Interaction of Osmium(II) redox probe with DNA: Insights from theory.

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Supporting Information

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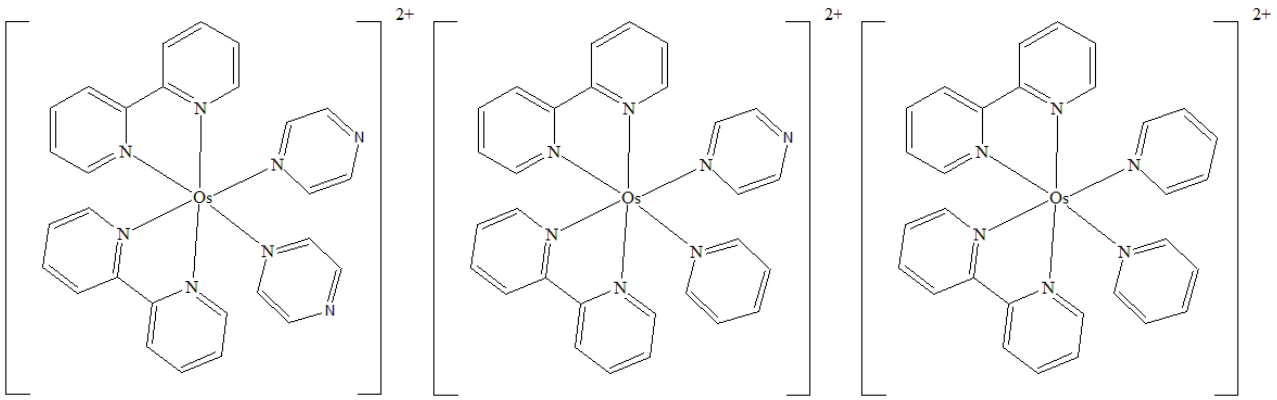
I. Molecular Dynamics simulation of the B-DNA dodecamer

The initial structure of the B-DNA dodecamer (Drew–Dickerson dodecamer)[1] with 12 base pairs (bp) d(CGCGAATTCGCG)$_2$ was obtained from Nucleic Acid Database (http://ndbserver.rutgers.edu/)[2] with PDB code 1BNA. The structure of the DNA was subjected to molecular dynamics simulation for energy minimization by GROMACS.v.5.0.5 simulation tool[3] (www.gromacs.org) using the PARMBSC0 refinement of the parm99 force field[4]. The DNA was inserted into a cubic box of 1.5 nanometer on each side of the DNA, using periodic boundary conditions and simulation box was solvated with 13408 water molecules using TIP3P/SPC water model[5] . The negative charge of the phosphate groups (-22) in the DNA was neutralized by adding 22 Na^+ counterions , while other 25 Na^+ and Cl^- ions were added to set the solution ionic strength to about 100 mM. Furthermore, complete system was set to energy minimization for 1000 steps using steepest descent method to remove excessive strain. Minimized system was further subjected to three steps real molecular dynamics simulations. First, the system was heated to constant temperature of 298.15 K via NVT (Constant number of particles N, volume V and temperature T) ensemble dynamics for 100 picoseconds (ps) (time steps, dt=0.002 and nsteps =50000) with leap-frog integrator. During the dynamics, temperature was kept constant at 298.15 K with the help of Berendsen thermostat[6]. Second, the NVT was continued with NPT (Constant number of particles N, pressure P and temperature T) ensemble dynamics for 100 ps where the pressure coupling of 1 bar was provided with Parrinello-Rahman method[7]. Third, the well equilibrated system was then subjected to final production molecular dynamics for 10 nanosecond (ns). The total number of atoms in the system was 41198 for Molecular dynamics.

II. Parameterization of the Os(II) probes for MD simulations:

The General Amber Force Field (GAFF) parameters[8] for Os(II) probes were developed by using the Paramfit program[9] that is designed to address derivation of bonded and dihedral terms in the AMBER[10, 11] equation. Paramfit program is able to refine parameters in the bonded terms such as bond k_r and angle force constants k_θ, equilibrium bond length r_{eq}, equilibrium bond angle θ_{eq}, dihedral barrier height V_n, phase γ and periodicity n.

In this parametrization process, we have considered six different compounds, $Os[(bpy)_2dppz]^{2+}$, $Os[(bpy)_2phen]^{2+}$ and $Os[(bpy)_3]^{2+}$ as well as three other complexes represented on Figure S.1. It is important to note that there is no X-Ray structure available in the literature for Os complexes with an octahedral arrangement and we will thus use quantum mechanical calculations (DFT calculations) as reference data.



$Os[(bpy)_2(pz)_2]^{2+}$ $Os[(bpy)_2(py)(pz)]^{2+}$ $Os[(bpy)_2(py)_2]^{2+}$

Figure S.1. Os(II) complexes used for parametrization (with py= pyridine and pz=pyrazine).

In the first step of the parameterization process for the Os(II) probes by Paramfit, we considered each Os complex separately. The initial *frcmod* topology file was created containing the guess parameters to be fit. These guess parameters for the Os(II) probe were obtained from the reported Ruthenium parameters for $[Ru(phen)_3]^{2+}$ compound[12]. The geometry of the Os(II) complexes were optimized with the help of DFT calculations carried out with Gaussian 09 suite. We used the B3LYP exchange-correlation functional with the 6-31G(d) basis set on C, H, and N atoms and the LANL2DZ basis set and corresponding effective core potential for Osmium. These optimized structures were used to calculate, with the same level of theory, the Electrostatic Surface Potential (ESP) fit[13] relying on the electrostatic charge computing method developed by Merz and

Kollman[14, 15]. It uses a Connolly surface algorithm to calculate a number of shells with radii of 1.5 times the van der Waals radius of the constituent atoms in the molecule. This ESP was further used to calculate the Restrained Electrostatic Potential (RESP) charges of Os(II) probes as described by the[16]. These Gaussian outputs were invoked to xleap program for generating initial parameter files *prmtop* using the initial *frcmod* file.

Next, for each complex, a variety of molecular structures were generated by molecular dynamics simulations in vacuum These MD simulations were completed in two steps:(1) Simulation at 600 K (t = 100000 and dt = 0.001), and (2) Simulation at 1000 K (t = 100000 and dt = 0.001) where force constants were halved in order to explore a large conformation space. These molecular structures (Total = 2000) were further subjected to single-point QM energy calculations, using the computational strategy described above. We further run the Paramfit process to conduct least squares fitting to QM energies. During the fitting process, Paramfit program optimizes parameters so that the least squares difference between the input quantum energies and calculated AMBER energies over all the input structures is minimized, using the following equation:

$$f(N, E_{QM}, K) = \sum_{i=1}^{N} \left[(E_{MM}(i) - E_{QM}(i) + K)^2 \right] \qquad \text{(Eq 1)}$$

Where N is the input set of structures, E_{QM} is the set of quantum energies of those structures, E_{MM} is the calculated AMBER energy of those structures, and K is a system-dependent constant term. The fit was conducted using the genetic algorithm (GA) with the following important settings: the number of generation to converged was set to 10, mutational rate 0.05, search space for parameter search 0.5, bond limit 0.1, angle limit 0.3141 and dihedral span of 12. After the fitting process by GA, we obtained the fitness function R^2 close to 0.95-0.96 for the parameters. To improve the fitness function, we performed the “weighting structure Paramfit” meaning that a weight of 0 was assigned to the structures presenting a large deviation in the energies from the average of QM energies. These structures were ignored during the next steps of Paramfit process. After the weighted fit, the fitness function R^2 was improved to 0.96-0.97 for the parameters.

Subsequently, multiple molecule fits were conducted for these six Os(II) probes in order to generate more broadly applicable parameters that can describe a whole class of Os(II) molecules. After the weighted fit, the fitness function R^2 reached a 0.98-0.99 range for all the parameters.

Table S.1. Molecular Dynamics parameters (to be used with AMBER GAFF force fields) of the Os(II) compounds within octahedral complex. Atom type Os (Osmium , defined as Om in the force field in order to distinguish from the oxygen Os atom type), n_x, n_y and n_z are given to Osmium and nitrogen coordinating sphere, "ca" for aromatic carbon, "cp" for carbon connecting the pyridine ring and "h4" for the hydrogen atom attached to aromatic carbon.

Bond parameters: $\Sigma_{bonds}\ k_r\,(r-r_{eq})^2$

	force constant (k_r) kcal/(mol.Å^2)	equilibrium bond length (r_{eq}) (Å)
$[n_x\|n_y\|n_z]$-Os	203.94	2.14

Angle parameters: $\Sigma_{angles}\ k_\theta\,(\theta-\theta_{eq})^2$

	force constant (k_θ) kcal/(mol.rad^2)	equilibrium bond angle (θ_{eq}) degrees
Os-$[n_x\|n_y\|n_z]$-ca	61.22	120.54
Os-$[n_x\|n_y\|n_z]$-cp	63.11	122.15
$[n_x][n_y][n_z]$-Os-$[n_x][n_y][n_z]$	15.17	180.00
$[n_x\|n_y]$-Os-$[n_z]$; $[n_x\|n_z]$-Os-$[n_y]$; $[n_y\|n_z]$-Os-$[n_x]$	42.97	92.35

Dihedral parameters: $\Sigma_{dihedrals}\ V_n/2\ .\ [1 + cos(n\Phi - \gamma)]$

	multiplication factor	force constant ($V_{n/2}$)(kcal/mol)	phase angle (γ) degrees	periodicity (n)
Os-$[n_x\|n_y\|n_z]$-ca-h4	1	-0.63	180.00	-0.30
Os-$[n_x\|n_y\|n_z]$-ca-ca	1	0.05	180.00	1.56
Os-$[n_x\|n_y\|n_z]$-cp-ca	1	-4.93	180.00	2.91
Os-$[n_x\|n_y\|n_z]$-cp-cp	1	-0.18	180.00	0.61
$[[n_x\|n_y],[n_x\|n_z],[n_y\|n_z]$-Os-$[n_z],[n_y],[n_x]]$-cp	1	-1.72	180.00	1.44
$[[n_x\|n_y],[n_x\|n_z],[n_y\|n_z]$-Os-$[n_z],[n_y],[n_x]]$-ca	1	-0.74	180.00	1.04
$[[n_x][n_y][n_z]$-Os-$[n_x][n_y][n_z]]$-cp	1	1.04	180.00	1.42
$[[n_x][n_y][n_z]$-Os-$[n_x][n_y][n_z]]$-ca	1	0.25	180.00	1.71

r_{vdw} and ε_{well} parameters of the van der Waals term

Osmium Os(II)	r_{vdw} = 2.35 Å ε_{well}=0.691 kcal/mol	Mass = 190.23 g/mol

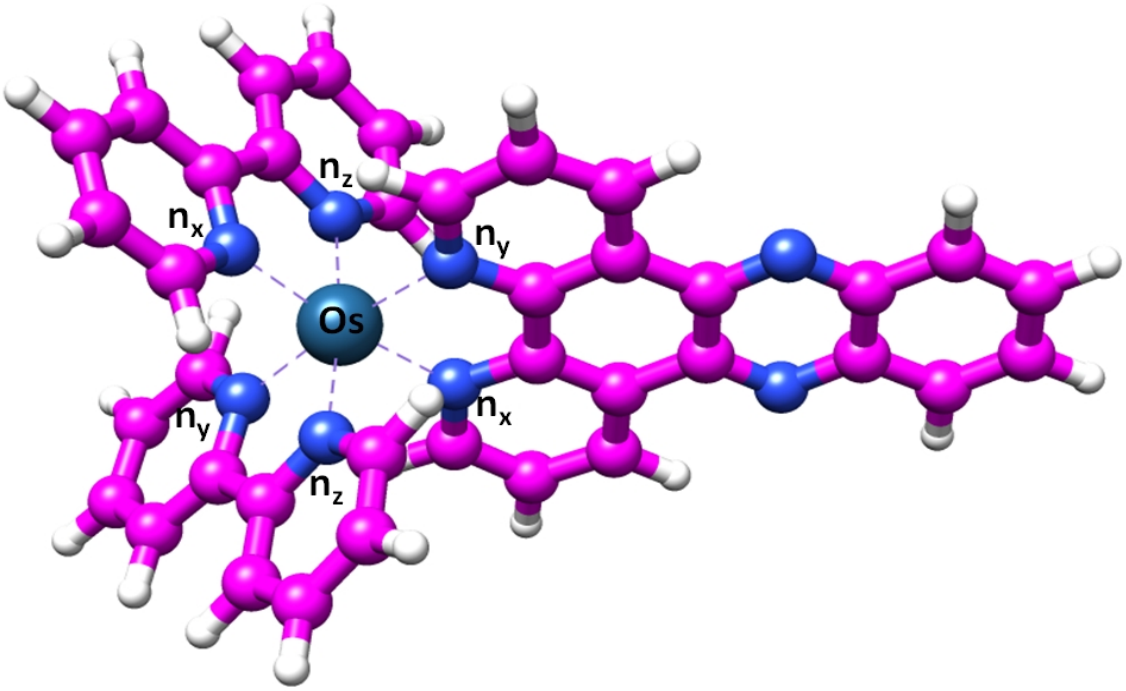


Figure S.2. 3D structure of the $Os[(bpy)_2dppz]^{2+}$ octahedral complex with "cross-Osmium" nitrogen atoms of atom type "n_x, n_y and n_z (light blue) ",of bpy and dppz group, "Os" for osmium (dark blue). All aromatic carbon atoms "ca and cp" are in magenta and hydrogen atoms "ha and h4" are in white.

III. Calculation of the binding energy with QM/QM' calculations

The interaction energy between DNA and Os(II) probe produced by QM/QM' calculation is described as:

$$\Delta E_{(\text{Interaction energy})} = E_{(\text{Probe/1BNA})} - E_{(\text{1BNA})} - E_{(\text{Probe})}$$

The calculation of the binding energy in the case of $Os[(bpy)_2dppz]^{2+}$ is given in Table S.2 for the probe intercalated into the major groove.

Table S.2. $Os[(bpy)_2dppz]^{2+}$: intercalation in the major groove: DFT energies (in Hartree), in vacuo and in water, for $Os[(bpy)_2dppz]^{2+}$, 1BNA and the complex $Os[(bpy)_2dppz]^{2+}$ / 1BNA. Thermal corrections of the enthalpy obtained by QM/QM' calculations of the harmonic vibrational frequencies are also given.

Model system	**DFT energy (vacuo)** **model system, high layer**	**DFT energy (solution)** **model system, high layer**	**Thermal correction to Enthalpy (vacuo)**
$Os[(bpy)_2dppz]^{2+}$	-1991.603127	-1991.781135	0.610
1BNA	-2763.365536	-2763.408081	0.686
$Os[(bpy)_2dppz]^{2+}$/ 1BNA	-4755.038715	-4755.209780	1.299

IV. Detailed analysis of intercalated binding modes for Os[(bpy)$_2$dppz]$^{2+}$ complex: time evolution

IV.1 . DNA structural properties:

IV.1.2. Major Groove

Figure S.3 shows that some degree of fluctuation was observed for the distances between the nitrogen atoms N1 of the Adenine bases and N3 atoms of thymine bases during the MD simulation of 10 ns, before and after the Os(II) probe intercalation in the major groove. MD simulation of the DNA alone predicts that the distances between the nitrogen atoms of the Adenine (Black) and thymine (Red) bases are found to be constant with average distance of 3.7 Å (Standard deviation = ± 0.3) with respect to MD simulation time of 10 ns. Note that the average was conducted for 2000 snapshots produced during MD simulation of 10 ns. Nevertheless, the nitrogen atoms distances underwent some fluctuation during the MD simulation, they explain same trends and the average distances remain constant between the nitrogen atoms of the Adenine (Black) and thymine (Red) bases.

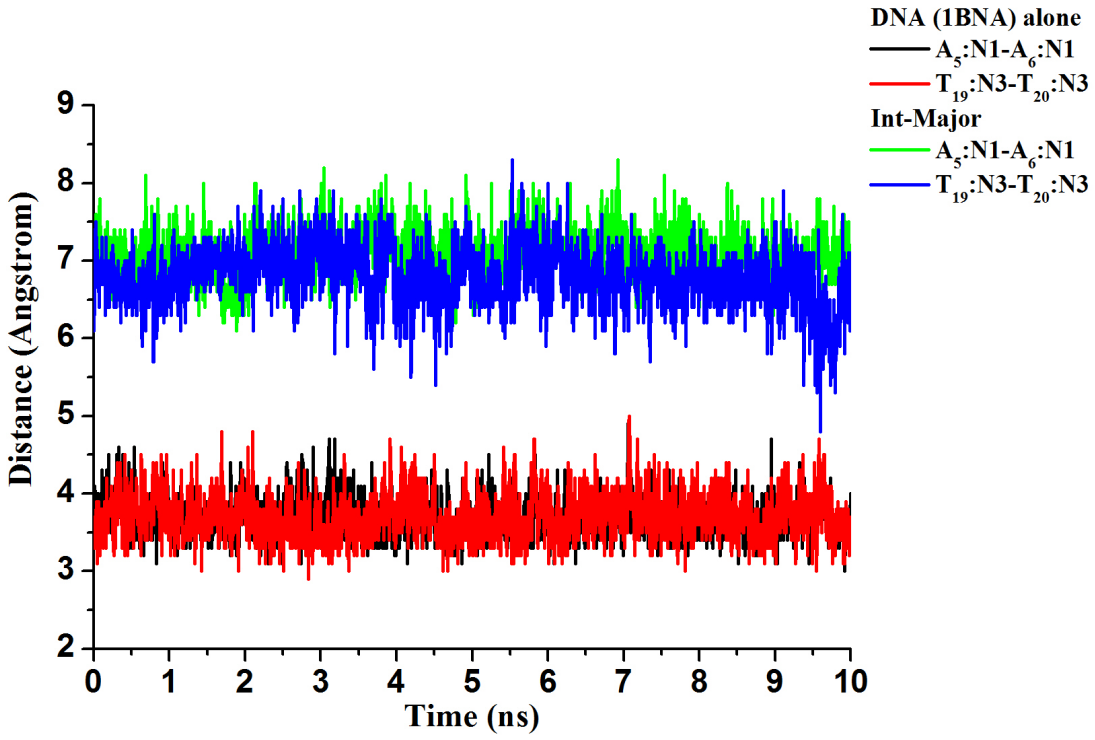


Figure S.3. Time evolution of the distances between the nitrogen atoms N1 of the Adenine bases and N3 atoms of thymine bases during the MD simulation, before and after the Os(II) probe intercalation in the major groove.

The distances, A_5:N1-A_6:N1 and T_{19}:N3-T_{20}:N3 recorded along the time of MD simulation of 10 ns shows that the average distance between the N1 atoms of adenine base is higher than the N3 atoms of the thymine base with order of 0.3 Å. This behavior is also reflected by Figure S.3, where the trends for T_{19}:N3-T_{20}:N3 distance (Blue) is lower than A_5:N1-A_6:N1 (Green). Therefore, it is revealed that the Os(II) probe spans more time closer to adenine bases A_5-A_6 than the thymine bases during the MD simulation**.**

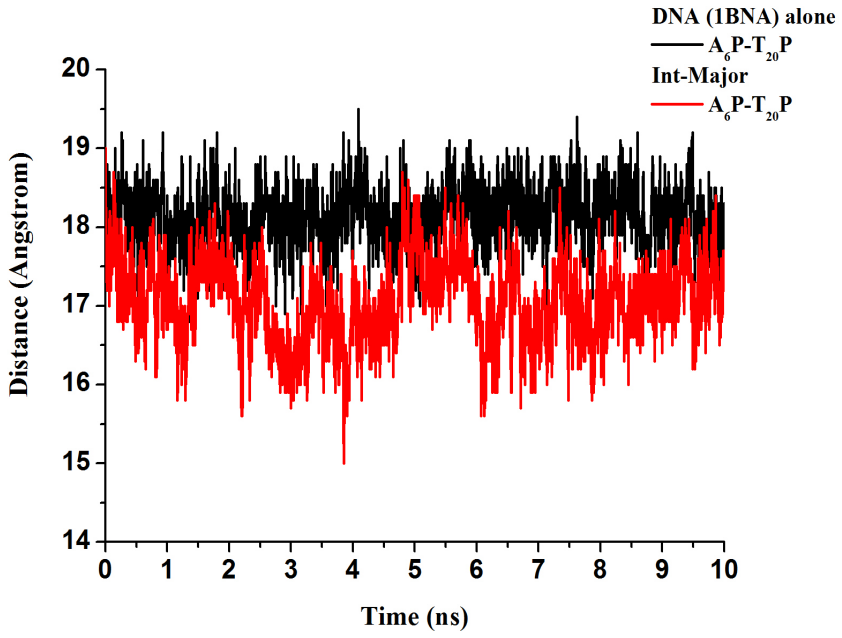


Figure S.4. Time evolution of the distances between the phosphate atoms of adenine and thymine residue (A_6P-T_{20}P) along the MD simulation of 10 ns before and after the Os(II) probe intercalation in the Major groove.

Figure S.4 demonstrates that the DNA structure also underwent conformational changes upon probe binding at the major groove site. The calculated distance between the phosphate atoms of adenine and thymine residue (A_6P-T_{20}P) along the MD simulation of 10 ns before and after the Os(II) probe intercalation at Major groove explained the horizontal deformation of the DNA structure. High degree of fluctuation was observed for distance between the phosphate atoms of adenine and thymine residue (A_6P-T_{20}P) when the Os(II) probe reside inside the intercalation pocket (Red) as compare to the MD simulation of the DNA alone (Black) (Figure S.4). Furthermore, the average distance for A_6P-T_{20}P is reduced from 18.1 Å (Standard deviation = ± 0.4) to 17.1 Å (Standard deviation = ± 0.6) upon probe binding. This distance contraction could be the consequence of the interaction between the phosphate groups and the intercalated Os(II) probe.

IV.1.3. Minor Groove

The Os(II) probe $Os[(bpy)_2dppz]^{2+}$ also found to be strongly intercalated in the minor groove of the DNA,1BNA between the base pairs 5'-A_5-A_6-3' and 5'-T_{19}-T_{20}-3' and also produced longitudinal and horizontal deformation in the DNA structure. Similar to intercalation in the major groove, the probe binding at the intercalation site in the minor groove of the DNA contributes increase in distances between two adenine A_5 and A_6 bases and two thymine T_{19} and T_{20} base pairs along the longitudinal axis. These distances are measured between the N1 atoms of the adenine bases and N3 atoms of the thymine bases. The MD simulation in the Figure S.5 demonstrates that the DNA structure underwent larger fluctuations as compare to the case of intercalation in major groove. The MD simulation curve shows that the distances between the nitrogen atoms N1 of the adenine (Black) and N3 of thymine (Red) bases remain constant over time of simulation of 10 ns . However, after intercalation of the probe, the DNA structure is deformed due of formation of intercalation « bubble ». The green and blue curves in Figure S.5 show the distances of the bases after the probe binding as compare to the DNA alone (black and red). The MD curve explains that the distances underwent high degree of fluctuations after probe binding over the simulation time. For initial 3 ns of the simulation, the distances decreased in both the cases, N1 for adenine (A5-A6) and N3 for thymine (T19-T20). After 3 ns, there is again increasing in nitrogen atoms distances until 7 ns. Finally, after 7 ns, the DNA/Probe complex becomes stable and the distances found to be constant until end of MD simulation. Therefore, it concludes that there are three conformations of the DNA/probe complex which span the MD simulation. We also predict that these three conformations are raised due to the flexibility of the probe within the intercalation pocket of minor groove which produces large deformation in the DNA structure along the horizontal axis. We measured the average distances for the nitrogen atoms between the bases (for 2000 snapshots) and found that distances are increased from 3.7 Å (Standard deviation = ± 0.3), DNA alone to 7.0-7.2 Å (Standard deviation = ± 0.4) after probe binding (Table 3). This variation is slightly larger than the case of intercalation in major groove.

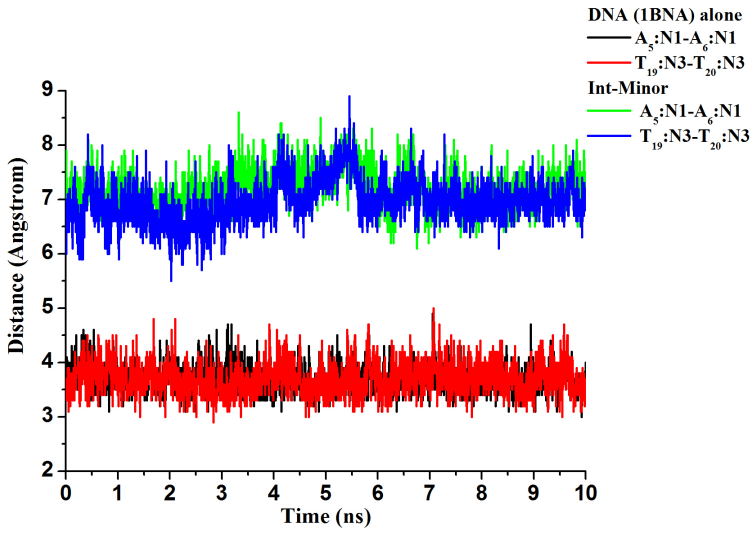


Figure S.5. Time evolution of the distances between the nitrogen atoms, N1 of the Adenine bases and N3 atoms of thymine bases during the MD simulation, before and after the Os(II) probe intercalation in the inor groove.

The horizontal deformation of the DNA structure has been measured by calculating the distance between the phosphate atoms of adenine and thymine residue (A_6P-$T_{20}P$) along the MD simulation of 10 ns before and after the Os(II) probe intercalation at minor groove. The MD simulation curve in the Figure S.6 shows that phosphate atoms distances remain almost constant over time of MD simulation without the probe (Black), however after intercalation of the Os(II) probe (Red), the DNA structure underwent high degree of fluctuation over the MD simulation time of 10 ns. These big deformations in the DNA structure can also justified by the A_6P-$T_{20}P$ average distances where the distances from the DNA alone of 18.1 Å (Standard deviation = ± 0.4) changed to 17.1 Å with large Standard deviation of ± 0.8 upon probe binding (Table 3). Nevertheless, the reduction in the phosphate atoms distances could be the consequence of the interaction between DNA and probe.

