.31299400  3.96954300
Na         9.25974300  -1.15204500  -2.3409700
Na        7.51125300    2.76307000  -1.32581700
O          -1.62884100    2.89140100  -2.97663000
H         -2.39070000    2.50901000  2.48789600
H  -1.25547400  2.11841200  3.42740900
O  -1.15582500 -5.14783800 -3.03367100
H  -1.81498000 -4.95072400 -2.32760800
Hg -0.66160500 -2.24791400 -1.43828500
Hg -0.74917000  0.54685800  0.74363200

\[ p_{TTTT} \]

C  -7.52411600  -2.37846000  3.30088000
C  -5.53391700  -1.46394700  2.04350300
C  -4.86682900  -2.84122200  1.95554800
N  -4.31225800  -3.03529200  0.61951500
C  -2.98100800  -2.69837600  0.36279100
O  -2.24929900  -2.28250800  1.28307900
N  -2.54423400  -2.86532200  -0.91456400
C  -3.32548700  -3.18471000  -1.95628900
O  -2.84082100  -3.47180200  -3.09626900
C  -4.73547900  -3.58012900  -1.6721700
C  -5.63621900  -4.01075900  -2.79434600
C  -5.16134900  -3.41707900  -0.39850100
C  -7.71882600  2.93768300  2.26904300
C  -6.33816500  3.61625100  2.31853600
C  -4.93797400  3.61835000  0.24045000
C  -4.30964100  2.30334500  0.71771400
N  -3.58029000  1.65166000  -0.54905000
C  -2.21179100  1.88519600  -0.49403600
O  -1.60512300  2.55338400  0.36687100
N  -1.59752100  1.32477200  -1.57386300
C  -2.25182800  0.62086700  -2.56661100
O  -1.61756800  0.16702800  -3.53913000
C  -3.69162300  0.41415000  -2.40468000
C  -4.43989100  -0.35730800  -3.45389600
C  -4.27772700  0.93234700  -1.29999100
H  -8.00309200  -1.97736400  4.19931100
H  -4.03776200  -2.85816500  2.66551800
H  -6.65816200  -4.17896200  -2.43996900
H  -5.27199800  -4.93564000  -3.25779300
H  -5.66448500  -3.25224200  -3.58580900
H  -6.19151200  -3.57226400  -0.08293200
H  -8.48956200  3.68189100  2.04683200
H  -7.95691000  2.53366600  3.25641900
H  -6.36517000  4.44348700  3.03538800
H  -3.60192000  2.51747200  1.52148800
H  -5.47900000  -0.52635900  -3.15386000
H  -3.96632200  -1.32634400  -3.63711000
H  -4.44217300  0.18424500  -4.08666000
H  -5.33079600  0.79141600  -1.07981300
O  -4.56061900  4.16300100  -0.79817800
H  -5.04396600  1.59425700  1.09159000
N  -5.93226500  4.14490400  1.01610000
C  -6.45217400  5.44537400  0.63983200
H  -6.51056300  5.51148000  -0.44856600
H  -7.46658600  5.55963500  1.03513900
C  -5.57063700  6.58304100  1.18803200
O  -4.65329900  6.37463300  1.97851900
N  -5.90867200  7.81531200  0.74184800
H  -5.39495600  8.62034600  1.07366200
H  -6.65552900  7.96689800  0.07867600
N  -7.82263400  1.90939100  1.25371700
H  -8.10606600  2.18363900  0.32530600
H  -5.58693100  2.91829500  2.68673200
C  -7.66096100  0.54905300  1.38388600
Cartesian Coordinates of optimized geometries of single canonical base pairs and mispair using B3LYP-D3/6-31G* level of theory in the gas phase:

**dTₚ**

| Atom | Cartesinon Coordinates |
|------|------------------------|
| P    | 9.11537200 -2.00351800 0.54970600 |
| O    | 10.13584500 -3.09686600 -0.81332000 |
| O    | 8.31314200 -2.23297100 0.73260800 |
| O    | 9.81967300 -0.54647200 -0.42663000 |
| C    | 9.65833900 0.56263200 -1.31410700 |
| C    | 8.72221200 1.60293000 -0.71521600 |
| O    | 7.36165700 1.15462500 -0.84903200 |
| C    | 8.94492050 1.80875300 0.80909000 |
| O    | 8.76433000 3.25832000 1.11565600 |
| C    | 7.78104400 1.13115500 1.44858500 |
| C    | 6.69944100 1.35199500 0.39042900 |
| N    | 5.55543200 0.45128600 0.44381400 |
| C    | 5.55399800 -0.93748600 0.49937000 |
| N    | 4.34367000 -1.45471300 0.44444900 |
| C    | 3.51660400 -0.36246800 0.33497300 |
| C    | 2.11550200 -0.27943000 0.23083300 |
| N    | 1.34092700 -1.37331000 0.23097500 |
| N    | 1.59734100 0.98923500 0.12720400 |
| C    | 2.43083000 2.08666400 0.13151000 |
| N    | 3.73341500 2.07523900 0.22640900 |
| C    | 4.24630000 0.82977600 0.32430000 |
| P    | -8.64289100 -2.29117600 0.39103900 |
| O    | -10.10372000 -2.62611000 0.16371300 |
| O    | -7.65750500 -3.03596400 -0.50002900 |
| O    | -8.34387600 -0.69812700 0.15370900 |
| C    | -8.94307800 0.27903900 1.01944700 |
| C    | -8.34305400 1.63531600 0.69065600 |
| O    | -6.92890700 1.60376600 0.95874800 |
| C    | -8.49701100 2.08008400 -0.77684480 |
| O    | -8.66732600 3.49261200 -0.74768100 |
| C    | -7.15291800 1.67638900 -1.39248700 |
| C    | -6.19401500 1.89907700 -0.21576300 |
| N    | -4.99670000 1.03754400 -0.23935600 |
| C    | -3.73706300 1.64302400 -0.23172000 |
| O    | -3.54081200 2.85038600 -0.29145600 |
\[ d_{GC_D} \]

\begin{align*}
O & \quad -7.757422400 -1.408167000 0.127107000 \\
C & \quad -7.710478000 -0.603872000 -1.046674000 \\
C & \quad -7.943724000 0.856618000 -0.642747000 \\
O & \quad -7.157910000 1.245636000 0.501036000 \\
C & \quad -7.494549000 1.832674000 -1.744323000 \\
O & \quad -8.064452000 3.119120000 -1.588482000 \\
C & \quad -5.997684000 1.978275000 -1.437990000 \\
C & \quad 5.949096000 1.975248000 0.094681000 \\
N & \quad -4.827701000 0.864938000 0.517230000 \\
C & \quad -3.530704000 1.220385000 0.244646000 \\
O & \quad -3.231791000 2.309998000 -0.340746000 \\
N & \quad -2.533380000 0.385649000 0.606932000 \\
C & \quad -2.739104000 -0.798787000 1.215268000 \\
N & \quad -1.663930000 -1.542387000 1.481619000 \\
C & \quad -4.079529000 -1.168409000 1.539003000 \\
C & \quad -5.074852000 -0.307879000 1.186973000 \\
P & \quad 7.159577000 -2.401705000 -1.258666000 \\
O & \quad 8.236573000 -2.637634000 -2.312392000 \\
O & \quad 6.344084000 -3.631560000 -0.917741000 \\
O & \quad 7.871646000 -1.853685000 0.132507000 \\
P & \quad 8.945089000 -0.914518000 0.017511000 \\
C & \quad 8.513971000 0.441550000 0.549914000 \\
O & \quad 7.360575000 0.917157000 -0.180907000 
\end{align*}
34

