

SUPPORTING INFORMATION

Role of Backbones of Nucleic Acids on the Stability of Hg²⁺ Mediated Canonical Base Pairs and Thymine-Thymine Mispair: A DFT Study

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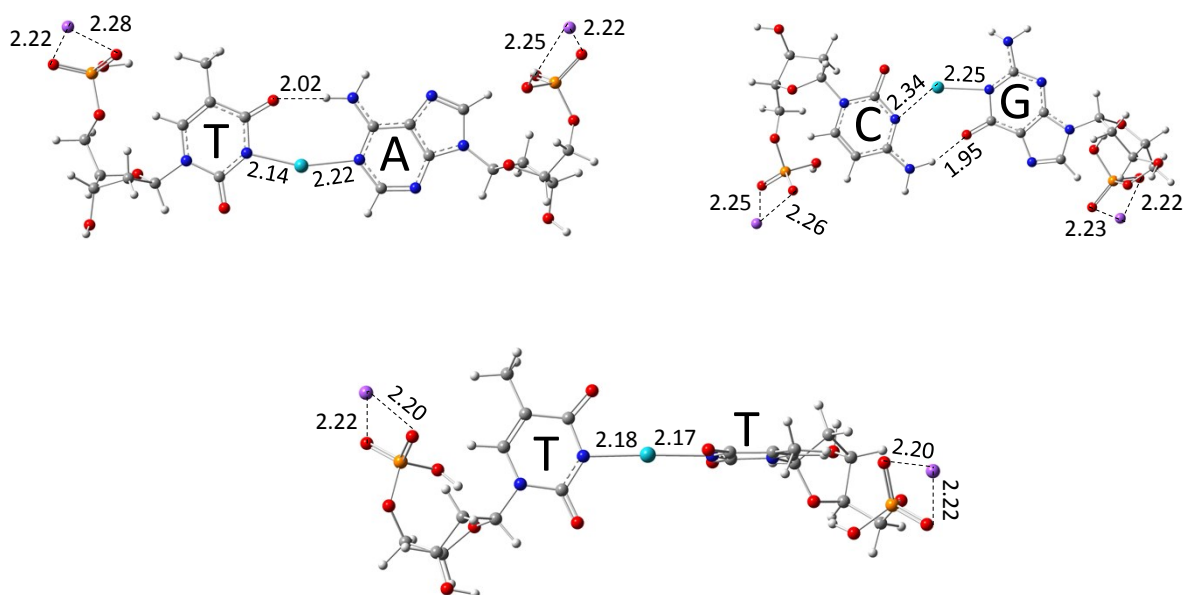


Figure S1: The optimized structure of canonical base pairs ${}_{\text{D}}\text{AT}_{\text{D}}$, ${}_{\text{D}}\text{GC}_{\text{D}}$, and mispair ${}_{\text{D}}\text{TT}_{\text{D}}$ mediated with Hg^{2+} in DNA using B3LYP-D3/6-31G* level of theory in the gaseous phase. The distances are given in Angstrom ($\text{\AA}$). Dark grey: Carbon, Red: Oxygen, White: Hydrogen, Blue: Nitrogen, Cyan: Mercury, Violet: Sodium.

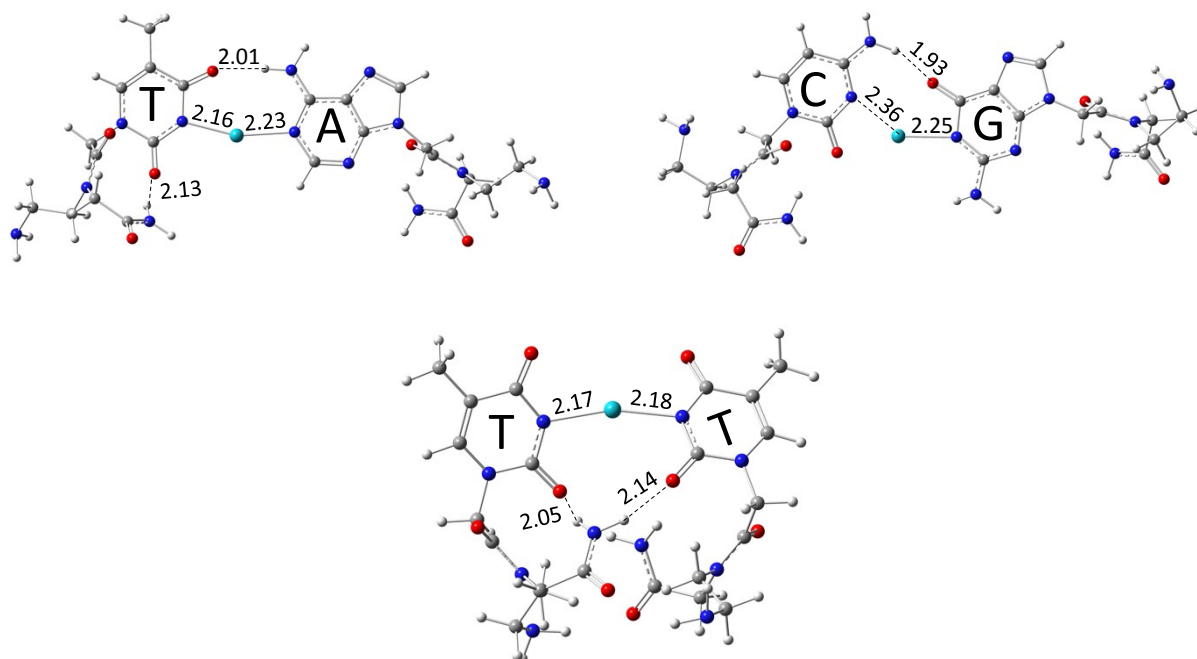


Figure S2: The optimized structure of canonical base pairs ${}_{\text{P}}\text{AT}_{\text{P}}$, ${}_{\text{P}}\text{GC}_{\text{P}}$, and mispair ${}_{\text{P}}\text{TT}_{\text{P}}$ mediated with Hg^{2+} in DNA using B3LYP-D3/6-31G* level of theory in the gaseous phase. The distances are given in Angstrom ($\text{\AA}$). 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.

Hg²⁺ mediated systems	B3LYP-D3/6-31G* ΔE	B3LYP-D3/6-31G* ΔG	BSSE corrected
_DAT_D	-49.8	-41.2	-42.8
_DGC_D	-59.4	-49.4	-51.5
_DTT_D	-145.7	-134.2	-136.8
_PAT_P	-17.6	-9.7	-10.9
_PGC_P	-44.5	-35.1	-37.0
_PTT_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.

Hg²⁺ mediated systems	B3LYP-D3/6-31G* ΔG
_DAT_D	-42.9
_DGC_D	-38.7
_DTT_D	-59.5
_PAT_P	-40.2
_PGC_P	-36.8
_PTT_P	-64.9
_DATGC_D	-106.2
_DTTTT_D	-138.2
_DTTTT_P	-140.6
_PTTTT_P	-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* ΔE (kcal/mol)	B3LYP-D3/6-31G* ΔG (kcal/mol)	B3LYP-D3/6-31G* ΔH (kcal/mol)
_DTTTT_D	-190.4	-146.3	-173.3
_DTTTT_P	-181.1	-136.0	-167.7
_PTTTT_P	-193.3	-148.2	-178.7

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

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

Where $E_{\text{mispair Complex}}$ refers to the energy of dimer mispair (_DTTTT_D, _DTTTT_P, and _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.

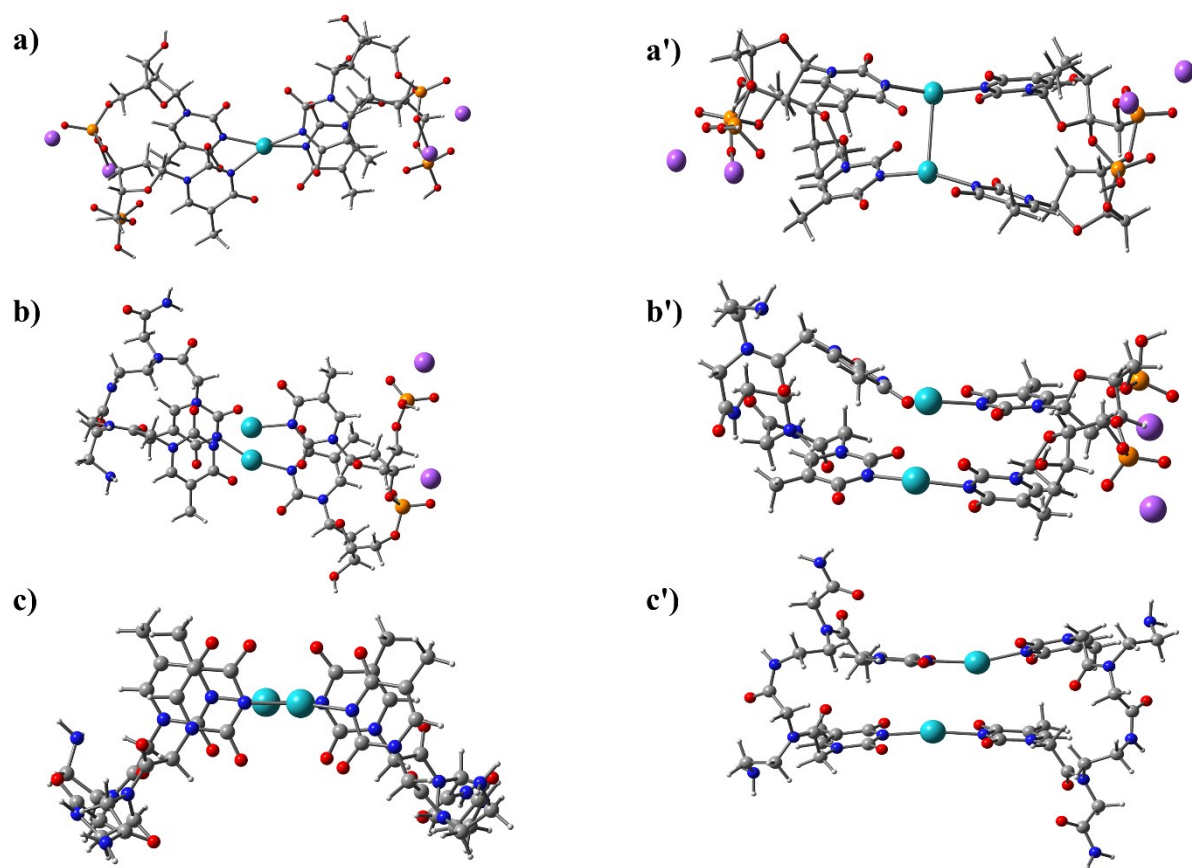
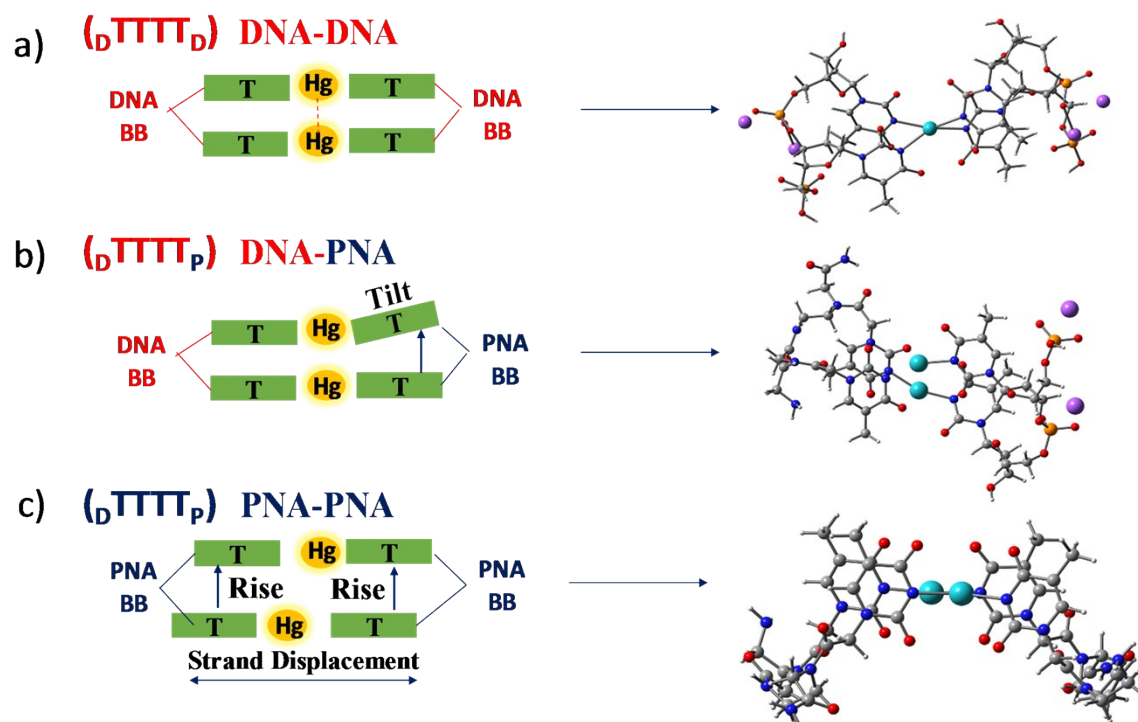