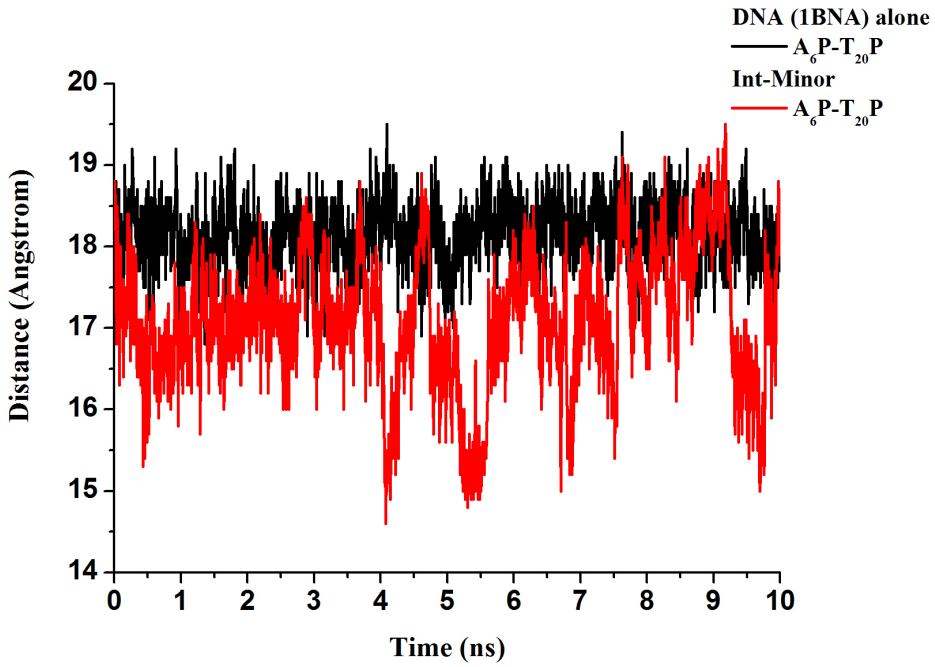


Figure S.6. Time evolution of the distances between the phosphate atoms of adenine and thymine residue (A_6P-$T_{20}P$) along the MD simulation of 10 ns before and after the Os(II) probe intercalation at Minor groove.

IV.2. DNA-Probe complex analysis

IV .2.1. Major Groove

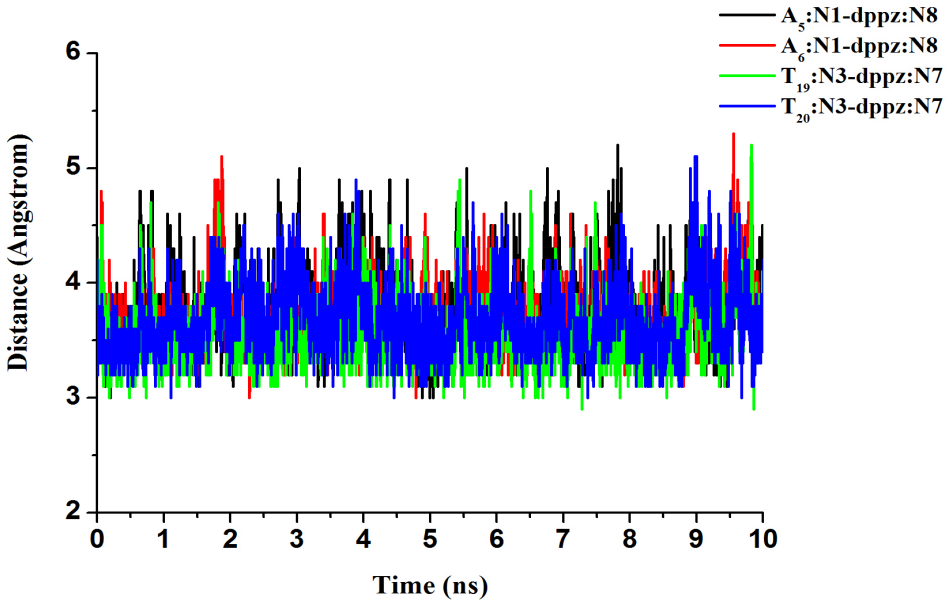


Figure S.7. Time evolution of the distances separating the nitrogen atoms of the adenine and thymine bases of the DNA and the nitrogen atoms of the dppz group of the probe over time of MD simulation.

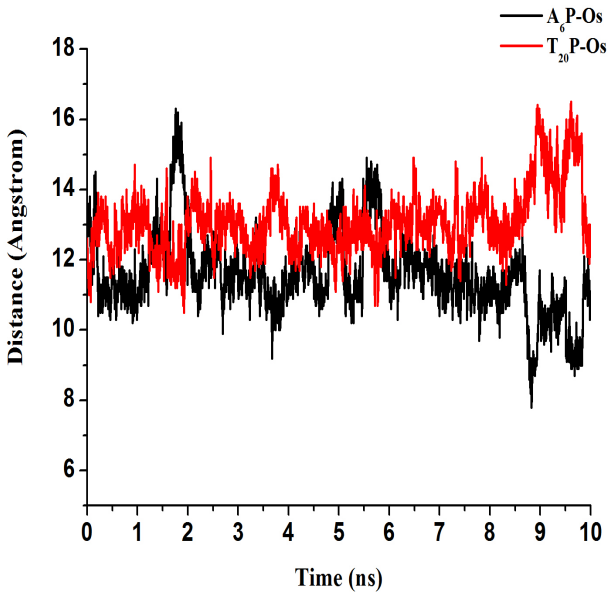


Figure S.8. Time evolution of the distances between the phosphate atoms of DNA bases (A6P and T20P) from Os metal of the probe over time of MD simulation.

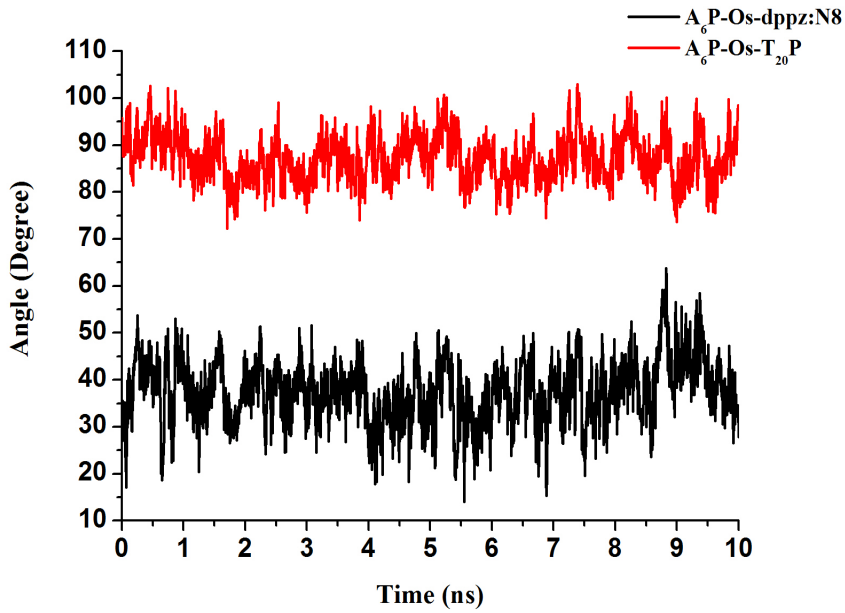
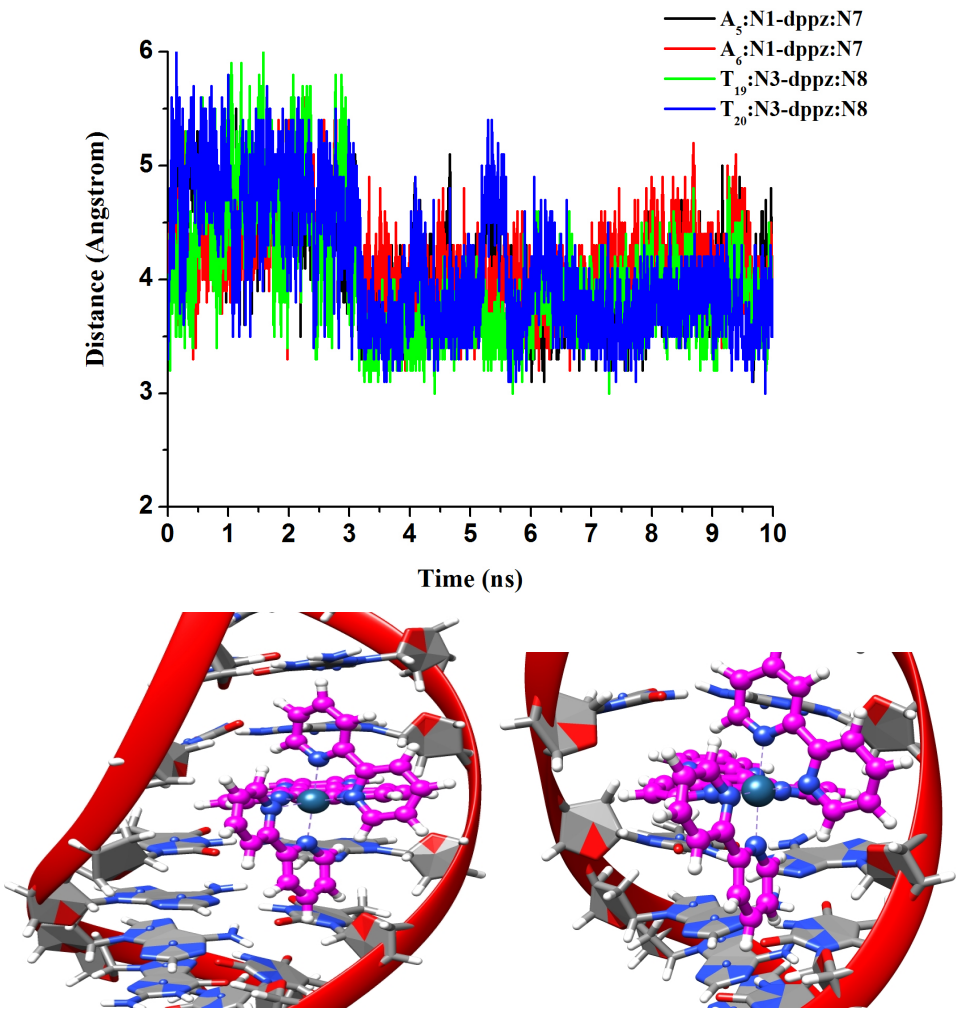


Figure S.9 Time evolution of the horizontal insertion angles of A_6P-Os-T_{20}P and A_6P-Os-dppz:N8 for the Os(II) probe, intercalation in the major groove, over the MD simulation time of 10 ns.

IV .2.2. Minor Groove

MD simulation in Figure S.10 shows that binding of the Os(II) probe in the intercalation pocket of the minor groove is not so stable as compare to the major groove. The DNA/Os[$(bpy)_2$dppz]$^{2+}$ adduct underwent more fluctuations during the simulation time. On comparison with the major groove complex, the distances between the DNA bases and dppz group are higher than the major groove. In major groove, the average distances vary between the 3.6-3.8 Å, but in minor groove the distances vary between 4.4-4.8 Å with standard deviation of ± 0.4-0.6 Å,, which explain that the DNA bases are slightly far from the probe in the case of intercalation in the minor groove and make a little weaker complex than the intercalation in the major groove. The MD simulation also reveals that the probe shows large movements between the DNA base pairs which leads to formation of many conformations. We extracted different snapshots to represent the kind of DNA/probe adduct formation during simulation. For, initial 2.5 ns, the Os(II) probe intercalated inside the minor groove with its dppz polycyclic rings between the adenine base pairs (A5-A6), later after 3 ns, the dppz moved towards middle of the DNA long axis and aligned equidistance with respect to the adenine and thymine base pairs. Therefore, these snapshots have us the understanding that the intercalation of the Os(II) probe inside the minor groove is not as stable as in the major groove. This behavior may exist because of steric hindrance created by the DNA backbone against the bpy arms of the probe which is making big movements of the probe inside the intercalation pocket.



Conformation 1 Conformation 2

2.5 ns **5 ns**

Figure S.10. Time evolution of the distances separating the nitrogen atoms of the adenine and thymine bases of the DNA and the nitrogen atoms of the dppz group of the probe over time of MD simulation. Different snapshots from MD simulation to show several types of conformations raised over time.

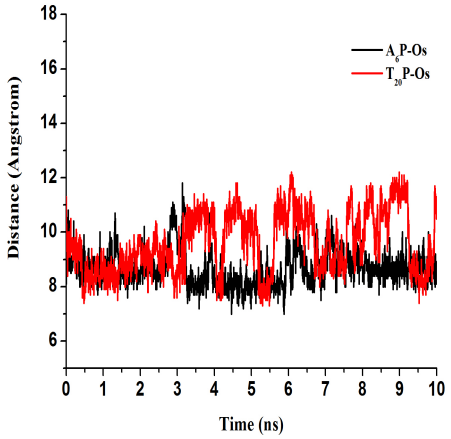


Figure S.11. Time evolution of the distances between the phosphate atoms of DNA bases (A6P and T20P) from Os metal of the probe over time of MD simulation.

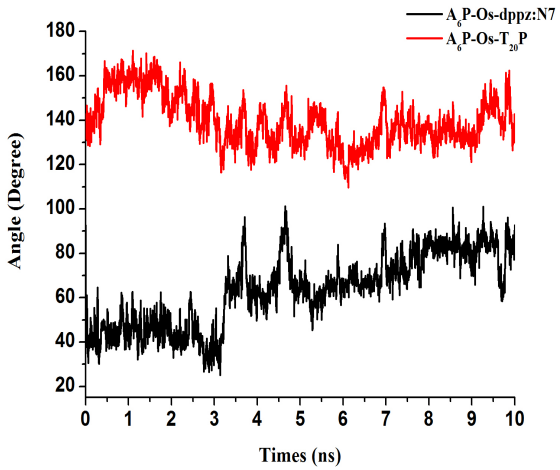


Figure S.12. Time evolution of the horizontal insertion angles of A_6P-Os-T_{20}P and A_6P-Os-*dppz*:N7 for the Os(II) probe, intercalation site in the major groove over the MD simulation time of 10 ns.

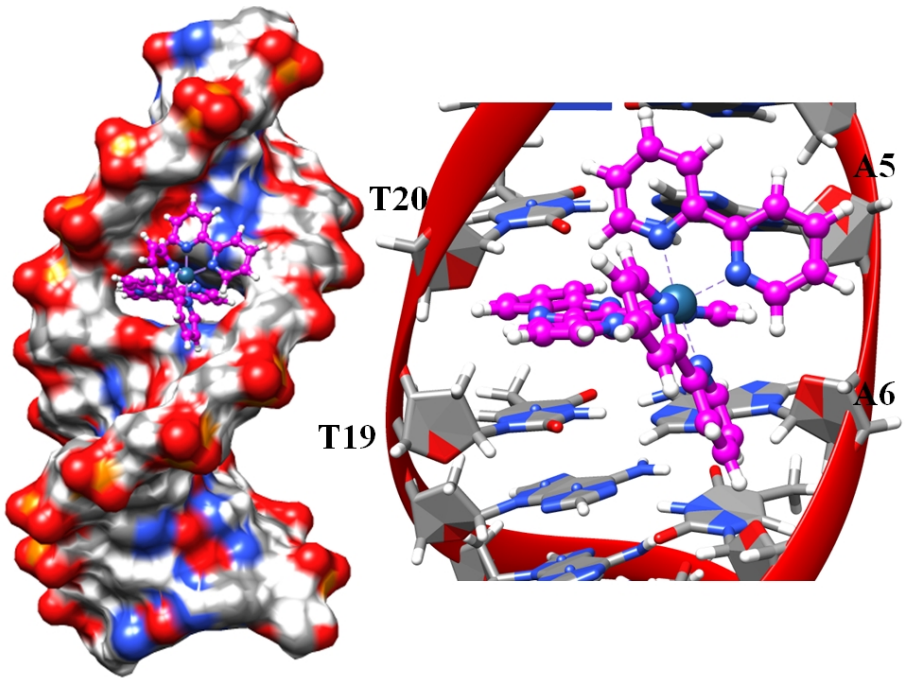


Figure S.13. Snapshot of the Os(II) probe intercalation at the minor groove side of the DNA, 1BNA at 10 ns.

V. Root-Mean Square Deviation (RMSD) for 1BNA/Os[(bpy)$_2$dppz]$^{2+}$ complex

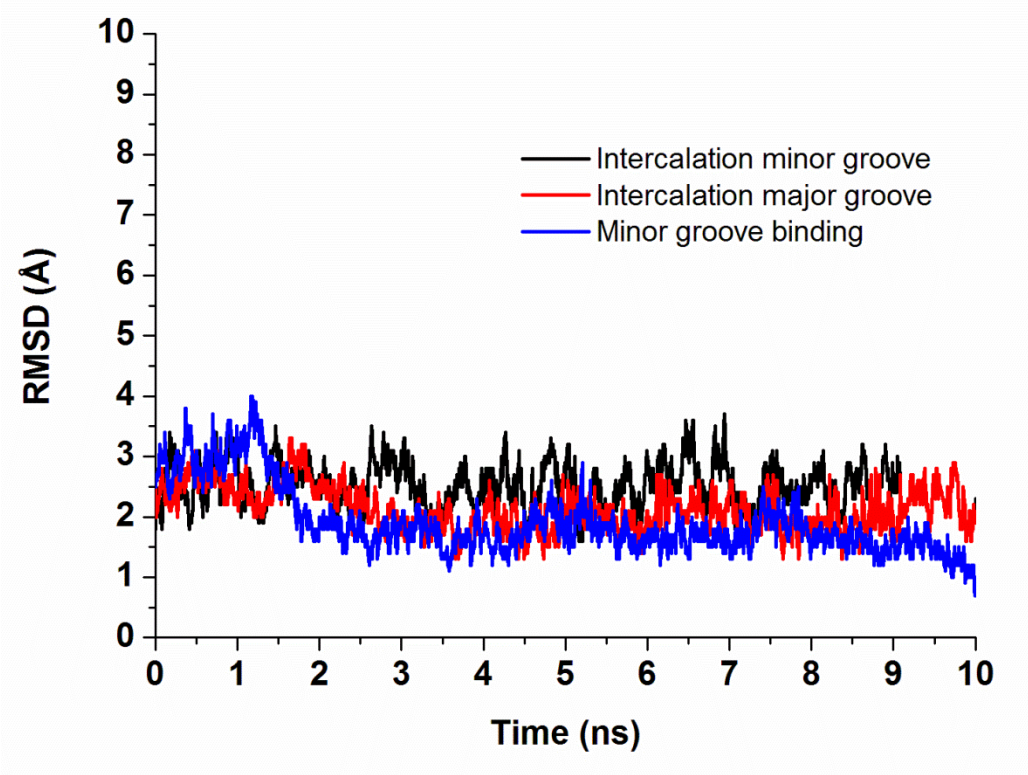


Figure S.14. Plot of the RMSD obtained for 1BNA/Os[(bpy)$_2$dppz]$^{2+}$ complex with respect to time, up to 10 ns of MD simulation, for different binding modes : Intercalation in Minor groove (Black), Intercalation in Major groove (Red) and Minor groove binding (Blue).

	RMSD(SD)$_a$ (Å)
1BNA DNA	2.0 Å (0.6 Å)
Complex 1BNA/Os[(bpy)$_2$dppz]$^{2+}$	
Intercalation major groove	2.5 Å (0.5 Å)
Intercalation minor groove	2.7 Å (0.5 Å)
Minor groove binding	2.0 Å (0.6 Å)

[a]*Average of Standard deviation*

Table S.3. Average (standard deviation) values of the RMSD in Å, relative to the starting structure , obtained within 10 ns of MD simulatiosn.

For the intercalation binding modes , the slightly higher RMSD value may be caused by structural distorsions of the DNA due to the formation of the intercalation pocket.

VI. Cartesian coordinates of the 1BNA / redox probe complexes

VI.1. Major groove intercalation

VI.1.1. 1BNA/ $Os[(bpy)_2dppz]^{2+}$

O	-18.80079000	8.39837800	-9.80181900
H	-19.22144900	7.53932100	-9.89437100
C	-19.50214200	9.25652000	-8.93055600
H	-20.56094700	8.97803700	-8.90647300
H	-19.43715200	10.26177900	-9.33912800
C	-18.82148400	9.29477500	-7.57120300
H	-19.23093600	10.16151800	-7.03790600
O	-19.11144600	8.07825100	-6.91493200
C	-18.00026300	7.50729200	-6.27035700
H	-17.84572500	7.96222600	-5.29385600
N	-18.19838400	6.05084100	-6.13619700
C	-17.82170800	5.09759000	-7.03465500
H	-17.29606700	5.26112100	-7.96924500
C	-17.97820000	3.78721500	-6.76110800
H	-17.79482400	3.01734600	-7.49341600
C	-18.42483200	3.37680400	-5.46512100
N	-18.82998200	2.11595400	-5.22015000
H	-18.27122500	1.47149000	-5.75405700
H	-19.19411300	1.90958200	-4.29894400
N	-18.90104100	4.27490700	-4.59751900
C	-18.79997200	5.57946300	-4.98329000
O	-19.06481000	6.31465300	-4.03965000
C	-17.30609800	9.47445600	-7.58218900
H	-16.89297300	9.75351700	-8.54829000
C	-16.92545100	8.04245200	-7.20672300
H	-16.93362800	7.47987300	-8.14210400

H	-15.91674000	7.98778200	-6.79137500
O	-17.03300700	10.46157200	-6.61698300
P	-15.56472000	10.81794400	-6.06586400
O	-15.50572500	12.21527000	-5.56776700
O	-14.64199200	10.48080600	-7.16614100
O	-15.25317400	9.80987200	-4.84777900
C	-16.09668400	9.79513000	-3.72738900
H	-17.10830900	9.85896300	-4.13999000
H	-15.82669800	10.71877200	-3.20912900
C	-15.98468700	8.59322400	-2.80257600
H	-16.74244900	8.68506700	-2.01965700
O	-16.19627100	7.35423400	-3.44470900
C	-15.81121200	6.37877900	-2.51233700
H	-16.56460100	6.25532400	-1.73467100
N	-15.62233200	5.05662800	-3.14387500
C	-15.23189200	4.74453300	-4.41920000
H	-15.01647300	5.48629400	-5.17264900
N	-15.24226900	3.47706000	-4.71636300
C	-15.58916900	2.92164900	-3.48616900
C	-15.92232100	1.58930800	-3.14473300
O	-16.09350900	0.65750200	-3.93145600
N	-16.16902800	1.31556800	-1.80130400
H	-16.43666300	0.38576000	-1.53181000
C	-16.26247300	2.32566500	-0.86478300
N	-16.41145300	1.93841900	0.41488300
H	-16.57687600	0.95082900	0.54868000
H	-16.56343200	2.56493500	1.18545500
N	-16.09839900	3.60644700	-1.21360700
C	-15.72477100	3.85496900	-2.48385900
C	-14.59726500	8.49844000	-2.17921600

H	-13.83266700	8.98958300	-2.78812300
C	-14.49066200	6.98086700	-2.02753000
H	-13.73205200	6.63628600	-2.73093200
H	-14.25963300	6.61382200	-1.03103400
O	-14.56205800	9.09779100	-0.90088200
P	-13.18660800	9.37189100	-0.10094000
O	-13.24008500	10.56641400	0.77241800
O	-12.05130300	9.27300400	-1.04232300
O	-13.04334700	8.09874200	0.87628400
C	-13.96635500	8.11701900	1.94778900
H	-14.98730100	8.09772000	1.58420000
H	-13.77868100	9.07475400	2.44701200
C	-13.87068300	6.97219700	2.95611800
H	-14.68777600	7.11311700	3.65797400
O	-14.11218800	5.73039800	2.32801700
C	-12.97090900	4.93730000	2.50767500
H	-13.17273300	4.25543000	3.33060900
N	-12.71468700	4.19266300	1.25868900
C	-12.45968500	4.84325500	0.08676500
H	-12.24963600	5.89969300	0.06191000
C	-12.32442100	4.21736600	-1.10418700
H	-12.02773500	4.79084800	-1.97458700
C	-12.66403600	2.83194900	-1.02947500
N	-12.59970500	2.06860600	-2.12836900
H	-12.28695500	2.32611700	-3.05625600
H	-12.79976700	1.10268400	-1.92156100
N	-13.07975500	2.19464600	0.07321400
C	-13.06043000	2.84984500	1.25758700
O	-13.49112100	2.29072100	2.26559800
C	-12.51316500	6.93457800	3.64831000

H	-11.93947800	7.85320600	3.55883600
C	-11.79647600	5.84594700	2.87053200
H	-11.36520200	6.29655300	1.97033400
H	-10.99318100	5.36550000	3.43257200
O	-12.60299700	6.57441000	5.00963700
P	-11.35706100	6.69945200	6.02383900
O	-11.89537000	7.32937300	7.24700000
O	-10.17424900	7.31134200	5.38302100
O	-10.94907400	5.19112900	6.42807700
C	-11.58621300	4.35115500	7.35300800
H	-12.66386800	4.54483500	7.27459200
H	-11.46217400	4.69265900	8.38431200
C	-11.28626500	2.86529400	7.20351000
H	-11.76784300	2.35203000	8.04091200
O	-11.83759400	2.33485800	6.02144700
C	-11.04796200	1.31701400	5.44901900
H	-11.66384400	0.42080200	5.34609500
N	-10.54218300	1.57053600	4.08383900
C	-9.98284600	2.70909400	3.57302800
H	-9.71131700	3.54250300	4.21193400
N	-9.80212100	2.74070300	2.27563000
C	-10.06570800	1.41110200	1.95347500
C	-10.08361200	0.83292700	0.65926000
O	-9.97594400	1.29376500	-0.47283400
N	-10.30248400	-0.53106400	0.71778500
H	-10.28530800	-1.07849600	-0.13199300
C	-10.62317300	-1.22891800	1.86846200
N	-10.75942100	-2.55612600	1.78269400
H	-10.56227200	-3.12311900	0.97069000
H	-11.17842700	-2.99678200	2.58988500

N	-10.73994000	-0.64376900	3.06932300
C	-10.42221400	0.67283800	3.05532300
C	-9.80838000	2.48468700	7.12871400
H	-9.22400400	3.19958400	6.56513000
C	-9.92882600	1.11605000	6.46968000
H	-9.01802500	0.82946400	5.95275700
H	-10.16547300	0.34803700	7.21537000
O	-9.35770000	2.45557300	8.46880300
P	-7.82766500	2.39105100	8.96046100
O	-7.79243200	2.42812900	10.43991500
O	-7.19352100	3.49222000	8.21682800
O	-7.19255000	0.99671800	8.46069700
C	-7.59799300	-0.27503300	8.92380000
H	-8.67466500	-0.22223400	9.06160500
H	-7.19525600	-0.51543600	9.89843300
C	-7.24926600	-1.38253100	7.92774100
H	-7.47779000	-2.37343300	8.29692600
O	-7.74370700	-1.21192800	6.61530000
C	-6.85262900	-1.82377100	5.70614700
H	-7.32289000	-2.76694200	5.44110300
N	-6.78965400	-0.94530400	4.5216150
C	-6.56380600	0.40847700	4.4748500
H	-6.48646000	0.99726100	5.3860740
N	-6.46682100	0.86735600	3.2548370
C	-6.63888500	-0.24936300	2.4519890
C	-6.54476900	-0.45437700	1.0606850
N	-6.20041000	0.51929900	0.1848160
H	-6.39455300	1.47469900	0.4497690
H	-6.21951200	0.28953600	-0.8130290
N	-6.72299700	-1.70028700	0.6038570