C  8.10115600  0.44166300  2.02603100
O  9.26555300  0.64886300  2.80341000
C  7.08008800  1.58866000  2.07489800
C  6.41592400  1.53900000  0.69109800
N  5.15298300  0.80493800  0.66968800
C  4.89521800 -0.52353600  1.02691500
N  3.63426400 -0.84794600  0.93932600
C  3.01331300  0.30233800  0.48790000
C  1.66317000  0.59746200  0.20015500
O  0.64320800 -0.14974900  0.30630400
N  1.43759500  1.90748700 -0.24075700
C  2.43306500  2.83153500 -0.37515400
N  2.05849500  4.09822100 -0.76293000
N  3.70924300  2.59746100 -0.11018100
C  3.94175000  1.33995300  0.31232300
H -8.49000900 -0.90767600 -1.75812600
H -6.73731300 -0.72413400 -1.53589600
H -8.98564800  1.00094000 -0.34349200
H -7.67056600  1.42727200 -1.75284000
H -9.02431000  3.05971700 -1.71718000
H -5.41310000  1.20473400 -1.94282500
H -5.62397600  2.95294000 -1.75026500
H -5.76814500  2.73223700  0.62893800
H -0.73394300 -1.22944200  1.18830700
H -4.33878400 -2.10823300  2.01014400
H -6.11554500 -0.51429000  1.39100500
H  9.78183800 -1.26626800  0.63210500
H  9.28776800 -0.84317500 -1.01955000
H  9.33839300  1.15763700  0.42621800
H  7.62948600 -0.51892800  2.27056100
H  9.07789700  0.39377400  3.71885800
H  6.35018900  1.51656700  2.88517000
H  7.63492500  2.52637000  2.18342800
H  6.17352100  2.52994600  3.01705000
H  5.69779200 -1.19779700  1.28835600
H  2.84215800  4.69041000 -1.00949000
H  1.28221500  4.16171800 -1.40811700
H -1.76218500 -2.44804400  1.91609000
P -7.16860400 -2.93399900  0.19453900
O -8.16527200 -3.97225700 -0.28814900
O -5.90344600 -2.85784500 -0.84741900
O -6.69339000 -3.12560800  1.62499900
O  6.17653600 -1.17187300 -1.65998400
H  6.56414200 -0.31794800 -1.37657400
Na 7.54387100 -4.75012800 -2.42909800
Na -8.15670200 -4.84721400  1.78887600
H -6.04984300 -3.50985900 -1.55255600
Hg -0.81482900  1.74852500 -0.23464200

\textbf{dTTD}

P  -8.23146300 -1.14083600  0.45794800
O  -9.31683000 -2.19956900  0.45899100
O  -7.92838700 -0.61084200 -0.95219400
O  -8.65312900  0.16450800  1.35918500
C  -8.05225700  0.48885300  2.61227200
C  -6.86556800  1.42629400  2.42228700
O  -5.77108400  0.71071700  1.80663100
C  -7.16484800  2.65331300  1.50708200
C  -6.84652500  3.88799200  2.13547800
C  -6.32602000  2.35935200  0.25364800
C  -5.14335900  1.59741900  0.85096200
N  -4.30965700  0.82981300 -0.04294900

34
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | -2.90715500 | 0.93832000 | 0.10746200 |
| O       | -2.38680300 | 1.71657500 | 0.90127300 |
| N       | -2.18115800 | 0.12053700 | -0.71430100 |
| C       | -2.67563600 | -0.80270500 | -1.61939800 |
| O       | -1.87240300 | -1.47850300 | -2.28120800 |
| C       | -4.12724600 | -0.89894300 | -1.71291700 |
| C       | -4.73725600 | -0.97788000 | -2.65424000 |
| P       | 8.27438800  | 1.02731300 | 0.54519200  |
| O       | 9.38603700  | 2.05634800 | 0.61679300  |
| O       | 7.94691400  | 0.61733000 | -0.89984700 |
| C       | 8.06174000  | -0.85417200 | 1.75611700  |
| C       | 6.84666100  | -3.98412000 | 1.75611700  |
| N       | 4.29062800  | -0.79064100 | -0.08305000 |
| C       | 2.88659000  | -1.09386800 | -1.34765800 |
| O       | 2.24826800  | -1.27624900 | 0.77408000  |
| C       | 5.11325100  | -1.64738500 | 0.73845200  |
| N       | 4.29062800  | -0.79064100 | -0.08305000 |
| C       | 8.27438800  | 1.02731300 | 0.54519200  |
| O       | 7.94691400  | 0.61733000 | -0.89984700 |
| O       | 8.67167300  | -0.35437900 | 1.33732100  |
| C       | 8.06174000  | -0.85417200 | 1.75611700  |
| C       | 6.84666100  | -3.98412000 | 1.75611700  |
| N       | 4.29062800  | -0.79064100 | -0.08305000 |
| C       | 2.88659000  | -1.09386800 | -1.34765800 |
| O       | 2.24826800  | -1.27624900 | 0.77408000  |
| C       | 5.11325100  | -1.64738500 | 0.73845200  |
| N       | 4.29062800  | -0.79064100 | -0.08305000 |
| C       | 8.27438800  | 1.02731300 | 0.54519200  |
| O       | 7.94691400  | 0.61733000 | -0.89984700 |
| O       | 8.67167300  | -0.35437900 | 1.33732100  |
| C       | 8.06174000  | -0.85417200 | 1.75611700  |
| C       | 6.84666100  | -3.98412000 | 1.75611700  |
| N       | 4.29062800  | -0.79064100 | -0.08305000 |
| C       | 2.88659000  | -1.09386800 | -1.34765800 |
| O       | 2.24826800  | -1.27624900 | 0.77408000  |

