

Modeling DNA oxidation in water

– Electronic Supporting Information (ESI) –

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Section S1: Adopted constraints in geometry optimizations

C1'-C1' distances and C1'-C3'...C3'-C1' dihedral angles involving consecutive ribose rings have been held fixed for all the steps in all the sequences.

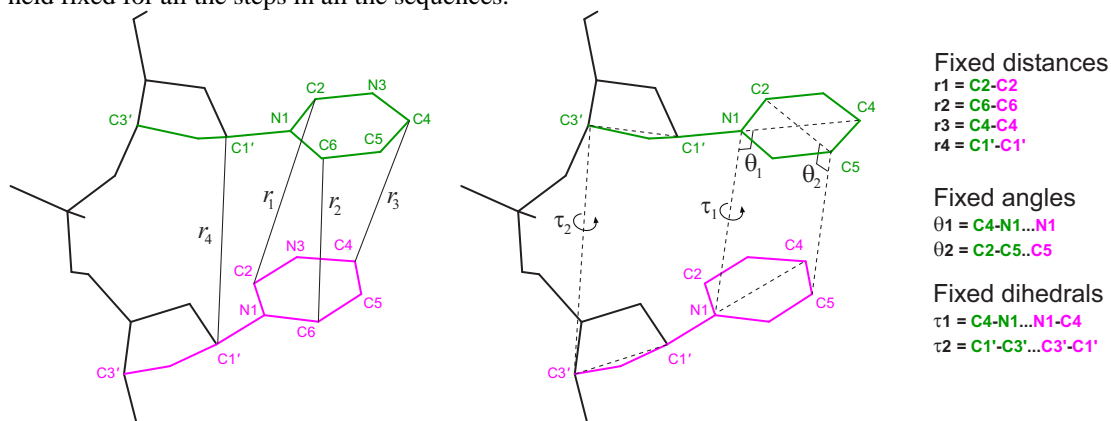


Figure S1: Internal coordinates held fixed in 5'-Pyrimidine-Pyrimidine-3' steps. C6 has to be replaced with N for 6-deaza uracil.

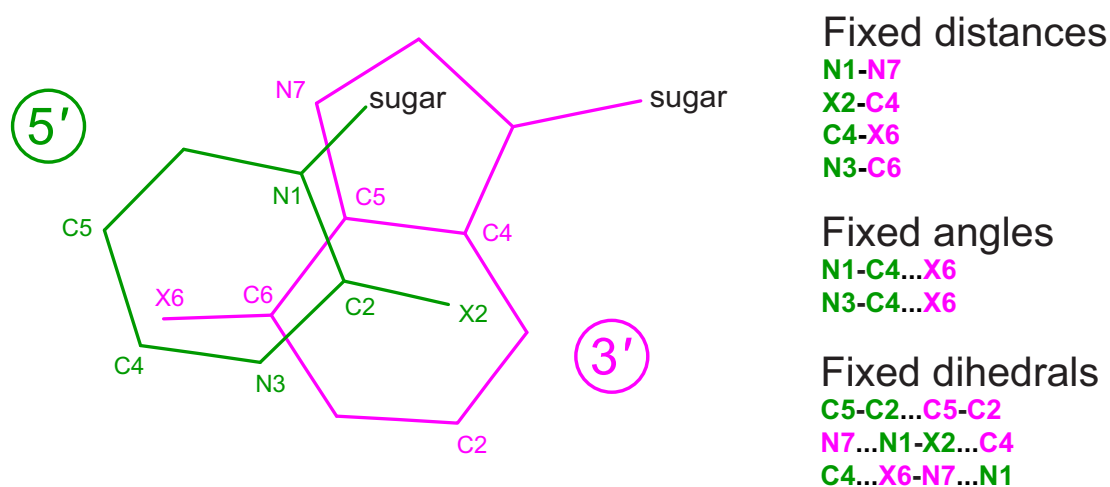


Figure S2: Constrained inter base coordinates for 5'-Pyrimidine-Purine-3' steps. X symbols denote heteroatoms.

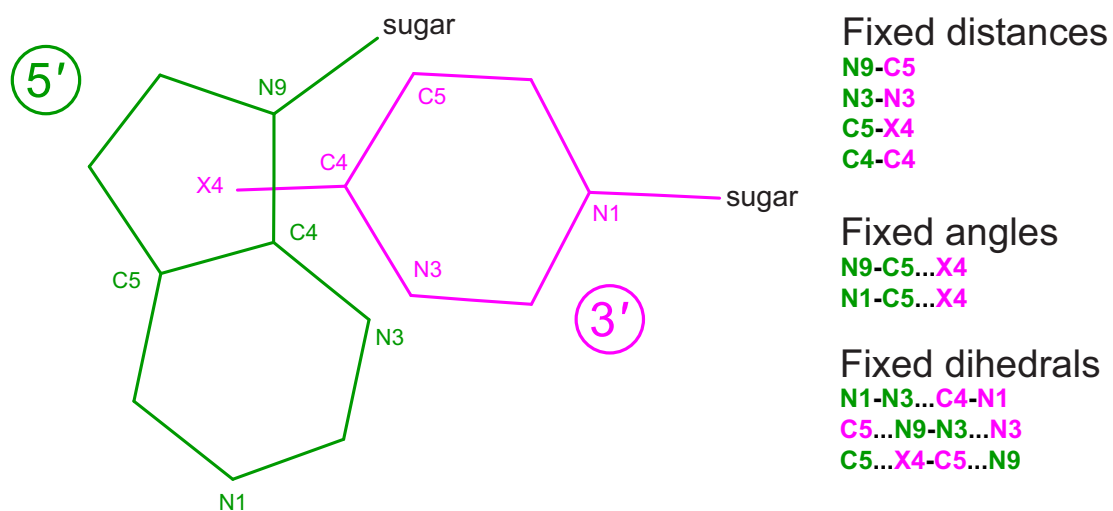


Figure S3: Constrained inter base coordinates for 5'-Purine-Pyrimidine-3' steps. X symbols denote heteroatoms.

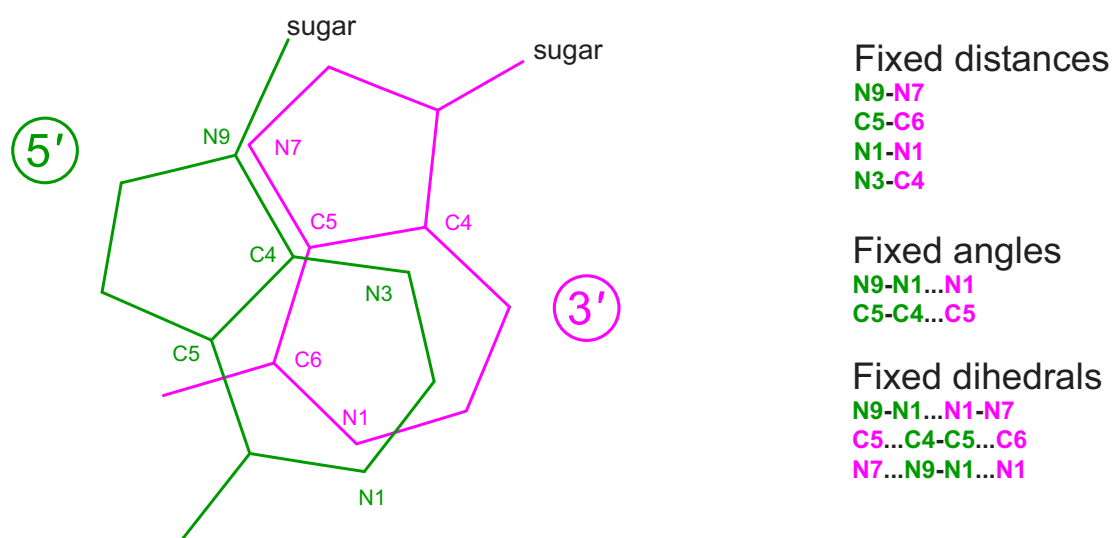


Figure S4: Constrained inter base coordinates for 5'-Purine-Purine-3' steps.

Section S2: Optimized geometries of free and embedded DNA nucleobases

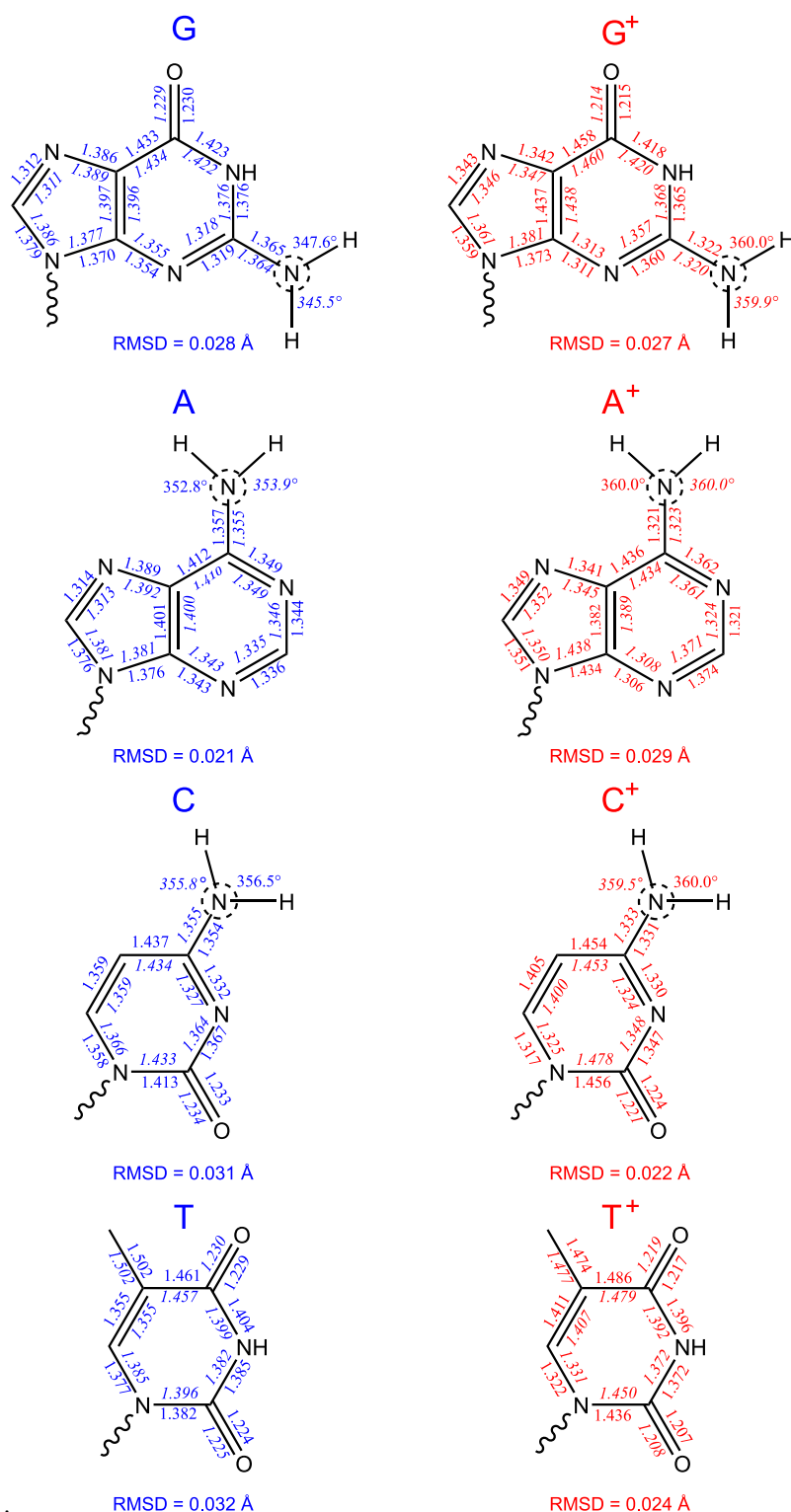


Figure S5: Geometric parameters (bond lengths in Å, angles in degrees) for neutral (blue) and singly ionized (red) free DNA nucleobases (roman font) and DNA nucleobases in XXYY single strands (italicized font) optimized at the PCM/B3LYP-D/TZVP level.