Figure S3. The comparison between the Hg^{2+} mediated DNA-DNA, DNA-PNA, and PNA-PNA duplexes in the mispair duplexes. a) $\text{D}^{\text{TTTT}}_{\text{D}}$ consecutive mispair from top view a') side view b) $\text{D}^{\text{TTTT}}_{\text{P}}$ consecutive mispair from top view b') side view c) $\text{P}^{\text{TTTT}}_{\text{P}}$ consecutive mispair from top view c') side view.

Helix Parametres

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 PNA₂/DNA is known to form a unique *P*-form helix, which is different from the well-known *A*- and *B*-form of duplexes.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.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.¹ The helix parameters such as X-displacement, tilt, rise, twist angles are different in DNA-DNA (_DTTTT_D), DNA-PNA (_DTTTT_P), and PNA-PNA (_PTTTT_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 unwounded 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 Hg²⁺ 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) _DTTTT_D, b) _DTTTT_P and c) _PTTTT_P with Hg²⁺ ion. BB depicts DNA/PNA backbone here.

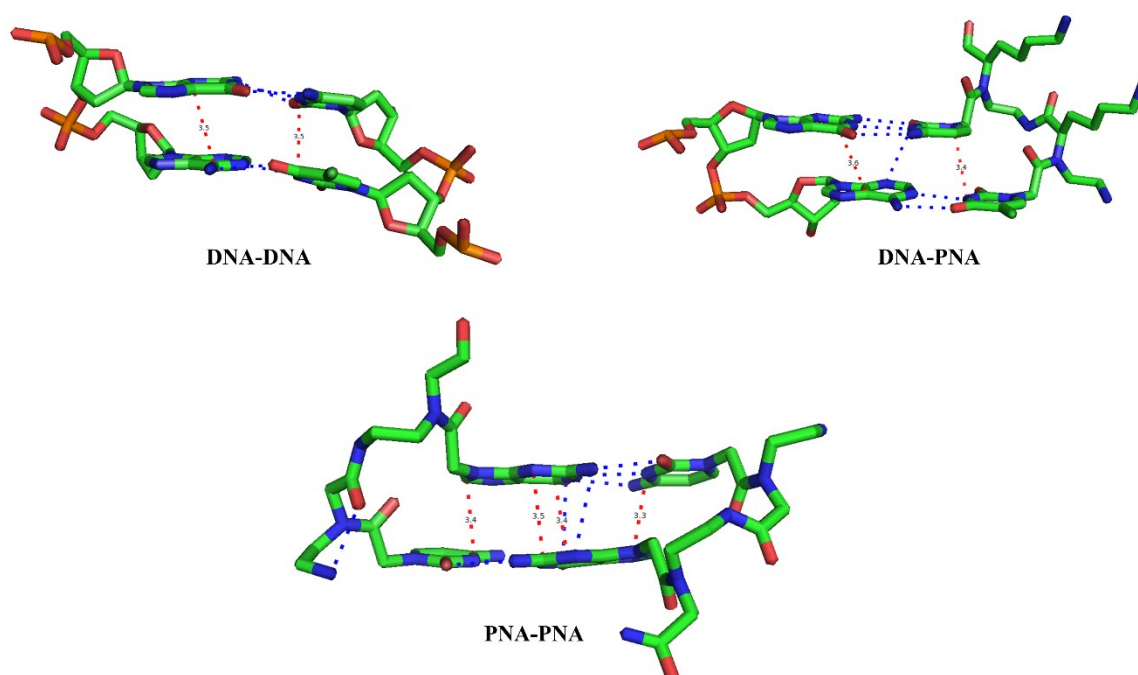


Figure S4. Stacking in DNA-DNA, DNA-PNA, and PNA-PNA duplexes. Duplexes are truncated by Discovery Studio software and images were captured from the PDB ID: 1BNA, 1NR8, and 1UNN. Dotted Blue color depicts the hydrogen bond interaction between the nucleobases and the red color depicts the stacking interaction 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:

dAT_D

P	8.71435900	-2.62888000	-0.37420700
O	10.09696300	-3.24783500	-0.35460700
O	7.62358900	-3.31856000	0.41483000
O	8.73270100	-1.08704500	0.18605800
C	9.48633800	-0.07545200	-0.49051000
C	8.96053700	1.28883000	-0.06841700
O	7.59688600	1.44015500	-0.50239200
C	8.95085000	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	5.46095100	-0.67750100	0.34170000
N	4.24744500	-1.11666800	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	1.51055500	-0.37278000
C	2.55668400	2.52995200	-0.19584200
N	3.85342400	2.45072100	0.05681300
C	4.27543900	1.17231400	0.12288100
P	-8.22706400	-2.79064100	0.43712400
O	-9.62230200	-3.31777600	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
O	-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	-1.16530500	-0.26082300
C	-3.95359800	-2.66305200	-0.38334600
C	-5.02680900	-0.41907200	-0.03967100
H	9.36808200	-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	6.32549000	-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

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	-2.42195500	-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	-4.63024900	-1.32055000
Na	9.21667300	-5.00716600	1.05951100
Hg	-0.68075600	2.07506600	-0.63304200

dGC_D

O	-8.42458700	1.20397700	-0.18773900
C	-7.50063200	1.60948100	-1.20266200
C	-6.69375500	2.77718200	-0.64885100
O	-5.99389100	2.41514500	0.56161100
C	-5.58784300	3.25912200	-1.60269900
O	-5.19607400	4.59732400	-1.31685900
C	-4.41611900	2.35343300	-1.21915200
C	-4.66589200	2.05442300	0.27512500
N	-4.45995700	0.60528800	0.59194400
C	-3.13756300	0.14262000	0.54636300
O	-2.23367800	0.95175400	0.29399300
N	-2.92002700	-1.19225500	0.77100400
C	-3.93577200	-2.02917600	1.04271700
N	-3.66475800	-3.32739500	1.24698000
C	-5.28207800	-1.55675900	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	-1.80003700
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	1.11887200
H	-0.24915800	1.20090800	0.81103400
H	-4.39764300	-3.96925300	1.51210000
P	-9.34758700	-0.13587300	-0.44408900
O	-9.72832900	-0.24070200	-1.90669800
O	-8.31599400	-1.36034600	-0.04967200
O	-10.45228400	-0.09330900	0.58268000
O	6.63262800	0.50634000	-2.03989800
H	6.50513200	1.07213100	-1.24419900
Na	9.26340500	-2.04930700	-3.82385100
Na	-12.04790700	-0.18721100	-1.22737600
H	-7.91917800	-1.73447400	-0.85395000
Hg	-0.52116700	-1.77010100	0.36213200

$\mathbf{dTT_d}$

P	-9.10080300	-0.89339000	0.24210500
O	-10.56881200	-0.53714200	0.19065600
O	-8.56654300	-1.87180900	-0.78065600
O	-8.16681600	0.45346800	0.09095700
C	-8.34170500	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	-6.01110300	2.19401800	-1.26990100
C	-5.10554900	2.00722800	-0.04368500
N	-4.35250200	0.75708100	-0.02383300
C	-2.94612500	0.79262700	0.03380700
O	-2.33980900	1.87339700	0.03387400
N	-2.31267600	-0.41671700	0.07607700
C	-2.94627800	-1.64393200	0.07530900
O	-2.28258600	-2.69566800	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	0.11787100	-0.12993200
C	8.35096000	1.09810600	-1.15760900
C	7.31112700	2.19291100	-0.97592200
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	0.09092900
C	2.85139700	-1.76860000	0.14153800
O	2.14214900	-2.79073900	0.17522700
C	4.31442700	-1.82965000	0.15288200
C	4.99281800	-3.16952500	0.21026200