**pATp**

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 7.96129500 | 2.10214000 | 2.46775600 |
| Element | X-Centre | Y-Centre | Z-Centre |
|---------|----------|----------|----------|
| N       | -1.283574 | -0.628638 | -0.305506 |
| C       | 0.203047  | 0.530081  | -0.345989 |
| N       | 3.296045  | 0.632704  | -0.650590 |
| C       | 3.862663  | -0.556579 | -0.941938 |
| C       | 3.225531  | -1.799438 | -0.944447 |
| C       | 1.858241  | -1.840886 | -0.606510 |
| N       | 1.171368  | -2.988613 | -0.582187 |
| C       | 5.237880  | -2.183559 | -1.475734 |
| N       | 5.151848  | -0.811359 | -1.313838 |
| O       | 8.532465  | 3.182069  | 2.423928  |
| C       | 9.829436  | 0.858316  | -1.321314 |
| N       | 5.151848  | -0.811359 | -1.313838 |
| O       | 6.166044  | -0.357785 | 1.100680  |
| C       | 6.252758  | 0.131322  | -1.251698 |
| H       | 1.4872790 | 1.437016  | -0.095430 |
| H       | 6.166086  | -2.057847 | -1.750340 |
| H       | 10.509761 | 0.475520  | -0.551162 |
| H       | 7.967681  | 1.985821  | -1.392925 |
| H       | 9.061236  | 2.519391  | -0.132649 |
| H       | 8.283813  | -0.060520 | 2.246580  |
| H       | 9.609949  | 0.984635  | 1.675530  |
| H       | 1.680719  | -3.833911 | -0.809151 |
| H       | 0.191870  | -0.083746 | -0.320486 |
| H       | 7.015560  | -0.170711 | -1.973209 |
| C       | 5.872238  | 1.113526  | -1.546785 |
| C       | -5.773884 | 3.135828  | -2.141315 |
| N       | -5.221043 | -1.135668 | 0.940899  |
| C       | -4.039687 | -0.405415 | 0.809617  |
| O       | -4.010181 | 0.824005  | 0.845971  |
| N       | -2.917586 | -1.174655 | 0.636031  |
| C       | -2.872069 | -2.545534 | 0.458119  |
| O       | -1.750762 | -3.061545 | 0.222748  |
| C       | -4.126080 | -3.253548 | 0.540546  |
| C       | -5.239152 | -2.490989 | 0.747348  |
| C       | -4.144787 | -4.744687 | 0.353603  |
| O       | -5.796098 | 3.934428  | -3.063552 |
| C       | -7.381788 | 2.424348  | 0.560432  |
| N       | -7.001130 | 1.578967  | -0.580605 |
| C       | -6.978841 | 2.209834  | -1.899408 |
| O       | -6.562607 | 0.295150  | -0.483156 |
| O       | -6.210589 | -0.387148 | -1.441600 |
| C       | -6.451499 | -0.340059 | 0.921599  |
| H       | -6.224462 | -2.946040 | 0.780491  |
| H       | -9.510988 | 2.172562  | 0.293377  |
| H       | -6.625712 | 2.356830  | 1.351886  |
| H       | -7.354160 | 3.460489  | 0.210895  |
| H       | -6.961906 | 1.427597  | -2.660296 |
| H       | -7.881787 | 2.801144  | -2.045719 |
| H       | -3.540087 | 5.242300  | 1.199930  |
| H       | -5.164249 | -5.136479 | 0.409306  |
| H       | -3.721383 | -5.018133 | -0.619024 |
| H       | -7.298047 | -1.010621 | 1.084561  |
| H       | -6.411674 | 0.377275  | 1.738998  |
| N       | -4.722792 | 2.997582  | -1.283043 |
| H       | -6.644176 | 2.281759  | -0.569807 |
| H       | -3.917006 | 3.581002  | -1.457472 |
| H       | -8.816214 | 1.068874  | 1.466058  |
| C       | -8.786062 | 2.108642  | 1.113504  |
| N       | -9.230393 | 2.971910  | 2.197518  |
| H       | -9.306555 | 3.938270  | 1.886785  |
| H       | -8.571955 | 2.958262  | 2.974111  |
| N       | 6.774302  | 1.878827  | 3.097178  |
| H       | 6.286682  | 2.679087  | 3.477561  |
\textbf{pGCp}