Section S3: local base steps coordinates and puckering conformations of single strands

XACX cation

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/A	0.13	0.43	3.20	6.64	2.40	33.15
2	A/C	0.48	0.44	3.38	4.00	0.97	36.76
3	C/X	0.49	0.58	3.33	4.88	0.89	36.96
~~~~~							
	ave.	0.37	0.48	3.30	5.17	1.42	35.63
	s.d.	0.20	0.09	0.09	1.35	0.85	2.14

*****

base Puckering

- 1 C2'-endo
- 2 C1'-exo
- 3 O4'-endo
- 4 C2'-endo

XACX neutral

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/A	0.12	0.40	3.21	6.33	2.11	33.03
2	A/C	0.46	0.44	3.38	3.85	2.44	36.95
3	C/X	0.49	0.56	3.39	3.97	1.10	37.10
~~~~~							
	ave.	0.36	0.47	3.33	4.72	1.89	35.70
	s.d.	0.21	0.08	0.10	1.40	0.70	2.31

base Puckering

- 1 C2'-endo
- 2 C1'-exo
- 3 O4'-endo
- 4 C2'-endo

XAGX cation

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/A	0.15	0.42	3.22	6.48	1.64	32.97
2	A/G	0.33	0.37	3.30	4.94	1.97	35.47
3	G/X	0.80	0.66	3.24	5.99	-1.16	39.33
~~~~~							
	ave.	0.43	0.48	3.25	5.81	0.82	35.92
	s.d.	0.33	0.15	0.04	0.79	1.72	3.20

*****

base Puckering

- 1 C2'-endo
- 2 C2'-endo
- 3 C1'-exo
- 4 C2'-endo

XAGX neutral

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/A	0.15	0.41	3.23	6.15	1.76	33.01
2	A/G	0.34	0.37	3.28	5.32	2.27	35.30
3	G/X	0.83	0.69	3.11	7.87	0.11	39.12
~~~~~							
	ave.	0.44	0.49	3.21	6.45	1.38	35.81
	s.d.	0.35	0.17	0.09	1.30	1.12	3.08

base Puckering

- 1 C2'-endo
- 2 C1'-exo
- 3 C1'-exo
- 4 C2'-endo

XATX cation

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/A	0.10	0.42	3.19	6.61	2.72	33.17
2	A/T	0.32	0.31	3.58	1.12	-0.80	36.02
3	T/X	0.61	0.52	3.33	4.57	1.08	39.03

```

~~~~~
ave.      0.34      0.42      3.37      4.10      1.00      36.07
s.d.     0.25      0.10      0.20      2.78      1.76      2.93
*****
base Puckering
1  C2'-endo
2  C1'-exo
3  O4'-endo
4  C2'-endo

XATX neutral
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1  X/A      0.09      0.40      3.19      6.68      2.20      33.00
2  A/T      0.36      0.37      3.46      2.92      0.01      36.01
3  T/X      0.62      0.49      3.33      4.52      0.76      39.20
~~~~~
ave.      0.36      0.42      3.33      4.71      0.99      36.07
s.d.     0.26      0.07      0.13      1.88      1.11      3.10
*****
base Puckering
1  C2'-endo
2  C1'-exo
3  O4'-endo
4  C2'-endo

XCAX cation
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1  X/C      0.28      0.48      3.27      4.86      2.68      33.39
2  C/A      0.41      0.48      3.27      5.47      2.63      37.05
3  A/X      0.63      0.62      3.30      5.19      -1.16     37.46
~~~~~
ave.      0.44      0.53      3.28      5.17      1.38      35.97
s.d.     0.18      0.08      0.02      0.30      2.21      2.24
*****
base Puckering
1  C2'-endo
2  C2'-endo
3  C1'-exo
4  C2'-endo

XCAX neutral
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1  X/C      0.27      0.47      3.30      4.51      2.69      33.32
2  C/A      0.43      0.48      3.30      5.14      2.90      36.85
3  A/X      0.67      0.67      3.15      7.19      0.52      37.15
~~~~~
ave.      0.46      0.54      3.25      5.61      2.04      35.77
s.d.     0.20      0.12      0.09      1.40      1.32      2.13
*****
base Puckering
1  C2'-endo
2  C1'-exo
3  O4'-endo
4  C2'-endo

XAAX neutral
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1  X/A      0.05      0.48      3.42      3.76      -1.64     33.22
2  A/A      0.37      0.45      3.31      4.79      1.99      35.97
3  A/X      0.59      0.66      3.18      8.73      -2.86     37.32
~~~~~
ave.      0.34      0.53      3.30      5.76      -0.83     35.50
s.d.     0.27      0.12      0.12      2.62      2.52      2.09
*****
base Puckering
1  C2'-endo
2  C2'-endo
3  C1'-exo
4  C1'-exo

XAAX cation
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist

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```

1 X/A      0.30    1.25    3.28    5.53    5.69    33.01
2 A/A      0.42    0.48    3.29    4.91    2.70    36.14
3 A/X      0.58    0.66    3.22    8.29   -3.04    37.20
~~~~~
ave.      0.44    0.80    3.26    6.24    1.78    35.45
s.d.      0.14    0.40    0.03    1.47    4.44    2.18
*****
base Puckering
1 C2'-endo
2 C2'-endo
3 C1'-exo
4 C1'-exo

XCCX cation
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/C      0.45    0.45    3.29    4.77    1.88    35.66
2 C/C      0.43    0.39    3.48    1.33    2.58    36.59
3 C/X      0.38    0.64    3.26    6.05    1.55    35.05
~~~~~
ave.      0.42    0.49    3.34    4.05    2.00    35.76
s.d.      0.04    0.13    0.12    2.44    0.52    0.78
*****
base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C1'-exo

XCCX neutral
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/C      0.42    0.46    3.28    4.79    2.47    35.32
2 C/C      0.43    0.45    3.41    2.69    2.64    36.25
3 C/X      0.42    0.57    3.31    5.29    1.07    35.77
~~~~~
ave.      0.42    0.49    3.33    4.25    2.06    35.78
s.d.      0.01    0.07    0.07    1.38    0.86    0.47
*****
base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C1'-exo

XCGX cation
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/C      0.32    0.50    3.24    5.43    2.67    33.99
2 C/G      0.19    0.45    3.25    5.64    3.07    34.08
3 G/X      0.82    0.64    3.32    4.92   -2.11    40.05
~~~~~
ave.      0.44    0.53    3.27    5.33    1.21    36.04
s.d.      0.33    0.10    0.05    0.37    2.88    3.47
*****
base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo

XCGX neutral
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/C      0.32    0.48    3.27    4.87    2.84    34.13
2 C/G      0.22    0.45    3.27    5.42    2.86    34.04
3 G/X      0.87    0.70    3.14    7.32   -0.46    39.66
~~~~~
ave.      0.47    0.54    3.23    5.87    1.74    35.94
s.d.      0.35    0.14    0.07    1.28    1.91    3.21
*****
base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo

```

XCTX cation

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/C	0.40	0.45	3.32	4.37	2.13	35.12
2	C/T	0.27	0.43	3.42	2.47	3.11	34.26
3	T/X	0.60	0.56	3.30	5.54	0.47	38.32
~~~~~							
	ave.	0.43	0.48	3.35	4.13	1.90	35.90
	s.d.	0.17	0.07	0.07	1.55	1.33	2.14

*****

base Puckering

- 1 C2'-endo
- 2 C1'-exo
- 3 O4'-endo
- 4 C2'-endo

XCTX neutral

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/C	0.36	0.48	3.29	4.52	3.11	34.71
2	C/T	0.28	0.46	3.36	3.75	2.76	34.05
3	T/X	0.63	0.51	3.34	4.73	0.25	38.97
~~~~~							
	ave.	0.43	0.48	3.33	4.33	2.04	35.91
	s.d.	0.18	0.02	0.04	0.51	1.56	2.67

base Puckering

- 1 C2'-endo
- 2 C1'-exo
- 3 O4'-endo
- 4 C2'-endo

XGAX cation

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/G	0.12	0.34	3.25	5.68	2.62	32.22
2	G/A	0.40	0.55	3.27	5.43	2.12	36.83
3	A/X	0.70	0.61	3.17	7.06	-0.24	38.39
~~~~~							
	ave.	0.41	0.50	3.23	6.05	1.50	35.81
	s.d.	0.29	0.14	0.05	0.88	1.53	3.21

*****

base Puckering

- 1 C2'-endo
- 2 C2'-endo
- 3 O4'-endo
- 4 C2'-endo

XGAX neutral

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/G	0.10	0.33	3.24	5.71	3.23	32.22
2	G/A	0.42	0.55	3.27	5.47	2.44	36.75
3	A/X	0.70	0.61	3.19	6.82	-0.38	38.48
~~~~~							
	ave.	0.41	0.50	3.23	6.00	1.76	35.81
	s.d.	0.30	0.15	0.04	0.72	1.90	3.23

base Puckering

- 1 C2'-endo
- 2 C2'-endo
- 3 O4'-endo
- 4 C2'-endo

XGCX cation

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/G	0.07	0.30	3.17	6.89	1.87	32.68
2	G/C	0.52	0.48	3.46	2.90	-0.24	38.03
3	C/X	0.49	0.56	3.33	4.81	0.66	37.02
~~~~~							
	ave.	0.36	0.45	3.32	4.87	0.77	35.91
	s.d.	0.25	0.13	0.14	2.00	1.06	2.85

*****

base Puckering

- 1 C2'-endo
- 2 C1'-exo
- 3 O4'-endo

4 C2'-endo

XGCX neutral

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/G	0.11	0.32	3.21	6.20	2.27	32.49
2 G/C	0.56	0.52	3.34	4.44	2.25	37.87
3 C/X	0.49	0.55	3.36	4.41	0.81	37.10
ave.	0.39	0.46	3.30	5.02	1.78	35.82
s.d.	0.24	0.12	0.08	1.02	0.84	2.91

*****

base Puckering

- 1 C2'-endo
- 2 C2'-endo
- 3 O4'-endo
- 4 C2'-endo

XGGX cation

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/G	-0.24	1.07	3.45	2.43	-3.36	32.95
2 G/G	0.35	0.46	3.27	5.38	-0.15	36.08
3 G/X	0.86	0.71	3.13	7.65	-0.59	39.56
ave.	0.32	0.74	3.28	5.15	-1.37	36.20
s.d.	0.55	0.31	0.16	2.62	1.74	3.31

*****

base Puckering

- 1 C2'-endo
- 2 C2'-endo
- 3 C1'-exo
- 4 C2'-endo

XGGX neutral

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/G	0.10	0.32	3.27	5.31	2.57	31.95
2 G/G	0.39	0.48	3.25	5.91	1.80	35.97
3 G/X	0.87	0.72	3.09	8.15	-0.00	39.30
ave.	0.45	0.51	3.20	6.46	1.46	35.74
s.d.	0.39	0.20	0.10	1.49	1.32	3.68

*****

base Puckering

- 1 C2'-endo
- 2 C1'-exo
- 3 C1'-exo
- 4 C2'-endo

XGTX cation

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/G	0.05	0.33	3.20	6.25	3.35	32.23
2 G/T	0.40	0.38	3.57	1.25	-1.67	37.07
3 T/X	0.61	0.50	3.29	5.08	0.77	39.12
ave.	0.35	0.40	3.36	4.19	0.82	36.14
s.d.	0.28	0.09	0.19	2.61	2.51	3.54

*****

base Puckering

- 1 C2'-endo
- 2 C1'-exo
- 3 O4'-endo
- 4 C2'-endo

XGTX neutral

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/G	0.09	0.33	3.22	5.89	3.04	32.25
2 G/T	0.44	0.43	3.45	2.99	-0.36	37.05
3 T/X	0.62	0.48	3.30	5.04	0.46	39.22
ave.	0.38	0.41	3.32	4.64	1.05	36.17
s.d.	0.27	0.08	0.11	1.49	1.77	3.57

*****

base Puckering

- 1 C2'-endo



2 C1'-exo  
 3 O4'-endo  
 4 C2'-endo

XXAX cation

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/X	0.45	0.51	3.32	5.04	-0.29	35.47
2	X/A	0.16	0.48	3.31	4.63	4.64	32.90
3	A/X	0.74	0.59	3.30	5.29	-1.62	38.81
~~~~~							
	ave.	0.45	0.53	3.31	4.99	0.91	35.73
	s.d.	0.29	0.05	0.01	0.33	3.30	2.96