C	-6.96304400	-2.70872600	1.4589980
H	-7.09943500	-3.67974100	0.9893190
N	-7.03106300	-2.64382600	2.7811000
C	-6.84728300	-1.39300600	3.2176260
C	-5.73617000	-1.27108100	7.74142800
H	-5.45417900	-0.24691300	7.50004900
C	-5.51313200	-1.98103300	6.41436100
H	-4.65431400	-1.58087500	5.88126000
H	-5.35156200	-3.05328200	6.55858200
O	-5.06350900	-1.81791500	8.85972900
P	-3.46536100	-1.70873500	8.98974000
O	-3.01424900	-1.83423200	10.39698900
O	-2.91919100	-0.50731100	8.32801700
O	-3.08957400	-3.02745000	8.14453300
C	-3.56683300	-4.30386600	8.51057500
H	-4.62723600	-4.26893100	8.25187500
H	-3.31757400	-4.56743100	9.54527500
C	-3.08875400	-5.34531400	7.50424100
H	-3.83766900	-6.11374200	7.30712300
O	-2.92666200	-4.79776600	6.21335000
C	-1.56353300	-4.85596700	5.85146000
H	-1.40567100	-5.56486400	5.03417700
N	-1.25378900	-3.54288100	5.2000660
C	-1.07150600	-2.30076400	5.7732010
H	-1.25582700	-2.13481900	6.8328860
N	-0.71756700	-1.37654100	4.9211370
C	-0.68524400	-2.03480600	3.7020950
C	-0.41878200	-1.58995000	2.3923050
N	-0.10829300	-0.29196300	2.1213040
H	0.40561600	0.17490900	2.8591450

H	0.22360200	-0.10407300	1.1727840
N	-0.54066800	-2.46480200	1.3828290
C	-0.84579600	-3.74716600	1.6677360
H	-0.88157500	-4.41222100	0.8088220
N	-1.09457200	-4.28089100	2.8555800
C	-1.02102500	-3.37869700	3.8418310
C	-1.73852300	-5.92951700	7.90045800
H	-1.60202800	-5.87335800	8.98674300
C	-0.73357800	-5.11851200	7.09834700
H	-0.60279300	-4.17960100	7.63644400
H	0.20965900	-5.63340600	6.90426700
O	-1.77446900	-7.25592900	7.40868700
P	-0.62111100	-8.27720900	7.88915500
O	-1.22402200	-9.62321300	7.88067200
O	0.19324800	-7.82593300	9.03185800
O	0.20404600	-8.19869000	6.50007300
C	-0.30092000	-8.73151800	5.30236600
H	-1.22225300	-8.17666100	5.09505100
H	-0.49963900	-9.77149200	5.57561600
C	0.57257500	-8.43889900	4.08771900
H	0.13598000	-8.88860100	3.19498700
O	0.57389200	-7.02451000	4.06711400
C	1.83800000	-6.67601800	3.55411900
H	2.01344500	-6.95382000	2.51853700
N	2.02448800	-5.21930000	3.7117840
C	2.02370800	-4.60425900	4.9418760
H	1.86147200	-5.27126200	5.7867840
C	2.20847600	-3.27407700	5.1013210
C	2.23511000	-2.57885700	6.4299600
H	3.23740400	-2.21379300	6.6595250

H	1.56679700	-1.71193100	6.3966640
H	1.90179400	-3.25152900	7.2243490
C	2.37278000	-2.45597500	3.9018010
O	2.56038100	-1.23825700	3.9218060
N	2.29628200	-3.13664200	2.7058370
H	2.35004200	-2.58089400	1.8273550
C	2.07019300	-4.48403100	2.5124520
O	1.95528500	-4.97302700	1.4107770
C	2.00991000	-8.93058700	4.26770700
H	2.07976200	-9.52705000	5.16678800
C	2.79755500	-7.62861700	4.25492900
H	3.06952600	-7.33392600	5.27177100
H	3.71717100	-7.67167200	3.66313700
O	2.31887500	-9.74044200	3.14664200
P	3.62198500	-10.59432400	2.75409800
O	3.18738800	-11.75774100	1.95086200
O	4.45481400	-10.92598100	3.94342500
O	4.46267400	-9.58833000	1.81894200
C	3.85502100	-9.28072900	0.58470600
H	2.84597000	-8.86498300	0.67564200
H	3.87922300	-10.12754400	-0.09619100
C	4.68861200	-8.16160300	-0.04361000
H	4.35550200	-7.99285300	-1.06940800
O	4.53968900	-6.93413900	0.61855000
C	5.59498600	-6.09969400	0.19223000
H	5.42606800	-5.90274700	-0.86265300
N	5.81783400	-4.90016800	1.01440700
C	5.83289800	-5.06311400	2.37518600
H	5.64708100	-6.02173500	2.82764400
C	5.98350300	-3.99101000	3.18172900

C	5.94709100	-4.31386500	4.65731000
H	5.39673500	-5.24582500	4.77961500
H	6.95300300	-4.49145500	5.00645500
H	5.48945400	-3.48939100	5.20768400
C	6.37230400	-2.69787600	2.66603500
O	6.66766000	-1.69911300	3.32469800
N	6.52294100	-2.71691300	1.28721500
H	6.68592600	-1.78541400	0.93743700
C	6.13404200	-3.70613900	0.38822100
O	6.15792600	-3.46815400	-0.81747100
C	6.19050600	-8.45301100	-0.09924600
H	6.51253900	-9.06155800	0.74364400
C	6.78247700	-7.06701500	0.16473900
H	7.28623500	-7.11931800	1.12873700
H	7.38913900	-6.68360400	-0.65285400
O	6.65177200	-9.11781400	-1.25136200
P	8.16486700	-9.37429300	-1.73938000
O	8.12392500	-10.46166200	-2.74275000
O	9.06468900	-9.44957900	-0.56970000
O	8.46769200	-7.97722300	-2.47463100
C	7.48559300	-7.56393100	-3.40289400
H	6.55561800	-7.33913600	-2.88220800
H	7.48889600	-8.30614900	-4.20007700
C	7.73853000	-6.20190900	-4.03773100
H	6.92102800	-6.01192300	-4.73808500
O	7.81109700	-5.11895300	-3.13172800
C	9.01612000	-4.43772600	-3.39771500
H	8.84377500	-3.69923600	-4.18760700
N	9.48616500	-3.79898300	-2.15350100
C	9.78417800	-4.59187700	-1.08513500

H	9.66584400	-5.66734000	-1.11795400
C	10.31704400	-4.08472100	0.04577000
H	10.52797000	-4.77982800	0.84109100
C	10.17769500	-2.66403100	0.18260000
N	10.45255000	-2.12646200	1.37519100
H	10.88911300	-2.78688600	2.00292700
H	10.32602300	-1.14342800	1.56580800
N	9.72430100	-1.87089500	-0.79656800
C	9.36158800	-2.44029100	-1.97619800
O	9.07086400	-1.68789200	-2.90171200
C	9.03279900	-6.30281600	-4.84009400
H	9.26134500	-7.36262400	-4.92117600
C	9.96827400	-5.48417000	-3.95714200
H	10.45343800	-6.07471500	-3.18327300
H	10.68339500	-4.96528900	-4.60186200
O	8.84107200	-5.75872900	-6.13071800
P	10.00278400	-5.79710000	-7.24599900
O	9.43089600	-5.62901100	-8.59581000
O	10.83989200	-6.97668300	-6.93707200
O	10.81445300	-4.44515300	-6.92657400
C	10.31157400	-3.16752900	-7.24436200
H	9.35763900	-3.03597800	-6.72928600
H	10.29459500	-3.07632700	-8.33137400
C	11.20672000	-2.06671000	-6.69027600
H	10.74417900	-1.16007700	-7.07468800
O	11.12983500	-2.13043100	-5.28477600
C	12.30354600	-1.53941000	-4.77321400
H	12.01953300	-0.51655000	-4.51847100
N	12.79976500	-2.06441800	-3.47801800
C	12.77635700	-3.32266200	-2.94587700

H	12.54379100	-4.20502500	-3.52574600
N	12.90212700	-3.36668600	-1.64593700
C	13.12900400	-2.03985300	-1.31709200
C	13.44111400	-1.32487600	-0.13071300
O	13.59072900	-1.91461100	0.93981400
N	13.69000600	0.03383200	-0.17616700
H	14.01325400	0.50866900	0.65806300
C	13.62293100	0.72841500	-1.36328800
N	14.05032500	1.99458300	-1.27467700
H	14.23596000	2.33043600	-0.34122000
H	14.08222900	2.65849100	-2.03593200
N	13.36776600	0.08819100	-2.52018200
C	13.16725800	-1.24442900	-2.43760100
C	12.65924200	-2.02418400	-7.14784500
H	12.91353500	-3.06603400	-7.33435300
C	13.36574300	-1.57295500	-5.86454900
H	14.24849500	-2.17119500	-5.66266400
H	13.66629700	-0.53360000	-6.02766800
O	12.79790600	-1.08726400	-8.19696500
P	14.11227100	-0.82493500	-9.09759100
O	13.84472300	0.14540800	-10.17951200
O	14.77855100	-2.09845500	-9.42119400
O	15.12987500	0.03577400	-8.19500600
C	14.96824400	1.38484400	-7.80643400
H	13.93969600	1.38881000	-7.45462100
H	15.15847700	1.97532900	-8.70088300
C	15.92580000	1.75786500	-6.68762100
H	15.85340300	2.81672400	-6.43767000
O	15.77260000	0.98670800	-5.51516800
C	17.01122900	0.90830500	-4.84947100

H	17.43267200	1.82662900	-4.44405000
N	16.86314500	-0.10365700	-3.77844200
C	16.43614400	-1.36701400	-4.05808100
H	16.24586900	-1.52731600	-5.10884200
C	16.24598200	-2.30467700	-3.09754600
H	16.05915800	-3.33118300	-3.36640000
C	16.52157000	-1.88776300	-1.75648900
N	16.47448900	-2.77159800	-0.75089600
H	16.38050900	-3.75100600	-0.96913500
H	16.52002500	-2.44280800	0.20310800
N	16.86554800	-0.62882500	-1.44096600
C	17.05277800	0.25802800	-2.45355600
O	17.24597600	1.44084800	-2.18971700
C	17.37629000	1.49279700	-7.10417800
H	17.42184300	1.03840600	-8.08863300
C	17.94049600	0.59135300	-6.01016200
H	17.90226500	-0.43535300	-6.37555700
H	18.95109000	0.85641300	-5.67648100
O	18.12820900	2.68224500	-7.17987700
P	19.66350600	2.93338400	-7.59023400
O	19.86333100	4.38261400	-7.80773000
O	20.01496300	1.89287500	-8.58844200
O	20.41372900	2.62491800	-6.20181300
C	20.12962300	3.27123400	-4.98207500
H	19.09264800	3.15442400	-4.63676800
H	20.24563600	4.34248900	-5.08333400
C	20.99668000	2.67115800	-3.88038400
H	20.90141700	3.23348700	-2.94469700
O	20.47365100	1.38376400	-3.63552300
C	21.42350400	0.41155700	-3.27986300

H	21.68696600	0.65759300	-2.25543500
N	20.96605400	-0.96927500	-3.49114700
C	20.81116500	-1.57985800	-4.71335700
H	21.12825200	-1.07051900	-5.60298100
N	20.36090600	-2.80912900	-4.65803800
C	20.18954000	-3.04076500	-3.30231700
C	19.59005200	-4.10362700	-2.57689400
O	19.02773100	-5.12345400	-2.97520000
N	19.63914100	-3.93173700	-1.20483600
H	19.35942100	-4.76368400	-0.69207700
C	20.17503900	-2.84843300	-0.53658100
N	19.96626500	-2.84223400	0.78696600
H	19.45318700	-3.57198600	1.25729800
H	20.26840800	-2.02747800	1.30211900
N	20.63060200	-1.80580100	-1.23799400
C	20.63276200	-1.95672100	-2.58922300
C	22.46104700	2.38173600	-4.20095000
H	22.75405700	2.74594800	-5.17808600
C	22.63709500	0.86866500	-4.09983200
H	22.62528800	0.49587700	-5.12613100
H	23.49614000	0.52488700	-3.53409600
O	23.14391100	3.08971000	-3.18037700
H	23.49344400	2.48785300	-2.51269800
O	23.78916000	-1.55992300	5.55383600
H	23.14466000	-1.31330100	4.88451000
C	24.49045400	-0.41518900	5.97415800
H	25.27469100	-0.20662100	5.23654500
H	24.97051900	-0.70495500	6.90425100
C	23.51422000	0.70526800	6.29748700
H	24.03294600	1.51132100	6.81662300

O	23.05204600	1.22198000	5.06610400
C	21.64740200	1.28116900	5.12585200
H	21.30962600	2.25985900	5.47092000
N	21.08212300	1.12226500	3.78171300
C	20.34427900	2.13328200	3.23023200
H	20.07905200	2.99598300	3.82082600
C	19.96157300	2.09392000	1.93586400
H	19.36282400	2.87861900	1.48603700
C	20.31200900	0.94402400	1.15590700
N	19.86290600	0.81888600	-0.10478600
H	19.31648100	1.51075700	-0.58989800
H	20.20177000	0.00551100	-0.59975300
N	21.05453900	-0.02745000	1.68965700
C	21.43529100	0.03936100	2.99960600
O	22.02866000	-0.94738700	3.42603400
C	22.33257000	0.27944800	7.15619600
H	22.51723200	-0.63710400	7.71578000
C	21.18697700	0.23997500	6.14503000
H	21.20547300	-0.75577000	5.70011500
H	20.24667100	0.36739800	6.68834200
O	22.07579300	1.28772400	8.10753500
P	20.86687300	1.17811800	9.15667700
O	21.33228300	1.77327200	10.43217200
O	20.45463300	-0.24238500	9.16214800
O	19.69485000	2.00833500	8.41999400
C	19.78002000	3.30876500	7.88546000
H	20.59838500	3.44097200	7.18396100
H	19.98942700	4.03315800	8.67653800
C	18.50274000	3.69096400	7.14824900
H	18.66650300	4.71690400	6.81190300

O	18.43158900	2.90417300	5.98381900
C	17.19869300	2.21977100	5.97592100
H	16.53317900	2.88704000	5.41010800
N	17.19029700	0.89600500	5.32248900
C	17.28200300	-0.33866700	5.89813900
H	17.33686800	-0.54899200	6.94945000
N	17.17608600	-1.25082100	4.96945400
C	16.92731600	-0.58943000	3.77309500
C	16.71463400	-1.02202800	2.44188300
O	16.65696200	-2.15027200	1.95769400
N	16.70064700	-0.01787400	1.47981200
H	16.57198900	-0.34299400	0.53459000
C	16.90419300	1.32229200	1.77582500
N	16.96288000	2.17351900	0.74569600
H	16.90090200	1.84992900	-0.20669500
H	17.25226700	3.11392600	0.97370900
N	16.98230300	1.75377300	3.04078500
C	17.05608200	0.75928000	3.96124200
C	17.28206200	3.44213600	8.03042200
H	17.56019900	3.23115800	9.06595500
C	16.74495800	2.14163300	7.43016200
H	17.13434600	1.26921300	7.95050900
H	15.66704200	2.07642600	7.37777500
O	16.28641200	4.43220900	7.89427000
P	16.38395500	5.93693600	8.43904600
O	17.82483400	6.12973400	8.74218900
O	15.35613100	6.09303300	9.48566500
O	16.00284700	6.88862300	7.18962600
C	14.67414600	6.88772600	6.72935300
H	14.22412000	7.83772700	7.01461400

H	14.09839500	6.09345600	7.20279400
C	14.60465600	6.59601300	5.22566600
H	15.17653200	7.38116100	4.74213600
O	14.97488800	5.30019700	4.80794500
C	14.13244600	4.95074700	3.73264200
H	14.45751400	5.21416400	2.72529700
N	13.84762100	3.49974700	3.64736400
C	13.61488900	2.82562900	4.81218200
H	13.65126600	3.33826500	5.76206700
C	13.28454600	1.52739000	4.82433200
H	12.91134300	1.03369300	5.71145200
C	13.27452400	0.89534900	3.53614500
N	13.05791700	-0.42521500	3.41576000
H	12.90705900	-1.00187000	4.23301900
H	13.12466500	-0.78933500	2.48031300
N	13.41360200	1.49194700	2.34853100
C	13.65721500	2.82448200	2.45763200
O	13.78891000	3.43449300	1.39949900
C	13.20638900	6.94183800	4.73632400
H	12.48343300	7.05985000	5.54168600
C	12.82512800	5.69983300	3.92418900
H	11.97496900	5.15627000	4.32589700
H	12.57075100	6.20420200	2.99091300
O	13.34139600	8.09739500	3.93697400
P	12.18392900	9.00578800	3.28261000
O	12.80446900	10.31985000	3.01583200
O	11.00716100	9.00643600	4.18006000
O	11.80218600	8.39763800	1.84795800
C	12.73107200	8.35698900	0.78451200
H	13.69466000	7.87081800	0.95313900

H	13.09176800	9.37768800	0.67463800
C	12.10496300	7.83509700	-0.50541700
H	12.71462100	8.14128000	-1.35345400
O	12.15943500	6.42934500	-0.56367900
C	10.85687200	5.91578900	-0.77860000
H	10.58599300	5.56321800	-1.78314900
N	10.68833700	4.78804900	0.14725000
C	10.51733200	4.80721000	1.50404400
H	10.52819700	5.75511400	2.03050200
N	10.30628500	3.66618400	2.10138700
C	10.45698600	2.80171500	1.03102200
C	10.20913700	1.39322800	1.06161100
O	10.09198000	0.61745400	1.99641000
N	10.17757200	0.88320000	-0.21958900
H	9.90051000	-0.08647600	-0.22762200
C	10.39760300	1.64375000	-1.35855800
N	10.28344800	1.03292000	-2.53671500
H	9.94459100	0.08507600	-2.50110600
H	10.32985600	1.59508400	-3.38005300
N	10.74041500	2.93575800	-1.40951100
C	10.68488200	3.44842600	-0.15671900
C	10.72977900	8.37178200	-0.87883000
H	10.39706000	9.20253200	-0.25324800
C	9.98108000	7.11372500	-0.42513200
H	9.83426200	7.18110300	0.65078800
H	9.00987200	7.14161000	-0.92978900
O	10.70012600	8.52057100	-2.28068000
P	9.43665200	9.04162700	-3.13883700
O	10.00586500	9.57809900	-4.39764400
O	8.58821100	9.90892800	-2.30857500

O	8.64429000	7.67936100	-3.47617300
C	9.17999100	6.81519100	-4.46669600
H	10.25259400	6.73427700	-4.36935600
H	8.95091600	7.15478700	-5.47877200
C	8.44075500	5.47933700	-4.47164600
H	8.99800200	4.86108700	-5.16745000
O	8.56209300	4.78846900	-3.23934000
C	7.45085500	3.92868500	-3.11555700
H	7.68958700	3.10870700	-3.80399200
N	7.21728200	3.47213100	-1.73081800
C	7.31648200	4.22111400	-0.59253700
H	7.60980400	5.26174500	-0.58552000
N	6.96643300	3.57110000	0.47659700
C	6.85516400	2.26255800	0.02733500
C	6.56414100	1.03583900	0.64366900
N	6.37522200	0.80325500	1.94751500
H	6.22357000	1.56062000	2.60955800
H	6.27610300	-0.12564300	2.31997300
N	6.44591000	-0.10135900	-0.05697400
C	6.64872300	-0.01712200	-1.36088000
H	6.73833500	-0.95156700	-1.89845000
N	6.96786100	1.04375100	-2.08586300
C	6.98959100	2.16852100	-1.33691800
C	6.94716800	5.47170400	-4.79311200
H	6.55672700	6.48272200	-4.90310600
C	6.24762300	4.60696000	-3.74251600
H	5.86061400	5.27887300	-2.97228400
H	5.58538900	3.80828800	-4.07443200
O	6.69332900	4.69745600	-5.93836500
P	5.33625500	4.73383900	-6.80803500

O	5.68678300	4.73152700	-8.24901500
O	4.44026800	5.76059600	-6.23255400
O	4.69099500	3.29206600	-6.50549600
C	5.29176600	2.11426800	-6.99952700
H	6.37180300	2.19986400	-6.86726600
H	5.17558800	2.06203100	-8.07733700
C	4.66813500	0.85035100	-6.42996900
H	5.20346500	0.00817000	-6.87522400
O	4.94774800	0.86114700	-5.04043700
C	4.17950500	-0.18239200	-4.48572700
H	4.76958700	-1.09650000	-4.45085700
N	3.81446000	0.25694200	-3.1157520
C	3.98974700	1.50874300	-2.5900720
H	4.35330200	2.32282400	-3.2127730
N	3.68822600	1.58273700	-1.3154900
C	3.30328900	0.29424900	-0.9854090
C	2.93954200	-0.30820300	0.2329560
N	2.89671300	0.38746800	1.4134740
H	3.56088800	1.14970100	1.4570700
H	2.86775100	-0.19623800	2.2540550
N	2.60736300	-1.60129600	0.2320270
C	2.66388700	-2.29270400	-0.9286550
H	2.36325200	-3.33421500	-0.8533570
N	3.03436700	-1.85035100	-2.1185210
C	3.36141300	-0.55132700	-2.0917620
C	3.16238500	0.60553800	-6.48273900
H	2.68836700	1.52631400	-6.16183700
C	2.97673400	-0.43557400	-5.39075500
H	2.08108400	-0.30331400	-4.77974900
H	2.95177800	-1.43808300	-5.82277000

O	2.66645700	0.24008700	-7.75596400
P	1.10872100	0.31409900	-8.12661500
O	0.99874300	0.40551300	-9.60433200
O	0.38998300	1.21912900	-7.21177300
O	0.43062600	-1.12131900	-7.80729900
C	0.92019700	-2.41275900	-8.07656400
H	2.00061700	-2.41950000	-7.89069500
H	0.55750200	-2.73821500	-9.05054100
C	0.31361000	-3.36248600	-7.04430100
H	0.77027600	-4.30039500	-7.36287400
O	0.81040600	-2.97067100	-5.78534000
C	-0.16820000	-3.28512800	-4.82771700
H	0.00464800	-4.27692100	-4.39389000
N	-0.06865200	-2.26012600	-3.7373120
C	0.09330500	-0.93468200	-4.0547940
H	0.18601500	-0.72173400	-5.1297380
C	0.16954300	0.04325200	-3.1196310
C	0.47662200	1.47057900	-3.4600400
H	-0.27340300	2.15508300	-3.0589610
H	1.44428700	1.76703500	-3.0422170
H	0.52045400	1.60113100	-4.5537890
C	0.02689700	-0.34090800	-1.7294170
O	0.08384100	0.45431600	-0.7808660
N	-0.23885600	-1.67336300	-1.4960280
H	-0.32207000	-1.97322100	-0.5071180
C	-0.26800800	-2.69730300	-2.4285640
O	-0.47374500	-3.85414900	-2.1193610
C	-1.20748600	-3.47195800	-6.94592000
H	-1.63562300	-2.69076000	-7.56714900
C	-1.53843400	-3.16111500	-5.49406700

H	-1.97261200	-2.16775900	-5.37304100
H	-2.22502300	-3.96701600	-5.24508900
O	-1.74265200	-4.67591800	-7.46570900
P	-3.20109100	-4.83449100	-8.12016400
O	-3.08969900	-5.84082900	-9.19583900
O	-3.67242800	-3.49321600	-8.50762100
O	-4.07289200	-5.41344600	-6.89506100
C	-3.71621800	-6.63073400	-6.27830100
H	-2.75166600	-6.73068700	-5.79513500
H	-3.79689900	-7.39565700	-7.05243600
C	-4.80772100	-6.95649400	-5.25723100
H	-4.50147300	-7.88522300	-4.78289800
O	-4.84556600	-6.01675000	-4.20908500
C	-6.16290000	-5.66840300	-3.81978000
H	-6.47603300	-6.30071900	-2.98905900
N	-6.09753100	-4.22131700	-3.5259920
C	-5.48187000	-3.38075800	-4.4350680
H	-5.10370800	-3.87256000	-5.3396170
C	-5.34454200	-2.05331200	-4.2298740
C	-4.69475100	-1.13889300	-5.2255210
H	-3.75246800	-0.72558500	-4.8444910
H	-4.45792000	-1.68385000	-6.1491020
H	-5.34051200	-0.29554500	-5.4682690
C	-5.83577000	-1.51330500	-2.9707730
O	-5.77611300	-0.31958400	-2.6563730
N	-6.40536200	-2.42715900	-2.1093090
H	-6.62597200	-2.09749400	-1.1477090
C	-6.48327800	-3.79578000	-2.2564440
O	-6.87393300	-4.53284700	-1.3740730
C	-6.25560700	-7.19304900	-5.67671500

H	-6.34223000	-7.09016800	-6.76736300
C	-6.99803500	-6.02722200	-5.03814800
H	-6.97020000	-5.17229500	-5.71284300
H	-8.05650100	-6.21004100	-4.82315500
O	-6.79476100	-8.43954200	-5.29413300
P	-8.23342200	-8.98797400	-5.79200400
O	-8.21491000	-10.45717300	-5.64031200
O	-8.44371300	-8.45907500	-7.16088900
O	-9.44645800	-8.40425400	-4.91222400
C	-9.47966200	-8.54140500	-3.50666800
H	-8.48297400	-8.40711100	-3.07914200
H	-9.75883800	-9.56664400	-3.29513700
C	-10.51551500	-7.60191200	-2.89768500
H	-10.73891400	-7.91378400	-1.87566300
O	-9.91689000	-6.32781400	-2.76306300
C	-10.92490700	-5.33960000	-2.83330900
H	-11.54571100	-5.37047000	-1.93256000
N	-10.31918200	-3.99466800	-2.85467400
C	-10.01859400	-3.44091000	-4.05567300
H	-9.93848000	-4.06804500	-4.93685600
C	-9.95451100	-2.09004900	-4.16182400
H	-9.84150700	-1.64225800	-5.13548300
C	-9.99721400	-1.33281600	-2.94676200
N	-9.73535400	-0.02079400	-2.89550800
H	-9.63367500	0.37535900	-3.81812700
H	-9.69851700	0.55058100	-2.06830000
N	-10.18270400	-1.92297700	-1.75705400
C	-10.48675200	-3.24775700	-1.70126900
O	-10.71718500	-3.75850100	-0.60575900
C	-11.81092600	-7.33128400	-3.64599800