C	4.99429400	-0.66183700	0.10114900
H	-8.25911400	1.18342900	2.03527600
H	-9.33144500	1.99685000	0.86435600
H	-7.46895900	3.44941100	1.38550000
H	-8.08739700	2.89850800	-1.26764100
H	-6.06385800	4.65376800	-0.36369200
H	-6.40402000	1.23071700	-1.60315900
H	-5.49051700	2.67501900	-2.10118500
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
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	2.58113700	1.91864900
H	6.52467000	1.08492800	1.49610500
H	4.46781300	2.59782300	-0.18218800
H	4.63302900	-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

pAT_p

P	-9.10080300	-0.89339000	0.24210500
O	-10.56881200	-0.53714200	0.19065600
O	-8.56654300	-1.87180900	-0.78065600
O	-8.16681600	0.45346800	0.09095700
C	-8.34170500	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	-6.01110300	2.19401800	-1.26990100
C	-5.10554900	2.00722800	-0.04368500
N	-4.35250200	0.75708100	-0.02383300
C	-2.94612500	0.79262700	0.03380700
O	-2.33980900	1.87339700	0.03387400
N	-2.31267600	-0.41671700	0.07607700
C	-2.94627800	-1.64393200	0.07530900
O	-2.28258600	-2.69566800	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	0.11787100	-0.12993200
C	8.35096000	1.09810600	-1.15760900
C	7.31112700	2.19291100	-0.97592200
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	0.09092900
C	2.85139700	-1.76860000	0.14153800
O	2.14214900	-2.79073900	0.17522700
C	4.31442700	-1.82965000	0.15288200
C	4.99281800	-3.16952500	0.21026200
C	4.99429400	-0.66183700	0.10114900
H	-8.25911400	1.18342900	2.03527600
H	-9.33144500	1.99685000	0.86435600
H	-7.46895900	3.44941100	1.38550000
H	-8.08739700	2.89850800	-1.26764100
H	-6.06385800	4.65376800	-0.36369200
H	-6.40402000	1.23071700	-1.60315900
H	-5.49051700	2.67501900	-2.10118500
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
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	2.58113700	1.91864900
H	6.52467000	1.08492800	1.49610500
H	4.46781300	2.59782300	-0.18218800
H	4.63302900	-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

pGCp

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	-3.50539300
N	-5.23002400	1.66077200	-0.62810800
C	-4.91359000	2.45129900	0.56715900
C	-6.14057300	3.18068100	1.12781600
N	-7.15209500	2.22602500	1.59550100
N	-4.87403000	-1.57071000	0.57300800
C	-5.21160800	-2.91005600	0.50477400
N	-4.17102200	-3.70318600	0.39632100
C	-3.08211300	-2.84078000	0.38049600
C	-1.66991000	-3.08615100	0.27051400
O	-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	0.15107300	1.56337800
H	-6.77940400	-0.77403200	0.79106500
H	-5.41217300	3.39260800	-1.80098900
H	-5.75938700	1.87614800	-2.63579200
H	-4.44641500	1.81348600	1.31986600
H	-4.15106500	3.18173600	0.27967300
H	-5.79517200	3.88492600	1.90200000
H	-6.58472600	3.78177200	0.32589600
H	-6.24712700	-3.22149600	0.54943900
H	0.32543400	0.29571800	-0.06063100
H	-1.00870700	1.29403300	0.29233600
C	4.53415000	1.94325000	-1.05764700
C	4.38836800	2.41718000	0.39728700
O	5.19511600	1.97857100	1.22105500
C	3.15544600	3.55035300	2.14419200
C	2.03145600	2.74338700	2.81554100
O	1.55171000	3.12977700	3.88149500
N	3.35113200	3.23064900	0.73558200
C	2.39843900	3.83462900	-0.20323900
C	2.91922300	5.14988100	-0.79370000
N	4.12117000	4.91774400	-1.60264800
N	4.62755500	0.47809800	-1.04306700
C	3.46669600	-0.22839300	-0.70452500
N	3.54831800	-1.58640300	-0.61413900
C	4.70934900	-2.23690300	-0.80484100
C	5.91043600	-1.51825500	-1.09444900
C	5.81847900	-0.16554100	-1.19062700
O	2.41553400	0.40402500	-0.49388800
N	4.72143000	-3.57159100	-0.70753100
H	3.72253400	2.22770900	-1.71791100
H	5.46195900	2.34862900	-1.45943400
H	2.91030600	4.60940500	2.26150100
H	4.08433200	3.35585000	2.68341000
H	2.14239800	3.11744800	-0.98625800
H	1.47244900	4.02088800	0.34889100
H	2.09333900	5.63026000	-1.34268100
H	3.18702400	5.81898700	0.03206400
H	6.85423200	-2.02897400	-1.23175500
H	6.67579400	0.46135200	-1.40190800
H	3.87136800	-4.09332900	-0.54430900
H	5.57051800	-4.09523700	-0.86398700
N	-2.76508200	1.59353000	-1.85776800
H	-2.99337500	0.98212400	-1.07355900
H	-1.84628000	1.51320500	-2.27276600
N	1.65766400	1.61085900	2.17999200
H	0.85260400	1.09915000	2.51599500
H	-6.90826600	1.90003200	2.52975000
H	-8.04780700	2.69918800	1.69539600
H	2.02075000	1.34675500	1.26957300
Hg	1.35954800	-2.52391300	0.12797500
H	4.60911200	5.79833100	-1.75280700
H	3.85189300	4.59024000	-2.52937300

pTTp

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	-0.22746300
C	-4.96493300	-1.24325000	0.06630600

C	-5.71717800	-3.54221200	-0.61971100
O	-0.17302500	3.43422600	-2.81531100
C	-3.09732900	4.37087300	1.57728900
C	-2.30295400	3.25314900	0.90040500
N	-2.84166800	2.85757400	-0.40571600
C	-2.22104300	3.46558400	-1.57608900
C	-3.73062300	1.84389100	-0.60870200
O	-4.07875500	1.47749800	-1.73343000
C	-4.30240200	1.08742000	0.60407600
H	-5.97645200	-0.85390100	0.03202900
H	-2.24298000	2.38634700	1.55544800
H	-1.27186100	3.57857300	0.74363100
H	-2.90828100	3.39914000	-2.42175900
H	-2.02595000	4.52276300	-1.38024700
H	-6.71861300	-3.10077700	-0.62860200
H	-5.50791000	-3.95053500	-1.61560600
H	-5.71865500	-4.39153800	0.07415500
H	-5.38710300	1.20699000	0.58374700
H	-3.93893800	1.43036300	1.57005000
C	1.08108300	2.82376700	1.99277500
N	3.97230800	-0.58295800	-0.39660900
C	2.60462500	-0.85462500	-0.44575900
O	1.80890600	0.07054700	-0.73038100
N	2.20038200	-2.11039700	-0.16001600
C	3.05100900	-3.14451300	0.18362300
O	2.59572600	-4.27320500	0.43222600
C	4.48086100	-2.83367700	0.25017600
C	4.86630400	-1.56449800	-0.02385800
C	5.43768400	-3.92626400	0.63145600
O	0.41109900	3.48765000	2.79218500
C	2.52756000	3.09196700	-0.92698800
N	3.03450300	2.69400600	0.39114300
C	2.44963200	3.36730100	1.54405700
C	3.85308100	1.62887000	0.62407400
O	4.16633700	1.26478300	1.75971800
C	4.38671300	0.81217000	-0.56641100
H	5.90380600	-1.25235700	0.02060100
H	2.42400300	2.21656600	-1.56432300
H	1.51485200	3.47678900	-0.78574800
H	3.13124200	3.28228800	2.39262100
H	2.31806700	4.42874400	1.32031700
H	5.38318700	-4.75790100	-0.08142900
H	6.46933700	-3.56239000	0.66155700
H	5.18449900	-4.33918100	1.61518900
H	5.47674000	0.84898200	-0.52543600
H	4.06969200	1.16812200	-1.54429500
H	-3.02969400	5.28212000	0.95795100
H	-4.15873900	4.08940200	1.60751400
N	-2.60460800	4.53136200	2.95115300
H	-1.58445700	4.55912400	2.94207800
H	-2.91815600	5.42526300	3.32452500
N	0.70946900	1.62689100	1.50168100
H	1.21321600	1.15813700	0.75056600
H	-0.21810200	1.26770100	1.69704000
C	3.38592000	4.14851900	-1.62328300
H	3.36520200	5.07747800	-1.02740300
H	4.43038500	3.80879200	-1.64025000
Hg	-0.08433200	-2.56508300	-0.00363900
N	-0.59467000	1.62117800	-1.49133600
H	0.31227700	1.20347600	-1.66770200
H	-1.12994100	1.20117900	-0.73343600
N	2.90916700	4.30068100	-3.00389700
H	1.89255400	4.39058000	-3.00059300
H	3.27740500	5.16353900	-3.39976800

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P	7.61672100	5.87341000	0.53571900
O	8.67325200	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	1.65365600	1.10578500
C	4.98878300	2.88674200	0.84235400
N	3.67742200	2.85455800	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	-2.49014500	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	-0.88333900	-2.09826200
O	7.93034900	-1.66081100	0.09235600
C	7.96547400	-2.49990400	1.25371400
C	7.37005200	-3.86666400	0.93648700
O	5.96612000	-3.75746700	0.62816900
C	7.99440900	-4.58222100	-0.27920000
O	7.86419700	-5.99961400	-0.17432800
C	7.09947400	-4.13495700	-1.43516000
C	5.72900900	-3.94093400	-0.76836700
N	4.95731000	-2.81693100	-1.28797200
C	5.38857200	-1.55295700	-1.66343300
N	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	5.33785400	-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	-1.76708100
C	-4.19566300	-0.26418700	-1.98561000
O	-4.64475100	-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