base Puckering

1 C2'-endo
 2 C2'-endo
 3 C1'-exo
 4 C2'-endo

XXAX neutral

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/X	0.44	0.50	3.33	4.94	-0.19	35.44
2	X/A	0.15	0.46	3.29	4.96	4.23	32.69
3	A/X	0.78	0.64	3.14	7.37	0.15	38.49
~~~~~							
	ave.	0.46	0.53	3.25	5.76	1.40	35.54
	s.d.	0.31	0.09	0.10	1.40	2.46	2.90

*****

base Puckering

1 C2'-endo  
 2 C2'-endo  
 3 C1'-exo  
 4 C2'-endo

XXCX cation

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/X	0.44	0.44	3.40	3.52	0.20	35.50
2	X/C	0.42	0.41	3.39	2.96	2.47	35.89
3	C/X	0.43	0.59	3.39	3.81	1.16	35.76
~~~~~							
	ave.	0.43	0.48	3.39	3.43	1.28	35.72
	s.d.	0.01	0.09	0.01	0.44	1.14	0.20

base Puckering

1 C2'-endo
 2 C2'-endo
 3 O4'-endo
 4 C2'-endo

XXCX neutral

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/X	0.44	0.45	3.39	3.85	-0.00	35.41
2	X/C	0.34	0.50	3.29	4.22	4.00	35.00
3	C/X	0.50	0.50	3.45	2.90	0.25	36.73
~~~~~							
	ave.	0.43	0.48	3.38	3.65	1.41	35.71
	s.d.	0.08	0.03	0.08	0.68	2.24	0.91

*****

base Puckering

1 C2'-endo  
 2 C2'-endo  
 3 C1'-exo  
 4 C2'-endo

XXGX cation

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	X/X	0.45	0.50	3.31	5.39	-0.31	35.24
2	X/G	0.14	0.38	3.31	4.36	4.91	32.28
3	G/X	0.78	0.61	3.34	4.67	-2.05	39.65
~~~~~							
	ave.	0.46	0.50	3.32	4.81	0.85	35.72
	s.d.	0.32	0.11	0.02	0.53	3.62	3.71

base Puckering
1 C2'-endo
2 C2'-endo
3 C1'-exo
4 C2'-endo

XXGX neutral

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/X	0.45	0.49	3.33	5.05	-0.26	35.36
2 X/G	0.16	0.39	3.32	4.46	4.65	32.27
3 G/X	0.84	0.68	3.12	7.57	-0.31	39.18
ave.	0.48	0.52	3.26	5.69	1.36	35.60
s.d.	0.34	0.15	0.12	1.65	2.85	3.46

base Puckering
1 C2'-endo
2 C2'-endo
3 C1'-exo
4 C2'-endo

XXTX cation

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/X	0.45	0.47	3.36	4.54	-0.18	35.50
2 X/T	0.28	0.43	3.38	3.23	3.14	33.72
3 T/X	0.56	0.58	3.29	5.50	1.03	37.94
ave.	0.43	0.49	3.34	4.42	1.33	35.72
s.d.	0.14	0.08	0.04	1.14	1.68	2.12

base Puckering
1 C2'-endo
2 C2'-endo
3 O4'-endo
4 C2'-endo

XXTX neutral

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/X	0.45	0.48	3.34	4.88	-0.28	35.43
2 X/T	0.20	0.50	3.29	4.62	4.09	32.66
3 T/X	0.63	0.49	3.35	4.47	0.23	39.04
ave.	0.43	0.49	3.33	4.66	1.35	35.71
s.d.	0.21	0.01	0.03	0.21	2.39	3.20

base Puckering
1 C2'-endo
2 C2'-endo
3 C1'-exo
4 C2'-endo

XTAX cation

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/T	0.23	0.47	3.24	5.58	2.43	32.50
2 T/A	0.35	0.45	3.27	5.43	3.44	36.53
3 A/X	0.71	0.57	3.29	5.26	-1.22	38.50
ave.	0.43	0.50	3.27	5.42	1.55	35.85
s.d.	0.25	0.06	0.03	0.16	2.45	3.06

base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo

XTAX neutral

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/T	0.23	0.46	3.25	5.42	2.42	32.40
2 T/A	0.36	0.45	3.27	5.53	3.24	36.33
3 A/X	0.74	0.62	3.15	7.18	0.29	38.22

ave.	0.44	0.51	3.22	6.04	1.98	35.65
s.d.	0.27	0.09	0.06	0.99	1.52	2.97

```
base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo
```

XTCX cation

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/T	0.26	0.45	3.29	5.03	2.17	32.82
2 T/C	0.55	0.39	3.41	2.15	3.24	38.74
3 C/X	0.48	0.59	3.31	5.61	-0.28	36.13

```
~~~~~
ave. 0.43 0.48 3.34 4.26 1.71 35.90
s.d. 0.15 0.10 0.06 1.85 1.80 2.97
```

```
base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo
```

XTCX neutral

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/T	0.22	0.47	3.25	5.48	2.69	32.30
2 T/C	0.55	0.43	3.37	3.02	3.33	38.49
3 C/X	0.52	0.55	3.34	5.04	-0.59	36.75

```
~~~~~
ave. 0.43 0.48 3.32 4.52 1.81 35.85
s.d. 0.18 0.06 0.06 1.31 2.11 3.19
```

```
base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo
```

XTGX cation

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/T	0.23	0.49	3.23	5.91	2.39	32.25
2 T/G	0.31	0.37	3.25	5.51	3.58	35.60
3 G/X	0.78	0.62	3.32	4.96	-1.91	39.65

```
~~~~~
ave. 0.44 0.49 3.27 5.46 1.35 35.84
s.d. 0.30 0.13 0.05 0.48 2.89 3.71
```

```
base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo
```

XTGX neutral

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/T	0.23	0.46	3.26	5.43	2.46	32.39
2 T/G	0.34	0.37	3.28	5.30	3.31	35.57
3 G/X	0.84	0.68	3.12	7.52	-0.17	39.22

```
~~~~~
ave. 0.47 0.51 3.22 6.08 1.87 35.73
s.d. 0.33 0.16 0.08 1.24 1.81 3.42
```

```
base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo
```

XTTX cation

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/T	0.28	0.44	3.30	4.62	2.00	33.61
2 T/T	0.42	0.32	3.44	2.10	2.15	36.45

```

3 T/X      0.61      0.61      3.30      7.47      -1.76      37.26
~~~~~
ave.      0.44      0.46      3.35      4.73      0.80      35.77
s.d.      0.16      0.15      0.08      2.69      2.22      1.91
*****
base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C1'-exo

XTTX neutral
Local base step parameters
step Shift Slide Rise Tilt Roll Twist
1 X/T 0.25 0.45 3.27 5.03 2.37 33.13
2 T/T 0.43 0.37 3.38 3.42 2.12 36.15
3 T/X 0.64 0.57 3.35 6.58 -1.67 38.01
~~~~~
ave. 0.44 0.46 3.33 5.01 0.94 35.76
s.d. 0.20 0.10 0.05 1.58 2.27 2.46
*****
base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C1'-exo

```

Section S4: results obtained by using the TZVP basis set

Table S1: Predicted (PCM-B3LYP-D/TZVP) adiabatic ionization potentials (eV) of nucleobases (Y) and of XXYX single stranded oligonucleotides

	Y	XXYX
G	5.79	5.82
A	6.20	6.25
C	6.55	6.50
T	6.55	6.52

Table S2: Adiabatic ionization potentials (eV, TZVP basis set) of 5'-XYZX-3' single strands

Y (5' side)	Z (3' side)			
	G	A	C	T
	5.73	5.77	5.76	5.78
	5.79	6.01	6.17	6.22
	5.75	6.15	6.38	6.38
	5.80	6.23	6.41	6.40

Table S3: Predicted electronic couplings (eV, TZVP basis set) for 5'-YZ-3' steps

Y (5' side)	Z (3' side)			
	G	A	C	T
	0.09	0.16	0.23	0.16
	0.12	0.24	0.16	0.10
	0.25	0.18	0.12	0.13
	0.13	0.08	0.10	0.12

Table S4: Hole energies (eV) relative to XXGX of single strands predicted by PCM/B3LYP-D/TZVP computations and by using the TB Hamiltonian. Deviations^a of TB from DFT results are in eV

ss	TB	DFT	ss	TB	DFT
XAGA	-0.08	-0.09	XCAC	0.28	0.29
AAGA	-0.09	-0.09	CCAC	0.28	0.28
TGAC	-0.08	-0.06	XTAT	0.38	0.39
TAGC	-0.11	-0.11	TTAT	0.38	0.39
XCGC	-0.14	-0.14	TCAT	0.31	0.32
CCGC	-0.14	-0.15	CTAC	0.34	0.34
XTGT	-0.06	-0.06	CAAC	0.14	0.14
TTGT	-0.06	-0.06	TAAT	0.18	0.19
AGGA	-0.13	-0.11	CAAT	0.15	0.14
CGGC	-0.16	-0.16	TAAC	0.16	0.17
TGGT	-0.12	-0.11	XTCT	0.52	0.52
TGGA	-0.12	-0.14	TTCT	0.51	0.52
CGGT	-0.14	-0.15	TCCT	0.49	0.49
MUE ^a	MSE	RMSD	L. dev. (seq)	R ²	intercept
7×10^{-3}	-2×10^{-3}	9×10^{-3}	2×10^{-2} (AGGA)	0.999	-4×10^{-4}

^aMUE/MSE denote mean unsigned/signed errors; RMSD is the root mean square deviation. Signed largest deviation is reported for the corresponding sequence. R^2 is the linear correlation coefficient between DFT and TB calculated hole energies. The linear fitting using DFT values as abscissa and TB ones as ordinate returns 0.99 and -4×10^{-4} eV as the slope and the intercept, respectively.