H	-11.84993400	-7.91900300	-4.56663100
C	-11.69965900	-5.85724700	-4.04024800
H	-11.22991800	-5.81824700	-5.01918700
H	-12.64175200	-5.30507600	-4.07856000
O	-13.02013600	-7.32147000	-2.92279900
P	-13.78605400	-8.66876700	-2.48091900
O	-12.80466100	-9.76129000	-2.34578100
O	-14.94391500	-8.71819100	-3.39907800
O	-14.25363700	-8.19949800	-1.01080000
C	-13.76445700	-8.70423800	0.20929900
H	-12.68266800	-8.81387600	0.12092200
H	-14.05037300	-9.73348100	0.42703900
C	-14.13210700	-7.67875600	1.27687600
H	-13.69527500	-8.11546700	2.17802000
O	-13.56723300	-6.38546000	1.12955500
C	-14.63441500	-5.48429700	0.92284700
H	-14.76773100	-4.85068300	1.79878100
N	-14.24250900	-4.54926700	-0.14253000
C	-13.96377400	-4.71541000	-1.47718500
H	-14.13409500	-5.65601500	-1.97873700
N	-13.72674800	-3.63662700	-2.16700000
C	-13.78495600	-2.69674200	-1.14087700
C	-13.46847300	-1.31417500	-1.19421700
O	-13.06783600	-0.68574900	-2.17404800
N	-13.62213200	-0.65563700	0.01393000
H	-13.26169700	0.29014100	0.08093600
C	-14.04839800	-1.25013900	1.18109100
N	-13.96196500	-0.47065200	2.27686900
H	-13.56975600	0.45857700	2.28716200
H	-14.20202300	-0.82111500	3.19149800

N	-14.37084300	-2.54227000	1.25407100
C	-14.16297000	-3.19304600	0.07755900
C	-15.63189700	-7.42693200	1.35758400
H	-16.08632500	-8.32676500	0.92828700
C	-15.93994400	-6.16861000	0.54626900
H	-15.96129200	-6.26521600	-0.53775600
H	-16.76920300	-5.51230200	0.82642800
O	-15.95694500	-7.26244200	2.72143400
P	-17.46197100	-7.53909100	3.21261800
O	-17.47129500	-7.91803900	4.64921500
O	-18.16664100	-8.38393900	2.22505900
O	-18.30460700	-6.18148800	3.14134200
C	-18.38217100	-5.22724000	4.17182400
H	-17.37015100	-5.10429600	4.54424900
H	-19.11580400	-5.58138800	4.90268800
C	-18.78176600	-3.90205500	3.51363800
H	-18.64200400	-3.16598300	4.30108000
O	-17.92247800	-3.53196400	2.46237400
C	-18.72154300	-2.94039100	1.46120600
H	-18.97820000	-1.93387800	1.79952200
N	-18.00239100	-2.88127600	0.17003400
C	-18.18374900	-3.82744400	-0.79804500
H	-18.76968700	-4.69604800	-0.56076100
C	-17.69383000	-3.67723900	-2.05379900
H	-17.87775100	-4.45859400	-2.77342200
C	-17.01709000	-2.44688300	-2.34577300
N	-16.47983100	-2.22081200	-3.54953600
H	-16.33033300	-2.93454700	-4.25020200
H	-16.01898700	-1.31750300	-3.56199300
N	-16.97522200	-1.46117600	-1.43917000

C	-17.39143800	-1.69009300	-0.17028900
O	-17.17680200	-0.75151600	0.60353600
C	-20.22111200	-3.74680500	3.03397100
H	-20.77581900	-4.62263400	3.36491600
C	-19.97409100	-3.80529700	1.52494500
H	-19.79442800	-4.85073800	1.27122500
H	-20.80623000	-3.44145600	0.92082200
O	-20.87403100	-2.51716000	3.26325300
P	-21.50678300	-2.15434700	4.69482200
O	-20.90229000	-2.83566300	5.86178300
O	-22.95825900	-2.30029700	4.44260100
O	-21.15028100	-0.59139800	4.59187100
C	-20.08369600	-0.12107900	5.39249300
H	-19.13993800	-0.58127800	5.08928100
H	-20.24897400	-0.48008700	6.41498800
C	-19.99408300	1.38791500	5.22276300
H	-19.28406500	1.72779100	5.97100000
O	-19.39203100	1.51492600	3.94491300
C	-20.13421800	2.30928900	3.05573000
H	-19.69693900	3.30613100	2.99748800
N	-20.22321000	1.82493500	1.66433500
C	-20.37933200	0.49257100	1.39261400
H	-20.72538000	-0.18525700	2.15825100
N	-20.30441300	0.30462700	0.09648000
C	-19.95801800	1.54121000	-0.42118100
C	-19.66133900	1.96589900	-1.74187000
O	-19.62977600	1.26483900	-2.75563500
N	-19.39832500	3.31519900	-1.92301500
H	-19.34402000	3.69950500	-2.85637500
C	-19.37125600	4.20778300	-0.86705000

N	-19.33103800	5.49248300	-1.25114600
H	-19.29483000	5.70119800	-2.23685700
H	-19.22638200	6.22665700	-0.56745300
N	-19.71956600	3.85446100	0.37920100
C	-19.86571100	2.51746600	0.53407100
C	-21.29143700	2.20271600	5.24202600
H	-22.07075800	1.58555900	5.67315800
C	-21.49912600	2.28364300	3.73202000
H	-22.16462500	1.52245200	3.30799300
H	-22.03928800	3.22873800	3.61027900
O	-21.20953800	3.46395100	5.85438000
H	-21.12106300	3.15774600	6.75149300
Os	-2.49696600	3.70797000	1.3960340
N	-4.53249500	4.07412700	1.1830880
C	-5.49794000	3.41656900	1.8439730
C	-6.84253900	3.69363100	1.6593010
C	-7.21056200	4.68600100	0.7521390
C	-6.21320700	5.37416300	0.0759480
C	-4.87468800	5.05135200	0.3106960
C	-3.73304500	5.74069100	-0.3122720
N	-2.50844000	5.32943700	0.1235390
C	-1.41069300	5.93324500	-0.3770780
C	-1.47429000	6.92654300	-1.3366500
C	-2.72304500	7.33527700	-1.8015750
C	-3.85843700	6.73813500	-1.2764770
N	-0.41975600	3.57250400	1.5727420
C	0.38903300	3.03204900	0.6467970
C	1.76843600	3.19091700	0.6847160
C	2.33153100	3.90857100	1.7376900
C	1.50190000	4.42717500	2.7226690

C	0.12437600	4.24719900	2.6149450
C	-0.85302200	4.80656100	3.5635620
N	-2.14528000	4.75878700	3.1458190
C	-3.10972700	5.23757400	3.9550250
C	-2.84368900	5.74712400	5.2133020
C	-1.52308600	5.77664000	5.6579430
C	-0.52154100	5.30948500	4.8202410
C	-4.18433500	-5.09195000	1.3323500
C	-3.89612700	-3.78574500	0.8570900
N	-3.83663500	-2.75783200	1.7302730
C	-3.55156700	-1.57129600	1.2361620
C	-3.36801200	-0.45084800	2.1615560
C	-3.40693700	-0.62062100	3.5506250
C	-3.12221200	0.45961500	4.3676510
C	-2.82202500	1.69043700	3.7827710
N	-2.79920600	1.87110600	2.4595420
C	-3.05597200	0.81357100	1.6564310
C	-2.95604700	1.03653100	0.2205020
C	-4.18671400	-6.14278400	0.4568110
C	-3.89223200	-5.95123500	-0.9228170
C	-3.61341100	-4.70751400	-1.4140400
C	-3.63124000	-3.59005000	-0.5357450
N	-3.39833900	-2.35821700	-1.0282450
C	-3.36607700	-1.36433800	-0.1650810
C	-3.10370500	-0.02207600	-0.6744980
C	-2.98750100	0.23608200	-2.0434840
C	-2.74288000	1.53193100	-2.4588780
C	-2.59669400	2.53628700	-1.5021420
N	-2.70016500	2.29860700	-0.1915120
H	-5.19427800	2.63173200	2.5295880

H	-7.57121100	3.10983500	2.2199600
H	-8.26037500	4.90680400	0.5836070
H	-6.47310100	6.15386500	-0.6250650
H	-0.46205600	5.55656900	-0.0082160
H	-0.55618600	7.34305700	-1.7289710
H	-2.80757800	8.08661200	-2.5715510
H	-4.84022400	7.02385600	-1.6269320
H	-0.08025000	2.44663100	-0.1409190
H	2.38566500	2.75313900	-0.1034970
H	3.40714100	4.05397500	1.7860950
H	1.91603100	4.98301500	3.5515780
H	-4.12476700	5.15054300	3.5770190
H	-3.66736500	6.06487400	5.8410300
H	-1.28558400	6.12235000	6.6526890
H	0.50686000	5.28072200	5.1521710
H	-4.37057100	-5.21008300	2.3937660
H	-3.61268300	-1.61071700	3.9555620
H	-3.08666100	0.35475500	5.4538810
H	-2.59040600	2.55473200	4.3966200
H	-4.39949400	-7.14071500	0.8150650
H	-3.89023500	-6.80316100	-1.5933860
H	-3.37760000	-4.53268700	-2.4624620
H	-3.07885700	-0.59230800	-2.7400450
H	-2.62361900	1.76594500	-3.5129570
H	-2.37101000	3.55821900	-1.7900970

VI.1.2. 1BNA/ Os[(bpy)$_2$phen]$^{2+}$

O	23.02184100	-7.72348500	1.05710000
H	22.86642600	-7.30785300	0.21276800
C	21.95041800	-7.57836500	1.95642900
H	22.24562900	-7.83687200	2.97531200

H	21.10319700	-8.20164500	1.68013300
C	21.42510800	-6.14069900	1.96469800
H	22.30749400	-5.54629300	2.19069800
O	21.01132900	-5.66332700	0.71142000
C	20.20907400	-4.51599800	0.86769700
H	20.87689400	-3.65257200	0.84291900
N	19.25615300	-4.38763200	-0.24803700
C	18.29630500	-5.27504800	-0.63634900
H	18.31078800	-6.20381000	-0.07315200
C	17.32466600	-4.95720900	-1.51407200
H	16.57125500	-5.65023000	-1.85771800
C	17.41343500	-3.66816500	-2.11647400
N	16.53212500	-3.29201800	-3.05199800
H	15.81476900	-3.95402500	-3.31666200
H	16.65053300	-2.35760000	-3.41219800
N	18.35131700	-2.77602600	-1.76810200
C	19.30014500	-3.16235200	-0.88092800
O	20.20598700	-2.35194600	-0.70487200
C	20.21433300	-5.87197000	2.86264500
H	19.44264000	-6.64477800	2.87013900
C	19.53937100	-4.65536100	2.24104200
H	18.46220400	-4.77988400	2.17773900
H	19.75317200	-3.80358700	2.88770400
O	20.74086000	-5.52394800	4.12650700
P	19.80712300	-5.37526700	5.42624900
O	20.74515300	-5.68482500	6.52623600
O	18.54668600	-6.14472000	5.30482800
O	19.51046900	-3.78714300	5.53187200
C	20.53295100	-2.82224300	5.52184700
H	21.17457600	-3.05740800	4.66796400

H	21.05975500	-2.85926400	6.47211300
C	20.06123500	-1.38413900	5.30289800
H	20.93554600	-0.73388900	5.33213300
O	19.63386600	-1.12825900	3.98833200
C	18.32218300	-0.61156200	4.02719400
H	18.50279400	0.46262000	3.96228400
N	17.52092300	-1.07458400	2.88579400
C	17.09412600	-2.33807700	2.59299500
H	17.32155000	-3.21503200	3.17791200
N	16.46618300	-2.50777100	1.45607300
C	16.31211600	-1.20152000	0.97423100
C	15.74906600	-0.63013700	-0.19084200
O	15.23084800	-1.22896200	-1.13591300
N	15.84685600	0.75696100	-0.24079200
H	15.26525900	1.23935400	-0.91045000
C	16.58773600	1.51149300	0.64531000
N	16.45213200	2.84424100	0.52700200
H	15.81056700	3.19313200	-0.17554300
H	17.02420900	3.45271000	1.10058000
N	17.07153400	0.98049200	1.76360200
C	17.01830800	-0.37587800	1.80519800
C	19.00492600	-0.91745900	6.30455800
H	18.87443100	-1.56855200	7.17562000
C	17.79389800	-1.03246600	5.39462100
H	17.40260300	-2.05536200	5.38616800
H	16.96919000	-0.41372500	5.76111200
O	19.27889300	0.37725300	6.78274200
P	18.59691000	0.96875200	8.12159600
O	19.50349800	2.00735900	8.66223900
O	18.15507200	-0.12035200	9.02444200

O	17.28208800	1.69570500	7.52856800
C	17.31750600	2.66100300	6.50409500
H	18.08882900	2.34075600	5.80167000
H	17.60031400	3.66440100	6.80775900
C	16.06107000	2.88471800	5.66420200
H	16.21324100	3.80879300	5.09893400
O	15.89381000	1.93238800	4.64455000
C	14.49939400	1.73219600	4.62158000
H	13.91459400	2.57701600	4.27446700
N	14.09970900	0.59250100	3.76767800
C	14.09970000	-0.66605600	4.29733100
H	14.42080200	-0.83552200	5.31501200
C	13.57427700	-1.68863900	3.58652000
H	13.47772200	-2.69796500	3.94336700
C	13.12342100	-1.38564900	2.26036500
N	12.65140500	-2.38183600	1.48840500
H	12.34213800	-3.23054200	1.93589100
H	12.55409800	-2.03407400	0.53640100
N	13.21902800	-0.17109500	1.69549900
C	13.64338000	0.84612100	2.49380900
O	13.65171900	1.95070300	1.96890200
C	14.79804600	2.98154500	6.51296400
H	15.09583800	2.92934600	7.56234300
C	14.12350800	1.66717200	6.10001900
H	14.48821500	0.82453900	6.69361700
H	13.04139300	1.66464500	6.23163300
O	14.05883600	4.10616800	6.09608400
P	12.85056300	4.77410700	6.91969400
O	13.40243400	5.79398800	7.83346700
O	12.11053500	3.67882400	7.59771700

O	11.84078900	5.55419000	5.93484700
C	12.26190900	6.63154600	5.12963700
H	13.28052000	6.53461000	4.74827400
H	12.18904500	7.47282500	5.81252800
C	11.34187300	6.85593700	3.93206300
H	11.69930100	7.69064500	3.33097600
O	11.35807500	5.59941800	3.29881900
C	10.07945500	5.03784800	3.12686000
H	9.58747100	5.22969000	2.16574100
N	10.22511200	3.57689100	3.28206000
C	10.83500500	2.85241800	4.26555900
H	11.29789300	3.25878500	5.15319600
N	10.94188000	1.58835200	3.94459900
C	10.19169100	1.45613300	2.78419700
C	9.67814400	0.29395200	2.13797200
O	9.71832800	-0.86571400	2.53954400
N	8.96510100	0.56207300	0.98446400
H	8.45565900	-0.23481200	0.61454200
C	8.61921100	1.84591100	0.61798800
N	7.61139300	1.94402800	-0.26841900
H	7.35116900	1.17794300	-0.86919200
H	7.45231200	2.89239300	-0.57193400
N	9.06315800	2.96153800	1.22436600
C	9.82040000	2.69317300	2.31347900
C	9.88572400	7.12922400	4.29198600
H	9.82198100	7.52982500	5.30581800
C	9.31045700	5.72145500	4.25656100
H	9.43934700	5.17660300	5.19033000
H	8.28560500	5.79342100	3.90230300
O	9.23776300	8.07462600	3.46321500

P	7.74699400	8.56145100	3.83739000
O	7.59340300	9.90993800	3.25011500
O	7.42212000	8.34947800	5.26288100
O	6.78343000	7.49546200	3.11953500
C	7.08680600	6.87958000	1.88586100
H	8.12703700	6.57787600	1.77634700
H	6.92151500	7.63603300	1.11731800
C	6.17644900	5.69674500	1.56059100
H	6.41859100	5.41699200	0.53052900
O	6.40071600	4.59508700	2.40352100
C	5.42822500	4.55677500	3.41960800
H	5.01013600	3.55133500	3.53558200
N	6.12190100	4.73109000	4.7502440
C	6.32160800	5.81406700	5.5858410
H	5.93315400	6.80375700	5.3449350
N	7.05790300	5.55183200	6.6358350
C	7.39998200	4.21641200	6.4809250
C	8.32483200	3.39097900	7.1383020
N	9.12584700	3.86157900	8.1769700
H	9.26961600	4.86214600	8.0680950
H	10.03487400	3.38509700	8.1487330
N	8.45059900	2.12076300	6.7607320
C	7.76143400	1.71705900	5.6750620
H	7.91864100	0.68225400	5.3827020
N	6.95375400	2.42432300	4.9011590
C	6.82215000	3.68227400	5.3282390
C	4.69776000	6.06648000	1.67639300
H	4.54673800	7.14071600	1.62612900
C	4.32585800	5.54530500	3.05365100
H	4.45438100	6.42930500	3.67589500

H	3.28658600	5.24743100	3.20183800
O	3.97416900	5.37951300	0.67611300
P	2.81576800	5.95846000	-0.27332300
O	3.00869000	7.39126500	-0.54544600
O	1.48872900	5.59158200	0.28789700
O	3.11244800	5.16521900	-1.64447200
C	4.38022200	5.13853900	-2.26972400
H	5.15983600	5.14900100	-1.50795600
H	4.50426700	6.02623100	-2.89142800
C	4.63545500	3.88964600	-3.09611400
H	5.51515700	4.07921400	-3.71521700
O	5.02199600	2.87527700	-2.19182500
C	4.25913000	1.70381800	-2.40659300
H	5.05068800	0.97984900	-2.54697000
N	3.49145500	1.42693700	-1.1620250
C	3.49113000	2.16003500	0.0068210
H	3.95545300	3.14513500	0.0507930
N	2.88470700	1.56180600	0.9980200
C	2.46168000	0.36045500	0.4553610
C	1.77627300	-0.73858700	1.0040420
N	1.41383100	-0.79334300	2.3179940
H	1.25316400	0.10772000	2.7466360
H	0.76772500	-1.53808100	2.5716710
N	1.53897800	-1.79359000	0.2213610
C	1.94423600	-1.76291600	-1.0706240
H	1.69994800	-2.65417900	-1.6396230
N	2.58674600	-0.79295300	-1.6942310
C	2.82450400	0.25148600	-0.8854340
C	3.49570500	3.36921200	-3.96801900
H	2.55014000	3.84064000	-3.72274000

C	3.42361700	1.86905100	-3.67016500
H	2.44977100	1.42083000	-3.52311900
H	3.87042800	1.33910200	-4.51687500
O	3.79485400	3.59741800	-5.32736800
P	2.58606100	3.81349700	-6.37213200
O	3.03186900	3.92096100	-7.77634200
O	1.73489700	4.88810700	-5.83451500
O	1.68072300	2.49251600	-6.17320500
C	1.94191700	1.35903300	-6.97420000
H	2.95166600	1.07284300	-6.67453200
H	2.07525900	1.78297800	-7.97134200
C	0.99412700	0.16089200	-6.99278000
H	1.49064000	-0.52411900	-7.68987300
O	0.82816900	-0.23204000	-5.64854500
C	-0.52780200	-0.39700400	-5.31293500
H	-0.94746500	-1.36866700	-5.54759000
N	-0.62042400	-0.13093700	-3.8585250
C	-0.14295300	1.04156800	-3.2953070
H	0.27833100	1.75472900	-4.0102780
C	-0.19344800	1.29287400	-1.9694270
C	0.26854700	2.57533700	-1.3429920
H	-0.57287500	3.20005200	-1.0292850
H	0.86383000	2.38737400	-0.4448050
H	0.88136600	3.16536700	-2.0362530
C	-0.72498700	0.24632500	-1.0964910
O	-0.84662900	0.34309300	0.1256740
N	-1.10455500	-0.91993500	-1.7356740
H	-1.40206800	-1.72244100	-1.1469440
C	-1.07111000	-1.19588600	-3.0814770
O	-1.44367500	-2.26256000	-3.5384180

C	-0.40490600	0.50022400	-7.49771300
H	-0.32781500	1.47082200	-7.98113600
C	-1.25230100	0.57835600	-6.23627400
H	-1.18336400	1.60122200	-5.85275100
H	-2.31147000	0.36866500	-6.39716500
O	-0.93145500	-0.38728700	-8.45983000
P	-2.32168100	-0.21861000	-9.27021300
O	-2.02159700	-0.88808000	-10.55097700
O	-2.82372500	1.17402900	-9.26754600
O	-3.41994000	-1.14283200	-8.54520300
C	-3.38316200	-2.54410900	-8.64354300
H	-2.34904800	-2.90024500	-8.59088400
H	-3.72509500	-2.89923600	-9.61918000
C	-4.20444100	-3.18081100	-7.52608600
H	-4.13657900	-4.26000700	-7.63847800
O	-3.93853300	-2.75630300	-6.21000000
C	-5.15197800	-2.60831700	-5.49512000
H	-5.48838900	-3.60164800	-5.20978000
N	-4.96061800	-1.67621600	-4.37343800
C	-4.48632500	-0.42880600	-4.66449500
H	-4.40982500	-0.19005000	-5.71237000
C	-4.26794000	0.44675800	-3.65449700
C	-3.95991100	1.88557700	-3.99672200
H	-4.18818600	2.55176700	-3.15893900
H	-2.88212300	1.94294300	-4.06939600
H	-4.38592200	2.25408700	-4.92565400
C	-4.46603900	0.06816900	-2.27336400
O	-4.38589400	0.76601700	-1.26594800
N	-4.88252400	-1.24490400	-2.10699400
H	-5.33113700	-1.37422400	-1.21709300

C	-5.17156400	-2.16593600	-3.09853500
O	-5.72890200	-3.24079700	-2.87910600
C	-5.66181700	-2.85314300	-7.82254900
H	-5.73318700	-2.09624700	-8.61514900
C	-6.21465700	-2.25498300	-6.53640200
H	-6.32028900	-1.18415100	-6.69215900
H	-7.13565400	-2.69528300	-6.16210200
O	-6.37896100	-3.98369900	-8.26543300
P	-7.85534500	-3.86718900	-8.88938700
O	-8.05752600	-4.93719000	-9.89373800
O	-8.17663300	-2.45400400	-9.21153600
O	-8.78459000	-4.11073500	-7.59594600
C	-8.85738800	-5.34033500	-6.90516000
H	-7.81658800	-5.62644800	-6.76276700
H	-9.43621600	-6.10233300	-7.43309600
C	-9.36400700	-5.21185000	-5.47214700
H	-9.25467000	-6.21144400	-5.03459000
O	-8.77687000	-4.25799300	-4.61311900
C	-9.70470400	-3.70417500	-3.70685800
H	-9.72103800	-4.38531300	-2.85205800
N	-9.16072000	-2.42634500	-3.23895600
C	-8.65456600	-1.48657100	-4.08467000
H	-8.81164900	-1.56319100	-5.15656300
C	-8.07433700	-0.35936400	-3.59442700
H	-7.65879900	0.29822800	-4.33354900
C	-8.15861900	-0.14164200	-2.17781300
N	-7.55663700	0.94780800	-1.68647300
H	-7.19890700	1.67106300	-2.30090800
H	-7.45241300	0.96809600	-0.68481100
N	-8.66811000	-1.06276000	-1.35309600

C	-9.14044000	-2.22397100	-1.87164700
O	-9.65663600	-2.92819900	-1.01508400
C	-10.83969900	-4.84331100	-5.54839500
H	-11.19007300	-4.67198600	-6.55977300
C	-10.96690200	-3.67017200	-4.58104600
H	-11.10624400	-2.73066600	-5.12438000
H	-11.82489400	-3.82525400	-3.93475000
O	-11.56897300	-5.94312000	-5.05709100
P	-13.17332800	-5.98166500	-5.19836300
O	-13.50135600	-7.32956000	-5.70568700
O	-13.56606300	-4.82882700	-6.04531300
O	-13.71637000	-5.85624700	-3.69560800
C	-13.59290600	-6.82292000	-2.67855300
H	-12.57391600	-7.04745000	-2.35414000
H	-14.04731800	-7.75855700	-2.98999400
C	-14.29786600	-6.40518300	-1.39518700
H	-14.24403500	-7.24934500	-0.70591700
O	-13.82334500	-5.22438700	-0.79290000
C	-14.70235000	-4.13904800	-0.97480400
H	-14.98680900	-3.78694100	0.01196000
N	-14.06140400	-3.01416500	-1.67745900
C	-13.88721400	-2.73806300	-3.01249700
H	-14.32685900	-3.34520500	-3.79645600
N	-13.24367400	-1.62435700	-3.23968600
C	-12.90131800	-1.14424500	-1.98159900
C	-12.16235300	0.03206100	-1.67299400
O	-11.61906400	0.88110000	-2.36708900
N	-12.04456000	0.17701200	-0.29599900
H	-11.48789800	0.95911600	-0.00386900
C	-12.67232700	-0.62618900	0.64276400

N	-12.48521500	-0.27481000	1.91591900
H	-11.96799000	0.56717900	2.13416700
H	-12.93517300	-0.79316700	2.66039400
N	-13.39499900	-1.69875500	0.29991300
C	-13.52600400	-1.92689200	-1.03458800
C	-15.78958400	-6.13117900	-1.58146600
H	-16.09816200	-6.78020000	-2.39488500
C	-15.93090400	-4.61772600	-1.74786400
H	-15.90856600	-4.39500200	-2.82042900
H	-16.86416900	-4.21982900	-1.36031200
O	-16.34995300	-6.56157500	-0.36025900
P	-17.91678400	-6.88787300	-0.21068700
O	-18.13205700	-7.82433600	0.90609300
O	-18.34789000	-7.35005600	-1.55304900
O	-18.53482300	-5.44329600	0.14233300
C	-18.48951900	-4.99709900	1.47464500
H	-17.48418500	-5.08396600	1.88544500
H	-19.16535400	-5.53390800	2.14336200
C	-18.80293200	-3.50653600	1.56292400
H	-18.77450100	-3.28700400	2.62983300
O	-17.80744500	-2.90035800	0.77168600
C	-18.33584900	-1.76734100	0.10967200
H	-18.62745000	-0.98800400	0.81038800
N	-17.50471600	-1.18454700	-0.96199400
C	-17.67736100	-1.42079900	-2.29708900
H	-18.39577200	-2.18905000	-2.55120500
C	-17.01532900	-0.75477500	-3.25840300
H	-17.26128300	-0.93206400	-4.30084000
C	-16.08823400	0.26254800	-2.85423900
N	-15.45978800	1.09260500	-3.70256700