\begin{tabular}{ccc}
\hline
& \textbf{C} & \\
\hline
\textbf{H} & -6.08445700 & 0.11716900 & 1.36863900 \\
\textbf{C} & -6.92152700 & -0.11913700 & 0.09150600 \\
\textbf{O} & -6.43833700 & -0.75729200 & -0.84420200 \\
\textbf{C} & -8.97268400 & 0.17835900 & -1.14991600 \\
\textbf{O} & -8.64395700 & 1.28456600 & -2.16482200 \\
\textbf{N} & -8.18269300 & 0.38821000 & 0.07360400 \\
\textbf{C} & -7.84948000 & 1.32542200 & 1.05789200 \\
\textbf{H} & -9.38349800 & -0.46588200 & 2.76002800 \\
\textbf{C} & -8.41180500 & -0.61557500 & 1.29832500 \\
\textbf{C} & -5.81888500 & -1.26321400 & 0.73250000 \\
\textbf{C} & -1.50759400 & -1.04539800 & 0.24746200 \\
\textbf{O} & -0.54516500 & -1.86586500 & -0.15094200 \\
\textbf{N} & -1.25305100 & 0.26913600 & -0.16149500 \\
\textbf{C} & -2.18467400 & 1.26643800 & -0.97063000 \\
\textbf{N} & -1.78013200 & 2.52172800 & -0.48450400 \\
\textbf{N} & -3.41925700 & 1.10537500 & 0.35619100 \\
\textbf{C} & -3.67363900 & -0.15274300 & 0.75886500 \\
\textbf{H} & -5.83797800 & 1.17824400 & 1.46828400 \\
\textbf{H} & -6.63958700 & -0.18661500 & 2.25974000 \\
\textbf{H} & -10.03138300 & 0.25562000 & -0.90082500 \\
\textbf{H} & -8.75912600 & -0.81926200 & -1.53764100 \\
\textbf{H} & -7.94866500 & 1.73541900 & 1.67857900 \\
\textbf{H} & -9.17829400 & 2.16372300 & 0.49565500 \\
\textbf{H} & -10.23363300 & 1.43208200 & 2.61170600 \\
\textbf{H} & -10.65128300 & 0.32358200 & 1.31919000 \\
\textbf{H} & -5.44238600 & -2.58556200 & 1.93242300 \\
\textbf{H} & -1.10167400 & 2.57324000 & -1.23243100 \\
\textbf{H} & -2.54062000 & 3.18445100 & -0.57252700 \\
\textbf{C} & 6.00547400 & -0.47268400 & -0.98550900 \\
\textbf{C} & 6.30337600 & 0.29341000 & 0.32200800 \\
\textbf{O} & 5.50940100 & 0.22557300 & 1.26446600 \\
\textbf{C} & 7.76412200 & 1.74012000 & 1.59885900 \\
\textbf{C} & 7.13398300 & 3.13838000 & 1.50723600 \\
\textbf{O} & 7.74734100 & 4.07788400 & 1.02208100 \\
\textbf{N} & 7.45989200 & 0.99691300 & 0.36744900 \\
\textbf{C} & 8.35847900 & 1.21569200 & -0.77760700 \\
\textbf{C} & 9.57973500 & 0.28471000 & -0.73999500 \\
\textbf{N} & 9.15592300 & -1.12153400 & -0.65300000 \\
\textbf{N} & 4.89946400 & -1.39770400 & -0.74105800 \\
\textbf{C} & 3.61204700 & -0.90652900 & -0.71588800 \\
\textbf{C} & 2.61370000 & -1.71062100 & -0.29249400 \\
\textbf{C} & 2.80289700 & -2.96320700 & 0.14939300 \\
\textbf{C} & 4.13928300 & -3.48623500 & 0.15875900 \\
\textbf{C} & 5.13492500 & -2.66499400 & -0.27064700 \\
\textbf{O} & 3.22354200 & 0.25873400 & -1.09824600 \\
\textbf{N} & 1.73156400 & -0.64198600 & 0.55498600 \\
\textbf{H} & 5.70009800 & 0.21990000 & -1.77267300 \\
\textbf{H} & 6.88486200 & -1.03384100 & -1.31335200 \\
\textbf{H} & 8.84570000 & 1.86071400 & 1.67598500 \\
\textbf{H} & 7.39568100 & 1.16971100 & 2.45340300 \\
\hline
\end{tabular}
|      |          |          |          |
|------|----------|----------|----------|
| H    | 7.80850800 | 1.06143800 | -1.70815300 |
| H    | 8.66394800 | 2.26492500 | -0.75378400 |
| H    | 10.13693100 | 0.43247400 | -1.67157100 |
| H    | 10.24893300 | 0.58899900 | 0.08087900 |
| H    | 8.99229000 | -1.35919400 | 0.32354800 |
| H    | 9.91230200 | -1.72779800 | -0.96411100 |
| H    | 4.35453800 | -4.88944500 | 5.05834000 |
| H    | 6.17516500 | -2.97043300 | -0.27670100 |
| H    | 0.80493500 | -3.20441500 | 0.51970500 |
| N    | -7.58468600 | 1.00165800 | -2.97390300 |
| H    | -7.23444900 | 1.74936500 | -3.55813200 |
| H    | -6.96468000 | 0.23816800 | -2.72821200 |
| H    | 5.33776700 | 4.05812600 | 1.80017900 |
| Hg   | 0.94537600 | -0.05500000 | -0.57065200 |