Section S5: Statistical analysis for the symmetric couplings

Table S5: Hole energies (eV) relative to XXGX of single strands predicted by PCM/B3LYP-D/TZV+P computations and by using the TB Hamiltonian with symmetric 5'-YZ-3' couplings, see Eq. (5) in the main text. Deviations of TB from DFT results are in eV

ss	TB	DFT	ss	TB	DFT
XGAX	-0.05	-0.05	XACX	0.34	0.35
XAGX	-0.05	-0.03	XCAX	0.34	0.33
AAGA	-0.10	-0.10	CCAC	0.28	0.28
TGAC	-0.07	-0.06	XATX	0.40	0.40
TAGC	-0.11	-0.11	XTAX	0.40	0.41
XGCX	-0.07	-0.08	TTAT	0.38	0.38
XCGX	-0.07	-0.07	TCAT	0.32	0.32
CCGC	-0.14	-0.14	CTAC	0.33	0.34
XGTX	-0.03	-0.04	CAAC	0.14	0.14
XTGX	-0.03	-0.02	TAAT	0.18	0.19
TTGT	-0.05	-0.06	CAAT	0.16	0.14
AGGA	-0.13	-0.11	TAAC	0.16	0.17
CGGC	-0.16	-0.16	XCTX	0.57	0.56
TGGT	-0.11	-0.11	XTCX	0.57	0.58
TGGA	-0.12	-0.14	TTCT	0.50	0.52
CGGT	-0.14	-0.15	TCCT	0.49	0.49
MUE ^a	MSE	RMSD	L. dev. (seq)	R ²	intercept
8 x 10 ⁻³	-8 x 10 ⁻⁴	1 x 10 ⁻²	-2 x 10 ⁻² (TTCT)	0.999	5 x 10 ⁻⁴

^aMUE/MSE denote mean unsigned/signed errors; RMSD is the root mean square deviation. Signed largest deviation is reported for the corresponding sequence. R² is the linear correlation coefficient between DFT and TB calculated hole energies. The linear fitting using DFT values as abscissa and TB predictions as ordinate returns 0.99 and 5 x 10⁻⁴ eV as the slope and the intercept, respectively.

Cartesian coordinates

XAAX							
O	-9.85446	0.10734	0.23297	H	-10.09257	-1.84058	-0.49185
C	-9.67437	-0.86705	-0.79043	H	-10.16045	-0.55730	-1.72748
C	-8.18980	-1.05570	-1.05577	H	-8.06597	-1.91484	-1.72593
O	-7.64945	0.12011	-1.69258	H	-7.95055	-1.67397	1.04509
C	-7.35306	-1.27422	0.22122	H	-7.56224	0.74291	0.93358
O	-6.29748	-2.20087	-0.11703	H	-5.60822	0.09489	-1.32224
C	-6.78674	0.11769	0.48886	H	-4.63298	4.14784	-2.86651
C	-6.51840	0.56363	-0.94262	H	-5.89238	0.09666	1.10928
N	-6.34247	1.99750	-1.13757	H	-3.98302	-4.74062	-1.51267
C	-5.43338	2.41660	-2.12268	H	-4.87698	-3.20964	-1.70604
O	-4.81975	1.63354	-2.82990	H	-2.38592	-3.27933	-2.37250
N	-5.30544	3.79304	-2.19285	H	-1.91853	-4.20774	0.24972
C	-6.02398	4.72131	-1.44239	H	-2.55074	-2.05663	1.21278
O	-5.85430	5.92542	-1.55581	H	-1.01681	-0.84679	-1.14984
C	-6.97928	4.08623	-0.51564	H	-3.70838	-0.18543	1.45351
N	-7.11482	2.81199	-0.38989	H	-0.19075	3.29547	-2.65446
P	-5.45986	-2.90502	1.10358	H	-3.64562	4.69430	1.05254
O	-6.35889	-3.81257	1.91977	H	-2.79864	5.79131	0.03478
O	-4.71148	-1.86689	1.92851	H	-0.76171	-1.89463	1.08512
O	-4.42844	-3.82285	0.24078	H	2.64698	-3.75777	-3.14114
C	-4.08167	-3.71225	-1.15003	H	1.11743	-2.93161	-2.74944
C	-2.75965	-2.99034	-1.38161	H	3.22293	-1.51472	-3.00794
O	-2.96434	-1.56439	-1.35246	H	4.36025	-3.20824	-0.99149
C	-1.68348	-3.30239	-0.31561	H	3.20356	-2.03986	0.77714
O	-0.41662	-3.46592	-0.98739	H	3.48779	0.46954	-0.95177
C	-1.69088	-2.03390	0.53750	H	1.23545	-1.22092	1.63250
C	-1.92255	-0.99262	-0.55003	H	2.36089	4.74933	-0.46619
N	-2.32699	0.31294	-0.10572	H	-1.05459	2.83753	2.99973
C	-3.21471	0.61139	0.90739	H	-0.93577	4.47043	2.53092
N	-3.39572	1.90019	1.07941	H	4.68438	-1.01599	0.62871
C	-2.58359	2.49730	0.12101	H	7.70023	0.61480	-3.67601
C	-2.29580	3.83627	-0.20907	H	6.07721	0.39976	-2.97462
N	-2.83449	4.88219	0.47800	H	7.46328	2.52010	-2.43998
N	-1.45567	4.08660	-1.23249	H	9.32976	0.65948	-1.26964
C	-0.88174	3.03613	-1.85506	H	7.98753	0.44304	0.70752
N	-1.04678	1.73148	-1.62441	H	7.15587	3.34873	0.22245
C	-1.92589	1.52080	-0.63615	H	3.77527	3.78695	3.13854
P	0.82716	-4.10095	-0.11714	H	8.95426	1.89716	1.16101
O	0.52954	-5.53583	0.27051	H	10.29338	2.68965	-0.77049
O	1.20239	-3.20137	1.05082	H	-10.80687	0.18107	0.39620
O	1.98037	-4.11731	-1.26697	H	-7.60198	4.72739	0.09880
C	2.10574	-3.20356	-2.36804	H	5.00651	-0.25458	3.38585
C	2.89423	-1.94294	-2.05078	Na	-5.82689	-2.58735	3.96096
O	2.05855	-0.98890	-1.37545	Na	0.77665	-4.98707	2.64228
C	4.14876	-2.14840	-1.15739	Na	7.67416	-3.96419	0.44988
O	5.25461	-1.52463	-1.83854	XACX			
C	3.79527	-1.39321	0.12343	O	9.82464	0.05178	0.29694
C	2.89473	-0.29989	-0.44294	C	9.61883	1.08220	-0.66494
N	2.06658	0.39704	0.51023	C	8.13210	1.21754	-0.94685
C	1.26010	-0.14686	1.49267	O	7.66472	0.05735	-1.66857
N	0.55896	0.75176	2.14954	C	7.26596	1.31556	0.32896
C	0.91664	1.95250	1.56016	O	6.19431	2.24184	0.05079
C	0.50255	3.27047	1.79003	C	6.73296	-0.10281	0.47567
N	-0.45048	3.59752	2.70947	C	6.52445	-0.46339	-0.99172
N	1.05505	4.24190	1.04195	N	6.39563	-1.89423	-1.25434
C	1.95371	3.91437	0.09999	C	5.48094	-2.32423	-2.22829
N	2.40174	2.70076	-0.24412	O	4.83744	-1.54933	-2.91737
C	1.85144	1.75750	0.53707	N	5.38651	-3.70358	-2.31038
P	6.78142	-1.90508	-1.36345	C	6.05457	-4.62323	-1.50177
O	7.15529	-3.29729	-1.83858	O	5.84241	-5.82431	-1.56452
O	6.97616	-1.66793	0.12236	C	7.01897	-3.97857	-0.59143
O	7.60763	-0.83145	-2.27276	N	7.16310	-2.70408	-0.49432
C	7.14635	0.44146	-2.74797	P	5.31740	2.82514	1.30774
C	7.41949	1.61589	-1.81611	O	6.17549	3.69416	2.20563
O	6.35026	1.76967	-0.86444	O	4.58308	1.71060	2.04016
C	8.73801	1.54002	-0.99977	O	4.27373	3.77528	0.49660
O	9.46365	2.74237	-1.27114	C	3.95498	3.73876	-0.90349
C	8.23896	1.47461	0.44884	C	2.68168	2.96634	-1.21209
C	6.95030	2.28041	0.32798	O	2.94394	1.55009	-1.25615
N	6.00394	2.14813	1.42820	C	1.54133	3.17119	-0.18244
C	5.20461	3.24982	1.77628	O	0.33245	3.36327	-0.93950
O	5.24915	4.32533	1.20579	C	1.51333	1.83999	0.55485
N	4.36847	3.01043	2.86103	C	1.86489	0.88660	-0.58693
C	4.18131	1.78803	3.49512	N	2.30092	-0.42496	-0.17529
O	3.38187	1.63005	4.40430	C	3.20550	-0.71501	0.82722
C	5.06506	0.73918	2.95502	N	3.44969	-1.99889	0.96238
N	5.90400	0.92634	1.99582	C	2.66259	-2.60439	-0.01280