H	-15.54739600	0.83661100	-4.66863900
H	-14.85695000	1.86101900	-3.42994000
N	-15.86028300	0.47659000	-1.55719400
C	-16.53781900	-0.25505500	-0.63267100
O	-16.22924900	-0.03819100	0.53023600
C	-20.09722400	-3.02885800	0.91660200
H	-20.78610900	-3.83817700	0.66893000
C	-19.64180800	-2.38609700	-0.39452500
H	-19.36021600	-3.10946500	-1.15823000
H	-20.42678100	-1.73171300	-0.77425800
O	-20.63534200	-2.02996300	1.75632500
P	-21.89126900	-2.34704400	2.71246600
O	-21.88085800	-3.76175800	3.13028800
O	-23.07509300	-1.80439500	2.02058900
O	-21.55417400	-1.35707700	3.93861200
C	-20.37750100	-1.46198900	4.70622800
H	-19.74664000	-2.18370300	4.18378700
H	-20.53557600	-1.90588300	5.68957400
C	-19.61780700	-0.16660000	4.96493900
H	-18.98937500	-0.34891600	5.82710900
O	-18.86196600	0.42968300	3.93627600
C	-19.38707700	1.67520600	3.52611600
H	-18.66136800	2.39790900	3.89101200
N	-19.39234300	1.77262100	2.06082400
C	-20.16051600	1.00650100	1.22591500
H	-20.84554900	0.27686500	1.63902800
N	-19.91155600	1.29911900	-0.02059700
C	-19.05754300	2.38742700	-0.00850500
C	-18.50167500	3.16163300	-1.06638900
O	-18.66273100	3.00457000	-2.27580600

N	-17.73643100	4.22996000	-0.61976100
H	-17.42352100	4.96169600	-1.23859000
C	-17.58412800	4.53385100	0.71198700
N	-17.00070800	5.69287600	1.04900800
H	-16.53822700	6.21914800	0.32862600
H	-16.70283800	5.83151900	2.01075100
N	-18.03861200	3.76089500	1.71676800
C	-18.67399200	2.65384000	1.28177200
C	-20.58761500	0.93603300	5.35579700
H	-21.55535600	0.55275200	5.70245700
C	-20.79290100	1.78519400	4.10444400
H	-21.57788700	1.38800200	3.44760800
H	-20.97849300	2.78322900	4.48730300
O	-20.11170200	1.66614200	6.46234500
H	-19.24373200	2.06267400	6.36240300
O	-14.57880400	11.67078000	-5.95036000
H	-13.70667200	12.02503800	-5.76465200
C	-15.52970400	12.19532400	-5.04739600
H	-16.53791900	12.18733300	-5.47534400
H	-15.35713300	13.26361200	-4.97337900
C	-15.56942400	11.55845300	-3.66373500
H	-16.12302300	12.20481600	-2.98238200
O	-16.13282500	10.28749300	-3.87478000
C	-15.51825100	9.43181900	-2.94192300
H	-15.83393900	9.57123800	-1.91056300
N	-15.60815700	7.99375400	-3.25286100
C	-15.60691800	7.56483900	-4.54863500
H	-15.55311500	8.30687400	-5.32670400
C	-15.90916600	6.29472200	-4.89568900
H	-15.92905600	5.95424800	-5.91900900

C	-16.25612700	5.40837400	-3.81823600
N	-16.37221400	4.10005400	-4.06688100
H	-16.61777800	3.72574700	-4.97009300
H	-16.62093000	3.54305200	-3.26489100
N	-16.21119100	5.82359800	-2.54196400
C	-15.97113400	7.12020600	-2.23769400
O	-16.11524100	7.47877500	-1.07697800
C	-14.19463500	11.40766100	-3.02552100
H	-13.34099000	11.90449400	-3.49129700
C	-14.06270100	9.88302000	-3.05808600
H	-13.60611500	9.49206600	-3.96383600
H	-13.50613700	9.55105200	-2.18411000
O	-14.26990900	11.88200600	-1.70619100
P	-13.01071500	12.07721000	-0.72312300
O	-13.31374900	13.27687800	0.08617700
O	-11.78841900	12.18790500	-1.55248200
O	-12.93570800	10.80646500	0.26959100
C	-13.86758900	10.70526000	1.31842500
H	-14.85325000	10.80496700	0.86828000
H	-13.70027700	11.57484200	1.95019600
C	-13.79706500	9.43249300	2.14811800
H	-14.50511800	9.60450100	2.96596600
O	-14.22018300	8.29146900	1.43964300
C	-13.32677500	7.23775000	1.69498300
H	-13.68454700	6.64565800	2.54027800
N	-13.25102200	6.42190200	0.46268600
C	-12.66995400	6.70829800	-0.74687500
H	-12.18495000	7.63968300	-1.00608900
N	-12.79140400	5.77022400	-1.63730600
C	-13.47605800	4.79515700	-0.92794500

C	-13.91954900	3.51760800	-1.37346500
O	-13.88814800	3.14672500	-2.54626400
N	-14.39089300	2.68424100	-0.38158000
H	-14.85265500	1.81798200	-0.62068300
C	-14.49090300	3.13863700	0.92395500
N	-15.13970100	2.26888500	1.72119600
H	-15.38550800	1.33256100	1.44267300
H	-15.38237600	2.51971400	2.67800900
N	-14.18595100	4.34992200	1.38023900
C	-13.66499400	5.11379100	0.38539900
C	-12.46450300	9.16116500	2.84787600
H	-11.86153400	10.03767100	2.64498700
C	-12.01835900	7.88529600	2.13864100
H	-11.55854900	8.29082400	1.23519100
H	-11.49443600	7.25183900	2.85469700
O	-12.71712100	8.84290600	4.19602200
P	-11.63028500	8.94709600	5.37327800
O	-10.65824100	9.94619100	4.89679100
O	-10.93023500	7.49731500	5.40268000
C	-11.50073900	6.38486700	6.04803700
H	-12.51111200	6.23663400	5.66728200
H	-11.53190800	6.50187100	7.13810000
C	-10.81375900	5.06732800	5.69215900
H	-11.24668100	4.32041100	6.34514800
O	-11.08602900	4.67601200	4.36847400
C	-9.91745800	4.11767400	3.82002100
H	-9.74649800	3.13491800	4.25322100
N	-10.00509100	3.97183300	2.36123700
C	-9.76795200	4.99964200	1.49361100
H	-9.46261200	5.95498700	1.88435600

C	-9.87907200	4.81737800	0.15860800
H	-9.63012200	5.62208300	-0.50905400
C	-10.38261900	3.55081500	-0.26760600
N	-10.49145900	3.24365200	-1.57106600
H	-10.09252600	3.80162400	-2.31033500
H	-10.91086000	2.34012200	-1.74523400
N	-10.67568700	2.55345400	0.56928100
C	-10.49835000	2.76584000	1.90147700
O	-10.78138700	1.86826100	2.69207200
C	-9.29455000	5.17327000	5.83064300
H	-8.97842100	6.06235300	6.37036000
C	-8.82805700	5.02940100	4.39033500
H	-8.71543200	6.00209700	3.91265700
H	-7.89414600	4.45419500	4.35952100
O	-8.80950800	4.00637400	6.45991900
P	-8.69074600	4.01831400	8.07102100
O	-9.91462400	4.59886300	8.65752500
O	-7.34377300	4.59450200	8.30226100
O	-8.69986500	2.42244600	8.29287900
C	-9.91714800	1.77168100	8.57488300
H	-10.67730100	2.24260700	7.95198900
H	-10.23576100	1.88848600	9.61519200
C	-9.92217500	0.25701200	8.41100900
H	-10.82084000	-0.15703700	8.88128900
O	-9.84358600	-0.00799600	7.02949000
C	-8.56652600	-0.42899600	6.59535200
H	-8.53131700	-1.47435500	6.28959900
N	-8.29439000	0.40574300	5.40772800
C	-7.57571300	1.56693900	5.32510400
H	-7.18768200	2.10127500	6.17640800

N	-7.31297500	1.89941400	4.08323900
C	-7.93596700	0.89916200	3.34109500
C	-7.80291600	0.53873200	1.97091700
O	-7.29303600	1.20391200	1.08066000
N	-8.44263300	-0.62081800	1.54712000
H	-8.47436700	-0.94235100	0.59014000
C	-9.07363700	-1.44251500	2.46043800
N	-9.73322800	-2.54060300	2.08488500
H	-9.79818100	-2.72605200	1.09216600
H	-10.16708300	-3.27516600	2.63469100
N	-9.10015600	-1.21821200	3.77846200
C	-8.52586500	-0.05066700	4.13402900
C	-8.73988700	-0.49303600	9.01410100
H	-8.45867800	-0.04644600	9.96635000
C	-7.73328000	-0.36199200	7.87512300
H	-7.13845100	0.54577200	7.81561000
H	-7.02460100	-1.19187900	7.92052300
O	-9.12835800	-1.83990900	9.19361600
P	-8.16295800	-2.89127900	9.92541300
O	-9.02448800	-3.77980500	10.73977700
O	-7.07483500	-2.16724300	10.62445400
O	-7.64473900	-3.71856100	8.64122000
C	-8.65594700	-4.39317200	7.93576900
H	-9.47274900	-3.66965000	7.83209300
H	-8.97445100	-5.20934400	8.58524400
C	-8.13971900	-4.87168200	6.57124200
H	-8.97815400	-5.37870800	6.11107800
O	-7.70722100	-3.74816900	5.85286500
C	-6.72599200	-4.16832700	4.93305100
H	-7.12015000	-4.86442800	4.19617800

N	-6.09797900	-2.95116900	4.38112100
C	-5.37658400	-2.00737300	5.05746400
H	-5.46953300	-1.90514700	6.13468700
N	-4.86641500	-1.05939900	4.32318000
C	-5.13609200	-1.57973200	3.06543200
C	-4.95936800	-1.02507900	1.78698500
N	-4.24053600	0.07513900	1.51679400
H	-3.85854500	0.68696500	2.23787100
H	-4.02279300	0.32132400	0.56738300
N	-5.33211800	-1.69308100	0.68112500
C	-6.00477400	-2.80698900	0.93181400
H	-6.37808000	-3.26541000	0.03131700
N	-6.42517100	-3.42815100	2.01842500
C	-5.86807100	-2.73854800	3.03797800
C	-6.91835200	-5.78201500	6.62562500
H	-6.59396900	-6.00522900	7.64265500
C	-5.83998800	-5.01100100	5.85337600
H	-5.24683500	-4.40822300	6.54238200
H	-5.27402200	-5.64739000	5.17892000
O	-7.24546900	-6.97319300	5.93353500
P	-6.28691400	-8.26928700	5.94410800
O	-7.05793900	-9.50631500	6.18676000
O	-5.13388400	-7.96590000	6.83060800
O	-5.65064000	-8.46953200	4.48388300
C	-6.41464300	-8.90469000	3.38037200
H	-7.25858300	-8.25373600	3.14032200
H	-6.86417000	-9.86906800	3.62368300
C	-5.59612300	-9.12956800	2.10744000
H	-6.07501400	-9.79954200	1.39772300
O	-5.36564500	-7.89819300	1.45032800

C	-3.98947900	-7.63254400	1.35337200
H	-3.55926400	-7.77103500	0.36179000
N	-3.73328200	-6.22470200	1.7365290
C	-3.75113100	-5.65832200	2.9927450
H	-4.17976200	-6.18704400	3.8392730
N	-3.23085000	-4.46221500	3.0367000
C	-2.84035200	-4.21479900	1.7295580
C	-2.18632800	-3.12421000	1.1083500
N	-1.73957000	-2.04115300	1.7728610
H	-2.02677500	-1.92867800	2.7339110
H	-1.44196600	-1.21940600	1.2374210
N	-1.95637300	-3.20552000	-0.2106550
C	-2.32421000	-4.30120000	-0.8915740
H	-2.10511700	-4.27052500	-1.9559630
N	-2.91020300	-5.39304000	-0.4142620
C	-3.14565500	-5.29035500	0.8978990
C	-4.23713800	-9.79502800	2.30038200
H	-4.26864200	-10.33123400	3.24826900
C	-3.26195700	-8.62244600	2.26331800
H	-3.32316400	-8.38595400	3.32144200
H	-2.19124200	-8.82182600	2.15415100
O	-3.97642400	-10.64592600	1.20758800
P	-2.57486900	-11.43346500	1.09477900
O	-2.79297500	-12.57623100	0.18071300
O	-2.07455500	-11.66144100	2.47017300
O	-1.67507100	-10.33858900	0.33385000
C	-1.92559800	-9.98967500	-1.01188200
H	-2.89734400	-9.50633900	-1.11384000
H	-2.09552500	-10.88598800	-1.60031000
C	-0.84753400	-9.04828700	-1.56602000

H	-0.97160900	-8.85136400	-2.62871700
O	-0.85697200	-7.91464800	-0.73820700
C	0.47302500	-7.46905000	-0.56316100
H	0.82447600	-7.02334400	-1.48988900
N	0.44468100	-6.49542100	0.5437040
C	-0.06436800	-6.82010600	1.7848840
H	-0.42035900	-7.84616500	1.8851550
C	-0.10536100	-5.93630000	2.8032170
C	-0.59347600	-6.26233300	4.1832250
H	0.22818200	-6.24793000	4.9009840
H	-1.32745200	-5.51238500	4.4917260
H	-1.07170000	-7.24725900	4.1990520
C	0.31566000	-4.55414100	2.5400690
O	0.33430900	-3.68060300	3.3999740
N	0.71556100	-4.29301000	1.2420490
H	0.94115600	-3.30521900	0.9548500
C	0.77176100	-5.17423200	0.1897080
O	1.12653100	-4.86573700	-0.9286980
C	0.56635600	-9.58735500	-1.39332900
H	0.42748400	-10.63165100	-1.12751200
C	1.27447300	-8.75133000	-0.33435300
H	0.99890000	-9.14652100	0.64426000
H	2.32624800	-8.51786100	-0.48455900
O	1.22014600	-9.41342200	-2.62864600
P	2.66403900	-10.06916000	-2.96447200
O	2.76400300	-10.06757200	-4.43637700
O	2.74573000	-11.38772300	-2.29155300
O	3.71766400	-9.01298900	-2.36490800
C	3.92070300	-7.75597300	-2.96638000
H	3.03510600	-7.13779800	-2.86687900

H	4.25491000	-7.87947900	-3.99598700
C	5.12763600	-7.00283500	-2.42185800
H	5.17131200	-6.01021900	-2.86169600
O	5.09677300	-6.94448600	-1.01347400
C	6.42324400	-7.09465300	-0.56617300
H	7.03889100	-6.21027500	-0.74533200
N	6.28865000	-7.43034300	0.8882070
C	5.08717000	-7.17563400	1.5303270
H	4.34346600	-6.64596300	0.9205080
C	4.82225200	-7.54136700	2.8065970
C	3.51298900	-7.24646700	3.4782850
H	2.85705100	-6.68204600	2.8018450
H	2.99284400	-8.16768700	3.7543630
H	3.65613200	-6.65223100	4.3825760
C	5.84464800	-8.25708400	3.5377990
O	5.76632500	-8.69017400	4.6830240
N	7.02630700	-8.45503600	2.8151350
H	7.77120700	-8.93279200	3.2966180
C	7.31786100	-8.10859200	1.5001980
O	8.39531000	-8.40149200	1.0074740
C	6.35279300	-7.82537300	-2.80481600
H	6.11924300	-8.77349400	-3.27675200
C	6.95684600	-8.21422000	-1.45534700
H	6.68843700	-9.22383800	-1.16684400
H	8.04601400	-8.21791500	-1.48906800
O	7.37482800	-7.21063500	-3.55455900
P	7.30911600	-6.90521800	-5.13977200
O	6.42409200	-7.85886500	-5.82744200
O	8.71043600	-6.67139500	-5.55477600
O	6.70017300	-5.40742300	-5.14099100

C	5.34662700	-5.09812900	-5.39407400
H	4.74919800	-5.80745000	-4.83394900
H	5.18636300	-5.15815200	-6.46976600
C	5.20894600	-3.59694400	-5.14329700
H	4.20222100	-3.32529100	-5.45636500
O	5.42495200	-3.32681300	-3.77546300
C	6.34606200	-2.25582800	-3.68464400
H	5.87470300	-1.27782500	-3.70282800
N	7.23792800	-2.44435900	-2.51741100
C	7.87053700	-3.63420200	-2.32252800
H	7.71581300	-4.41236200	-3.06558100
C	8.71800600	-3.80710800	-1.28676700
H	9.29117100	-4.71779600	-1.24400000
C	8.70865700	-2.75903200	-0.30638500
N	9.18446000	-2.92550900	0.93703600
H	9.51233100	-3.84778000	1.16090300
H	9.52625600	-2.08775300	1.38896700
N	8.08564500	-1.58388900	-0.46822500
C	7.45284200	-1.39233100	-1.65488700
O	6.97440800	-0.28733300	-1.90203000
C	6.13809200	-2.75574800	-6.01046100
H	6.63988700	-3.35220000	-6.77259300
C	7.14494100	-2.23046200	-4.97976800
H	8.08803800	-2.77909600	-5.00748400
H	7.31731100	-1.20571100	-5.30638000
O	5.48878700	-1.63888000	-6.56283000
P	6.24294900	-0.69794200	-7.63743400
O	5.25449400	-0.07009500	-8.54184900
O	7.29935900	-1.52659300	-8.24631400
O	6.96536700	0.53167400	-6.89780300

C	6.24491100	1.64076800	-6.39794600
H	5.48993600	1.21452400	-5.73271800
H	5.67302200	2.11972500	-7.19603300
C	7.08538300	2.67102000	-5.65418100
H	6.37704900	3.43505100	-5.32949500
O	7.61299900	2.06038600	-4.49930100
C	9.02222900	2.19200900	-4.57771500
H	9.31440300	3.05084800	-3.96580700
N	9.65153700	0.95908500	-4.06813700
C	9.73180900	-0.30021900	-4.60925600
H	9.37220400	-0.52588300	-5.60993600
N	10.23133200	-1.18573400	-3.78941500
C	10.67130000	-0.41645600	-2.71855600
C	11.40327300	-0.78209800	-1.55945200
O	11.67768500	-1.92153700	-1.18665500
N	11.84568700	0.29237700	-0.78934100
H	12.49170000	0.06616500	-0.05470100
C	11.39263200	1.56483600	-1.06318200
N	11.88897300	2.46656100	-0.19794400
H	12.43240400	2.24225000	0.63089100
H	11.60462000	3.42065300	-0.37187500
N	10.63848400	1.96109100	-2.09630500
C	10.33789000	0.89913000	-2.87783200
C	8.18987100	3.27719500	-6.51036900
H	8.13226800	3.02237100	-7.57542600
C	9.38222300	2.44735000	-6.02740600
H	9.48413700	1.52276700	-6.59842100
H	10.32946700	2.95925000	-6.18984600
O	8.19530800	4.69167500	-6.52131400
P	9.30781500	5.64957500	-7.19008600

O	8.65309600	6.95353600	-7.39436400
O	9.95189700	4.94162000	-8.32157100
O	10.43597700	5.76600000	-6.04662900
C	10.15843700	6.43583100	-4.83580300
H	9.32028300	5.89728300	-4.38097800
H	9.84377700	7.44128600	-5.10216500
C	11.37885100	6.50310600	-3.93166600
H	11.17097200	7.13674900	-3.06888900
O	11.55963100	5.20335700	-3.39113700
C	12.95451400	4.95471200	-3.32887600
H	13.40493700	5.38825600	-2.44368700
N	13.23642000	3.51866300	-3.46849000
C	12.72049200	2.84335300	-4.53904000
H	12.13514600	3.38567000	-5.25963800
C	12.98060100	1.51730400	-4.65365500
H	12.51460900	0.93463200	-5.44026000
C	13.78778700	0.88841000	-3.65468400
N	13.96743100	-0.44252100	-3.61796600
H	13.58143600	-0.95521300	-4.40273200
H	14.38342100	-0.86239800	-2.79976300
N	14.24375900	1.53755400	-2.56928000
C	13.97097300	2.85774800	-2.49595500
O	14.58957300	3.38667100	-1.57179400
C	12.62686000	6.99181300	-4.65784600
H	12.44126100	7.13474600	-5.72063600
C	13.54962900	5.79174900	-4.46100000
H	13.56018900	5.29051800	-5.42243500
H	14.57217800	6.07267300	-4.22147100
O	13.15620900	8.10816000	-3.98817800
P	14.39502300	8.96454300	-4.54813400

O	14.34078600	10.26241300	-3.83399900
O	14.39934300	8.93992400	-6.02812600
O	15.74151800	8.22943100	-4.04359500
C	15.92508400	8.18269200	-2.63781500
H	14.98428100	7.94628000	-2.14588200
H	16.26048500	9.17429800	-2.32441000
C	16.97278000	7.17323200	-2.18667900
H	17.07530200	7.38242400	-1.12167800
O	16.48785200	5.87218500	-2.43692700
C	17.65095300	5.08210800	-2.46647200
H	18.08136700	4.90852000	-1.47934900
N	17.36123600	3.80940000	-3.15121700
C	16.60242800	3.60728100	-4.26757700
H	16.17051400	4.45597300	-4.77843000
N	16.55606100	2.35678400	-4.63785900
C	17.34122700	1.69752400	-3.70047400
C	17.72075700	0.33315600	-3.58234600
O	17.27182800	-0.64714700	-4.17248900
N	18.63468700	0.04382800	-2.58438800
H	18.55551500	-0.93509200	-2.34617200
C	19.19318600	1.03972000	-1.80729200
N	19.72484000	0.59303500	-0.65026300
H	19.98639500	-0.38112900	-0.62390300
H	19.89790400	1.16125300	0.16052400
N	18.89864600	2.33875000	-1.93982800
C	17.94536900	2.60239800	-2.85909600
C	18.32416400	7.31441500	-2.88562800
H	18.36090600	8.07034000	-3.66769400
C	18.63754100	5.88558800	-3.30959700
H	18.58735700	5.70381400	-4.37760400

H	19.68508200	5.70459000	-3.05582500
O	19.22764000	7.74456300	-1.89446500
H	19.15684100	8.69381000	-1.82086600

VI.2. Minor groove intercalation

VI.2.1. 1BNA/ Os[(bpy)$_2$dppz]$^{2+}$

O	-20.48619400	7.53438700	-7.98049900
H	-20.89180100	7.02919800	-7.27412300
C	-20.91045100	8.87196500	-7.85443500
H	-22.00771300	8.93872500	-7.84187900
H	-20.48459800	9.45655500	-8.67119900
C	-20.22647400	9.43472300	-6.60945300
H	-20.65426100	10.42138400	-6.39945500
O	-20.55566700	8.59170500	-5.52873400
C	-19.35446900	8.40014400	-4.81843300
H	-19.17220000	9.32359800	-4.28111500
N	-19.34566300	7.22065800	-3.93404800
C	-18.94126700	7.44443900	-2.65260900
H	-18.65588400	8.42880300	-2.31618200
C	-18.86764500	6.39527300	-1.79848300
H	-18.59684800	6.50363600	-0.75501500
C	-19.20164700	5.12142400	-2.33574500
N	-19.04041000	4.05885400	-1.52682800
H	-19.08059000	4.15204400	-0.52413100
H	-19.44106700	3.18919300	-1.85080900
N	-19.60685900	4.87688300	-3.58606600
C	-19.72756900	5.96870700	-4.39368500
O	-20.14709200	5.75892200	-5.51835900
C	-18.71229600	9.59724600	-6.62521500
H	-18.48575800	9.52894200	-7.68997600
C	-18.28421000	8.32293000	-5.90879300
H	-18.43848300	7.51603400	-6.63434100
H	-17.25234700	8.39927500	-5.56407600
O	-18.38504200	10.84462900	-6.05115700

P	-17.03207000	11.61742800	-6.46738800
O	-17.08905900	13.02148300	-5.97883900
O	-16.64276600	11.34530900	-7.86631400
O	-16.10715500	10.82608900	-5.41571600
C	-16.11544100	11.04908200	-4.02029300
H	-17.17818500	10.97250400	-3.78110300
H	-15.68337700	12.02613500	-3.78451900
C	-15.52639500	9.86746000	-3.25387600
H	-15.59097100	10.03914900	-2.18016600
O	-16.09806700	8.60239700	-3.50228600
C	-15.08903700	7.62689800	-3.62211200
H	-14.70886400	7.48269500	-2.61252100
N	-15.48681500	6.31816500	-4.15539700
C	-15.44149200	5.85825600	-5.45082300
H	-15.35487000	6.47443800	-6.32610400
N	-15.58412700	4.56211500	-5.52875700
C	-15.74949400	4.15818900	-4.20542900
C	-15.98682200	2.85063700	-3.68930600
O	-16.16887100	1.78495700	-4.26366200
N	-16.04220500	2.79093600	-2.31018800
H	-16.36677000	1.90784400	-1.93414800
C	-16.00946700	3.92016800	-1.51096000
N	-16.40927600	3.73761900	-0.24532700
H	-16.76658300	2.83872500	0.04540000
H	-16.58986000	4.59872600	0.23766800
N	-15.84807700	5.15415700	-2.00424000
C	-15.72413500	5.23012300	-3.34821500
C	-14.07893300	9.69350400	-3.69511500
H	-13.81184300	10.52467100	-4.34189500
C	-14.14063300	8.41071100	-4.52042500

H	-14.46244400	8.57758400	-5.55192500
H	-13.15806200	7.97354300	-4.39105400
O	-13.14517800	9.55331000	-2.64905200
P	-12.62700400	10.84334300	-1.83265100
O	-13.69991900	11.85507300	-1.69032900
O	-11.39083900	11.29025100	-2.50471600
O	-12.24746800	10.23972000	-0.38724800
C	-13.16733800	10.21927100	0.67403400
H	-14.14951400	10.28463400	0.20663900
H	-13.07346500	11.11166500	1.28150600
C	-13.08916100	8.96836100	1.54150800
H	-13.78322100	9.14461500	2.36716800
O	-13.59164500	7.85363000	0.82961900
C	-12.77393700	6.77869700	1.22009500
H	-13.25184600	6.26545300	2.05417200
N	-12.52498700	5.93610300	0.03461600
C	-12.13740200	6.56118400	-1.11605800
H	-12.02124700	7.63389100	-1.18467100
C	-12.07306200	5.88101500	-2.27835400
H	-11.85262800	6.35933100	-3.22282300
C	-12.44406500	4.50284600	-2.23704100
N	-12.50505300	3.63467300	-3.26132400
H	-12.27976600	3.93851200	-4.19995500
H	-12.68456800	2.70274800	-2.92370200
N	-12.76198000	3.83360800	-1.11078600
C	-12.86499200	4.60072000	-0.00718900
O	-13.32402700	4.07048400	1.00564800
C	-11.70668600	8.79303600	2.15813200
H	-11.03889200	9.47039500	1.63455400
C	-11.44187400	7.36433900	1.66823400