C	-4.55054000	2.06999400	-1.44210400
P	-10.08545800	-0.69329200	0.26473500
O	-11.24729000	-1.47706600	-0.30090700
O	-10.34196900	0.19910100	1.45833500
O	-8.85922800	-1.70597400	0.69741300
C	-8.48663400	-2.73318500	-0.23222400
C	-7.28516200	-3.48716800	0.29986000
O	-6.12691800	-2.63490900	0.25116800
C	-7.40928600	-3.99136800	1.76147200
O	-7.04879800	-5.37203300	1.74875600
C	-6.38053200	-3.13261000	2.51197400
C	-5.34329200	-2.90412600	1.41119600
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	-2.67279400	0.32678800	1.70872200
N	-1.82111100	1.35127800	1.75197300
C	-4.08381500	0.55349200	1.83590500
C	-4.89688700	-0.52718700	1.78508900
H	9.16233500	4.21425600	2.15519400
H	10.16658400	4.05118100	0.69013300
H	9.86259600	1.89808200	1.85455700
H	9.60895000	2.05062400	-0.88714200
H	7.22537800	2.44500200	-0.80029600
H	7.26456500	0.69912700	-1.13012200
H	6.96799500	0.18607900	1.23118400
H	5.58574500	3.75727600	0.60342300
H	4.36726100	-2.91381900	1.71268600
H	7.35927600	-2.01609800	2.02516100
H	8.99063600	-2.62427100	1.61589900
H	7.45532900	-4.48917300	1.83516200
H	9.03945000	-4.28423400	-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	-4.06706900	-0.86933900
H	-9.21370500	3.95125800	-1.39368000
H	-7.98803600	4.07113400	-2.68524900
H	-9.17858500	1.87742700	-2.67003100
H	-8.96628300	1.85389800	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	3.59989500	-0.22682800
H	-3.45872100	4.35391300	-0.66990700
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	-1.20299400
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	-4.72649000	-3.79339100	1.26996600
H	-0.81598700	1.26485800	1.55381700
H	-4.48143800	1.55126100	1.96653700
H	-5.96956100	-0.44295700	1.87839400
H	2.69903900	-3.01558300	1.58155500
H	2.16847300	0.84058100	-2.07410200
O	-6.37327500	5.97287100	-1.85043000
H	-5.51866000	5.61933900	-2.15174200
H	-2.19323300	2.28822000	1.82013500

O	7.39796800	5.97849200	2.16289900
H	8.04029800	6.60755800	2.53079400
Na	7.09859900	7.70382600	-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

dTTTT_D

P	8.62650400	-3.06131500	0.11641800
O	9.82396000	-2.16099100	0.35738000
O	7.50550800	-3.11241900	1.12379900
O	7.91462200	-2.68730800	-1.32095400
C	8.53408200	-1.90592800	-2.34925600
C	7.93620900	-0.49784800	-2.37939300
O	6.53816700	-0.57353500	-2.68724500
C	8.07436400	0.20998000	-1.02274100
O	8.57105400	1.55651400	-1.21129600
C	6.66839300	0.16753700	-0.42883100
C	5.73997700	-0.01573500	-1.63574000
N	4.59524500	-0.88689500	-1.37854400
C	3.30430100	-0.47791000	-1.76586300
O	3.11748600	0.62206100	-2.30595800
N	2.29095600	-1.35576500	-1.50787100
C	2.44127500	-2.59453700	-0.92463100
O	1.45011100	-3.32863800	-0.74126400
C	3.79301200	-2.99137500	-0.54635900
C	4.01111000	-4.30419200	0.14824800
C	4.79831900	-2.12525300	-0.80236900
P	9.07707800	2.34305700	0.13715200
O	10.08757300	3.38080100	-0.28959700
O	9.50577900	1.36012500	1.21683600
O	7.70420600	3.04147400	0.69629300
C	7.07501000	4.04025400	-0.12301700
C	5.63836900	4.22456300	0.31552800
O	4.88460600	3.04462500	0.03358200
C	5.41909900	4.47393500	1.81734600
O	5.74966900	5.78349600	2.23960800
C	3.94886900	4.05510200	1.99146700
C	3.70152200	3.04216800	0.84559400
N	3.45199900	1.67450100	1.28538200
C	2.18727400	1.10457400	1.06903400
O	1.28718200	1.75814900	0.51782100
N	2.00761800	-0.17056300	1.51333000
C	2.96547200	-0.92928000	2.15604100
O	2.70320300	-2.07392500	2.56468000
C	4.28234700	-0.30814400	2.35096500
C	5.38039200	-1.10068100	3.00043900
C	4.44481600	0.96570700	1.93038900
P	-8.74930600	-3.51192500	0.55079700
O	-10.26443800	-3.53343500	0.53489200
O	-8.02390300	-3.86973900	-0.72518800
O	-8.18756400	-2.02586400	0.97347000
C	-8.55859000	-1.44807400	2.23198400
C	-7.82246600	-0.12714300	2.40437700
O	-6.42634400	-0.35062800	2.65225100
C	-7.91388400	0.78786500	1.17217200
O	-8.07333100	2.13951900	1.64755700
C	-6.57317400	0.57086900	0.46894200
C	-5.61340000	0.19660200	1.60769700
N	-4.59560000	-0.79404700	1.25224600
C	-3.23017100	-0.48003500	1.35117100

O	-2.85653300	0.68051700	1.58370400
N	-2.35629300	-1.51509600	1.18161300
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	-9.71655300	2.66532600	-0.30799600
O	-7.40389500	3.69691600	-0.27723800
C	-6.36397600	4.45148000	0.36328500
C	-5.16287000	4.52348700	-0.55634700
O	-4.52401400	3.23704800	-0.60312000
C	-5.48874000	4.91462800	-2.02178500
O	-4.55522200	5.92872100	-2.39527600
C	-5.25192700	3.60122400	-2.78190600
C	-4.10304700	3.02113500	-1.95956200
N	-3.75072400	1.62858800	-2.13306300
C	-2.39189300	1.27754500	-1.94955200
O	-1.54511600	2.15874900	-1.75605200
N	-2.08633300	-0.04937300	-2.01642300
C	-3.00305900	-1.06094000	-2.22897200
O	-2.63651300	-2.24664000	-2.29841800
C	-4.40783900	-0.66777000	-2.38098100
C	-5.44162800	-1.73203500	-2.61525900
C	-4.70517100	0.64916700	-2.32112100
H	8.33572100	-2.40891400	-3.30071000
H	9.61668600	-1.84058200	-2.19746000
H	8.44593800	0.08301700	-3.15898500
H	8.80030400	-0.31618600	-0.41053400
H	6.59146400	-0.66817300	0.26803000
H	6.42577900	1.08311800	0.10309800
H	5.31769500	0.93414700	-1.96289800
H	5.07446400	-4.45907300	0.35767300
H	3.63800700	-5.14412500	-0.45012800
H	3.46624800	-4.31372300	1.09984800
H	5.82272800	-2.36790100	-0.55829900
H	7.09847500	3.73689800	-1.17539800
H	7.60294200	4.99404200	-0.01378800
H	5.22958200	5.07935600	-0.25092300
H	6.08057000	3.81262400	2.38290900
H	5.16749800	6.40938900	1.77659100
H	3.73354700	3.62516700	2.97212600
H	3.30241200	4.92931500	1.85666500
H	2.83573300	3.31523500	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	6.17866100	-3.31412800
H	-4.99748700	3.75727200	-3.83347500

H	-6.14930800	2.98115500	-2.71044900
H	-3.19045300	3.58777700	-2.15204200
H	-5.49645400	-2.42276500	-1.76779600
H	-5.19083100	-2.33017500	-3.49955300
H	-6.43478000	-1.29476000	-2.76336800
H	-5.72177700	1.00326300	-2.43015800
O	9.24062900	-4.56352700	-0.15242000
H	8.52509000	-5.22078200	-0.11506500
O	-8.19627800	-4.45146000	1.78228000
H	-8.94357700	-4.72194600	2.34125700
Hg	0.10797800	-0.69072300	-1.74286600
Hg	-0.11000600	-1.00422900	1.22013100
Na	9.30841400	-0.76162500	2.08864300
Na	11.72909500	2.53306000	1.18922800
Na	-11.33295900	4.27376500	0.49368800
Na	-10.14783700	-4.11732700	-1.82056900

DTTTT_P

P	-9.30694200	-2.60565100	0.92108600
O	-10.80797900	-2.53890000	1.11718500
O	-8.78051400	-3.43790300	-0.22490400
O	-8.66011500	-1.10802200	0.71234900
C	-8.93108600	-0.08751700	1.68314600
C	-7.87976100	1.00738800	1.57408100
O	-6.61624900	0.52632700	2.06362800
C	-7.63241800	1.51098900	0.13995200
O	-7.40448800	2.93162300	0.23047500
C	-6.39165200	0.72714800	-0.27880900
C	-5.62095700	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	3.53802400	-0.08637600
C	-2.97706800	5.38129000	-1.54626000
O	-1.94857500	6.35621600	-1.36358300
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

H	-5.81179800	1.23615000	-1.04605100
H	-6.70469200	-0.24644900	-0.66155700
H	-4.93461600	1.39542700	1.20800400
H	-5.25751300	-4.98373400	1.77926300
H	-4.97627400	-4.94990900	0.04389400
H	-6.48362500	-4.26719000	0.70328200
H	-6.50179000	-1.83667400	0.91559500
H	-5.24876900	5.46465600	0.24304100
H	-4.82839400	3.93207600	1.05137800
H	-2.88470400	5.45752000	0.61271000
H	-3.87717200	5.83421500	-1.98045400
H	-1.72069900	6.71036800	-2.23849900
H	-1.84113900	4.44678200	-3.18564100
H	-3.34024100	3.60304900	-2.71974600
H	-0.73651700	3.78599100	-1.11226600
H	-3.64441100	-1.59919500	-3.17894300
H	-4.68478300	-0.49193700	-2.25844700
H	-3.83385100	-1.81518900	-1.44263500
H	-3.61672900	1.66531200	-1.61190800
O	-8.59701000	-3.07515900	2.32967800
H	-9.27963700	-3.16444700	3.01516600
Na	-8.47761200	5.00095100	-3.13742000
Na	-11.04279500	-3.99616800	-0.81471100
C	9.40375000	2.18440000	-2.10972000
C	7.58487200	0.66163600	-1.30245300
C	7.45439900	0.07159400	-2.71413000
N	6.40007200	-0.92452900	-2.76871400
C	5.07713300	-0.47838000	-2.62775600
O	4.84744100	0.73667100	-2.54390700
N	4.10511400	-1.43596800	-2.60132100
C	4.33408000	-2.78873400	-2.73833900
O	3.38944800	-3.59981600	-2.73199200
C	5.72788600	-3.21982700	-2.88122500
C	6.02503100	-4.68324600	-3.04142500
C	6.68854400	-2.26590200	-2.86787900
C	7.78587600	2.88994100	3.03133200
C	6.25336500	2.73907900	3.04249900
C	4.95997700	0.60444700	3.21297400
C	4.65576100	0.69608000	1.70773000
N	3.89941300	-0.46676900	1.27653300
C	2.51402300	-0.46807100	1.48694800
O	1.93643200	0.56866200	1.84550900
N	1.85962100	-1.64481900	1.24619600
C	2.48466000	-2.83421000	0.91421000
O	1.82338900	-3.87428100	0.73959300
C	3.94027000	-2.80696100	0.76740800
C	4.64764300	-4.07906100	0.40086900
C	4.57164200	-1.62551600	0.94951500
H	9.51134600	3.26862200	-2.00427500
H	7.22545600	0.87009700	-3.42422300
H	7.09593800	-4.85700800	-3.18860600
H	5.48511100	-5.09794000	-3.90101900
H	5.70205800	-5.25237600	-2.16213400
H	7.74302800	-2.50741000	-2.95403600
H	8.15129300	3.09821600	4.04051000
H	8.04001300	3.77017600	2.43311100
H	5.81237700	3.62632500	3.51263700
H	4.05194200	1.58435000	1.51213800
H	5.71502000	-3.90470100	0.23208000
H	4.21604600	-4.49818800	-0.51269700
H	4.53817800	-4.83334200	1.19047600
H	5.64038700	-1.50633800	0.81312200
O	4.47665700	-0.29622400	3.89884700
H	5.57024800	0.74993300	1.11529000
N	5.79471300	1.54574800	3.75071300
C	5.90981800	1.54954000	5.19805900
H	6.01706000	0.52425500	5.55769600