C	-4.95461	-3.37963	1.81751	N	2.29051	-0.41850	-0.16253
O	-4.98177	-4.45220	1.23853	C	3.22537	-0.71120	0.81001
N	-4.09602	-3.12475	2.87950	N	3.45576	-1.99652	0.94820
C	-3.89046	-1.89076	3.48400	C	2.62410	-2.60117	0.00980
O	-3.04699	-1.69883	4.34465	C	2.40563	-3.93672	-0.37910
C	-4.82282	-0.86674	2.98688	N	2.98873	-4.98730	0.25840
N	-5.69502	-1.07246	2.06112	N	1.56284	-4.17929	-1.40213
H	10.08459	2.02670	-0.32870	C	0.91530	-3.14202	-1.96907
H	10.20743	0.81790	-1.63348	N	1.00875	-1.84668	-1.67719
H	8.07583	2.12196	-1.60013	C	1.89621	-1.63471	-0.69533
H	7.93824	1.70036	1.16096	P	-0.99828	3.96143	-0.20714
H	7.54332	-0.68693	0.88971	O	-0.78946	5.38875	0.25534
H	5.66305	0.08445	-1.39183	O	-1.51771	3.01524	0.86437
H	7.55024	-4.57653	0.04273	O	-1.96180	4.00015	-1.52113
H	4.62018	-3.95770	-2.95345	C	-2.07490	2.92384	-2.46654
H	5.86758	-0.06012	1.05417	C	-2.86172	1.71151	-1.98373
H	3.94584	4.91125	-1.22316	O	-2.03047	0.80531	-1.26235
H	4.89347	3.42907	-1.50804	C	-4.06468	2.02601	-1.06772
H	2.42146	3.45078	-2.18509	O	-5.23293	1.99748	-1.90077
H	1.87587	4.21084	0.49082	C	-3.98426	0.95455	0.04670
H	2.43705	1.99444	1.32366	C	-2.91822	-0.00594	-0.48143
H	1.07618	0.93453	-1.21380	N	-2.09740	-0.71770	0.48631
H	3.72939	0.22090	1.41693	C	-1.95657	-2.09822	0.33256
H	0.25678	-3.19096	-2.78380	O	-2.55720	-2.76410	-0.50300
H	3.72797	-4.66087	0.88523	N	-1.09495	-2.68232	1.24193
H	2.95550	-5.72031	-0.22688	C	-0.29743	-2.05829	2.21009
H	0.66073	1.84211	1.05853	O	0.48005	-2.70363	2.90909
H	-2.53653	3.67448	-3.21476	C	-0.48917	-0.61806	2.27824
H	-1.01013	2.88934	-2.73558	C	0.32507	0.15278	3.27773
H	-3.17689	1.49706	-2.86244	C	-1.34865	-0.01880	1.41862
H	-3.96378	3.28293	-0.62169	P	-6.73507	2.12880	-1.24997
H	-3.51200	1.71275	0.98468	O	-7.62219	2.74295	-2.31141
H	-3.33664	-0.51228	-1.08436	O	-6.70063	2.78615	0.11124
H	-1.27301	1.13197	1.69190	O	-7.12290	0.54564	-1.01707
H	-0.70672	-5.21676	0.90014	C	-7.02621	-0.31834	-2.15841
H	-3.21187	-4.74465	-1.47069	C	-7.30675	-1.74656	-1.74436
H	-2.33997	-5.89502	-0.57933	O	-6.25286	-2.21406	-0.87801
H	-4.84919	0.73401	0.30440	C	-8.63520	-1.94390	-0.98402
H	-7.82444	0.20333	-2.80104	O	-9.21330	-3.15846	-1.46750
H	-6.07858	-0.05385	-2.53166	C	-8.17257	-2.07017	0.46498
H	-7.42163	-2.14222	-2.48768	C	-6.83760	-2.79053	0.28304
H	-9.32345	-0.82095	-0.91731	N	-5.92135	-2.64284	1.40870
H	-7.88392	-0.70178	1.02144	C	-5.17946	-3.74585	1.85090
H	-6.96593	-3.54509	0.37062	O	-5.29965	-4.87300	1.40462
H	-4.76349	0.13065	3.40890	N	-4.27881	-3.42764	2.85868
H	-3.47573	-3.88741	3.13551	C	-4.06257	-2.16964	3.41339
H	-8.77060	-2.22296	1.36261	O	-3.22128	-1.96610	4.27574
H	-10.00717	-3.03036	-0.57415	C	-4.92951	-1.14361	2.81740
H	10.82383	-0.01839	0.46925	N	-5.78237	-1.38426	1.88172
Na	5.67522	2.46027	4.13130	H	9.98140	2.00477	-0.49763
Na	-1.34730	4.84653	2.65743	H	10.09768	0.79678	-1.80382
Na	-8.07426	4.84649	-0.78122	H	7.93910	2.05567	-1.71445
XATX				H	7.88071	1.63003	1.04645
O	9.83257	0.01039	0.11733	H	7.54159	-0.76982	0.78276
C	9.60445	1.03211	-0.84907	H	5.57965	-0.04203	-1.44418
C	8.11120	1.16778	-1.09430	H	7.60946	-4.65362	-0.05721
O	7.62428	0.00166	-1.79311	H	4.59068	-4.10803	-2.97881
C	7.28003	1.27782	0.20338	H	5.85601	-0.18490	0.99471
O	6.20011	2.20128	-0.05032	H	3.80612	4.77693	-1.22851
C	6.75000	-0.13904	0.37615	H	4.78949	3.32324	-1.53613
C	6.49917	-0.50808	-1.08258	H	2.32798	3.28149	-2.21704
N	6.35211	-1.93832	-1.33460	H	1.74614	4.04845	0.44915
C	5.40392	-2.36742	-2.27660	H	2.33001	1.83708	1.29832
O	4.74163	-1.59029	-2.94531	H	1.00883	0.74779	-1.24859
N	5.30337	-3.74635	-2.35141	H	3.71359	0.08947	1.35706
C	5.98174	-4.66394	-1.54841	H	0.22937	-3.40641	-2.77151
O	5.75296	-5.86284	-1.59040	H	3.77737	-4.78518	0.85910
C	6.98032	-4.02077	-0.67383	H	3.02722	-5.86574	-0.24308
N	7.13785	-2.74718	-0.59257	H	0.56077	1.67237	1.01374
P	5.37007	2.79970	1.23176	H	-2.61131	3.35582	-3.31587
O	6.27208	3.65537	2.09914	H	-1.07960	2.60835	-2.79521
O	4.64394	1.69698	1.99019	H	-3.25061	1.19981	-2.87796
O	4.31283	3.76002	0.45122	H	-3.97678	3.01935	-0.62876
C	3.96810	3.73239	-0.94294	H	-3.64888	1.42915	0.97127
C	2.68924	2.96232	-1.23069	H	-3.38057	-0.77023	-1.11135
O	2.94353	1.54422	-1.26319	H	-1.48920	1.05873	1.38380
C	1.55980	3.18322	-0.19228	H	-0.97716	-3.68409	1.13190
O	0.34685	3.37629	-0.94203	H	-4.93303	0.44282	0.21393
C	1.52760	1.85797	0.55525	H	-7.75529	-0.01561	-2.92088
C	1.86470	0.89477	-0.58105	H	-6.01905	-0.25500	-2.58575
				H	-7.32258	-2.36231	-2.65269

H	-9.31655	-1.09783	-1.13425
H	-7.99498	-1.07810	0.88488
H	-6.98034	-3.86397	0.14633
H	-4.84299	-0.12174	3.17026
H	-3.71070	-4.19704	3.20068
H	-8.87266	-2.62917	1.09288
H	-10.01501	-3.31994	-0.94446
H	10.78743	-0.02538	0.27900
H	0.07476	1.21783	3.24562
H	0.14746	-0.22298	4.29300
H	1.39777	0.03913	3.07332
Na	5.83861	2.24523	4.03571
Na	-1.51614	4.78114	2.51746
Na	-8.27481	4.49836	-0.70648

XCAX

O	-9.85940	0.07286	0.10011
C	-9.64620	-0.98459	-0.83095
C	-8.15573	-1.13331	-1.08178
O	-7.67662	0.01226	-1.82230
C	-7.31847	-1.20098	0.21838
O	-6.26188	-2.16688	0.01403
C	-6.75314	0.20679	0.31698
C	-6.51558	0.50259	-1.16144
N	-6.29942	1.91069	-1.47284
C	-5.37374	2.26323	-2.46681
O	-4.74255	1.45460	-3.12461
N	-5.24044	3.63633	-2.62532
C	-5.90705	4.63060	-1.90998
O	-5.73720	5.82082	-2.12097
C	-6.80640	4.06531	-0.89443
N	-6.99244	2.80181	-0.72276
P	-5.48166	-2.73710	1.34104
O	-6.42460	-3.55637	2.20084
O	-4.77242	-1.61740	2.09120
O	-4.40148	-3.73251	0.64022
C	-4.01974	-3.79543	-0.74261
C	-2.73264	-3.04376	-1.04502
O	-2.99211	-1.63570	-1.15566
C	-1.61750	-3.20117	0.02208
O	-0.39252	-3.43777	-0.69414
C	-1.60025	-1.83325	0.69899
C	-1.91429	-0.94382	-0.50275
N	-2.34882	0.41681	-0.23313
C	-1.81064	1.49175	-1.00881
O	-0.98590	1.24742	-1.89237
N	-2.23022	2.75713	-0.71885
C	-3.08213	2.96955	0.27758
N	-3.47482	4.24911	0.49723
C	-3.64987	1.91882	1.06058
C	-3.25900	0.65339	0.75500
P	0.95519	-3.92701	0.10507
O	0.75660	-5.30241	0.71042
O	1.46175	-2.87086	1.07423
O	1.92578	-4.09654	-1.19519
C	2.02535	-3.13253	-2.25590
C	2.80971	-1.87319	-1.91295
O	1.98507	-0.92114	-1.24236
C	4.04638	-2.09611	-1.01443
O	5.19584	-2.06275	-1.87430
C	3.95847	-0.96765	0.03645
C	2.87164	-0.05415	-0.53219
N	2.08976	0.70717	0.41374
C	1.28409	0.20882	1.42063
N	0.51965	1.11972	1.98299
C	0.82510	2.28486	1.28953
C	0.40371	3.62554	1.42069
N	-0.48841	4.03747	2.35743
N	0.93252	4.55625	0.60396
C	1.84062	4.17419	-0.30697
N	2.33382	2.95115	-0.53390
C	1.79930	2.05215	0.31242
P	6.69984	-2.26780	-1.24323
O	7.54882	-2.90569	-2.32167
O	6.64678	-2.94184	0.10932
O	7.16101	-0.70814	-0.99279
C	7.13829	0.16472	-2.13200
C	7.41897	1.58535	-1.69014
O	6.32059	2.06431	-0.88896
C	8.69608	1.74993	-0.83986
O	9.32564	2.96043	-1.26492

C	8.13903	1.86454	0.57936
C	6.84577	2.62841	0.31044
N	5.83645	2.53052	1.35838
C	5.02043	3.64431	1.61444
O	5.09973	4.69632	1.00500
N	4.12143	3.44784	2.65456
C	3.89748	2.25186	3.32278
O	3.04139	2.12484	4.18296
C	4.82466	1.18739	2.89620
N	5.71101	1.33331	1.97294
H	-10.02348	-1.94213	-0.44078
H	-10.14766	-0.78144	-1.78873
H	-7.98611	-2.04120	-1.67298
H	-7.92706	-1.49271	1.07836
H	-7.52295	0.87703	0.70200
H	-5.62448	-0.02099	-1.51867
H	-7.37174	4.74662	-0.26745
H	-4.57360	3.93206	-3.33192
H	-5.85336	0.25645	0.92468
H	-3.85740	-4.85656	-0.95847
H	-4.82336	-3.41911	-1.38091
H	-2.35207	-3.41854	-2.00506
H	-1.81208	-4.02821	0.71019
H	-2.40919	-1.79315	1.43322
H	-1.05045	-0.86781	-1.16380
H	-3.67783	-0.21462	1.25788
H	-4.38226	2.11055	1.83492
H	-2.98342	4.99052	0.01614
H	-3.98478	4.49019	1.33481
H	-0.63962	-1.61737	1.16197
H	2.55843	-3.65185	-3.05737
H	1.02597	-2.85981	-2.60915
H	3.15870	-1.43721	-2.86196
H	4.00826	-3.06780	-0.52298
H	3.62343	-1.38917	0.98661
H	3.31095	0.68318	-1.21666
H	1.31089	-0.85025	1.64593
H	2.22731	4.96792	-0.94313
H	-1.07095	3.33073	2.78773
H	-0.92536	4.93698	2.20282
H	4.90401	-0.43976	0.17154
H	7.90121	-0.14732	-2.85614
H	6.15341	0.12304	-2.61134
H	7.50743	2.20743	-2.59002
H	9.37236	0.89441	-0.95485
H	7.90786	0.87171	0.96937
H	7.03972	3.69366	0.17249
H	4.74445	0.21491	3.36971
H	3.50618	4.23002	2.85864
H	8.81004	2.39399	1.26223
H	10.09443	3.09848	-0.68861
H	-10.81152	0.11468	0.27587
Na	-5.99978	-2.15313	4.12867
Na	1.46819	-4.47522	2.89396
Na	8.06610	-4.75381	-0.76317

XCCX

O	-9.87828	0.35066	0.12502
C	-9.69104	-0.63156	-0.89000
C	-8.20415	-0.81277	-1.14360
O	-7.67220	0.37181	-1.77338
C	-7.37989	-1.02643	0.14553
O	-6.33687	-1.97952	-0.15984
C	-6.79055	0.36016	0.39417
C	-6.51129	0.77043	-1.04510
N	-6.24619	2.18125	-1.27210
C	-5.32012	2.53386	-2.26689
O	-4.72204	1.72303	-2.95331
N	-5.13525	3.90186	-2.39332
C	-5.76588	4.89552	-1.65282
O	-5.55450	6.08535	-1.82597
C	-6.69075	4.33246	-0.65316
N	-6.90857	3.07065	-0.49620
P	-5.51662	-2.66074	1.08755
O	-6.42977	-3.55312	1.90539
O	-4.78073	-1.60838	1.90563
O	-4.47187	-3.59865	0.26405
C	-4.07670	-3.49949	-1.11413
C	-2.75941	-2.76127	-1.31333
O	-2.98416	-1.34145	-1.28985
C	-1.69138	-3.05813	-0.22931