H	-10.71262100	7.37461900	0.85547000
H	-11.07732300	6.78052200	2.51909300
O	-11.80715000	9.01427600	3.54354200
P	-10.45811000	9.16768800	4.42038600
O	-10.72237700	9.81744500	5.73068300
O	-9.36755300	9.69103300	3.56733600
O	-10.03615100	7.67822600	4.86135400
C	-10.88013900	6.99588800	5.75940700
H	-11.93661900	7.03181600	5.50180300
H	-10.92349900	7.49827400	6.72973100
C	-10.48639800	5.52687800	5.92727200
H	-11.01124400	5.17837800	6.82503800
O	-11.01420300	4.75268600	4.87953600
C	-10.03854500	3.83639700	4.46734000
H	-10.47638800	2.87248700	4.73186000
N	-9.72157100	4.01112500	3.03685100
C	-9.02818300	5.04441000	2.47503600
H	-8.67383500	5.89535100	3.04882700
N	-8.91755700	4.94892000	1.17378900
C	-9.44221300	3.68860700	0.89121800
C	-9.57991600	2.91670100	-0.29258900
O	-9.32648500	3.35073100	-1.42320400
N	-10.11966000	1.64928600	-0.17538200
H	-10.32365100	1.04713300	-0.95845200
C	-10.52585300	1.20322700	1.06531900
N	-11.02625800	-0.03816000	0.98561100
H	-11.01941900	-0.52443200	0.09899300
H	-11.57713300	-0.35229000	1.76744200
N	-10.53183200	1.90606600	2.20570600
C	-9.95601200	3.11646500	2.01605700

C	-9.01486900	5.17023100	6.15532000
H	-8.37198800	5.93259600	5.72636400
C	-8.79425400	3.88477000	5.35812600
H	-7.85747200	3.84574900	4.80070600
H	-8.81866600	2.99503100	5.98826000
O	-8.70069300	5.00614600	7.51626400
P	-7.15199600	4.91948800	7.95538400
O	-7.12038300	5.24935600	9.39423300
O	-6.24467500	5.70425800	7.08555400
O	-6.80768700	3.35452700	7.74622100
C	-7.45776500	2.31049900	8.43054700
H	-8.50663600	2.58946000	8.38991600
H	-7.01915500	2.25000800	9.42682100
C	-7.27193000	0.90571600	7.86455200
H	-7.76415700	0.20771900	8.53321600
O	-7.82642300	0.69841500	6.58374000
C	-6.93433600	-0.07956700	5.8181640
H	-7.35631600	-0.99452000	5.40876600
N	-6.58929600	0.74004100	4.6175710
C	-6.11096900	2.03849200	4.5557840
H	-5.99786800	2.64254600	5.4578440
N	-5.83276900	2.41908300	3.3396500
C	-6.12689000	1.32002500	2.5577990
C	-5.99257700	1.08489300	1.1691240
N	-5.54489500	2.00750300	0.3116670
H	-5.45053400	2.95923700	0.6373520
H	-5.56517800	1.81629400	-0.6899700
N	-6.30210200	-0.14704600	0.7135770
C	-6.75173800	-1.07104900	1.5753390
H	-6.97195000	-2.03353700	1.1193150

N	-6.94084800	-0.96506100	2.8842140
C	-6.59936400	0.26251400	3.3243650
C	-5.77533800	0.58354100	7.76597500
H	-5.21142900	1.48087800	7.53104500
C	-5.68994100	-0.42767000	6.62760100
H	-4.76376300	-0.30798100	6.06010400
H	-5.82838300	-1.46899500	6.91581600
O	-5.37900800	-0.01626100	8.98620500
P	-3.84762100	0.11406000	9.46679600
O	-3.73815400	-0.06181800	10.93662100
O	-3.19946600	1.30620200	8.89408900
O	-3.25647900	-1.13293900	8.63749300
C	-3.63333600	-2.45316500	8.94226000
H	-4.63020100	-2.65825800	8.55755500
H	-3.63017700	-2.61132500	10.01942100
C	-2.65957400	-3.46457000	8.34444800
H	-3.07613600	-4.47052800	8.43042700
O	-2.61478500	-3.24607900	6.95526700
C	-1.24984000	-3.25235700	6.6141570
H	-0.87656900	-4.22236700	6.27559500
N	-1.08508200	-2.26857600	5.5063800
C	-1.19632100	-0.89135600	5.6031930
H	-1.51923400	-0.41975400	6.5317190
N	-0.91498700	-0.26651200	4.4924960
C	-0.60267500	-1.27643600	3.5993910
C	-0.31316100	-1.25718900	2.2114120
N	-0.19568700	-0.12502300	1.4958730
H	0.05413800	0.70698900	2.0139320
H	0.16539700	-0.19719700	0.5387770
N	-0.24040500	-2.43770500	1.5704660

C	-0.33820600	-3.57210500	2.2732040
H	-0.22491000	-4.48370200	1.6917410
N	-0.55321500	-3.71059500	3.5796020
C	-0.71156600	-2.52832800	4.1969880
C	-1.30683000	-3.40410000	9.04368500
H	-1.31611000	-2.65736400	9.83728400
C	-0.48606900	-2.86215100	7.87461900
H	-0.35698600	-1.78844100	7.99660400
H	0.57174800	-3.10334100	7.78643200
O	-0.97196100	-4.66976300	9.54812700
P	0.43639100	-5.00154300	10.26350500
O	0.22602600	-6.17430800	11.13698600
O	1.02523300	-3.74758500	10.76525500
O	1.23930300	-5.42907100	8.92920600
C	1.07797600	-6.61505500	8.18515200
H	0.03261600	-6.74433400	7.91402700
H	1.37199400	-7.47973100	8.78572500
C	1.92168500	-6.63700200	6.91362800
H	1.78213000	-7.51989200	6.28559000
O	1.70946200	-5.53980500	6.06862900
C	2.81036300	-5.33458300	5.2060710
H	2.75004000	-6.08457000	4.42454300
N	2.72871300	-3.96548300	4.6724990
C	2.62424100	-2.87343500	5.5115400
H	2.61031900	-3.11196400	6.5737760
C	2.53437000	-1.60872000	5.0525960
C	2.40689400	-0.39792800	5.9266090
H	3.26864800	0.26015500	5.7995180
H	1.51792100	0.17323600	5.6387940
H	2.32077100	-0.68506400	6.9776230

C	2.55869600	-1.39430100	3.6036880
O	2.49414600	-0.28638900	3.0815990
N	2.62678300	-2.54323900	2.8305330
H	2.65870000	-2.40935900	1.8000880
C	2.63000900	-3.84885300	3.2741630
O	2.56523900	-4.80333600	2.5272230
C	3.42314500	-6.58879300	7.17476000
H	3.62620500	-6.25903300	8.19384100
C	4.00747600	-5.73839700	6.05102000
H	4.54992000	-4.89216200	6.48199600
H	4.61639400	-6.29386800	5.33648000
O	3.88488700	-7.90809000	6.93011800
P	5.34743800	-8.49571200	7.25127900
O	5.01188800	-9.84806100	7.76064800
O	6.11180600	-7.56143200	8.09066300
O	6.02214000	-8.56893600	5.78686200
C	5.41361700	-9.28962200	4.74378500
H	4.33074000	-9.30242000	4.86753300
H	5.73743600	-10.33425000	4.77196900
C	5.72511500	-8.64589500	3.39146000
H	5.20859000	-9.24370000	2.63844500
O	5.40727100	-7.29652000	3.16505100
C	6.43698700	-6.61751900	2.47531000
H	6.38524600	-6.87839200	1.41939000
N	6.36104900	-5.15167100	2.54826000
C	6.30260500	-4.44209100	3.71105000
H	6.17479100	-4.98620400	4.63333300
C	6.27879600	-3.09499800	3.75434200
C	6.47545200	-2.46018100	5.10853300
H	7.18804400	-1.65461900	4.91910600

H	5.55221200	-1.96073400	5.42075100
H	6.88352700	-3.19957500	5.79568000
C	6.28777400	-2.33480500	2.51998900
O	6.12836400	-1.12451100	2.40740100
N	6.32830800	-3.09884200	1.37181500
H	6.30513700	-2.62005400	0.47269100
C	6.46149800	-4.48159900	1.33652100
O	6.62228300	-5.06367400	0.26790600
C	7.19994400	-8.73151700	3.03236700
H	7.69968100	-9.35419900	3.77407400
C	7.66709400	-7.28252200	3.09224500
H	7.71928100	-6.98074800	4.13690200
H	8.58196800	-7.09601500	2.52724800
O	7.48026800	-9.33456300	1.78579000
P	8.95553200	-9.81308700	1.33168600
O	8.83621300	-11.15622400	0.73776000
O	9.97824900	-9.51862700	2.36156100
O	9.21386900	-8.82068800	0.09811200
C	8.64273400	-8.91233300	-1.18952400
H	7.66316800	-8.44048700	-1.19284600
H	8.66743700	-9.96332800	-1.46265300
C	9.48420200	-8.13902500	-2.21012500
H	9.13642600	-8.41638800	-3.20447000
O	9.34626800	-6.75874800	-1.97094000
C	10.55578800	-6.08097000	-1.69913600
H	11.02301400	-5.68697000	-2.59376600
N	10.22604600	-5.03161900	-0.72490100
C	10.14744600	-5.33755400	0.61144700
H	10.26207200	-6.34548300	0.95106500
C	9.97513800	-4.33213100	1.51229900

H	10.07099200	-4.49504600	2.57586400
C	10.01565500	-2.98558200	1.02346000
N	10.02855400	-1.97959600	1.90704800
H	10.24201800	-2.23227100	2.86239500
H	9.90250500	-1.05063000	1.54658500
N	10.13366900	-2.69842000	-0.27296200
C	10.23063300	-3.72287100	-1.16598900
O	10.29985500	-3.38716300	-2.34132200
C	10.97753200	-8.43579200	-2.16329200
H	11.16965500	-9.38707100	-1.66815900
C	11.43630400	-7.26386600	-1.29870200
H	11.19166300	-7.56530200	-0.27220900
H	12.50020300	-7.05190500	-1.31256900
O	11.42435100	-8.46539600	-3.50496200
P	12.98631400	-8.58161900	-3.89182700
O	13.04602300	-9.01524200	-5.30430900
O	13.54763400	-9.50347500	-2.87570500
O	13.48494700	-7.07003400	-3.68331800
C	13.00665000	-6.04197700	-4.52357400
H	11.91832200	-6.04328400	-4.41158400
H	13.16370000	-6.18464500	-5.59478000
C	13.46330800	-4.61123900	-4.26405500
H	13.21425900	-3.95899800	-5.10158600
O	12.95925200	-4.01662800	-3.08360400
C	13.82966100	-2.94456700	-2.80508600
H	13.64598900	-2.08115900	-3.43253500
N	13.83787800	-2.63396100	-1.35720600
C	13.41647400	-3.34657600	-0.25939100
H	13.07784900	-4.36605700	-0.29928500
N	13.46874500	-2.65840600	0.85666900

C	13.87062900	-1.38584800	0.45969800
C	13.88037900	-0.21127300	1.26286500
O	13.68636500	0.01505800	2.44997600
N	14.26708900	0.87686800	0.48858800
H	14.17453000	1.78917700	0.92128500
C	14.60408100	0.84202600	-0.84981400
N	14.98645700	1.99229400	-1.42529100
H	15.00735800	2.86689900	-0.91194000
H	14.95222400	2.04662600	-2.42792600
N	14.48899300	-0.27522200	-1.58214800
C	14.15018700	-1.38526100	-0.88549600
C	14.97526400	-4.43632100	-4.18162700
H	15.39464100	-5.35360000	-3.76711300
C	15.25131300	-3.33222300	-3.17105100
H	15.89470300	-3.53678000	-2.31694000
H	15.64836500	-2.45114700	-3.68471900
O	15.47978000	-4.34193100	-5.49690400
P	17.06336200	-4.38559600	-5.80587200
O	17.29219100	-4.62476100	-7.25129100
O	17.69420600	-5.25679200	-4.78947800
O	17.47185900	-2.87548000	-5.44645400
C	16.91032300	-1.80879200	-6.17635300
H	15.82770600	-1.77061700	-6.05394100
H	17.12436100	-2.02779000	-7.22950400
C	17.58392600	-0.48083100	-5.82867700
H	17.28819500	0.17022300	-6.64572800
O	17.00900900	-0.05958500	-4.61470800
C	18.06001800	0.37870200	-3.78057100
H	18.15288800	1.46948500	-3.83773500
N	17.80629800	0.13691300	-2.35138800

C	17.53018600	-1.12103500	-1.89638100
H	17.45029300	-1.94329600	-2.59488100
C	17.32540800	-1.39773600	-0.59204200
H	17.23365400	-2.43788300	-0.32431900
C	17.37294100	-0.28345600	0.31328700
N	17.19742300	-0.37932800	1.63620100
H	17.02402500	-1.31561800	1.95821800
H	16.74438300	0.36602900	2.14087700
N	17.71123400	0.94414900	-0.08963300
C	17.97351900	1.13801200	-1.39952800
O	18.42300800	2.25556100	-1.63836700
C	19.10611200	-0.44447300	-5.71630600
H	19.51432000	-1.39756500	-6.07152700
C	19.36664500	-0.27708300	-4.21917400
H	19.55843400	-1.23192500	-3.71035900
H	20.26566600	0.29426900	-4.02651500
O	19.63594500	0.63449600	-6.43831800
P	21.08381500	0.52253800	-7.13383300
O	21.09747000	1.44367800	-8.28960800
O	21.60098900	-0.85356900	-7.28959300
O	22.00906300	1.27417500	-6.04573500
C	21.96957300	2.66547400	-5.81589600
H	20.90753900	2.89506500	-5.79661700
H	22.37288100	3.22785900	-6.66092000
C	22.65217500	3.12923200	-4.53095200
H	22.53915000	4.20760200	-4.42826300
O	21.98368200	2.47366500	-3.47546700
C	22.94691300	2.26362300	-2.46880400
H	23.06796500	3.25181500	-2.01844400
N	22.52531900	1.34417600	-1.40293600

C	22.90623500	0.04626100	-1.14696800
H	23.56124500	-0.45410600	-1.84603500
N	22.28042000	-0.54503700	-0.17603000
C	21.62501400	0.53882400	0.40456500
C	20.91512100	0.53135600	1.62783800
O	20.58143800	-0.37683500	2.39180400
N	20.41203600	1.80063800	1.90229900
H	19.90722300	1.89066700	2.76858900
C	20.60315700	2.90469200	1.09816100
N	20.25554200	4.08756800	1.62434200
H	19.72184200	4.08508000	2.47314000
H	20.45500300	4.96317600	1.16290300
N	21.17404200	2.89558600	-0.11089100
C	21.70556800	1.67792100	-0.35659800
C	24.12158800	2.71125900	-4.47241600
H	24.30217500	2.17029000	-5.39097000
C	24.24408800	1.89670700	-3.19054300
H	24.22922900	0.85085200	-3.49984300
H	25.17877200	2.02629900	-2.62967600
O	24.92499700	3.85598500	-4.27893300
H	24.84776700	4.38474000	-5.07865400
O	19.62465800	6.59405500	11.12758400
H	18.71048800	6.49681500	11.43079600
C	19.92143900	5.67112900	10.10507400
H	19.56531500	4.66440400	10.32389100
H	20.99500800	5.66368200	9.88081000
C	19.14960900	6.04425500	8.84588600
H	19.58463200	6.96341600	8.44538900
O	19.41561400	5.04476700	7.89039300
C	18.51144600	5.15245100	6.80734900

H	18.85506300	5.89481400	6.08083400
N	18.40977600	3.81280000	6.20014300
C	17.96055200	2.75143800	6.93601600
H	17.50023600	2.93979500	7.89478100
C	18.02425500	1.50600500	6.43778100
H	17.58512200	0.72364700	7.04191400
C	18.73314200	1.28588000	5.21367900
N	18.90897100	0.09433300	4.62257800
H	18.41073300	-0.67302000	5.03914500
H	19.44808200	0.00058400	3.77077400
N	19.23316300	2.32268300	4.52381200
C	19.01476800	3.59314300	4.97362900
O	19.28530700	4.49728200	4.19245000
C	17.64886200	6.30742800	8.86321300
H	17.16576100	5.74819600	9.66325800
C	17.28524300	5.73007000	7.49798800
H	16.47506300	5.01899300	7.68040700
H	16.92959700	6.48642600	6.79461000
O	17.31181500	7.67544600	8.97009600
P	15.79761400	8.18472700	8.86846900
O	15.69843000	9.43586700	9.65237600
O	14.87648800	7.09763700	9.27915500
O	15.65644900	8.54869200	7.30798700
C	16.61653600	9.35659600	6.65743100
H	17.61861500	9.04171800	6.96530800
H	16.47607300	10.39664600	6.93950400
C	16.55393300	9.41513900	5.13626200
H	17.35205800	10.01381500	4.70500400
O	16.87410800	8.08549300	4.76852800
C	15.80541300	7.66742500	3.95384400

H	16.13036600	7.95920200	2.94872100
N	15.59444000	6.21540000	4.05291300
C	15.01871500	5.50767100	5.08245700
H	14.62514800	6.00358700	5.96215600
N	15.05820800	4.22482200	4.87355500
C	15.81733700	4.01035000	3.72524100
C	16.20314100	2.82917700	3.04694600
O	15.96611100	1.65473600	3.32731100
N	16.98667900	3.07846100	1.93230400
H	17.22199200	2.28296600	1.34347900
C	17.21796300	4.34296900	1.41944200
N	17.70927900	4.41169300	0.17024800
H	18.04993200	3.56147700	-0.24022600
H	18.09020500	5.29607400	-0.14561000
N	16.82618700	5.43368900	2.08865100
C	16.18006400	5.24420300	3.26607200
C	15.15722700	9.79471400	4.67481300
H	14.50013900	10.21265800	5.44737900
C	14.55258900	8.43917300	4.33625400
H	14.03422900	7.95771700	5.17762300
H	13.92057700	8.42104400	3.44634900
O	15.28541600	10.64143100	3.54630200
P	14.09354600	11.61239400	3.08307700
O	14.72486800	12.82181000	2.49253200
O	13.27490600	11.77987200	4.29810000
O	13.38223600	10.72330100	1.95708700
C	14.09653700	10.51539000	0.75091700
H	15.16080000	10.38446400	0.90356900
H	14.02302500	11.38759900	0.10652000
C	13.73283300	9.23410500	-0.00096700

H	14.42207600	9.20862300	-0.83863900
O	13.92703300	8.15356200	0.87716400
C	13.32488300	7.05089300	0.23176700
H	13.91067200	6.84988000	-0.66145400
N	13.16142000	5.84554000	1.06866800
C	12.39654100	5.93578400	2.19179600
H	11.94287400	6.86460500	2.51035100
C	12.20011900	4.85685600	2.98042200
H	11.61869700	4.75774400	3.87598000
C	12.82230000	3.63415300	2.56019800
N	12.61679100	2.50120500	3.23220700
H	12.12276600	2.53091500	4.11959500
H	12.96289400	1.63949900	2.83349100
N	13.51253900	3.50830300	1.41135900
C	13.82665200	4.66957300	0.79322900
O	14.59935700	4.57168500	-0.17090100
C	12.29380800	9.09546500	-0.48147200
H	11.58303200	9.64907900	0.14239500
C	11.99325300	7.61176000	-0.26127700
H	11.19087500	7.35315600	0.41924700
H	11.84124900	7.19996300	-1.25662500
O	12.33262600	9.54876700	-1.81695400
P	11.06122900	9.46303200	-2.79122200
O	11.25698200	10.53222600	-3.80167000
O	9.81243100	9.39405000	-1.99910800
O	11.16771500	7.99385200	-3.43439700
C	12.43767800	7.66329300	-3.97191400
H	13.34344100	7.83252300	-3.40142900
H	12.46708600	8.28113000	-4.87008600
C	12.60204500	6.20219400	-4.37037600

H	13.55447200	6.03682700	-4.87992200
O	12.75602600	5.44762500	-3.18905600
C	12.07886700	4.22625600	-3.36287700
H	12.70358000	3.45223000	-3.80505200
N	11.55569200	3.79233700	-2.05608700
C	10.96884000	4.46387300	-1.02572600
H	10.92711500	5.53960600	-1.00969300
N	10.50961500	3.72680600	-0.04483600
C	10.80257400	2.43090900	-0.47753400
C	10.49524300	1.16395100	0.07669000
O	9.86405800	0.86208900	1.08633600
N	10.64915900	0.08687300	-0.79211000
H	10.34924900	-0.82374500	-0.48841900
C	11.21574600	0.22203400	-2.03678200
N	11.25928000	-0.83007100	-2.87253400
H	10.83982900	-1.72232600	-2.64006600
H	11.71938200	-0.65930000	-3.75238800
N	11.51640200	1.41511600	-2.56655600
C	11.27713000	2.46950000	-1.75691100
C	11.46897700	5.58625700	-5.18700200
H	10.65189100	6.26082500	-5.43323200
C	10.90047200	4.48838700	-4.29543900
H	10.02984600	4.88888400	-3.78113100
H	10.69543800	3.57650200	-4.84491700
O	12.03236300	5.15716200	-6.40329700
P	11.14753500	4.72018700	-7.67888800
O	11.95987000	4.45869200	-8.88931500
O	10.10902700	5.76292800	-7.76884700
O	10.41175600	3.32194000	-7.35203200
C	10.99819500	2.05397300	-7.48524700

H	11.87247300	1.94631700	-6.85608300
H	11.22432300	1.92106300	-8.54491800
C	9.98504000	0.97876400	-7.08832900
H	10.48783700	0.11341200	-7.52071800
O	9.98645800	0.74435200	-5.70216600
C	8.76452300	0.09058700	-5.43446200
H	8.83390600	-0.98060200	-5.64598000
N	8.45612500	0.40758100	-4.02918400
C	8.39765100	1.67529800	-3.50309100
H	8.76800400	2.47516600	-4.12626800
N	7.90841500	1.79744900	-2.30645900
C	7.55584300	0.46983700	-2.05418600
C	7.06462200	-0.21225500	-0.92819700
N	6.64336200	0.41127400	0.17409800
H	6.83263400	1.40695200	0.17491300
H	5.95755300	-0.03252800	0.77268500
N	6.83867200	-1.53080600	-0.90436400
C	7.28206700	-2.19673500	-1.97330800
H	7.20258200	-3.27192100	-1.99215400
N	7.77821400	-1.73652900	-3.10580400
C	7.88733100	-0.39220300	-3.06730100
C	8.54761300	1.01380200	-7.60396000
H	8.30269100	1.96825800	-8.06300900
C	7.71461200	0.69748500	-6.36180400
H	7.27625900	1.60484800	-5.96075600
H	7.03327400	-0.12537800	-6.52695300
O	8.48369300	-0.04230200	-8.53839100
P	7.17606900	-0.19310600	-9.45740000
O	7.56881000	-1.03774500	-10.61797800
O	6.53067100	1.10089300	-9.76469100

O	6.18098100	-1.08655800	-8.55954500
C	6.56375300	-2.37411800	-8.13272800
H	7.60770000	-2.42858600	-7.83640500
H	6.38782700	-3.12141700	-8.90906300
C	5.76619100	-2.99518400	-6.98369700
H	6.04414700	-4.01762900	-6.71696600
O	5.78283000	-2.20909600	-5.80646100
C	4.73309700	-2.56748200	-4.9386800
H	4.97050700	-3.48440100	-4.39694900
N	4.48306700	-1.54968500	-3.8886560
C	4.65729300	-0.18645000	-3.8611030
H	5.07143900	0.33944700	-4.7132300
N	4.28536000	0.36274200	-2.7306410
C	3.84875600	-0.70137900	-1.9612540
C	3.34724700	-0.79242100	-0.6396110
N	3.16620900	0.29095300	0.1465370
H	3.58023900	1.15874000	-0.1587160
H	3.00090000	0.14090600	1.1402260
N	3.01704400	-2.00150200	-0.1575850
C	3.17980500	-3.07770600	-0.9579510
H	2.90074600	-4.02615200	-0.5047320
N	3.62736400	-3.12088800	-2.1998140
C	3.96406800	-1.90060700	-2.6543890
C	4.25846700	-2.94421400	-7.20453300
H	4.06270700	-2.05844300	-7.80452500
C	3.54620600	-2.84445800	-5.85838400
H	2.81073300	-2.03054500	-5.86166900
H	3.16420200	-3.80058200	-5.51006700
O	3.77411300	-4.03826000	-7.94713800
P	2.26093000	-4.19530800	-8.47079100

O	2.36226800	-5.19713900	-9.54785400
O	1.78116100	-2.86717800	-8.94057000
O	1.39251300	-4.77283500	-7.24636800
C	1.07090000	-6.14240800	-7.09197700
H	1.92091000	-6.81385200	-7.01954600
H	0.53669500	-6.39724800	-8.01191200
C	0.30634900	-6.37134800	-5.79615600
H	0.13127700	-7.43651100	-5.67585400
O	0.97199200	-5.71334000	-4.73879900
C	0.05439200	-5.42087700	-3.7128610
H	0.26936700	-6.12683100	-2.91209000
N	0.30147400	-4.05323300	-3.1631940
C	0.74103900	-3.00401600	-3.9447880
H	1.01280000	-3.28374500	-4.9690570
C	0.82956600	-1.73711800	-3.4798450
C	1.31766500	-0.58700900	-4.3064540
H	0.49683600	0.07513200	-4.5882610
H	2.04232400	0.00584300	-3.7442520
H	1.79916400	-0.95739200	-5.2256100
C	0.46669800	-1.48909200	-2.0874110
O	0.47717800	-0.39206100	-1.5354550
N	0.04582300	-2.60832200	-1.3763630
H	-0.08207100	-2.50126400	-0.3571760
C	-0.09670400	-3.88876400	-1.8456420
O	-0.56637900	-4.78888500	-1.1564370
C	-1.10002500	-5.76975700	-5.79802300
H	-0.97420000	-4.81061300	-6.30528200
C	-1.34671700	-5.50029800	-4.32324200
H	-1.92127200	-4.56998000	-4.27034500
H	-1.89643000	-6.35867500	-3.94623500

O	-2.10535900	-6.54029300	-6.42522100
P	-2.75787500	-6.26281400	-7.86720900
O	-2.99925600	-7.49661700	-8.65490500
O	-2.01498800	-5.18620200	-8.56271200
O	-4.25501600	-5.69352500	-7.69697600
C	-4.51764800	-4.78795200	-6.65622600
H	-5.32183100	-4.11498500	-6.96103000
H	-3.65203300	-4.13107700	-6.50057800
C	-5.00108000	-5.45398600	-5.36506300
H	-4.27617500	-6.23875500	-5.14978600
O	-4.92047700	-4.42878300	-4.40905300
C	-6.20623000	-4.09398200	-3.9365710
H	-6.36765000	-4.75938500	-3.08325500
N	-6.20217600	-2.65177000	-3.6398680
C	-5.88749100	-1.73449200	-4.6255590
H	-5.78982800	-2.15014400	-5.6234210
C	-5.71032900	-0.42120900	-4.3760920
C	-5.40264000	0.60088500	-5.4274800
H	-6.22733300	1.30540100	-5.5341670
H	-4.51969300	1.17104900	-5.1241500
H	-5.19710500	0.11892700	-6.3853170
C	-5.76908500	0.02962100	-2.9858980
O	-5.59645600	1.18961900	-2.6345400
N	-6.02098300	-0.96491200	-2.0530960
H	-6.09171500	-0.66720800	-1.0537970
C	-6.21142800	-2.30127700	-2.2897490
O	-6.38565200	-3.10441700	-1.3844240
C	-6.45672200	-5.92926200	-5.44394900
H	-6.67116400	-6.25323600	-6.46911100
C	-7.19687700	-4.70510300	-4.91660200