H	6.80765100	2.09966800	5.49381900
C	4.68375400	2.21253100	5.85447400
O	3.85151100	2.83622900	5.20039200
N	4.62476900	2.07167200	7.19929500
H	3.86157700	2.49696500	7.70806100
H	5.29964300	1.52854700	7.71899900
N	8.51349900	1.71844200	2.55163500
H	8.88385100	1.08799700	3.25214800
H	5.88481900	2.71188200	2.01901100
C	8.91753300	1.42751200	1.28439700
O	9.67700900	0.49134500	1.04482200
C	8.38505400	2.35300900	0.17892000
H	9.00634400	3.25307200	0.14804200
H	7.36484600	2.66833600	0.40985000
N	8.39265400	1.74246800	-1.14226300
H	9.04195500	2.00677400	-3.12545200
C	10.76410500	1.50334800	-1.90660700
H	11.52556900	2.09196700	-2.44369700
H	11.00831200	1.53285300	-0.84124100
N	10.70809000	0.09529800	-2.32217900
H	11.47849100	-0.41826600	-1.89955800
H	10.85231500	0.03369000	-3.32921900
O	6.93625700	0.19682800	-0.36069400
H	8.40383900	-0.38748300	-2.99419600
Hg	1.96420000	-0.74923000	-2.03395600
Hg	-0.43188700	-1.63181500	1.26654800

pTTTT_p

C	8.17531100	3.30381300	1.14640800
C	6.52540900	1.66819900	0.20725600
C	6.40682200	2.52163100	-1.06315100
N	5.47863100	1.92228100	-2.00381600
C	4.11541100	1.93545500	-1.67058000
O	3.74030000	2.53248200	-0.65171700
N	3.26862100	1.28443100	-2.52004700
C	3.66264400	0.63368200	-3.67164100
O	2.82651900	0.08172900	-4.41124300
C	5.09670700	0.61612700	-3.97359800
C	5.57172600	-0.08111300	-5.21613400
C	5.93044900	1.24527300	-3.11256000
C	6.68989200	-0.76158700	4.43325600
C	5.17069600	-0.94241700	4.26337700
C	4.04854000	-2.34461200	2.52103500
C	3.75345700	-1.06678500	1.71756600
N	3.08000500	-1.39830000	0.47398200
C	1.69694000	-1.61675300	0.51313400
O	1.04807800	-1.32624000	1.52961200
N	1.12563500	-2.13425700	-0.61553100
C	1.82345100	-2.50266300	-1.75041300
O	1.22580800	-2.97011900	-2.73711200
C	3.27457500	-2.30545400	-1.73546000
C	4.06655100	-2.69177400	-2.95093200
C	3.82631500	-1.76097700	-0.62726400
H	8.19372600	3.79937800	2.12217400
H	6.05170100	3.52129900	-0.80165700
H	6.65409100	0.02588700	-5.34153900
H	5.07762500	0.32750600	-6.10574400
H	5.33317500	-1.15042600	-5.18638300
H	7.00525700	1.26719900	-3.26100000
H	7.07285500	-1.47851900	5.16449600
H	6.87226800	0.22983200	4.85908800
H	4.69270200	-0.86779200	5.24745600

H	3.09412800	-0.41547000	2.29469000
H	5.12305500	-2.42960600	-2.83394600
H	3.67808600	-2.17525600	-3.83363300
H	3.99488900	-3.76989600	-3.14222600
H	4.88486800	-1.53984400	-0.54918000
O	3.63143200	-3.43911200	2.14180400
H	4.66844400	-0.52191600	1.48098400
N	4.80330000	-2.21911900	3.65486900
C	4.91918800	-3.40464100	4.48466700
H	5.11618900	-4.27385400	3.85385900
H	5.76627200	-3.29146500	5.16744300
C	3.64232600	-3.63243300	5.31609200
O	2.77028600	-2.77304200	5.41894300
N	3.58462500	-4.83318300	5.93796600
H	2.79390100	-5.04483200	6.53138400
H	4.29962400	-5.53844500	5.82851600
N	7.47009000	-0.94525300	3.21198400
H	7.91619200	-1.84523500	3.08283300
H	4.77098000	-0.12886700	3.66120300
C	7.86676400	-0.00402200	2.31090000
O	8.69204800	-0.25158000	1.43466800
C	7.23379400	1.38752800	2.46952100
H	7.78687000	1.93677600	3.23738700
H	6.20096400	1.29511800	2.81367100
N	7.24579300	2.17182800	1.24308200
H	7.78736300	4.03720100	0.43508100
C	9.59699700	2.88146100	0.75078900
H	10.28416100	3.70183800	1.01435800
H	9.87433900	2.00805900	1.34773000
N	9.65410000	2.50098800	-0.66764300
H	10.48740800	1.94218400	-0.83936900
H	9.75999600	3.33878000	-1.23843900
O	5.94369300	0.58282900	0.29253100
H	7.39174400	2.60524500	-1.52550100
C	-8.80860700	-1.24682900	2.55659400
C	-6.43694900	-0.99131500	1.74329400
C	-6.27420000	-2.50222200	1.53517900
N	-5.49051900	-2.75181300	0.33321000
C	-4.09024000	-2.71555400	0.41741100
O	-3.52857300	-2.66209000	1.51972900
N	-3.41019000	-2.75756600	-0.76803500
C	-3.99865700	-2.87457700	-2.01145500
O	-3.30184200	-2.93160600	-3.04305300
C	-5.46203100	-2.91021300	-2.05701100
C	-6.15189900	-3.04494200	-3.38483500
C	-6.13204600	-2.81242400	-0.88484100
C	-6.72009300	3.78119500	2.55633200
C	-5.19345000	3.79630000	2.74972500
C	-3.73162800	3.62431000	0.71564900
C	-3.64484400	2.10733900	0.94296000
N	-3.08027700	1.45179100	-0.22327900
C	-1.68932400	1.45589000	-0.38309000
O	-0.94851200	1.79787400	0.55017400
N	-1.21185900	1.05187700	-1.59694400
C	-1.99774300	0.69241700	-2.67480100
O	-1.47813600	0.37611600	-3.76024600
C	-3.44877600	0.68930200	-2.46653300
C	-4.33643700	0.25845500	-3.59764200
C	-3.91344700	1.07771600	-1.25659200
H	-9.29701000	-0.79798600	3.42666600
H	-5.72205600	-2.89857800	2.39033600
H	-7.23915000	-3.08524000	-3.26196200
H	-5.82915000	-3.95679800	-3.90199800
H	-5.91139600	-2.20579400	-4.04704900
H	-7.21609300	-2.76882700	-0.82284800
H	-7.09425900	4.80470500	2.45689200
H	-7.19589100	3.36595000	3.44772600

H	-4.93745700	4.40370400	3.62426800
H	-2.99020900	1.91732800	1.79715800
H	-5.39024600	0.27111300	-3.30078200
H	-4.07597700	-0.75646700	-3.91374300
H	-4.21237800	0.91620600	-4.46691900
H	-4.97199500	1.09494500	-1.01614200
O	-3.12471800	4.16010000	-0.21206900
H	-4.61246600	1.65488000	1.14949000
N	-4.50288800	4.34577000	1.58299200
C	-4.44951500	5.79143400	1.47038500
H	-4.40826900	6.07373800	0.41641600
H	-5.36001300	6.22513100	1.89545500
C	-3.22909700	6.36488700	2.21576500
O	-2.52375100	5.67102900	2.94361000
N	-3.02323500	7.68758500	2.01435900
H	-2.25923700	8.14753100	2.49068200
H	-3.60391700	8.24115700	1.40036000
N	-7.13904500	3.04614100	1.36752500
H	-7.11902900	3.54738300	0.48724900
H	-4.83493900	2.78782000	2.95497300
C	-7.53895200	1.75065600	1.25593900
O	-7.88244300	1.27258000	0.17587300
C	-7.56199400	0.93354500	2.55999300
H	-8.46034300	1.19772200	3.12525400
H	-6.69575600	1.18920800	3.17588500
N	-7.56183300	-0.50445100	2.32919200
H	-8.57740700	-2.27726500	2.83729100
C	-9.76788300	-1.21325600	1.35841200
H	-10.77664300	-1.46560300	1.72290100
H	-9.79704400	-0.19076900	0.97201400
N	-9.30442800	-2.09529200	0.27780400
H	-9.78453100	-1.85768900	-0.58788200
H	-9.57054300	-3.05698200	0.48607700
O	-5.50465500	-0.24225100	1.43372400
H	-7.22194000	-3.02404900	1.44280000
Hg	1.07059800	1.05012600	-1.86490100
Hg	-1.17252800	-2.21757000	-0.70292900

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:

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P	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	7.30660200	0.15040100	-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	3.92444200	3.75231800	0.69499400
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	2.49417100	-1.27416700	2.35803900
C	4.23785100	0.17413900	1.65171600
C	5.29748800	-0.87281500	1.83218100
C	4.51702600	1.43703400	1.25792800
P	-8.45066500	-3.33867900	0.24616800
O	-9.14451400	-2.36948000	-0.69139100
O	-7.30189600	-4.19176500	-0.20943800
O	-7.87954200	-2.53950300	1.57130500
C	-8.67911700	-1.65706500	2.36321100
C	-8.15734800	-0.22537300	2.25912400
O	-6.80593700	-0.16266200	2.74373700
C	-8.14755700	0.29038600	0.81246200
O	-8.62322400	1.65713200	0.79380300
C	-6.68620300	0.16782300	0.39746200
C	-5.91231400	0.27460400	1.71521100
N	-4.69724400	-0.53916000	1.74817000
C	-3.44789900	0.06538200	1.94588900
O	-3.35327200	1.29128100	2.12827600
N	-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
P	-8.94663500	2.33721800	-0.66170000
O	-9.91730300	3.46996600	-0.42886300
O	-9.35006900	1.28215700	-1.68118300
O	-7.48501100	2.89265300	-1.15359500
C	-6.80163000	3.83366000	-0.30747500
C	-5.36786400	3.97772000	-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	-1.90968400	-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	-0.02728700	-3.55560800
H	7.24837000	-0.47072600	-0.67242600
H	5.28063600	0.97814900	-1.17315300

H	6.04377900	1.48291100	-2.68966000
H	4.69693300	-0.25974600	-3.55901500
H	5.81263200	-4.97076200	-0.41732700
H	4.20134300	-5.68828600	-0.65317200
H	4.59932700	-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	-1.42876800
H	6.65944400	5.62772200	1.08899700
H	4.09982700	6.55174600	0.32521200
H	5.60416600	3.72021100	2.07477800
H	4.39143800	4.96084600	2.46865400
H	2.98608600	4.30240300	0.60656100
H	6.27929800	-0.47256900	1.56886900
H	5.09833100	-1.74716700	1.20426700
H	5.32832700	-1.22803400	2.87014000
H	5.52640700	1.76311800	1.04089900
H	-9.73164600	-1.68687000	2.05898900
H	-8.60946300	-1.99533200	3.40244000
H	-8.78738400	0.42215900	2.88151800
H	-8.80431400	-0.31402500	0.19137100
H	-6.37648500	0.94497200	-0.29608800
H	-6.52765400	-0.80571700	-0.06942300
H	-5.58795600	1.29657500	1.91044800
H	-3.24968100	-4.41388100	0.29604300
H	-4.87037100	-4.47513900	1.02262100
H	-3.41895800	-4.79718600	2.01358100
H	-5.80587600	-2.26914100	1.39472300
H	-7.30319600	4.80750500	-0.35093400
H	-6.81009200	3.47615800	0.72820400
H	-4.89690200	4.77240800	-0.18205600
H	-6.14997500	4.63235400	-2.73079200
H	-4.12705000	5.63802700	-3.26604400
H	-4.03371900	3.21354200	-3.76764800
H	-5.47314800	2.37790400	-3.13290100
H	-2.89624600	3.03682900	-1.59301300
H	-4.79698500	-2.99022300	-3.00809600
H	-6.08515900	-1.78357100	-2.79935500
H	-5.54841500	-2.76798300	-1.42881200
H	-5.40487000	0.50900000	-2.30536400
O	9.90116900	-4.30481300	-0.35435000
H	9.27511600	-5.03625200	-0.21686200
O	-9.67386700	-4.23817800	0.88634600
H	-9.30532300	-4.94140300	1.44724400
Na	9.14530000	-0.95462000	1.96388100
Na	11.19960700	2.56074200	1.58707300
Na	-11.45792700	2.60543000	-2.00684400
Na	-9.07693700	-0.86818900	-2.32794000
O	-1.28034700	3.35452200	2.33112500
H	-0.49129600	3.18473900	1.78138300
H	-1.94260100	2.69291900	2.05634400
O	-0.13911500	-4.42745100	-1.85826500
H	-0.90751200	-3.84612500	-1.68757900
H	0.47895300	-4.26843100	-1.11686700
Hg	0.25619900	-1.28015300	-0.65535800
Hg	-0.28990000	0.17371400	1.86290200

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P	6.41009700	5.38752100	0.47741700
O	7.57276100	6.27130300	0.88357400
O	5.88548200	5.52759200	-0.93438600

O	6.76273800	3.79593600	0.64680800
C	7.10466900	3.25190500	1.92762300
C	6.69928500	1.78469600	1.96909100
O	5.26919600	1.67558300	1.93931000
C	7.21204000	0.94676500	0.78483300
O	7.41942600	-0.38756000	1.28736000
C	6.03775000	0.98285300	-0.18832700
C	4.84678600	0.94646100	0.77160000
N	3.60811800	1.52940600	0.27872600
C	2.39196300	0.88252600	0.58457600
O	2.38080200	-0.21013800	1.16635100
N	1.24790300	1.52571600	0.20734000
C	1.19676800	2.76415500	-0.39951000
O	0.10489900	3.28085800	-0.69918900
C	2.47446900	3.43601700	-0.64532600
C	2.47112300	4.80553600	-1.26388200
C	3.60725300	2.79570400	-0.27664900
P	8.20435000	-1.49118600	0.36560800
O	9.63703600	-1.06260100	0.11440500
O	7.43013000	-1.82098600	-0.90323600
O	8.20912000	-2.73893200	1.40985900
C	7.25628200	-2.96964700	2.46135400
C	6.03344600	-3.76468200	2.03180500
O	5.09417300	-2.92165200	1.34876600
C	6.32102000	-4.97833000	1.09094100
O	5.73271100	-6.18291100	1.58420600
C	5.58345100	-4.59156100	-0.19030000
C	4.43672900	-3.75115700	0.37697900
N	3.69210900	-2.92555000	-0.55083100
C	2.28413400	-3.00583500	-0.55429900
O	1.68969900	-3.80439900	0.18447000
N	1.63091400	-2.18764800	-1.42796600
C	2.23679800	-1.23830100	-2.22315200
O	1.55838200	-0.48355300	-2.94584700
C	3.69759300	-1.17500000	-2.18639400
C	4.39009900	-0.17123900	-3.06462000
C	4.35278200	-2.01380200	-1.35031400
H	8.18425700	3.34946700	2.09512400
H	6.57123700	3.78361900	2.72288300
H	7.07262800	1.35439700	2.90640000
H	8.14613400	1.33238300	0.36487700
H	6.07415200	1.91081500	-0.75953400
H	6.04910200	0.13539000	-0.86597700
H	4.60624600	-0.07957300	1.04929000
H	3.48723400	5.20485000	-1.33190100
H	1.85803400	5.49655000	-0.67191100
H	2.02816600	4.77976900	-2.26776700
H	4.57814800	3.25915600	-0.39104900
H	7.79646500	-3.55159000	3.21452500
H	6.94498800	-2.02126000	2.90638500
H	5.55981400	-4.15164400	2.94790000
H	7.39706900	-5.10857700	0.93005200
H	6.17354300	-6.41079400	2.41871400
H	6.23041800	-3.96975700	-0.81349000
H	5.24385200	-5.46783200	-0.74730200
H	3.69982300	-4.39100100	0.86674600
H	5.47585700	-0.30622000	-3.04542900
H	4.16515000	0.85420000	-2.74365100
H	4.04606600	-0.26071700	-4.10134400
H	5.43403500	-2.00688100	-1.24711700
O	5.18483400	5.58054300	1.55903100
H	5.47537100	6.18647000	2.26040600
C	-8.25658700	2.37432700	2.99710300
C	-7.21180500	0.28703600	2.08453000
C	-5.95765900	0.53492600	2.93160100
N	-4.82969400	-0.29094900	2.51562700
C	-3.70702800	0.32598800	1.95760800

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	-4.85534600	-1.65899000	2.70203200
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	-5.09150300	-3.26704900	-0.92583600
C	-5.87958500	-4.51871300	-0.66580300
C	-5.63852100	-2.02904700	-0.90328500
H	-8.72573800	3.21784000	2.47970100
H	-5.62279700	1.56827300	2.87352800
H	-4.78821700	-4.30477000	2.89441400
H	-3.05395300	-4.27680700	3.29199100
H	-3.56081800	-4.42036000	1.61129900
H	-5.79373000	-2.05117300	3.07295500
H	-8.87636900	3.34941400	-1.46747000
H	-8.58917700	3.07838500	0.24350200
H	-6.59198400	4.03278500	-0.98836600
H	-4.81690400	1.02878000	-0.35495700
H	-6.94409000	-4.29641600	-0.54105400
H	-5.52526200	-5.02372000	0.24045300
H	-5.76753700	-5.23266000	-1.49023900
H	-6.68396800	-1.85660700	-0.67849200
O	-5.40240600	0.63568700	-3.37541800
H	-6.42158400	0.29364000	-0.42481600
N	-6.31986800	2.36004200	-2.20685500
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	-3.82360900
O	-5.27179000	5.15814300	-3.69292800
N	-4.26710200	3.19520800	-4.29178100
H	-3.37168300	3.64457800	-4.43211700
H	-4.31280500	2.18161800	-4.25705900
N	-8.69920300	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	-0.01680100	1.88761000
H	-10.14037300	1.69131700	1.50475400
N	-8.18161700	1.24712300	2.05525400
H	-7.24696500	2.69496700	3.25884900
C	-9.05462400	2.04699300	4.26668700
H	-9.20265600	2.98823600	4.81979900
H	-10.04982500	1.68969400	3.98037700
N	-8.39403100	0.99251800	5.04418700
H	-9.05469300	0.58706500	5.70387100
H	-7.65425500	1.40315400	5.61228000
O	-7.33379500	-0.75919200	1.44002200
H	-6.22070400	0.31299400	3.96954300
Na	9.25974300	-1.15204500	-2.23409700
Na	7.51125300	7.26330700	-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	-1.30036200	-4.42694500	-3.66595800
H	-1.81419800	-4.95072400	-2.32760800
Hg	-0.66160500	-2.24791400	-1.43828500
Hg	-0.74791700	0.54685800	0.74363200

pTTTT_P

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	-2.86653200	-0.91456400
C	-3.32548700	-3.31847100	-1.95829500
O	-2.84028100	-3.47180200	-3.09626900
C	-4.73569700	-3.58012900	-1.67271700
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	1.65616600	-0.35864400
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	-3.53931300
C	-3.69162300	0.41415000	-2.40460800
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	-3.58589000
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	-5.47908000	-0.52635900	-3.15386000
H	-3.96632200	-1.32634400	-3.63671100
H	-4.44217300	0.18424500	-4.40866000
H	-5.33079600	0.79141600	-1.07981300
O	-4.56061900	4.16100100	-0.79817800
H	-5.04396600	1.59425700	1.09159000
N	-5.93226500	4.14490400	1.01611000
C	-6.45217400	5.44537400	0.63983200
H	-6.51056300	5.51148000	-0.44856600
H	-7.46658600	5.55963500	1.03513900
C	-5.57003700	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	1.89393100	1.25371700
H	-8.10606600	2.18363900	0.32530600
H	-5.58693100	2.91829500	2.68673200
C	-7.66069100	0.54905300	1.38388600