C	8.10455	1.73565	0.59873
C	6.80617	2.50218	0.36729
N	5.80966	2.37073	1.42442
C	4.98529	3.47010	1.70622
O	5.02508	4.52424	1.09482
N	4.12722	3.25857	2.77686
C	3.89959	2.04400	3.41166
O	3.04715	1.88851	4.27068
C	4.82740	0.99687	2.95647
N	5.70226	1.16393	2.02458
H	4.75976	0.01508	3.41236
H	-10.10600	-1.82229	-0.47871
H	-10.20231	-0.61572	-1.78803
H	-8.07859	-1.93906	-1.72396
H	-7.98664	-1.49235	1.04063
H	-7.53884	0.88349	0.74862
H	-5.65775	0.03201	-1.50459
H	-4.54065	4.01737	-3.18797
H	-5.88099	0.22168	0.94369
H	-3.95541	-4.80865	-1.17148
H	-4.89683	-3.33584	-1.52003
H	-2.41234	-3.34904	-2.11454
H	-1.94081	-4.07342	0.59271
H	-2.46316	-1.85557	1.38762
H	-1.08465	-0.86683	-1.17566
H	-3.70623	-0.27302	1.25998
H	-4.40485	2.02626	1.92312
H	-2.94699	4.96211	0.25506
H	-3.94941	4.42016	1.54314
H	-0.69105	-1.70987	1.11626
H	2.50600	-3.76780	-3.06137
H	0.98023	-2.95266	-2.63324
H	3.13053	-1.56339	-2.84244
H	3.98067	-3.26532	-0.57124
H	3.48413	-1.67012	1.00596
H	3.34920	0.50669	-1.12024
H	1.26086	-1.00170	1.70992
H	0.80330	5.33569	0.68528
H	3.37429	4.73075	-1.58885
H	2.48526	5.92778	-0.78146
H	4.84093	-0.71354	0.32978
H	7.82485	-0.22154	-2.84637
H	6.08026	0.04570	-2.57708
H	7.43134	2.13229	-2.56229
H	9.32741	0.81868	-0.97649
H	7.88335	0.73124	0.96339
H	6.99634	3.57189	0.26220
H	3.51509	4.03526	3.00930
H	8.78175	2.24964	1.28726
H	10.02523	3.02656	-0.66090
H	-10.83345	0.23100	0.30746
H	-7.35149	4.78643	-0.12363
Na	-6.06635	-2.25235	4.03380
Na	1.08571	-4.63113	2.87997
Na	8.05464	-4.83528	-0.78109

XCTX

O	9.82177	-0.20335	0.14732
C	9.64191	0.83821	-0.80831
C	8.15904	1.00146	-1.09375
O	7.67904	-0.15328	-1.81815
C	7.29532	1.10984	0.18537
O	6.25242	2.07747	-0.06807
C	6.71539	-0.29117	0.30892
C	6.50262	-0.61981	-1.16554
N	6.28419	-2.03131	-1.45440
C	5.35029	-2.40128	-2.43551
O	4.70413	-1.60529	-3.09417
N	5.23391	-3.77737	-2.58520
C	5.90731	-4.76047	-1.85955
O	5.75658	-5.95355	-2.06800
C	6.78202	-4.17677	-0.83257
N	6.96091	-2.91018	-0.67590
P	5.42007	2.67023	1.21715
O	6.32735	3.50537	2.09927
O	4.67840	1.56576	1.95806
O	4.38101	3.66004	0.44976
C	3.99886	3.63103	-0.93436
C	2.71723	2.85651	-1.19887
O	2.98197	1.44498	-1.24606
C	1.59682	3.06194	-0.14289

O	0.38694	3.33314	-0.87435
C	1.52619	1.70686	0.54737
C	1.87283	0.78180	-0.61939
N	2.27717	-0.57350	-0.27463
C	1.76813	-1.68687	-1.02333
O	0.94252	-1.48587	-1.91699
N	2.21412	-2.93328	-0.69093
C	3.08446	-3.09772	0.30073
N	3.54315	-4.35207	0.52753
C	3.60028	-2.01079	1.07331
C	3.18799	-0.76509	0.72489
P	-0.94671	3.88672	-0.09478
O	-0.73220	5.29436	0.42339
O	-1.45240	2.89744	0.94417
O	-1.92925	3.98269	-1.39179
C	-2.06248	2.94477	-2.37603
C	-2.85896	1.72400	-1.93216
O	-2.03222	0.78121	-1.25519
C	-4.05063	2.01537	-0.99313
O	-5.22570	2.01388	-1.81682
C	-3.95980	0.91096	0.08945
C	-2.92257	-0.04676	-0.49602
N	-2.10196	-0.82181	0.42242
C	-1.94335	-2.18553	0.15493
O	-2.54951	-2.78707	-0.72416
N	-1.07456	-2.83447	1.00785
C	-0.28325	-2.27866	2.01543
O	0.46953	-2.98940	2.67719
C	-0.43297	-0.83330	2.15962
C	0.41603	-0.13566	3.18265
P	-1.31741	-0.18122	1.36721
C	-6.72562	2.12613	-1.15901
O	-7.61275	2.78005	-2.19661
O	-6.68810	2.73420	0.22461
O	-7.11677	0.53627	-0.98545
C	-7.02735	-0.28210	-2.16105
C	-7.31621	-1.72485	-1.80635
O	-6.26134	-2.23792	-0.96786
C	-8.63880	-1.94205	-1.04357
O	-9.22321	-3.14116	-1.55649
C	-8.16419	-2.11121	0.39903
C	-6.84616	-2.84889	0.17731
N	-5.90836	-2.77367	1.29057
C	-5.15066	-3.90307	1.62811
O	-5.27035	-4.99060	1.09258
N	-4.23961	-3.66307	2.64788
C	-4.02021	-2.45184	3.29671
O	-3.17512	-2.31593	4.16855
C	-4.88457	-1.38037	2.78183
N	-5.74922	-1.54911	1.84135
H	10.02402	1.79828	-0.42922
H	10.16023	0.60954	-1.75128
H	8.01524	1.89818	-1.70842
H	7.88703	1.41974	1.05099
H	7.47141	-0.95827	0.72525
H	5.62258	-0.09736	-1.55032
H	7.33634	-4.84660	-0.18374
H	4.56994	-4.08498	-3.28941
H	5.80200	-0.31819	0.89798
H	3.82838	4.67593	-1.21311
H	4.80786	3.22547	-1.54747
H	2.33483	3.18319	-2.17559
H	1.81385	3.88955	0.53756
H	2.29964	1.66260	1.31744
H	1.03327	0.69105	-1.31033
H	3.59421	0.12451	1.19924
H	4.33217	-2.16109	1.85722
H	3.08664	-5.12226	0.05725
H	4.06209	-4.55947	1.36880
H	0.54516	1.52326	0.97331
H	-2.60065	3.41444	-3.20402
H	-1.07370	2.63027	-2.72479
H	-3.26244	1.25189	-2.84158
H	-3.95659	2.99571	-0.52687
H	-3.59230	1.35580	1.01666
H	-3.41233	-0.77023	-1.15278
H	-1.45216	0.89672	1.40001
H	-0.96322	-3.82785	0.83560
H	-4.91187	0.40882	0.26774
H	-7.75533	0.05670	-2.90918
H	-6.02044	-0.20841	-2.58716

H	-7.34387	-2.30090	-2.74004
H	-9.31973	-1.09074	-1.16322
H	-7.96622	-1.13321	0.84203
H	-7.01640	-3.91155	-0.00454
H	-4.78321	-0.38543	3.20138
H	-3.66610	-4.45527	2.92235
H	-8.86659	-2.67591	1.01918
H	-10.02036	-3.31699	-1.03105
H	10.76933	-0.25345	0.34423
H	0.19427	0.93581	3.20646
H	0.24349	-0.55651	4.18107
H	1.48159	-0.26821	2.95483
Na	5.86349	2.10835	4.02463
Na	-1.43197	4.60074	2.66270
Na	-8.24853	4.49065	-0.54542

XGAX

O	9.82725	0.10236	0.31938
C	9.64031	1.11891	-0.66116
C	8.15652	1.27254	-0.95001
O	7.67317	0.10693	-1.65188
C	7.28934	1.40656	0.32145
O	6.22904	2.34083	0.02450
C	6.73790	-0.00119	0.49479
C	6.52618	-0.38706	-0.96555
N	6.37860	-1.82076	-1.20079
C	5.46532	-2.25344	-2.16969
O	4.85326	-1.48380	-2.89332
N	5.33661	-3.63312	-2.21485
C	5.98661	-4.55340	-1.38845
O	5.78400	-5.75453	-1.46039
C	6.93953	-3.90606	-0.47357
N	7.11168	-2.63217	-0.40619
P	5.38040	2.96748	1.28094
O	6.26958	3.84529	2.14004
O	4.64933	1.87896	2.05397
O	4.33167	3.90879	0.46680
C	4.00672	3.86654	-0.93202
C	2.71850	3.11148	-1.22459
O	2.96119	1.69195	-1.25909
C	1.59700	3.34014	-0.18161
O	0.37276	3.52442	-0.91403
C	1.58068	2.02196	0.58473
C	1.89363	1.04970	-0.54961
N	2.32383	-0.26196	-0.13998
C	3.21461	-0.56009	0.87972
N	3.43181	-1.84537	1.01610
C	2.65075	-2.44210	0.02692
C	2.41747	-3.82105	-0.27363
O	2.87246	-4.83461	0.25694
N	1.53372	-3.94381	-1.37528
C	0.84664	-2.90508	-1.97228
N	-0.03487	-3.23745	-2.95952
N	1.04100	-1.63746	-1.66892
C	1.96596	-1.46375	-0.69697
P	-0.96029	4.09445	-0.14141
O	-0.73429	5.50836	0.35492
O	-1.46928	3.12155	0.90980
O	-1.94296	4.17701	-1.43993
C	-2.07775	3.12459	-2.40787
C	-2.86299	1.90790	-1.93718
O	-2.02503	0.99807	-1.22368
C	-4.07018	2.21494	-1.01975
O	-5.24122	2.13006	-1.84691
C	-3.95859	1.16960	0.10989
C	-2.89851	0.20353	-0.41929
N	-2.09743	-0.48425	0.56658
C	-1.27995	0.07189	1.53762
N	-0.51480	-0.80680	2.15192
C	-0.85094	-2.01193	1.54911
C	-0.37761	-3.31411	1.73650
N	0.60679	-3.63190	2.62414
N	-0.90497	-4.28839	0.96324
C	-1.81722	-3.97065	0.03431
N	-2.31448	-2.76572	-0.26618
C	-1.80860	-1.82879	0.54660
P	-6.74103	2.28448	-1.19393
O	-7.62978	2.87652	-2.26653
O	-6.69371	2.97659	0.14957
O	-7.13625	0.71026	-0.91880
C	-7.06069	-0.18467	-2.03802