H	-7.38342000	-3.97119400	-5.69477900
H	-8.06689400	-4.92188000	-4.29991100
O	-6.63189700	-7.02394100	-4.57851000
P	-7.91038800	-7.99688600	-4.67305800
O	-7.77495900	-9.16470400	-3.76792800
O	-8.19635900	-8.28966600	-6.09383200
O	-9.13840200	-7.12797200	-4.09662900
C	-9.42336900	-6.92387100	-2.72749200
H	-8.50010500	-6.76478900	-2.16653200
H	-9.95082700	-7.78730600	-2.31473500
C	-10.29761200	-5.72388200	-2.39973000
H	-10.42125900	-5.77518800	-1.31244900
O	-9.84181300	-4.40386600	-2.62222700
C	-10.96242200	-3.62613000	-2.95862400
H	-11.68536900	-3.54239400	-2.15045600
N	-10.58886500	-2.25939900	-3.36099400
C	-10.40688600	-1.83897400	-4.65038400
H	-10.69063400	-2.46167800	-5.48460600
C	-10.18720500	-0.53229900	-4.90404200
H	-10.06391900	-0.13549900	-5.90865600
C	-10.04716400	0.37300200	-3.79507100
N	-9.63845600	1.62722600	-3.99199800
H	-9.25862400	2.00085600	-4.85752000
H	-9.80903200	2.27770500	-3.23471200
N	-10.14200900	-0.07802500	-2.53345300
C	-10.46491700	-1.37710400	-2.30957100
O	-10.79880500	-1.70665800	-1.17563400
C	-11.56122300	-5.90200800	-3.22976500
H	-11.52005500	-6.73845000	-3.92169700
C	-11.63053500	-4.56330400	-3.96452200

H	-11.03807000	-4.69044200	-4.88219300
H	-12.67073100	-4.29753800	-4.13263100
O	-12.71777100	-6.01664500	-2.43998300
P	-13.29055100	-7.43036500	-1.92314700
O	-12.21562800	-8.41549900	-1.64919100
O	-14.33885400	-7.86384900	-2.87291100
O	-13.96343000	-7.10878800	-0.48902000
C	-13.11461000	-6.77326600	0.57654600
H	-12.15145300	-6.40928900	0.20512900
H	-12.94592000	-7.72010200	1.08688300
C	-13.74747100	-5.87888700	1.64189700
H	-13.35503200	-6.27242400	2.57223000
O	-13.26753500	-4.57989000	1.37065900
C	-14.41658500	-3.85377100	1.00550700
H	-14.61229800	-3.19296300	1.85257800
N	-14.18353700	-2.97312700	-0.15546400
C	-14.05029800	-3.31072100	-1.48267100
H	-14.11895800	-4.36408900	-1.71484100
N	-13.83011200	-2.34112200	-2.32111900
C	-13.86811900	-1.23946600	-1.46501800
C	-13.59100100	0.14023000	-1.69094800
O	-13.36789500	0.75550400	-2.72393400
N	-13.65400400	0.94310400	-0.56244200
H	-13.55116200	1.95280600	-0.56739100
C	-14.05419200	0.45534300	0.66023500
N	-14.27344200	1.40860800	1.58290200
H	-13.97019400	2.35746800	1.39157900
H	-14.44122000	1.13038300	2.53691500
N	-14.30887500	-0.83103500	0.93294300
C	-14.15391600	-1.59838100	-0.16944900

C	-15.26750700	-5.98607300	1.67192800
H	-15.72563700	-6.90505200	1.32639100
C	-15.54023900	-4.84071500	0.70643800
H	-15.37429500	-5.24464700	-0.30103500
H	-16.57590700	-4.53348000	0.84890800
O	-15.76452600	-5.76892500	2.97351100
P	-17.31151400	-5.89462600	3.41467600
O	-17.22456400	-6.44176800	4.78725600
O	-18.07714000	-6.67627300	2.41036300
O	-18.00570000	-4.44102200	3.49859600
C	-17.55012100	-3.50799800	4.45437500
H	-16.49238500	-3.69916600	4.62772300
H	-17.96654500	-3.70965400	5.43688600
C	-17.75932500	-2.04816100	4.04742500
H	-17.34257800	-1.47563200	4.86451300
O	-17.05461600	-1.76132900	2.85293300
C	-17.83013600	-0.85883300	2.10428700
H	-17.73678200	0.14591100	2.50712000
N	-17.46237000	-0.92556500	0.67793000
C	-17.64816800	-2.09409300	-0.00370200
H	-18.05645500	-2.95575000	0.50013100
C	-17.44406600	-2.14987200	-1.34349000
H	-17.64861800	-3.04456000	-1.91040500
C	-17.08356500	-0.90623200	-1.95365400
N	-16.71264200	-0.81620100	-3.23677900
H	-16.33654200	-1.64581300	-3.67756700
H	-16.42463400	0.10670900	-3.52294100
N	-16.93188000	0.25594400	-1.29643400
C	-17.14762600	0.26653600	0.03860900
O	-17.16316700	1.32674800	0.66519400

C	-19.24349800	-1.74739200	3.85567800
H	-19.85190200	-2.63460500	4.01907100
C	-19.27142200	-1.27890500	2.41288900
H	-19.50734200	-2.09039400	1.72069900
H	-19.86647400	-0.37311100	2.34924100
O	-19.60231200	-0.78048800	4.82234800
P	-21.07201300	-0.17027300	5.06238100
O	-21.08110400	0.57160800	6.34442300
O	-22.03333800	-1.28826900	4.95971700
O	-21.48475900	0.83676400	3.88203500
C	-20.73927100	1.99450700	3.58779300
H	-19.69099400	1.76685400	3.41519400
H	-20.86445900	2.71666500	4.39409000
C	-21.18543400	2.65326200	2.28668600
H	-20.78926200	3.67465100	2.33578900
O	-20.66769800	1.88722000	1.23002600
C	-21.70439200	1.63108000	0.31211600
H	-21.68302400	2.40139300	-0.45883200
N	-21.44576900	0.35999900	-0.37808000
C	-21.84613300	-0.90837500	-0.04576300
H	-22.21079700	-1.20864600	0.92694300
N	-21.67230200	-1.80116400	-0.99033300
C	-21.07989000	-1.01589300	-1.97734600
C	-20.58917600	-1.32705800	-3.27433400
O	-20.57511800	-2.41515700	-3.84243700
N	-19.93869100	-0.32687400	-3.98468800
H	-19.52695000	-0.60891100	-4.85940200
C	-19.83950800	0.97159100	-3.52714000
N	-19.29199200	1.92189000	-4.28954200
H	-18.69867700	1.57751400	-5.03719400

H	-19.35581500	2.91047600	-4.08478500
N	-20.29918700	1.30183800	-2.31944300
C	-20.79446200	0.27012100	-1.58428100
C	-22.66705300	2.83674900	1.96212900
H	-23.12919100	2.77675300	2.95118400
C	-23.06019600	1.70745200	1.01522500
H	-23.32024200	0.82156900	1.59676300
H	-23.94626000	1.97318800	0.42694500
O	-22.91537900	4.12572600	1.46587000
H	-23.83907800	4.25370400	1.22817000
Os	-5.35382900	-5.48594700	2.6439150
N	-7.12720700	-4.57690500	1.9594300
C	-7.53577200	-4.55421500	0.6835050
C	-8.72084300	-3.94284700	0.2942900
C	-9.51507700	-3.34191200	1.2626690
C	-9.09751500	-3.37287400	2.5889790
C	-7.89682000	-3.99909600	2.9118220
C	-7.37103000	-4.12023800	4.2849100
N	-6.27512800	-4.91023500	4.4223960
C	-5.74532100	-5.08909400	5.6466220
C	-6.25837700	-4.47678000	6.7771700
C	-7.36892700	-3.64533400	6.6416560
C	-7.93087100	-3.47345700	5.3853750
N	-3.67134600	-6.49804900	3.3250790
C	-2.51781100	-5.91727800	3.6961560
C	-1.38968300	-6.64328900	4.0449020
C	-1.46286400	-8.03535900	4.0234230
C	-2.65502200	-8.64246800	3.6571870
C	-3.75004500	-7.85291700	3.3051040
C	-5.05645000	-8.38097700	2.8927610

N	-5.98809300	-7.42604600	2.5956140
C	-7.22129900	-7.83135000	2.2129500
C	-7.56624300	-9.16013700	2.0782980
C	-6.61202400	-10.13824900	2.3641570
C	-5.35244200	-9.73776300	2.7777830
C	-2.30781700	-0.98413800	-4.4149890
C	-2.60316100	-1.27215600	-3.0518320
N	-2.91264500	-2.53165600	-2.6941070
C	-3.18975200	-2.74597200	-1.4218370
C	-3.60428000	-4.08764100	-1.0211700
C	-3.67788300	-5.14386400	-1.9362970
C	-4.15764400	-6.36905900	-1.5135760
C	-4.56103300	-6.51690000	-0.1855740
N	-4.51279300	-5.51169900	0.6913990
C	-4.03423400	-4.31009600	0.2854760
C	-4.00133600	-3.23642000	1.2688710
C	-2.00269900	0.29573700	-4.7818500
C	-1.97140700	1.34777000	-3.8168910
C	-2.24957800	1.10371500	-2.5030330
C	-2.57241600	-0.21674300	-2.0849360
N	-2.84966100	-0.45380100	-0.7899500
C	-3.15295600	-1.69480400	-0.4577400
C	-3.51216300	-1.97481000	0.9303460
C	-3.41209500	-1.00132600	1.9387760
C	-3.79357800	-1.33619700	3.2229020
C	-4.32612500	-2.60641600	3.4697000
N	-4.44283200	-3.53109200	2.5170440
H	-6.87203300	-4.99850600	-0.0487960
H	-8.98269300	-3.90675500	-0.7642260
H	-10.43425100	-2.83568600	0.9755670

H	-9.69021000	-2.89232600	3.3550610
H	-4.84788400	-5.69937800	5.6800360
H	-5.76175000	-4.61132600	7.7293870
H	-7.76865400	-3.11339500	7.4963730
H	-8.77057800	-2.80403200	5.2426580
H	-2.49533000	-4.83175400	3.6936150
H	-0.48305900	-6.09384900	4.2999880
H	-0.59567200	-8.63121500	4.2777830
H	-2.72945800	-9.71807600	3.6247870
H	-7.91642700	-7.03266800	1.9760220
H	-8.55523700	-9.41690200	1.7230180
H	-6.84078400	-11.18347200	2.2348000
H	-4.58562000	-10.46855100	2.9849050
H	-2.30996000	-1.81150800	-5.1217440
H	-3.39291600	-4.95168600	-2.9747450
H	-4.25756300	-7.20149100	-2.2040860
H	-4.96668000	-7.45501500	0.1770020
H	-1.75341000	0.51381000	-5.8150510
H	-1.70109700	2.34577500	-4.1361150
H	-2.21817000	1.87624400	-1.7443050
H	-3.00678500	-0.02300700	1.6906510
H	-3.68836500	-0.62517200	4.0397500
H	-4.66229600	-2.88067500	4.4673140

VI.2.2. 1BNA/ $Os[(bpy)_2phen]^{2+}$

O	-14.30253800	13.66256400	-6.20619400
H	-14.97559300	14.33877600	-6.31903700
C	-15.04153600	12.47268600	-6.00877900
H	-14.42825100	11.57756600	-5.97213900

H	-15.75001600	12.31442100	-6.82118800
C	-15.80248300	12.51288300	-4.68622600
H	-16.36066400	13.44922000	-4.59185100
O	-16.71345300	11.43907300	-4.67816300
C	-16.30279200	10.54236600	-3.66048200
H	-16.85202300	10.74392900	-2.74183300
N	-16.60739200	9.18998700	-4.16633900
C	-16.09939400	8.73948200	-5.34272500
H	-15.56975800	9.41335200	-6.00112100
C	-16.21086200	7.43508000	-5.69302400
H	-15.69658500	7.10277400	-6.57873900
C	-16.97583200	6.61275100	-4.79887800
N	-16.99393500	5.28873600	-4.96397900
H	-16.49441700	4.93150800	-5.76389700
H	-17.71812400	4.67956400	-4.61048200
N	-17.63299300	7.06786400	-3.72607300
C	-17.45023600	8.37665000	-3.41934900
O	-17.92062300	8.83312300	-2.38278300
C	-14.80736100	12.29975000	-3.55008900
H	-13.82076300	12.65881800	-3.84367600
C	-14.81857500	10.77986900	-3.38626800
H	-14.15386600	10.31868800	-4.11686600
H	-14.48535600	10.34761900	-2.44397100
O	-15.18992400	12.99422700	-2.38032500
P	-14.14415700	13.31383200	-1.19494600
O	-14.86865800	14.33722900	-0.40922600
O	-12.86015000	13.59412300	-1.86819500
O	-14.00193300	11.96551600	-0.33598400
C	-14.84927700	11.70595400	0.76457800
H	-15.84876200	11.97126500	0.44125000

H	-14.52924500	12.39009400	1.54286600
C	-14.83178600	10.24120900	1.20810600
H	-15.50995800	10.18343400	2.05954300
O	-15.24461100	9.32386800	0.21323900
C	-14.96427500	8.06448400	0.78844800
H	-15.72656800	7.88817200	1.53853000
N	-14.84286700	7.03357100	-0.26638800
C	-14.64647400	7.31798300	-1.59177000
H	-14.40163900	8.29569000	-1.96264000
N	-14.70444500	6.26804600	-2.36596200
C	-15.08338600	5.24122100	-1.51259500
C	-15.55137100	3.93456400	-1.81299000
O	-15.62882300	3.42054600	-2.91856100
N	-15.88514600	3.21615600	-0.67111200
H	-16.20789000	2.25677000	-0.78386900
C	-15.71039900	3.66720100	0.62172300
N	-15.92244600	2.86762000	1.66771900
H	-16.37974900	1.97809300	1.53462200
H	-15.82063900	3.33218500	2.56030800
N	-15.39917100	4.94395000	0.88296500
C	-15.07221600	5.68480500	-0.21044000
C	-13.46727600	9.72179200	1.65095900
H	-12.75364600	10.14043500	0.94891200
C	-13.59065800	8.21803600	1.44700500
H	-12.82795400	7.87334500	0.74845600
H	-13.58189700	7.68768100	2.39939500
O	-13.25708000	10.12234700	2.97835200
P	-11.84651400	10.14399300	3.75064300
O	-12.02619700	10.82366300	5.04658400
O	-10.89184600	10.72167000	2.78193300

O	-11.51986400	8.58355600	4.01792000
C	-12.17670600	7.86937700	5.04017600
H	-13.22937000	8.10808300	4.88879000
H	-11.87093900	8.34736300	5.97175200
C	-11.99012500	6.36948500	5.24732800
H	-12.57285400	6.11162200	6.12233300
O	-12.50717800	5.67039900	4.14291200
C	-11.53170200	4.84835500	3.52413000
H	-11.36029400	3.89646500	4.03238600
N	-11.77985000	4.58273200	2.10002700
C	-11.28793100	5.38246300	1.10572000
H	-10.71969100	6.26696100	1.35784400
C	-11.39990400	5.03840800	-0.19069300
H	-11.06767800	5.59197100	-1.06252700
C	-12.09123000	3.81389900	-0.47184700
N	-12.36947500	3.54556800	-1.75039300
H	-12.10414400	4.13708400	-2.52130700
H	-12.84118700	2.69489000	-2.00872100
N	-12.58114500	3.00811500	0.48841100
C	-12.30929500	3.34300300	1.77236900
O	-12.66738200	2.61179500	2.69188400
C	-10.49594000	6.07286000	5.37625900
H	-9.92870100	6.96038400	5.64540700
C	-10.26946900	5.58919100	3.94249600
H	-10.00074300	6.43174600	3.30336700
H	-9.38682500	4.95663700	3.89544500
O	-10.38418900	5.07874900	6.37016800
P	-9.03725300	4.69950900	7.17474100
O	-9.07841200	5.20470700	8.56271900
O	-7.84603200	5.05511500	6.37103800

O	-9.13921500	3.08480000	7.21498100
C	-10.17414700	2.46772600	7.94514200
H	-11.03817700	3.10150200	7.74049500
H	-10.12379400	2.55860000	9.03036400
C	-10.46538200	0.98701900	7.72133700
H	-11.29330000	0.67247100	8.35703400
O	-10.68416200	0.91440900	6.32338700
C	-9.67215400	0.17294400	5.68068200
H	-9.99085400	-0.85979900	5.56945700
N	-9.42219000	0.84692100	4.39492400
C	-8.81181700	2.05724100	4.14518700
H	-8.38639600	2.68544900	4.90437800
N	-8.85152200	2.39282700	2.89079200
C	-9.51521100	1.34797900	2.26213500
C	-9.80605400	1.11118200	0.89500800
O	-9.79488800	1.86859800	-0.07308100
N	-10.29789300	-0.17349500	0.66566200
H	-10.39707200	-0.39306500	-0.31732000
C	-10.64808500	-1.05267800	1.65894000
N	-11.08643300	-2.23664600	1.21512600
H	-11.22071500	-2.39287400	0.22469100
H	-11.37376800	-2.92666700	1.89652900
N	-10.33327400	-0.86785700	2.95448400
C	-9.76945600	0.34407300	3.16575700
C	-9.15740500	0.28246300	8.06455300
H	-8.59175800	0.91263600	8.74354000
C	-8.52261900	0.23951400	6.68219900
H	-7.90701400	1.11811600	6.52698800
H	-7.91900500	-0.66440600	6.64934800
O	-9.48925900	-0.98845200	8.59403200

P	-8.43530800	-1.77110700	9.52356800
O	-9.22952600	-2.61076500	10.44844300
O	-7.30732300	-0.88630800	9.87907000
O	-7.75677500	-2.79011800	8.48178600
C	-8.45768800	-3.83841400	7.85155100
H	-9.41181500	-3.52102500	7.42177800
H	-8.60888500	-4.64845700	8.56230400
C	-7.56046500	-4.44932000	6.77944900
H	-7.94782900	-5.44712300	6.56399600
O	-7.59780200	-3.59272100	5.66166800
C	-6.31926800	-3.44439100	5.0878930
H	-6.12040600	-4.31224600	4.44916400
N	-6.31393400	-2.15286700	4.3854640
C	-6.08951600	-0.91662100	4.9666440
H	-5.91260500	-0.82278300	6.0329580
N	-6.11653000	0.07004000	4.1182400
C	-6.39441400	-0.53549400	2.9108050
C	-6.45421800	-0.00388200	1.6036930
N	-6.24336500	1.29084300	1.3305890
H	-6.34678100	1.96689000	2.0777190
H	-6.31826600	1.61291700	0.3684490
N	-6.65768200	-0.87215700	0.5961020
C	-6.76805000	-2.18221000	0.8674630
H	-6.93163900	-2.79896100	-0.0094700
N	-6.69967000	-2.79834200	2.0418870
C	-6.52336000	-1.91810300	3.0410170
C	-6.09285800	-4.63045800	7.15647100
H	-5.97188100	-4.51930300	8.24226200
C	-5.42362300	-3.54906200	6.31088300
H	-5.44812800	-2.57421500	6.78173700

H	-4.42018900	-3.82665500	5.98981800
O	-5.67545600	-5.94329600	6.83294400
P	-4.38840700	-6.61428700	7.53314100
O	-4.47567800	-8.03065500	7.11019100
O	-4.47527200	-6.27686100	8.97175100
O	-2.98752100	-5.97708600	7.06176900
C	-2.05620600	-6.85297500	6.46170900
H	-2.52840600	-7.42058700	5.65962100
H	-1.69366600	-7.54515700	7.21698800
C	-0.81904800	-6.13198800	5.93056100
H	-0.06440700	-6.75065000	5.45058700
O	-1.19040000	-5.05187100	5.10578800
C	-0.28569600	-3.99240400	5.3407630
H	0.72918500	-4.24969200	5.02915700
N	-0.70037600	-2.75212500	4.6761410
C	-1.15879500	-1.59378600	5.2742040
H	-1.49202300	-1.58530900	6.3023340
N	-1.14211700	-0.55731100	4.4815690
C	-0.63418200	-1.04697400	3.2936850
C	-0.43765700	-0.45178700	2.0260510
N	-0.74204600	0.82751700	1.7459250
H	-0.78748400	1.48318500	2.5117080
H	-0.42033500	1.16827400	0.8408620
N	-0.00410200	-1.24002300	1.0305960
C	0.26371100	-2.52662500	1.2706560
H	0.65030900	-3.07969100	0.4127580
N	0.11608800	-3.19640900	2.4109750
C	-0.34900400	-2.40703900	3.3865880
C	0.00982200	-5.49860600	7.04738900
H	-0.36274400	-5.70802600	8.05537700

C	-0.24706900	-4.00613500	6.86678800
H	-1.25058700	-3.82020200	7.25632600
H	0.56275900	-3.35883500	7.19879500
O	1.40082000	-5.59033500	6.88124400
P	2.20826200	-6.80927000	7.54489800
O	1.23513200	-7.84085600	7.97646300
O	3.13134800	-6.15920200	8.49396300
O	3.05324000	-7.27638100	6.25032500
C	2.63575000	-8.26857400	5.33897800
H	1.55255900	-8.28236500	5.31879300
H	2.95721100	-9.25002600	5.66748300
C	3.05633300	-8.08093100	3.87952600
H	2.51815900	-8.74771300	3.20279000
O	2.57750500	-6.81532400	3.47361500
C	3.59036200	-6.12233100	2.7815270
H	3.53711200	-6.33696100	1.71813400
N	3.35485000	-4.66673000	2.9741100
C	3.12649600	-4.13487800	4.2281750
H	3.11724800	-4.86224200	5.0455920
C	2.91203400	-2.81657600	4.4210910
C	2.65539800	-2.19860100	5.7625240
H	1.72999000	-1.61472000	5.7344900
H	2.57389300	-2.97927100	6.5286320
H	3.46228800	-1.51630300	6.0325250
C	2.89883200	-1.93517100	3.2548800
O	2.62937500	-0.74012600	3.3142440
N	3.20007500	-2.53531800	2.0415250
H	3.12156500	-1.93312900	1.1917440
C	3.33508700	-3.88115900	1.8112160
O	3.43070200	-4.35354300	0.6909210

C	4.55380500	-8.09752400	3.63580300
H	5.12008200	-8.40777800	4.51726300
C	4.92061200	-6.64394600	3.34022900
H	5.31312000	-6.11094600	4.19664600
H	5.59184300	-6.73940600	2.48038400
O	4.69374800	-9.10655000	2.66627500
P	6.03361200	-9.55079000	1.87842100
O	5.85220700	-10.90167000	1.31493600
O	7.09364000	-9.23070900	2.85309500
O	6.21684300	-8.57067300	0.61066800
C	5.54362500	-8.78169000	-0.60145800
H	4.47934900	-8.92482800	-0.46830800
H	5.96771200	-9.71723100	-0.95644300
C	5.92719300	-7.72160200	-1.63668200
H	5.34772500	-7.89778900	-2.53816700
O	5.57182100	-6.41997200	-1.23113300
C	6.63353500	-5.60761400	-1.68899500
H	6.35592000	-5.16162100	-2.64221100
N	6.78175000	-4.53821400	-0.67799800
C	7.11207900	-4.83662000	0.61038800
H	7.27142700	-5.84569900	0.95775900
C	7.28491800	-3.83507500	1.50567300
C	7.66822600	-4.26189300	2.90224100
H	6.94606500	-3.74589000	3.53747600
H	7.64927700	-5.31368800	3.17622600
H	8.59189100	-3.86564300	3.31495100
C	7.00219300	-2.46932000	1.13462000
O	7.10440200	-1.43712200	1.79121700
N	6.85100800	-2.24565900	-0.22391600
H	6.77801300	-1.28692500	-0.53375800

C	6.62927000	-3.25339800	-1.15622100
O	6.39620000	-2.95671700	-2.32697200
C	7.37480200	-7.85453600	-2.09761100
H	7.79718500	-8.60507200	-1.42241700
C	7.90059200	-6.43609000	-1.88417500
H	8.55527700	-6.29888100	-1.02419800
H	8.38487100	-5.96905900	-2.73167500
O	7.53807700	-8.28362500	-3.42731900
P	8.96437900	-8.43843900	-4.16168500
O	8.71421500	-9.16028200	-5.42843700
O	9.97290600	-8.94499400	-3.20754800
O	9.50948400	-6.99406600	-4.65071200
C	8.61567600	-6.34181900	-5.52414300
H	7.68646000	-6.37560900	-4.95019700
H	8.36959400	-6.94067100	-6.39547600
C	8.98814800	-4.91925500	-5.94896700
H	8.42703600	-4.50970200	-6.78903900
O	8.63414100	-4.13031800	-4.83543300
C	9.44877900	-2.98622800	-4.87928300
H	8.75611500	-2.20637600	-5.19966900
N	9.86342900	-2.85631900	-3.47411800
C	10.42051900	-3.87079900	-2.73819600
H	10.47737700	-4.85595600	-3.19408300
C	10.67367500	-3.72314900	-1.42792400
H	10.99783400	-4.53018600	-0.78371000
C	10.35144000	-2.43721900	-0.88253500
N	10.47388600	-2.39716700	0.45092000
H	10.70055400	-3.24532900	0.94986100
H	10.10936900	-1.55249700	0.86668400
N	9.90120500	-1.39600100	-1.59930000

C	9.72372900	-1.59977100	-2.92450900
O	9.45683600	-0.59222000	-3.58338000
C	10.43430200	-4.62066500	-6.30461000
H	11.15575300	-5.21128700	-5.74597400
C	10.59074200	-3.16386600	-5.89065100
H	11.56765900	-2.86351300	-5.51062200
H	10.35251300	-2.50320600	-6.72111800
O	10.69056900	-4.66153500	-7.69786400
P	12.20057000	-4.63908400	-8.25910700
O	12.15356800	-4.98378300	-9.69255500
O	13.03213900	-5.58988300	-7.48310800
O	12.92326800	-3.22761700	-7.98584900
C	12.82847300	-2.16145500	-8.90346200
H	11.77133900	-1.89350100	-9.01332000
H	13.11836700	-2.55301300	-9.87995700
C	13.71963500	-0.98426200	-8.54339500
H	13.59801100	-0.25680700	-9.35537900
O	13.22454700	-0.49118800	-7.32095300
C	14.22083000	-0.54199800	-6.31346100
H	14.62361100	0.46485400	-6.22792800
N	13.78452100	-0.96754800	-4.97710700
C	13.67882300	-2.22811300	-4.41853500
H	13.85020700	-3.12076000	-4.98985800
N	13.47800700	-2.18509300	-3.13400300
C	13.43002300	-0.82741400	-2.81431000
C	13.35025500	-0.27424100	-1.50762000
O	13.35123000	-0.84037300	-0.42010300
N	13.25723100	1.10446100	-1.62898100
H	13.07836000	1.67600100	-0.81304800
C	13.55994700	1.81285300	-2.77678000