O	-7.86946300	-0.21901700	0.44645800
C	-7.21666600	0.05093200	2.77161600
H	-8.07636800	0.07744000	3.44729400
H	-6.45463000	0.71970200	3.18131000
N	-6.68992600	-1.30658700	2.74144500
H	-6.88964800	-3.20046200	3.63977100
C	-8.60201400	-2.88996700	2.33515800
H	-9.38191000	-3.39007100	2.93141400
H	-9.06052100	-2.02912400	1.84055500
N	-8.02289400	-3.75440600	1.29812000
H	-8.69695500	-3.88565700	0.54624700
H	-7.85462900	-4.68308700	1.68370300
O	-4.97368900	-0.50344900	1.50683200
H	-5.54179000	-3.66573300	2.16804000
C	8.35620000	3.53565300	1.61090000
C	6.05345600	2.48426900	1.53874700
C	5.56666700	3.40588400	0.41725600
N	4.92216000	2.60081400	-0.61925000
C	3.53468100	2.43728400	-0.61451300
O	2.84224100	3.00322200	0.25454500
N	3.00709300	1.66185800	-1.60189000
C	3.74160200	1.05289000	-2.60335900
O	3.17309100	0.42869600	-3.51643900
C	5.19742800	1.18372600	-2.52931200
C	6.04747500	0.50494100	-3.56416400
C	5.71587500	1.94736300	-1.53995800
C	6.48659000	-0.89779300	4.35963200
C	4.99566000	-0.94350000	3.98931400
C	4.28462200	-2.34369900	2.01215400
C	4.48139600	-1.14588100	1.06444400
N	3.88919200	-1.44781200	-0.22827100
C	2.49530800	-1.44401800	-0.30195400
O	1.83220700	-1.00026300	0.66120000
N	1.92468500	-1.94339200	-1.42794000
C	2.63403200	-2.48227100	-2.48367500
O	2.04480500	-2.93714500	-3.47982500
C	4.09267300	-2.51983000	-2.35838900
C	4.88984400	-3.11716600	-3.48085600
C	4.64376600	-2.01901700	-1.23007900
H	8.89948000	3.82542700	2.51629400
H	4.81372900	4.07833700	0.83048600
H	7.10877100	0.72450100	-3.40910500
H	5.76928300	0.82958400	-4.57414500
H	5.90973600	-0.58025400	-3.53251200
H	6.78416800	2.11319100	-1.40360500
H	6.76307200	-1.76404600	4.96855000
H	6.68624800	-0.01364900	4.96675500
H	4.37785700	-0.84855100	4.88762300
H	4.01820300	-0.24463200	1.45632400
H	5.96088700	-3.12121400	-3.25429800
H	4.73422300	-2.55363100	-4.40897300
H	4.57204900	-4.14732000	-3.68098600
H	5.71469800	-2.01793500	-1.05603600
O	3.84708300	-3.41138900	1.57988700
H	5.54329100	-0.92597200	0.92912400
N	4.63411500	-2.19963300	3.32527700
C	4.33421700	-3.32837200	4.19223100
H	4.60091200	-4.26024400	3.69053200
H	4.93869600	-3.25309700	5.10149100
C	2.84860000	-3.33041600	4.59818300
O	2.16720200	-2.30874000	4.56204500
N	2.38571300	-4.52002600	5.04934000
H	1.41565100	-4.59409800	5.32534000
H	2.92283200	-5.37241900	4.97717500
N	7.34046800	-0.90076200	3.17352900
H	7.38741000	-1.78786300	2.68205800
H	4.77433100	-0.09447200	3.34510800

C	7.66585000	0.15209000	2.37131600
O	8.03011900	-0.02130000	1.20713100
C	7.67844900	1.55758700	2.99628200
H	8.69867600	1.74890900	3.33964700
H	7.01605500	1.63169300	3.85929500
N	7.31808600	2.58092200	2.01968600
H	7.88653600	4.44773500	1.23678800
C	9.34501700	2.97284400	0.58210200
H	10.26479700	3.57743300	0.62987000
H	9.60037000	1.94949500	0.87153400
N	8.74965400	2.92786400	-0.75935800
H	9.32833900	2.35635100	-1.37213500
H	8.75244900	3.86202700	-1.16774700
O	5.27192500	1.63500200	1.98460800
H	6.36047100	3.98711200	-0.04589200
O	0.36253500	-3.32147700	1.58216500
H	0.91162800	-2.53980200	1.37391900
H	-0.55183100	-2.97483000	1.51835600
O	0.45191000	4.42852600	-0.34868100
H	1.27880500	3.95242600	-0.12488500
H	-0.25099600	3.80606500	-0.07038700
Hg	-0.38780400	-2.17571600	-1.45886300
Hg	0.70981900	1.37297600	-1.65599000

Cartesian Coordinates of optimized geometries of single canonical base pairs and mispair using B3LYP-D3/6-31G* level of theory in the gas phase:

dAT_D

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	1.60293800	-0.71521600
O	7.36165700	1.15462500	-0.84903200
C	8.94520200	1.88075300	0.80090900
O	8.76643300	3.25832000	1.11565600
C	7.78104400	1.13115300	1.44858500
C	6.69944100	1.35199500	0.39042900
N	5.55543200	0.45128600	0.44381400
C	5.55399800	-0.93748600	0.49903700
N	4.34367000	-1.45471300	0.44444900
C	3.51660400	-0.36246800	0.33497300
C	2.11550200	-0.27944300	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	4.24630900	0.82977600	0.32430000
P	-8.64289100	-2.29117600	0.39103900
O	-10.10037200	-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	-0.77664800
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	-0.29146500

N	-2.69620000	0.73894500	-0.15885200
C	-2.76628400	-0.63774500	-0.07353800
O	-1.68910100	-1.27555300	0.01290800
C	-4.09504600	-1.20746400	-0.09166600
C	-4.26475600	-2.70016000	-0.01979800
C	-5.13693800	-0.33188700	-0.15969700
H	9.27339800	0.23848800	-2.28489800
H	10.65299300	1.00096600	-1.45045000
H	8.83880200	2.54136800	-1.27725300
H	9.91930400	1.51026600	1.14168100
H	9.48820400	3.76626200	0.71351000
H	8.01750700	0.06717400	1.53529700
H	7.52411400	1.54978800	2.42380700
H	6.28499400	2.36433600	0.45729700
H	6.48234700	-1.49789600	0.57968000
H	0.32441400	-1.37869400	0.15871400
H	1.92960000	3.04673900	0.04652500
H	-10.02975600	0.29551200	0.87204400
H	-8.72979400	0.02521900	2.06317700
H	-8.80588500	2.39050800	1.33612000
H	-9.34568300	1.58047100	-1.26320600
H	-8.75188400	3.80998700	-1.66037500
H	-6.88326000	2.28057300	-2.26366700
H	-7.17743100	0.62266000	-1.68165800
H	-5.81908600	2.92327100	-0.18754300
H	-3.67902600	-3.18992000	-0.80619800
H	-5.31604900	-2.97914100	-0.14101300
H	-3.89279000	-3.08999500	0.93605000
H	-6.16370000	-0.67843900	-0.14698200
H	1.81368100	-2.26501800	0.30695300
O	8.11173900	-1.84868500	-1.82907200
H	8.41876300	-2.44405700	-2.53272700
O	-8.28928100	-2.50755800	1.97183100
H	-7.33071700	-2.61699800	2.08463100
Na	-9.46986400	-4.12656700	-1.35872600
Na	9.57444700	-4.05853800	1.11653900
Hg	-0.61240300	1.22736500	-0.04917200

dGC_D

O	-7.75742400	-1.40816700	0.12710700
C	-7.71047800	-0.60387200	-1.04667400
C	-7.94372400	0.85661800	-0.64274700
O	-7.15791000	1.24563600	0.50103600
C	-7.49454900	1.83264700	-1.74493200
O	-8.06445200	3.11912000	-1.58848200
C	-5.99768400	1.97827500	-1.43799000
C	-5.94090600	1.79524800	0.09468100
N	-4.82770100	0.86493800	0.51723000
C	-3.53070400	1.22038500	0.24464600
O	-3.23179100	2.30099800	-0.34074600
N	-2.53338000	0.38564900	0.60693200
C	-2.73910400	-0.79878700	1.21526800
N	-1.66393000	-1.54238700	1.48161900
C	-4.07952900	-1.16840900	1.53900300
C	-5.07485200	-0.30787900	1.18697300
P	7.15957700	-2.40170500	-1.25866600
O	8.23657300	-2.63763400	-2.31239200
O	6.34408400	-3.63156000	-0.91774100
O	7.87164600	-1.85368500	0.13250700
C	8.94508900	-0.91451800	0.01751100
C	8.51397100	0.44155000	0.54991400
O	7.36057500	0.91715700	-0.18090700

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	-7.67055600	1.42727200	-2.75284000
H	-9.02431000	3.05977100	-1.71718000
H	-5.41310000	1.20473400	-1.94282500
H	-5.62397600	2.95294000	-1.75026500
H	-5.76841500	2.73233700	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	2.52996400	0.30170500
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

$\mathbf{dT_Td}$

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
O	-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