C	-7.32208	-1.60390	-1.57902
O	-6.24181	-2.04567	-0.73286
C	-8.62356	-1.78574	-0.77161
O	-9.20304	-3.02358	-1.18925
C	-8.11529	-1.85148	0.66833
C	-6.79082	-2.58251	0.46831
N	-5.82522	-2.41152	1.54842
C	-4.98658	-3.48335	1.88607
O	-5.02024	-4.57175	1.33903
N	-4.12139	-3.19557	2.93162
C	-3.94164	-1.95528	3.53350
O	-3.11036	-1.76227	4.40482
C	-4.86887	-0.93995	3.01021
N	-5.72993	-1.17058	2.07940
H	10.02046	2.08939	-0.30708
H	10.15701	0.86894	-1.59964
H	8.01528	2.15663	-1.58323
H	7.86983	1.76160	1.17743
H	7.50994	-0.63504	0.93266
H	5.61907	0.07751	-1.35939
H	7.53268	-4.53368	0.18289
H	4.66368	-3.99560	-2.88367
H	5.82502	-0.03017	1.08586
H	3.86782	4.90948	-1.23519
H	4.82877	3.43309	-1.50687
H	2.35986	3.43622	-2.21012
H	1.78829	4.21182	0.44950
H	2.40063	2.01393	1.30867
H	1.02490	0.90699	-1.20118
H	3.67833	0.23581	1.45175
H	1.30167	-4.89914	-1.62547
H	-0.68608	-2.49987	-3.19897
H	-0.44813	-4.16138	-2.93855
H	0.62399	1.83780	1.06787
H	-2.62610	3.57725	-3.23882
H	-1.08987	2.81087	-2.75999
H	-3.24953	1.40299	-2.83589
H	-4.00998	3.22108	-0.60575
H	-3.58869	1.66131	1.01180
H	-3.36299	-0.58393	-1.02656
H	-1.30033	1.14251	1.69731
H	-2.18886	-4.80246	-0.56046
H	1.18840	-2.85780	2.92370
H	1.12388	-4.47646	2.40329
H	-4.90156	0.66154	0.31709
H	-7.80922	0.09361	-2.79076
H	-6.06384	-0.12763	-2.48997
H	-7.36373	-2.24213	-2.47095
H	-9.31904	-0.95302	-0.93125
H	-7.92667	-0.84329	1.04144
H	-6.94388	-3.65828	0.36541
H	-4.81747	0.06596	3.41237
H	-3.49373	-3.94703	3.20241
H	-8.79533	-2.38426	1.33953
H	-9.98716	-3.17130	-0.63637
H	10.77671	0.05429	0.50740
Na	5.83235	2.46970	4.09848
Na	-1.42523	4.84317	2.60890
Na	-8.17743	4.73449	-0.73065

XGCX

O	9.81689	0.04859	0.34101
C	9.62501	1.04426	-0.65982
C	8.14063	1.18347	-0.95310
O	7.66500	0.00181	-1.63343
C	7.27168	1.33624	0.31506
O	6.20630	2.25849	0.00133
C	6.72723	-0.07141	0.51333
C	6.51818	-0.48286	-0.94024
N	6.37151	-1.91841	-1.15101
C	5.45541	-2.37816	-2.10352
O	4.82050	-1.63784	-2.83671
N	5.34685	-3.76036	-2.13362
C	6.00380	-4.66318	-1.29747
O	5.80377	-5.86615	-1.34225
C	6.96895	-3.99397	-0.41242
N	7.12835	-2.71675	-0.36229
P	5.34430	2.89620	1.24350
O	6.22092	3.79557	2.09317
O	4.61767	1.81414	2.02942
O	4.29244	3.81477	0.40745

C	-1.79385	-1.74256	0.56760
P	-6.68439	2.37346	-1.23048
O	-7.56347	2.94816	-2.32049
O	-6.62787	3.10255	0.09289
O	-7.10387	0.81396	-0.91232
C	-7.06675	-0.10605	-2.01332
C	-7.34487	-1.51104	-1.51940
O	-6.25679	-1.95591	-0.68505
C	-8.63077	-1.65195	-0.68157
O	-9.22339	-2.90300	-1.03646
C	-8.09431	-1.66140	0.74999
C	-6.78515	-2.42010	0.55566
N	-5.78768	-2.21019	1.60183
C	-4.93589	-3.27304	1.94062
O	-4.94810	-4.35696	1.38267
N	-4.07995	-2.98638	2.99705
C	-3.89944	-1.74053	3.58489
O	-3.05804	-1.51890	4.44054
C	-4.83847	-0.73670	3.05749
N	-5.70336	-0.96998	2.13167
H	10.09941	2.04075	-0.32221
H	10.22645	0.78782	-1.58430
H	8.10316	2.10539	-1.61423
H	7.93888	1.77566	1.15755
H	7.53329	-0.61589	0.96386
H	5.67559	0.08137	-1.35970
H	4.67245	-4.02194	-2.80223
H	5.85874	0.02311	1.08986
H	3.94748	4.88679	-1.35998
H	4.89085	3.39120	-1.58271
H	2.41058	3.40211	-2.25128
H	1.88688	4.24203	0.40451
H	2.45669	2.05221	1.29975
H	1.07181	0.91783	-1.19220
H	3.72251	0.26815	1.46728
H	1.30306	-4.88146	-1.54628
H	-0.70233	-2.47893	-3.08361
H	-0.62062	-4.09932	-2.62492
H	0.67802	1.89339	1.05641
H	-2.54610	3.64607	-3.25438
H	-1.01805	2.86722	-2.76988
H	-3.18217	1.47423	-2.85100
H	-3.97135	3.32230	-0.66395
H	-3.50293	1.80358	0.98735
H	-3.34578	-0.48356	-1.01459
H	-1.27284	1.23479	1.70691
H	-0.69435	-5.13297	1.07638
H	-3.07112	-4.70602	-1.43131
H	-2.19047	-5.83964	-0.53300
H	-4.84757	0.80607	0.34948
H	-7.82371	0.17142	-2.75774
H	-6.07739	-0.07811	-2.48448
H	-7.41512	-2.16661	-2.39667
H	-9.32525	-0.82253	-0.86155
H	-7.88731	-0.64022	1.07356
H	-6.95493	-3.49731	0.51060
H	-3.45159	-3.73649	3.26974
H	-8.76712	-2.15496	1.45741
H	-9.99187	-3.02844	-0.45679
H	10.81947	0.01777	0.54887
H	7.54581	-4.52601	0.26473
H	-4.79059	0.27022	3.45789
Na	5.72749	2.59658	4.07397
Na	-1.28799	4.97255	2.57818
Na	-8.07978	4.85984	-0.84511

XGTX

O	9.83258	0.00197	0.17153
C	9.62219	0.98872	-0.83467
C	8.13186	1.13063	-1.09475
O	7.63754	-0.05697	-1.75079
C	7.29613	1.29909	0.19371
O	6.22787	2.22582	-0.09632
C	6.74925	-0.10427	0.41691
C	6.50191	-0.52552	-1.02788
N	6.33396	-1.96010	-1.22634
C	5.38703	-2.41667	-2.15395
O	4.73121	-1.66946	-2.86143
N	5.27651	-3.79724	-2.18352
C	5.94598	-4.69945	-1.35677
O	5.74621	-5.90239	-1.40072

C	6.92211	-4.03113	-0.47850
N	7.09447	-2.75646	-0.44117
P	5.39834	2.86989	1.16492
O	6.30236	3.75408	2.00125
O	4.67217	1.79503	1.96134
O	4.34247	3.80503	0.35222
C	3.98843	3.72228	-1.03746
C	2.70283	2.94981	-1.28805
O	2.94929	1.53027	-1.27571
C	1.58290	3.21069	-0.24877
O	0.36335	3.37664	-0.99520
C	1.55442	1.91328	0.54608
C	1.87403	0.91040	-0.56031
N	2.29601	-0.39171	-0.10398
C	3.22507	-0.66688	0.88704
N	3.43675	-1.95000	1.05508
C	2.60858	-2.56932	0.12424
C	2.40313	-3.95446	-0.17255
O	2.86929	-4.95952	0.36098
N	1.49943	-4.09021	-1.26330
C	0.79029	-3.07441	-1.86570
N	-0.09503	-3.42720	-2.84407
N	0.97331	-1.80640	-1.57336
C	1.89400	-1.61523	-0.60132
P	-0.97079	4.00177	-0.27439
O	-0.74140	5.44201	0.13593
O	-1.49484	3.10096	0.83312
O	-1.94314	4.00596	-1.58258
C	-2.06270	2.90814	-2.50202
C	-2.85275	1.71061	-1.98895
O	-2.02483	0.82356	-1.24022
C	-4.05922	2.05167	-1.08637
O	-5.22615	1.98175	-1.91857
C	-3.97459	1.02316	0.06673
C	-2.91408	0.04148	-0.43177
N	-2.09506	-0.64018	0.55932
C	-1.94566	-2.02249	0.44349
O	-2.51735	-2.71218	-0.39411
N	-1.11333	-2.58002	1.39614
O	-0.29390	-1.92438	2.32637
C	0.48482	-2.54442	3.04620
C	-0.48212	-0.48427	2.34493
C	0.33610	0.31968	3.31489
C	-1.34506	0.08719	1.46953
P	-6.72908	2.14021	-1.27354
O	-7.61054	2.73063	-2.35289
O	-6.68837	2.83619	0.06814
O	-7.12545	0.56672	-0.99651
C	-7.01927	-0.33486	-2.10769
C	-7.29587	-1.75020	-1.64823
O	-6.24241	-2.18786	-0.76563
C	-8.62472	-1.92658	-0.88402
O	-9.19702	-3.15961	-1.32589
C	-8.16390	-2.00102	0.56934
C	-6.82872	-2.72636	0.41358
N	-5.91280	-2.54254	1.53407
C	-5.16698	-3.62966	2.00784
O	-5.28161	-4.76929	1.59272
N	-4.26933	-3.27968	3.00773
C	-4.06005	-2.00604	3.52888
O	-3.22369	-1.77590	4.38921
C	-4.92735	-1.00013	2.90059
N	-5.77717	-1.27018	1.97025
H	10.00750	1.96993	-0.51779
H	10.11904	0.71176	-1.77627
H	7.97269	1.99560	-1.74987
H	7.89830	1.67477	1.02555
H	7.53149	-0.72816	0.85109
H	5.59065	-0.06063	-1.41250
H	7.53542	-4.64536	0.17215
H	4.58201	-4.17176	-2.82311
H	5.85107	-0.11708	1.03081
H	3.83216	4.75552	-1.36445
H	4.80344	3.28336	-1.61812
H	2.33537	3.23823	-2.28160
H	1.77497	4.09897	0.35853
H	2.36534	1.91480	1.28007
H	1.01026	0.74930	-1.21389
H	3.71628	0.14376	1.41419
H	1.30308	-5.05067	-1.52546
H	-0.76691	-2.70205	-3.06531

H	0.02800	-0.35650	2.88395
H	0.29045	-4.01647	2.64950
H	0.77392	-2.60576	3.52179
H	-5.00624	0.49911	0.27905
H	-7.88540	0.19299	-2.84110
H	-6.15877	-0.13924	-2.53632
H	-7.58225	-2.17138	-2.62173
H	-9.46374	-0.83965	-1.02174
H	-8.08436	-0.92948	0.95805
H	-7.25106	-3.75272	0.13532
H	-4.84333	-0.21950	3.20568
H	-3.93474	-4.34791	3.09765
H	-9.04092	-2.43312	1.16379
H	-10.26965	-3.02814	-0.85191
H	10.32581	-1.57121	0.91011
Na	7.04494	4.62923	3.06458
Na	-1.15821	4.60766	2.74652
Na	-8.12337	4.73254	-0.63376