**PTTP**

|      |          |          |          |
|------|----------|----------|----------|
| C    | -0.86937800 | 2.97482000 | -1.84759000 |
| N    | -3.93452300 | -0.25126500 | 0.54462600 |
| C    | -2.60698900 | -0.64246000 | 0.56565200 |
| O    | -1.69882500 | 0.13633300 | 0.92016800 |
| N    | -2.33250100 | -1.90816300 | 0.15396700 |
| C    | -3.23983700 | -2.80467500 | -0.40489300 |
| O    | -2.83587100 | -3.88512000 | -0.83539100 |
| C    | -4.62763600 | -2.33893500 | -0.45056000 |
| C    | -4.89365200 | -1.08792000 | -0.00387500 |
| C    | -5.66220000 | -3.25787700 | -1.03239600 |
| O    | -0.12729300 | 3.62843600 | -2.57887100 |
| C    | -2.83263800 | 4.27921900 | 1.94543300 |
| C    | -2.12432000 | 3.22922300 | 1.08704800 |
| N    | -2.77431400 | 2.94109700 | -0.19598400 |
| C    | -2.20493400 | 3.58187300 | -1.37732300 |
| C    | -3.74441500 | 1.99706000 | -0.38101400 |
| O    | -4.23399100 | 1.72767500 | -1.47463800 |
| C    | -4.21862100 | 1.16319800 | 0.82871200 |
| H    | -5.88973400 | -0.66349900 | -0.04967200 |
| H    | -2.02425100 | 2.31420600 | 1.66739000 |
| H    | -1.10635100 | 3.56169500 | 0.87448700 |
| H    | -2.91814800 | 3.49547600 | -2.19989400 |
| H    | -2.02765800 | 4.64234500 | -1.18124900 |
| H    | -6.65155300 | 2.79036700 | -1.04533500 |
| H    | -5.39210300 | 3.53853100 | -2.05605050 |
| H    | -5.72062700 | 4.18896900 | -0.45702200 |
| H    | -5.30148000 | 1.27890700 | 0.90370000 |
| H    | -3.77284000 | 1.42713000 | 1.78553000 |
| C    | 1.40675600 | 2.80829100 | 1.83748500 |
| N    | 3.85241500 | -0.92151000 | -0.54961700 |
| C    | 2.47352200 | -1.05402300 | -0.60975900 |
| O    | 1.74583700 | -0.11936900 | -0.99589000 |
| N    | 1.95615600 | -2.24240500 | -0.20042000 |
| C    | 2.66386000 | -3.28201000 | 0.39519800 |
| O    | 2.04717700 | -4.26047700 | 0.82392800 |
| C    | 4.11156900 | -3.08834100 | 0.48198800 |
| C    | 4.62089900 | -1.91471000 | 0.03580700 |
| C    | 4.93629000 | -4.17649900 | 1.10598400 |
| O    | 0.79894800 | 3.60549300 | 2.55060400 |
| C    | 2.70521100 | 2.86363600 | -1.09405100 |
| N    | 3.26940300 | 2.41326600 | 0.18721300 |
| Element | X | Y | Z |
|---------|---|---|---|
| C       | 2.83208300 | 3.15123600 | 1.36829300 |
| C       | 4.06841900 | 1.32239700 | 0.37588400 |
| O       | 4.49838400 | 0.97413600 | 1.47292500 |