N	13.56591300	3.15126200	-2.67369200
H	13.59531200	3.54162600	-1.74867800
H	13.90557400	3.67683000	-3.46962400
N	13.70445100	1.26810900	-3.98130200
C	13.70942700	-0.08292700	-3.93465500
C	15.22996800	-1.20454900	-8.39184200
H	15.49321500	-2.13822800	-8.88585000
C	15.36215500	-1.38103600	-6.87834300
H	15.31950800	-2.45117900	-6.70234700
H	16.35475500	-1.09004300	-6.53097100
O	15.94168600	-0.13156300	-8.95775700
P	17.52898300	0.13571400	-8.83549000
O	18.04683500	0.83582900	-10.03376700
O	18.27026600	-1.08181400	-8.45205100
O	17.63099300	1.16765600	-7.60321900
C	16.88465600	2.35973300	-7.49489800
H	15.84754300	2.10588300	-7.31697200
H	16.97358100	3.03531300	-8.34400600
C	17.23447200	3.17915800	-6.25725100
H	16.84422600	4.17462000	-6.45132300
O	16.63843900	2.61960900	-5.10618700
C	17.67079200	2.66652000	-4.14918900
H	17.69400700	3.63789300	-3.65089600
N	17.48575100	1.53895600	-3.21363600
C	17.48769100	0.25724700	-3.69051900
H	17.48141900	0.08612400	-4.75300500
C	17.29487000	-0.75233600	-2.82926300
H	17.32602200	-1.80070600	-3.11095600
C	17.04315800	-0.40094200	-1.46157800
N	16.76344300	-1.37429300	-0.59425700

H	16.95320500	-2.30756300	-0.93994200
H	16.55115200	-1.17900400	0.37470900
N	16.92919900	0.85756900	-1.01653300
C	17.09296600	1.85108400	-1.91775900
O	16.92910400	3.00358600	-1.52141700
C	18.74230900	3.35183300	-6.08172500
H	19.19616300	2.91933900	-6.97080700
C	19.06472800	2.63629100	-4.77251000
H	19.48719400	1.65840700	-4.99671200
H	19.80065600	3.17863400	-4.17948900
O	19.01154000	4.73403500	-5.94743200
P	20.48659600	5.34662000	-5.76981000
O	20.41546300	6.80190100	-6.06796600
O	21.48311200	4.51293700	-6.47926700
O	20.76163300	5.36617500	-4.18877500
C	19.86167300	5.91583100	-3.23517600
H	18.84784500	5.78897300	-3.63060100
H	20.01876300	6.99631200	-3.21831100
C	20.15989600	5.41509300	-1.82460100
H	19.51330200	6.00781000	-1.17506000
O	19.80400000	4.06105500	-1.68705600
C	20.63091200	3.44676000	-0.71270600
H	20.21212700	3.98000100	0.14290600
N	20.55688900	1.98398000	-0.58622900
C	20.43784600	1.00349300	-1.52908300
H	20.61631500	1.20955100	-2.57726600
N	20.21211700	-0.20514000	-1.10428600
C	20.17445700	0.00690800	0.27140200
C	20.02621900	-0.95563900	1.30900900
O	20.08457000	-2.17597100	1.14172400

N	19.94240500	-0.43194700	2.58545800
H	19.93093600	-1.00687200	3.41535600
C	19.87060800	0.93737900	2.80769800
N	19.84744500	1.39843000	4.05773700
H	19.66896700	0.62625500	4.69553900
H	19.77224700	2.36295900	4.35761600
N	20.09949600	1.83900500	1.83853300
C	20.25059100	1.33180400	0.58660800
C	21.60194900	5.43894200	-1.35629000
H	22.21115300	5.86890200	-2.15460300
C	22.01191100	4.00132800	-1.04133200
H	22.36157100	3.62300000	-1.99904100
H	22.74855200	3.84017700	-0.25858700
O	21.82568400	6.28687100	-0.24860800
H	22.65163500	6.70098200	-0.48507700
O	18.22228000	-3.78269100	11.95534600
H	18.43234600	-4.22677300	12.78676800
C	18.88401600	-2.53744800	12.00199100
H	19.85652800	-2.63886400	12.47668400
H	18.31225200	-1.98623100	12.75142200
C	18.99795700	-1.77344500	10.68634700
H	19.58095800	-0.86402500	10.85267500
O	19.62532500	-2.46567900	9.63044900
C	19.27346300	-1.87156500	8.39395400
H	19.90525000	-0.97787600	8.33099400
N	19.42694000	-2.63889500	7.14729800
C	19.04669500	-3.94448200	6.99285000
H	18.77716500	-4.42231300	7.93127000
C	19.12272100	-4.60678900	5.82282000
H	18.95846300	-5.67767600	5.82732300

C	19.45245200	-3.81502400	4.67941100
N	19.50424200	-4.40695500	3.48369500
H	19.34981200	-5.40653000	3.41735900
H	19.55262800	-3.69700800	2.75531700
N	19.50435100	-2.47167300	4.70208900
C	19.53186200	-1.95049100	5.95616800
O	19.76394300	-0.74616000	5.96130200
C	17.65995800	-1.40078000	10.06555900
H	16.94983100	-2.21641500	10.22163400
C	17.87916100	-1.27974800	8.55910500
H	17.06601100	-1.77705900	8.04164100
H	17.84689900	-0.19936100	8.35338300
O	17.07796200	-0.24611500	10.62487000
P	15.63576900	0.33547700	10.23100300
O	15.02230400	0.81065800	11.49665000
O	14.94753800	-0.66218200	9.38105200
O	15.90801600	1.60375200	9.27556600
C	16.59856600	2.72037900	9.81080800
H	17.53196100	2.38589400	10.26002200
H	16.02471800	3.14355500	10.63574500
C	16.85878700	3.76737500	8.73540900
H	17.46405100	4.50030400	9.26923500
O	17.44381200	3.27057800	7.55416500
C	16.57765900	3.27044400	6.44003800
H	16.89420300	3.93620600	5.62956900
N	16.65192900	1.97975800	5.73405300
C	16.29661000	0.73334400	6.19318300
H	15.93379600	0.56398100	7.20049700
N	16.43512700	-0.21392500	5.31244800
C	16.52872000	0.48458600	4.11298000

C	16.53412100	0.05861100	2.76167800
O	16.25811800	-1.05488000	2.32663800
N	16.68744600	1.08920100	1.83562400
H	16.65362100	0.92343000	0.84105100
C	16.80396200	2.42005800	2.19913800
N	16.83775200	3.32135000	1.20680200
H	16.86851100	3.15241500	0.21659300
H	16.64282800	4.25816000	1.53980700
N	16.81490000	2.82079300	3.47365500
C	16.69452300	1.82416000	4.37211500
C	15.55928800	4.43057700	8.28256700
H	14.77052500	4.39068500	9.04208100
C	15.21844900	3.59424400	7.06020200
H	14.62284300	2.71736300	7.31026600
H	14.69614400	4.16276000	6.28813500
O	15.65307900	5.80030700	7.95646300
P	14.38942100	6.77598000	7.74974500
O	14.88915800	8.11836000	8.11027100
O	13.24991100	6.31339000	8.58138600
O	13.82133300	6.78402700	6.24053700
C	14.40219000	7.68590000	5.33316100
H	15.48194700	7.56182200	5.41877200
H	14.12125900	8.68591000	5.65574100
C	13.95713600	7.53009600	3.87794500
H	14.54453400	8.22324900	3.27238600
O	14.15810300	6.20535900	3.42630000
C	13.26927900	5.76316500	2.41879900
H	13.62311800	6.05227500	1.42491100
N	13.15487300	4.29442400	2.49696800
C	12.92941900	3.68542600	3.69625600

H	12.81921400	4.22203300	4.61642400
C	12.89736500	2.33220200	3.67062700
H	12.86397000	1.84478700	4.63639700
C	13.12552200	1.61461800	2.45476600
N	13.25022400	0.29130200	2.46828900
H	13.38060000	-0.18739200	3.35403900
H	13.03212400	-0.06311400	1.54339900
N	13.17765100	2.27893900	1.29417900
C	13.20554400	3.63267600	1.29010300
O	13.05590600	4.22786400	0.22391400
C	12.46325700	7.69514800	3.64907200
H	11.95340400	7.80286100	4.60434600
C	11.99204200	6.45655700	2.89584600
H	11.38503100	5.81612600	3.53199500
H	11.29821600	6.76456500	2.11300700
O	12.28742600	8.81971000	2.80441600
P	10.98118300	9.74329600	2.89227200
O	11.21427700	10.99451400	2.13727500
O	10.68052700	9.89315000	4.33402400
O	9.80361000	8.87751100	2.20740800
C	9.58267900	9.10787800	0.83182800
H	10.46242000	9.18260700	0.19482600
H	9.12796500	10.07650900	0.63285800
C	8.65495500	8.06511200	0.21663000
H	8.59617100	8.31377700	-0.84134500
O	9.19374300	6.76207300	0.30378500
C	8.20851600	5.88930800	0.80038400
H	7.56303900	5.67520200	-0.04538100
N	8.78795300	4.62575000	1.29995700
C	9.06044100	4.27680600	2.60567100

H	8.94950800	4.95179500	3.43070700
N	9.42490200	3.03211600	2.74855200
C	9.47765800	2.49841000	1.46618200
C	9.92875000	1.23488600	1.00075300
O	10.39282200	0.25287200	1.57858200
N	9.89755300	1.15934900	-0.37976100
H	10.10766300	0.29157100	-0.84162200
C	9.51914600	2.21906600	-1.18369500
N	9.67140700	2.07986500	-2.50685000
H	9.90028200	1.17398600	-2.88447200
H	9.31148600	2.76044700	-3.17180500
N	9.02466300	3.38286900	-0.74420900
C	9.07142900	3.47904100	0.60418400
C	7.27068600	7.89846400	0.85202600
H	7.12793100	8.76307000	1.50637900
C	7.44589800	6.72853200	1.81044100
H	8.07815800	6.92880300	2.68138300
H	6.48966200	6.25093300	2.02703300
O	6.18064200	7.70976900	-0.01854800
P	5.37528100	8.85106600	-0.81512400
O	6.17308400	10.04686800	-1.14523000
O	4.17548300	9.13192300	0.00414700
O	4.95768600	8.09354200	-2.17349500
C	5.82567900	8.13326600	-3.28074900
H	6.85418600	8.15095200	-2.92966400
H	5.56861000	9.05837100	-3.80103300
C	5.57677400	7.03056000	-4.31524700
H	6.19583700	7.16206500	-5.20089200
O	6.09525100	5.85837800	-3.71802900
C	5.11742400	4.86410800	-3.51070800

H	5.16774000	4.08767100	-4.26841100
N	5.18186100	4.27691600	-2.16313500
C	4.79709600	4.77050700	-0.94603900
H	4.39555500	5.76674700	-0.81197700
N	5.05111900	4.01957500	0.08937100
C	5.62367600	2.89895800	-0.51179300
C	6.04173300	1.62314700	-0.10764700
N	5.96159500	1.18699800	1.15169800
H	5.70531200	1.85322700	1.87575500
H	6.40979800	0.31491900	1.35661600
N	6.53457000	0.68292500	-0.93353800
C	6.54172300	0.98917100	-2.21520200
H	6.86516800	0.26658800	-2.94290800
N	6.19144500	2.15116000	-2.76546400
C	5.70850900	3.04019200	-1.87115100
C	4.12300100	6.80861900	-4.70791300
H	3.44559100	7.63884400	-4.48421300
C	3.81145200	5.56261100	-3.88797300
H	3.29304900	5.83418000	-2.96233400
H	3.18017700	4.84612300	-4.41450500
O	4.15484000	6.51315300	-6.08086100
P	2.80380400	6.25621000	-6.91942000
O	3.08189000	6.56918100	-8.33318000
O	1.68204900	6.95002000	-6.24533200
O	2.65328900	4.64815900	-6.88909600
C	3.55689700	3.76602900	-7.51904700
H	4.59481600	4.06751300	-7.37645800
H	3.31426200	3.76732000	-8.57910700
C	3.59596700	2.35568100	-6.94294700
H	4.34452100	1.77484100	-7.48874200

O	3.82472800	2.40835800	-5.54674000
C	3.15065800	1.28009100	-5.0510160
H	3.85083700	0.45157800	-4.99173400
N	2.76760400	1.53814100	-3.6312790
C	2.35621100	2.70063700	-3.0249910
H	2.22774700	3.60945800	-3.6060670
N	2.16644200	2.58079100	-1.7363520
C	2.47131400	1.25918500	-1.4776380
C	2.51791900	0.51078800	-0.2833620
N	2.21951700	1.07345000	0.9165460
H	2.35342400	2.07668500	0.9585740
H	2.48450000	0.53999400	1.7438460
N	2.83420100	-0.79207700	-0.3494880
C	3.12182300	-1.32416500	-1.5583970
H	3.35907700	-2.38435300	-1.5460660
N	3.14798400	-0.71915700	-2.7336500
C	2.83401100	0.58250600	-2.6378060
C	2.29512200	1.61190300	-7.20446900
H	1.44126500	2.22700500	-7.48155700
C	1.92531700	0.94020100	-5.88505100
H	0.94910000	1.28359300	-5.53364900
H	1.91797000	-0.14110600	-6.01043400
O	2.39780400	0.66067900	-8.24520500
P	1.15014900	0.14818000	-9.12622700
O	1.71517600	-0.35033800	-10.40232400
O	0.10035500	1.18892400	-9.19682600
O	0.61359900	-1.09961100	-8.25460000
C	1.20837900	-2.38638600	-8.31976200
H	2.28163200	-2.26015600	-8.43762900
H	0.89436100	-2.98584700	-9.17148900

C	0.83764600	-3.22948300	-7.11090100
H	1.27224900	-4.22176000	-7.27309000
O	1.36914700	-2.83617400	-5.86903200
C	0.49911500	-3.17831300	-4.8138990
H	0.97238000	-3.97034300	-4.23402800
N	0.15685300	-2.00276600	-3.9796520
C	-0.27221300	-0.81766300	-4.5440860
H	-0.29955900	-0.80998800	-5.6380440
C	-0.64638400	0.24784800	-3.8022560
C	-1.17723400	1.53070000	-4.3669750
H	-1.19498200	1.50160100	-5.4625140
H	-2.18986900	1.71849000	-4.0017190
H	-0.56146500	2.37594600	-4.0432010
C	-0.53706600	0.15180100	-2.3507430
O	-0.87775200	1.03301600	-1.5698910
N	-0.06459600	-1.06309300	-1.8724270
H	0.03373900	-1.11668600	-0.8436200
C	0.23535100	-2.18760900	-2.6001110
O	0.49822900	-3.26408000	-2.0794770
C	-0.66857400	-3.35876900	-6.91222200
H	-1.07651000	-2.34793600	-7.03960300
C	-0.69642500	-3.86504100	-5.47347700
H	-1.68481800	-3.71594500	-5.02835500
H	-0.49887100	-4.93806000	-5.43480500
O	-1.23577500	-4.41142800	-7.64543700
P	-2.54148200	-4.14368600	-8.54523900
O	-2.93639600	-5.29018800	-9.39845400
O	-2.38530200	-2.87617000	-9.29591300
O	-3.82019600	-3.73764000	-7.65888700
C	-4.63437300	-4.69219000	-7.02607700

H	-4.10174000	-5.16494700	-6.19994100
H	-4.76747900	-5.46621400	-7.77150900
C	-5.91623400	-4.13489400	-6.39588700
H	-6.39878900	-5.05286000	-6.06137300
O	-5.67030400	-3.29003500	-5.29813000
C	-6.65771200	-2.27900400	-5.1893510
H	-7.50789600	-2.80640300	-4.76977800
N	-6.23709800	-1.17967500	-4.3118190
C	-5.67388400	-0.00339800	-4.7684560
H	-5.40329300	0.00757600	-5.8217290
C	-5.47928400	1.06762600	-3.9689570
C	-4.90438300	2.37352700	-4.4313350
H	-4.44352200	2.27114500	-5.4176890
H	-5.67019300	3.14812400	-4.4646440
H	-4.13898700	2.71092400	-3.7246820
C	-5.83171600	0.94523700	-2.5507890
O	-5.70534000	1.84521300	-1.7305720
N	-6.31800600	-0.29230500	-2.1668600
H	-6.49995900	-0.44327400	-1.1449620
C	-6.53306900	-1.38565100	-2.9599030
O	-6.97790200	-2.43418300	-2.5192000
C	-6.83173500	-3.40421500	-7.37264300
H	-6.44492100	-3.34807700	-8.38190900
C	-6.92750000	-2.05346700	-6.67270100
H	-6.05580600	-1.51321500	-7.05816000
H	-7.86679600	-1.55641600	-6.89273700
O	-8.12537900	-3.96123900	-7.26164400
P	-8.59801700	-5.18999500	-8.19291900
O	-7.49099700	-6.17465200	-8.26402200
O	-9.27275700	-4.64131000	-9.38160300

O	-9.67148500	-5.72683400	-7.10923600
C	-9.30363500	-6.56472000	-6.03404600
H	-8.21381700	-6.57463800	-5.99163500
H	-9.52973800	-7.62312200	-6.18225100
C	-10.06361100	-6.26062200	-4.74073300
H	-9.75918200	-7.08778000	-4.09410200
O	-9.70152500	-4.97340500	-4.30802200
C	-10.88032600	-4.47885200	-3.68997700
H	-10.99489500	-5.05229400	-2.77831600
N	-10.71876800	-3.01625300	-3.59980300
C	-10.21418200	-2.21680000	-4.57569300
H	-10.05638100	-2.56169400	-5.58000700
C	-9.90495700	-0.93399800	-4.28040100
H	-9.59099500	-0.31788500	-5.11156500
C	-10.16410300	-0.45176900	-2.95990900
N	-9.93032800	0.82716400	-2.65074900
H	-9.77420100	1.48797900	-3.40516800
H	-9.98154200	1.21719800	-1.72454700
N	-10.62396100	-1.24451200	-1.97670500
C	-10.78452200	-2.55637000	-2.29332400
O	-11.03047500	-3.29437400	-1.34250600
C	-11.56655100	-6.31559600	-4.97213900
H	-11.93312100	-6.63969600	-5.94640100
C	-11.98959700	-4.87920600	-4.65913300
H	-11.85885100	-4.25943500	-5.54873300
H	-12.95448300	-4.90537000	-4.14739200
O	-12.09469300	-7.22464100	-4.02514200
P	-13.63683600	-7.69769600	-4.00243800
O	-13.63475400	-9.17248600	-3.93395900
O	-14.40382700	-7.11050000	-5.12703800

O	-14.29523100	-7.12764500	-2.64469800
C	-13.97789200	-7.60271400	-1.36091200
H	-12.91839900	-7.45251200	-1.14316700
H	-14.20792900	-8.66867100	-1.27305000
C	-14.76479100	-6.88845900	-0.26545400
H	-14.56185800	-7.48703700	0.62825900
O	-14.25021700	-5.59274000	-0.08959700
C	-15.25970500	-4.62921100	-0.30856500
H	-15.62616700	-4.31134000	0.67065000
N	-14.81525400	-3.43415400	-1.04701200
C	-14.54260700	-3.35583700	-2.39000500
H	-14.62192500	-4.26256100	-2.97358000
N	-14.15137600	-2.17705300	-2.78800600
C	-14.13110300	-1.42093600	-1.62311300
C	-13.69147900	-0.10464000	-1.30847900
O	-13.27135100	0.71818200	-2.11727900
N	-13.62108500	0.23522000	0.02735000
H	-13.22177800	1.11453700	0.34681200
C	-14.01713300	-0.61765000	1.03087300
N	-13.99563900	-0.28398500	2.32968300
H	-13.55093800	0.58616000	2.61233000
H	-14.40003800	-0.92082100	2.99473900
N	-14.51617400	-1.83148300	0.75326500
C	-14.51400900	-2.18838800	-0.54589400
C	-16.27277800	-6.86704900	-0.48136700
H	-16.65265500	-7.59567400	-1.20827800
C	-16.39477400	-5.42224300	-0.95099700
H	-16.33144800	-5.40598600	-2.03682600
H	-17.36162300	-4.99039900	-0.69700200
O	-16.93103700	-7.10811700	0.74451300

P	-18.53123900	-7.05752500	0.92915400
O	-18.74236700	-8.09706600	1.97087400
O	-19.16044800	-7.22629200	-0.39949700
O	-18.94753300	-5.62293100	1.53068500
C	-18.50089200	-5.26069500	2.81419500
H	-17.44803400	-5.49814000	2.89488200
H	-19.07399200	-5.75702400	3.60293700
C	-18.52135800	-3.74427800	3.02505300
H	-18.15934100	-3.62786400	4.05359200
O	-17.66610600	-3.01565700	2.17050300
C	-18.50214700	-1.98368900	1.70287400
H	-18.47566400	-1.19355500	2.45678800
N	-18.11045700	-1.38916600	0.41608700
C	-18.16259400	-2.04817100	-0.77969500
H	-18.65111400	-3.01022400	-0.77838300
C	-17.59164800	-1.50646400	-1.87032500
H	-17.46306100	-2.03277600	-2.80298800
C	-17.08697500	-0.15955500	-1.76289100
N	-16.54808700	0.47800200	-2.81370900
H	-16.63455500	0.09406300	-3.73735100
H	-16.00543300	1.32021000	-2.62606000
N	-16.99414500	0.47667700	-0.59003500
C	-17.33959600	-0.24447800	0.51640100
O	-17.09005000	0.27723500	1.60136300
C	-19.96687100	-3.27862900	2.96291900
H	-20.63044300	-4.09587300	2.65798400
C	-19.99450100	-2.32074200	1.77481600
H	-20.28131000	-2.83557000	0.85677900
H	-20.64655600	-1.49107600	2.03535100
O	-20.34847700	-2.78252400	4.22674500

P	-21.74478500	-2.13273200	4.69278700
O	-21.76611400	-2.20252000	6.17240700
O	-22.87611000	-2.71379200	3.94240400
O	-21.56891100	-0.62908400	4.16561600
C	-20.67221200	0.23957700	4.81581500
H	-19.75511700	-0.33760000	4.84905400
H	-21.05840400	0.53732500	5.79744700
C	-20.27249600	1.53076300	4.09876200
H	-19.59941900	2.03770100	4.79423400
O	-19.79709200	1.31575200	2.79635700
C	-20.07604000	2.47179100	2.03401700
H	-19.45840200	3.28409200	2.41936100
N	-19.88481900	2.34838700	0.58112100
C	-20.16324300	1.29867600	-0.25307600
H	-20.68725400	0.44936400	0.14902200
N	-20.05293500	1.61503200	-1.51871900
C	-19.39725000	2.83684700	-1.46826500
C	-18.99719400	3.67761100	-2.53988600
O	-18.99591200	3.49941500	-3.76513900
N	-18.53071500	4.91192900	-2.10924200
H	-18.25975800	5.58560300	-2.81219700
C	-18.61618900	5.35168900	-0.80034700
N	-18.25875900	6.61498000	-0.52224500
H	-18.14120500	7.26251900	-1.28832200
H	-18.44410600	7.11898200	0.34055800
N	-19.01358300	4.59183100	0.22180400
C	-19.35089600	3.35118300	-0.20011200
C	-21.49242000	2.41333300	3.88767600
H	-22.36511700	1.79288900	4.09346300
C	-21.54904000	2.66653400	2.38848200

H	-22.15056900	1.88898300	1.92742200
H	-21.78580300	3.71938600	2.18736600
O	-21.52261000	3.62376900	4.61639600
H	-20.64406400	4.00978500	4.65821600
Os	-3.59839200	-5.61444400	-0.2986570
N	-1.52783500	-5.83721900	-0.3472440
C	-0.69773500	-5.53365200	0.6582510
C	0.67711800	-5.65558700	0.5480820
C	1.22541800	-6.07096300	-0.6610240
C	0.36385500	-6.43132300	-1.6895000
C	-1.01263700	-6.32127100	-1.5022800
C	-2.02715700	-6.74952400	-2.4790840
N	-3.31370600	-6.71652000	-2.0279960
C	-4.29701700	-7.13252600	-2.8508020
C	-4.06630900	-7.51807200	-4.1596180
C	-2.75926900	-7.50047800	-4.6452180
C	-1.73395400	-7.13130100	-3.7879110
N	-5.67891700	-5.53051800	-0.2443090
C	-6.46537700	-4.95995600	-1.1702950
C	-7.84762600	-4.92248500	-1.0544310
C	-8.44091200	-5.48023300	0.0736780
C	-7.63293000	-6.09014100	1.0244550
C	-6.25424900	-6.11547400	0.8362060
C	-5.31382200	-6.81366700	1.7313430
N	-4.05535300	-6.95676700	1.2364580
C	-3.15172400	-7.64286100	1.9593510
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C	-4.68392000	-7.90413700	3.7865670
C	-5.64222500	-7.26362100	3.0124360
H	-3.46036900	0.47941500	1.5516580

C	-3.44149100	-0.39083300	0.9058460
C	-3.47986600	-1.68913100	1.5131590
C	-3.50910900	-1.87041300	2.9112790
C	-3.51230400	-3.14920000	3.4189700
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N	-3.54735700	-4.09685600	1.2189410
C	-3.48287100	-2.83768500	0.7044690
C	-3.41190600	-2.69561200	-0.7216760
H	-3.31620600	0.72860000	-0.9019640
C	-3.37057400	-0.25263300	-0.4419990
C	-3.34638400	-1.41030700	-1.2879210
C	-3.28604500	-1.32109600	-2.6948680
C	-3.31139600	-2.47187500	-3.4473000
C	-3.36712300	-3.71666500	-2.7954880
N	-3.40532600	-3.83189900	-1.4750590
H	-1.14559400	-5.14312800	1.5677240
H	1.28893900	-5.36899200	1.3978570
H	2.30419600	-6.08528200	-0.7867410
H	0.76174000	-6.77365700	-2.6349990
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H	-4.90198500	-7.77508700	-4.7962740
H	-2.54941400	-7.72907600	-5.6828380
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H	-3.49056000	-3.34258400	4.4915390
H	-3.54186500	-5.25183400	2.9337320
H	-3.23274400	-0.34278200	-3.1668870
H	-3.31931500	-2.44477100	-4.5390320
H	-3.40301600	-4.63455500	-3.3751490

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