C	-2.90715500	0.93832000	0.10746200
O	-2.38680300	1.71657500	0.90233300
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	-1.89758800	-2.65424000
C	-4.86601500	-0.08181700	-0.92634700
P	8.27438800	1.02731300	0.54519200
O	9.38603700	2.05634800	0.61679300
O	7.94691400	0.61733000	-0.89948700
O	8.67167300	-0.35437900	1.33732100
C	8.06174000	-0.76786900	2.56031700
C	6.84666100	-1.64972200	2.30272600
O	5.77083900	-0.85417200	1.75611700
C	7.09886900	-2.79791600	1.29160100
O	6.59405800	-3.98491100	1.90073200
C	6.27991100	-2.37022000	0.06660900
C	5.11325100	-1.64738500	0.73845200
N	4.29062800	-0.79064100	-0.08305000
C	2.88659000	-0.89339200	0.05129000
O	2.34828600	-1.72624900	0.77408000
N	2.17588100	0.00035300	-0.70499200
C	2.68494600	0.98635100	-1.53146000
O	1.89375800	1.72226300	-2.14190400
C	4.13809300	1.06923100	-1.61098000
C	4.76625300	2.12882100	-2.47036100
C	4.86143300	0.18074800	-0.88990000
H	-7.74523000	-0.41338800	3.15194600
H	-8.81436400	1.00646800	3.20393800
H	-6.54303000	1.79091000	3.40805100
H	-8.22879000	2.71620400	1.27440900
H	-5.89346500	3.90854200	2.32025500
H	-6.89079800	1.71321800	-0.42477900
H	-6.03075300	3.27548100	-0.26344700
H	-4.45624200	2.26343800	1.38080100
H	-5.82805900	-1.89120800	-2.56052900
H	-4.36786500	-2.90658800	-2.43765600
H	-4.46445200	-1.67872800	-3.69368300
H	-5.95109800	-0.12013600	-0.95292400
H	8.81037800	-1.35421100	3.10305700
H	7.78176300	0.09370300	3.17576800
H	6.51504600	-2.09244200	3.25071900
H	8.16639400	-2.89346200	1.05771600
H	6.71966400	-4.71784800	1.27804800
H	5.95350300	-3.21859100	-0.54262100
H	6.86553900	-1.67852700	-0.54632000
H	4.43639100	-2.35556700	1.21858300
H	4.49321400	1.99599600	-3.52424700
H	5.85673200	2.09837300	-2.37621000
H	4.41215200	3.12377500	-2.17687000
H	5.94680200	0.20318800	-0.91345400
O	-6.91262100	-1.72385900	1.19064000
O	6.97682400	1.58353500	1.33335600
H	-6.25860000	-1.00600000	1.34975700
H	6.30502000	0.87172600	1.44253400
Hg	-0.00086000	0.06373200	-0.75451600
Na	-9.45340700	-2.03236700	-1.73569800
Na	9.48668200	2.06949200	-1.58623000

pAT_P

C	7.96129500	2.10214000	2.46775600
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N	1.28357400	-0.62863800	-0.30550600
C	2.03014700	0.53008100	-0.34598900
N	3.29604500	0.63270400	-0.65059000
C	3.86266300	-0.55657900	-0.94193800
C	3.22553100	-1.79943800	-0.94444700
C	1.85824100	-1.84088600	-0.60651000
N	1.17136800	-2.98861300	-0.58218700
N	4.09498100	-2.80861600	-1.28226600
C	5.23288000	-2.18355900	-1.47573400
N	5.15184800	-0.81135900	-1.31383800
O	8.53246500	3.18206900	2.42392800
C	9.82943600	0.85831600	-1.32131400
C	8.67827700	1.62775400	-0.64083000
N	7.97760300	0.82755500	0.37603500
C	8.52647800	0.87266600	1.73991600
C	6.80225200	0.18253500	0.19428200
O	6.16604400	-0.35778500	1.10068000
C	6.25275800	0.13132200	-1.25169800
H	1.48727900	1.43701600	-0.09548300
H	6.16608600	-2.65784700	-1.75034000
H	10.50976100	0.47575200	-0.55116200
H	7.96768100	1.98582100	-1.39292500
H	9.06123600	2.51939100	-0.13264900
H	8.28381300	-0.06305200	2.24658000
H	9.60949400	0.98463500	1.67553000
H	1.68071900	-3.83399100	-0.80915100
H	0.19187000	-3.08374600	-0.32048600
H	7.01556000	-0.17071100	-1.97320900
H	5.87223800	1.11352600	-1.54678500
C	-5.77388400	3.13582800	-2.14131500
N	-5.22104300	-1.13566800	0.94089900
C	-4.03968700	-0.40541500	0.80961700
O	-4.01018100	0.82400500	0.84597100
N	-2.91758600	-1.17465500	0.63603100
C	-2.87206900	-2.54553400	0.45811900
O	-1.75076200	-3.06154500	0.22274800
C	-4.12608000	-3.25354800	0.54054600
C	-5.23915200	-2.49509800	0.74734800
C	-4.14478700	-4.74468700	0.35360300
O	-5.79609800	3.93442800	-3.06355200
C	-7.38187800	2.42434800	0.56043200
N	-7.00113000	1.57896700	-0.58060500
C	-6.97884100	2.20983400	-1.89940800
C	-6.56260700	0.29515000	-0.48315600
O	-6.21058900	-0.38714800	-1.44160000
C	-6.45149900	-0.34005900	0.92159900
H	-6.22446200	-2.94604000	0.78049100
H	-9.51098800	2.17256200	0.29337700
H	-6.62571200	2.35680300	1.35188600
H	-7.35416000	3.46048900	0.21089500
H	-6.96190600	1.42759700	-2.66029600
H	-7.88178700	2.80814400	-2.04571900
H	-3.54008700	-5.24230000	1.11999300
H	-5.16424900	-5.13647900	0.40930600
H	-3.72138300	-5.01813300	-0.61902400
H	-7.29804700	-1.01062100	1.08456100
H	-6.41167400	0.37727500	1.73899800
N	-4.72279200	2.99758200	-1.28304300
H	-4.66147600	2.28175900	-0.56980700
H	-3.91700600	3.58100200	-1.45747200
H	-8.81621400	1.06887400	1.46605800
C	-8.78606200	2.10864200	1.11350400
N	-9.23039300	2.97191000	2.19751800
H	-9.30655500	3.93827000	1.88678500
H	-8.57195500	2.95826300	2.97411100
N	6.77430200	1.87882700	3.09717800
H	6.28668200	2.67908700	3.47756100

H	6.25669800	1.02891700	2.90933100
H	9.42264200	-0.02514300	-1.83229100
N	10.60631500	1.63160600	-2.27713100
H	11.07455300	2.41229700	-1.82175500
H	10.01531100	2.02104900	-3.00894500
Hg	-0.88303900	-0.57070900	0.22903600

pGCp

C	-6.08445700	0.11716900	1.36863900
C	-6.92152700	-0.11913700	0.09150600
O	-6.43833700	-0.75729200	-0.84420200
C	-8.97268400	0.17835900	-1.14991600
C	-8.64395700	1.28456600	-2.16482200
O	-9.27605400	2.33147500	-2.18998800
N	-8.18269300	0.38821000	0.07360400
C	-8.74954800	1.32542200	1.05789200
C	-9.81971300	0.66396200	1.94801700
N	-9.38349800	-0.46588200	2.76002800
N	-4.84180500	-0.61557500	1.29832500
C	-4.64619100	-1.97345900	1.52700300
N	-3.44754600	-2.39178900	1.22309700
C	-2.81488500	-1.26321400	0.73250000
C	-1.50759400	-1.04539800	0.24746200
O	-0.54516500	-1.86585600	0.15094200
N	-1.25305100	0.26913600	-0.16149500
C	-2.18467400	1.26643800	-0.09700300
N	-1.78013200	2.52172800	-0.48450400
N	-3.41925700	1.10537500	0.35611000
C	-3.67363900	-0.15274300	0.75886500
H	-5.83797800	1.17824400	1.46828400
H	-6.63958700	-0.18661500	2.25974000
H	-10.03138300	0.25562000	-0.90082500
H	-8.75912600	-0.81926200	-1.53764100
H	-7.94866500	1.73541900	1.67857900
H	-9.17829400	2.16372300	0.49565500
H	-10.23363300	1.43208200	2.61170600
H	-10.65128300	0.32358200	1.31919000
H	-5.44146200	-2.58556200	1.93242300
H	-1.10167400	2.57324000	-1.23243100
H	-2.54062000	3.18445100	-0.57252700
C	6.00547400	-0.47268400	-0.98550900
C	6.30337600	0.29341000	0.32200800
O	5.50940100	0.22557300	1.26446600
C	7.76412200	1.74012000	1.59885900
C	7.13398300	3.13883800	1.50723600
O	7.74734100	4.07788400	1.02208100
N	7.45989200	0.99691300	0.36744900
C	8.35847900	1.21369200	-0.77760700
C	9.57973500	0.28761700	-0.73999500
N	9.15592300	-1.12153400	-0.65350000
N	4.89946400	-1.39770400	-0.74105800
C	3.61204700	-0.90652900	-0.71588800
N	2.61370000	-1.71062100	-0.29249400
C	2.80289700	-2.96320700	0.14939300
C	4.13928300	-3.48623500	0.15875900
C	5.13492500	-2.66499400	-0.27064700
O	3.32354200	0.25873400	-1.09824600
N	1.73156400	-3.64198600	0.55498600
H	5.70009800	0.21990000	-1.77276300
H	6.88486200	-1.03384100	-1.31335200
H	8.84570000	1.86071400	1.67598500
H	7.39568100	1.16971100	2.45340300

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	-4.48894500	0.50583400
H	6.17516500	-2.97043300	-0.27670100
H	0.80493500	-3.20441500	0.51970500
H	1.81340500	-4.58884800	0.89605700
N	-7.58468600	1.00165800	-2.97390300
H	-7.23444900	1.74936500	-3.55813200
H	-6.96468000	0.23816800	-2.72821200
N	5.85077100	3.20104700	1.95940100
H	5.33779600	2.34689800	2.13979000
H	-8.97197900	-1.19415300	2.18066700
H	-8.69717200	-0.18693100	3.45749100
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	-1.90861300	0.15396700
C	-3.23983700	-2.80467500	-0.40489300
O	-2.83587100	-3.88591200	-0.83539100
C	-4.62763600	-2.33893500	-0.45035600
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	-2.05650500
H	-5.72062700	-4.18899600	-0.45702200
H	-5.30148000	1.27809700	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	-0.20004200
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

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	2.93337300	2.19127300
H	2.85706900	4.22598200	1.17181500
H	4.83305300	-5.11176500	0.54384300
H	5.99561900	-3.90455200	1.14376900
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	2.93160400	3.57885700	-3.74121400
H	1.99455300	4.61575700	-2.93832500
Hg	-0.21308000	-2.37466800	-0.02669600

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