| C       | 4.40287200 | 0.41315100 | -0.82426600 |
| H       | 5.67678300 | -1.68301000 | 0.11242100 |
| H       | 2.52075300 | 2.00629900 | -1.73958300 |
| H       | 1.72068500 | 3.28951700 | -0.88671600 |
| H       | 3.51613700 | 0.32366700 | -0.87720000 |
| H       | 4.58977100 | -4.38292800 | 2.12474100 |
| H       | 5.48935900 | 0.32366700 | -0.87720000 |
| H       | 4.03143400 | 0.75251700 | -1.78869200 |
| N       | -0.61412500 | 1.70866500 | -1.44304200 |
| H       | 0.27571200 | 1.28578400 | -1.67272100 |
| H       | -1.13937000 | 1.26877300 | -0.69642100 |
| H       | -2.74428300 | 5.26744300 | 1.45722000 |
| H       | -3.90680300 | 4.04690200 | 1.98569400 |
| N       | -2.27339000 | 4.19507200 | 3.29449300 |
| H       | -1.25363000 | 4.17900000 | 3.24618400 |
| H       | -2.53980000 | 5.00842000 | 3.84409300 |
| N       | 0.92642500 | 1.60140700 | 1.45640000 |
| H       | 1.35484300 | 1.07277500 | 0.70589300 |
| H       | -0.02407600 | 1.35056400 | 1.69401000 |
| C       | 3.55727300 | 3.91237700 | -1.82844500 |
| H       | 3.70511500 | 4.78279200 | -1.17585400 |
| H       | 4.55736500 | 3.50252800 | -2.02527200 |
| N       | 2.97152300 | 4.36178400 | -3.08922700 |
| H       | 2.91604000 | 3.75885700 | -3.74121400 |
| H       | 1.99455300 | 4.61573700 | -2.93832500 |
| Hg      | -0.21308000 | -2.37466800 | -0.02669600 |

References

1. L. Betts, J. A. Josey, J. M. Veal and S. R. Jordan, *Science.*, 1995, 270, 1838.
2. S. Brown, S. Thomson, J. Veal and D. Davis, *Science.*, 1994, 265, 777–780.
3. C. M. Topham and J. C. Smith, *J. Mol. Biol.*, 1999, 292, 1017–1038.
4. W. He, E. Hatcher, A. Balaeff, D. N. Beratan, R. R. Gil, M. Madrid and C. Achim, *J. Am. Chem. Soc.*, 2008, 130, 13264–13273.
5. M. Eriksson and P. E. Nielsen, *Nat. Struct. Biol.*, 1996, 3, 410–413.
6. J. I. Yeh, E. Pohl, D. Truan, W. He, G. M. Sheldrick, S. Du and C. Achim, *Chem. - A Eur. J.*, 2010, 16, 11867–11875.
7. J. I. Yeh, B. Shivachev, S. Rapireddy, M. J. Crawford, R. R. Gil, S. Du, M. Madrid and D. H. Ly, *J. Am. Chem. Soc.*, 2010, 132, 10717–10727.
8. B. Petersson, B. B. Nielsen, H. Rasmussen, I. K. Larsen, M. Gajhede, P. E. Nielsen and J. S. Kastrup, *J. Am. Chem. Soc.*, 2005, 127, 1424–1430.
9. H. Rasmussen, T. Liljefors, B. Petersson, P. E. Nielsen and J. S. Kastrup, *J. Biomol. Struct. Dyn.*, 2004, 21, 495–502.