XXGX cation

O	9.51192	-1.20131	0.58484
C	9.82288	-0.27941	-0.45423
C	8.54906	0.38954	-0.94783
O	7.76505	-0.52244	-1.74075
C	7.63425	0.88196	0.18581
O	7.08425	2.14773	-0.22441
C	6.58227	-0.22586	0.28735
C	6.48490	-0.72243	-1.15476
N	6.13369	-2.14201	-1.29811
C	5.23077	-2.52495	-2.29850
O	4.62428	-1.73989	-3.00892
N	5.04424	-3.89873	-2.37701
C	5.69603	-4.87136	-1.62286
O	5.48389	-6.06535	-1.76043
C	6.64766	-4.27912	-0.66919
N	6.85780	-3.01285	-0.55179
P	6.24273	3.05559	0.86296
O	6.58512	4.50689	0.60266
O	6.41688	2.52538	2.26808
O	4.68877	2.75261	0.41661
C	4.28615	3.23710	-0.87244
C	2.88096	2.76184	-1.17885
O	2.89467	1.33176	-1.37443
C	1.84818	3.04292	-0.06201
O	0.60847	3.36777	-0.71852
C	1.75195	1.70015	0.64131
C	1.88647	0.75711	-0.55209
N	2.26282	-0.60582	-0.18511
C	1.68017	-1.68284	-0.86138
O	0.85659	-1.53441	-1.75048
N	2.13282	-2.91043	-0.40208
C	3.00859	-3.12256	0.66991
O	3.36502	-4.24081	1.00404
C	3.45773	-1.86674	1.28812
N	3.10667	-0.70495	0.86306
P	-0.67068	3.92101	0.14803
O	-0.36302	5.26050	0.78034
O	-1.19943	2.86906	1.11397
O	-1.69037	4.16988	-1.09833
C	-1.86709	3.25419	-2.19088
C	-2.75535	2.05666	-1.88783
O	-2.01349	1.01614	-1.23290
C	-3.98587	2.35627	-0.99867
O	-5.13278	2.30985	-1.85550
C	-3.93187	1.27133	0.09887
C	-2.95540	0.25696	-0.49130
N	-2.18868	-0.53618	0.47023
C	-1.34993	-0.06201	1.43104
N	-0.64184	-1.02666	2.04766
C	-1.01893	-2.16852	1.44058
C	-0.64031	-3.56305	1.64978
O	0.11311	-4.03246	2.47812
N	-1.32001	-4.41023	0.73558
C	-2.26254	-4.03379	-0.18149
N	-2.84700	-4.94505	-0.93725
N	-2.63848	-2.74208	-0.36017
C	-2.01420	-1.90590	0.43610
P	-6.63825	2.55450	-1.23184
O	-7.46594	3.21049	-2.31453
O	-6.56938	3.22647	0.12006
O	-7.12981	1.00428	-0.98515

C	-7.13061	0.13920	-2.13094
C	-7.48785	-1.26906	-1.70691
O	-6.43006	-1.80705	-0.88581
C	-8.79198	-1.38115	-0.88861
O	-9.46195	-2.56061	-1.33823
C	-8.27661	-1.52826	0.54047
C	-6.99960	-2.33300	0.30651
N	-6.02322	-2.23103	1.39039
C	-5.29730	-3.36973	1.76548
O	-5.38490	-4.44909	1.20590
N	-4.45506	-3.15962	2.85279
C	-4.15334	-1.92867	3.42480
O	-3.29222	-1.77855	4.27780
C	-5.00076	-0.85066	2.88956
N	-5.85347	-1.00793	1.93679
H	10.49894	0.51148	-0.09291
H	10.30620	-0.78125	-1.30554
H	8.83603	1.23427	-1.58434
H	8.17496	1.01095	1.12483
H	6.97423	-1.02166	0.92405
H	5.72096	-0.17762	-1.71283
H	7.23062	-4.94562	-0.04231
H	4.37871	-4.21125	-3.07790
H	5.62295	0.13056	0.66623
H	4.31381	4.33306	-0.88309
H	4.96597	2.85583	-1.64428
H	2.55170	3.24784	-2.10507
H	2.15033	3.86602	0.59171
H	2.60792	1.57874	1.30540
H	0.94472	0.67912	-1.09963
H	4.13829	-1.91742	2.13071
H	1.77424	-3.73035	-0.88344
H	0.81732	1.57775	1.18528
H	-2.35836	3.83911	-2.97361
H	-0.89499	2.91193	-2.55839
H	-3.12044	1.66949	-2.84940
H	-3.92306	3.34664	-0.54755
H	-3.50180	1.70911	1.00286
H	-3.47343	-0.47054	-1.12768
H	-1.26397	1.01021	1.59966
H	-1.09716	-5.39684	0.83992
H	-3.56853	-4.64651	-1.58413
H	-2.64595	-5.93558	-0.86410
H	-4.90623	0.83147	0.31473
H	-7.86466	0.49304	-2.86551
H	-6.13668	0.13742	-2.59317
H	-7.58242	-1.87979	-2.61356
H	-9.42592	-0.49558	-1.01548
H	-8.02301	-0.54658	0.94456
H	-7.21307	-3.39691	0.18988
H	-4.88144	0.14733	3.29751
H	-3.92794	-3.97123	3.16282
H	-8.98229	-2.03954	1.20173
H	-10.24840	-2.67134	-0.78012
H	10.34485	-1.60708	0.86895
Na	7.24321	4.73080	2.97741
Na	-0.94432	4.40261	3.00030
Na	-7.97166	5.06099	-0.74779

XXGX

O	9.52402	-1.16242	0.62998
C	9.82895	-0.22479	-0.39683
C	8.54802	0.42776	-0.89354
O	7.78254	-0.49413	-1.69288
C	7.62123	0.90103	0.23897
O	7.05569	2.16178	-0.16459
C	6.58405	-0.22192	0.32834
C	6.49833	-0.70511	-1.11858
N	6.15288	-2.12280	-1.28209
C	5.25617	-2.49675	-2.29211
O	4.65143	-1.70547	-2.99686
N	5.07815	-3.87061	-2.38993
C	5.72681	-4.85025	-1.64143
O	5.52562	-6.04346	-1.80023
C	6.65914	-4.26542	-0.66458
N	6.86627	-3.00001	-0.53283
P	6.20160	3.05288	0.92791
O	6.55060	4.50812	0.69828
O	6.35797	2.49852	2.32584
O	4.65400	2.76137	0.45523
C	4.27541	3.25515	-0.83781

C	-8.86607	-1.68621	-0.93490
O	-9.53285	-2.84734	-1.43418
C	-8.36774	-1.88422	0.49335
C	-7.07063	-2.65408	0.24761
N	-6.12104	-2.58220	1.35568
C	-5.42202	-3.73118	1.74930
O	-5.59917	-4.83623	1.27153
N	-4.48345	-3.48032	2.74412
C	-4.19845	-2.24839	3.32359
O	-3.27858	-2.09117	4.11550
C	-5.06375	-1.17783	2.81522
N	-5.93123	-1.35207	1.87751
H	10.40873	0.57529	-0.07764
H	10.27918	-0.71905	-1.29692
H	8.74123	1.24160	-1.59628
H	8.06238	0.99076	1.10942
H	6.92194	-1.07425	0.88455
H	5.68441	-0.23422	-1.76219
H	7.25814	-4.99062	-0.12140
H	4.41116	-4.28080	-3.16816
H	5.54064	0.04153	0.62087
H	4.13859	4.21386	-0.92418
H	4.84958	2.75927	-1.67637
H	2.43300	3.06330	-2.18105
H	1.97595	3.68209	0.51732
H	2.43130	1.40051	1.24396
H	0.88223	0.47277	-1.23017
H	4.08229	-2.08715	2.05506
H	1.73129	-3.92726	-0.94530
H	0.64830	1.38794	1.04116
H	-2.52625	3.48452	-3.09491
H	-1.03719	2.60948	-2.65804
H	-3.23117	1.29983	-2.88996
H	-4.00786	2.97859	-0.55168
H	-3.73019	1.29838	0.96727
H	-3.48377	-0.81811	-1.20997
H	-1.17797	-3.90385	0.99530
H	-5.03658	0.39468	0.14199
H	-7.96419	0.20166	-2.90198
H	-6.22913	-0.12079	-2.63366
H	-7.62470	-2.16683	-2.64090
H	-9.49747	-0.79580	-1.03784
H	-8.13538	-0.91670	0.94303
H	-7.26065	-3.71509	0.07553
H	-3.92948	-4.27960	3.03892
H	-9.07396	-2.43377	1.12235
H	-10.33218	-2.96968	-0.89721
H	-0.02219	0.94454	3.21928
H	0.13381	-0.58701	4.15661
H	1.30642	-0.21210	2.90526
H	-1.52889	0.92831	1.28580
H	-4.94078	-0.17539	3.21053
H	10.31314	-1.54576	0.88047
Na	7.04034	4.66228	2.97555
Na	-1.10128	4.28926	2.85968
Na	-8.03234	4.80161	-0.73549

XXTX

O	9.46417	-1.21844	0.56122
C	9.75274	-0.28953	-0.47835
C	8.46191	0.34210	-0.97675
O	7.70400	-0.59743	-1.76262
C	7.53453	0.81704	0.15445
O	6.95488	2.06799	-0.25841
C	6.51006	-0.31690	0.25963
C	6.42349	-0.81472	-1.18197
N	6.09220	-2.23655	-1.33342
C	5.18764	-2.62937	-2.32955
O	4.55769	-1.85132	-3.02680
N	5.03767	-4.00698	-2.42543
C	5.71457	-4.97375	-1.68435
O	5.54276	-6.17081	-1.84758
C	6.63303	-4.36863	-0.70668
N	6.81714	-3.09914	-0.57926
P	6.08729	2.95480	0.82678
O	6.40641	4.41354	0.57784
O	6.25942	2.42064	2.23064
O	4.54418	2.62596	0.36305
C	4.15748	3.08943	-0.93890
C	2.77017	2.58017	-1.26748
O	2.82020	1.14747	-1.43637

C	1.70492	2.86267	-0.17999
O	0.48216	3.18716	-0.87157
C	1.58473	1.52454	0.52392
C	1.78680	0.56942	-0.64992
N	2.16069	-0.78326	-0.24413
C	1.60656	-1.88429	-0.91464
O	0.79382	-1.79109	-1.81763
N	2.07149	-3.10556	-0.44639
C	2.96719	-3.30853	0.59959
O	3.37135	-4.41630	0.91634
C	3.37188	-2.04317	1.23070
N	3.00291	-0.88132	0.81077
P	-0.78289	3.82405	-0.03812
O	-0.45609	5.22053	0.44973
O	-1.28406	2.87752	1.04171
O	-1.83366	3.96110	-1.27522
C	-2.02784	2.98008	-2.30645
C	-2.88957	1.78639	-1.91685
O	-2.11762	0.79110	-1.24764
C	-4.09653	2.10063	-1.00048
O	-5.25934	2.08981	-1.84128
C	-4.03743	1.00470	0.08950
C	-3.04514	-0.00104	-0.49353
N	-2.25191	-0.78692	0.44205
C	-2.13881	-2.16084	0.21923
O	-2.76354	-2.77161	-0.63954
N	-1.28135	-2.80452	1.09129
C	-0.47319	-2.23715	2.08190
O	0.29299	-2.94367	2.73532
C	-0.60219	-0.79087	2.19963
C	0.25522	-0.08439	3.21013
C	-1.45985	-0.14023	1.37686
P	-6.76424	2.25632	-1.20100
O	-7.62283	2.91085	-2.26143
O	-6.71856	2.89427	0.16877
O	-7.19895	0.68194	-0.99455
C	-7.13737	-0.15977	-2.15556
C	-7.46811	-1.58698	-1.77608
O	-6.42718	-2.11618	-0.92987
C	-8.79896	-1.75700	-1.01263
O	-9.42553	-2.93315	-1.52944
C	-8.33305	-1.94558	0.42856
C	-7.02758	-2.71011	0.21433
N	-6.09999	-2.63670	1.33799
C	-5.38409	-3.77704	1.72359
O	-5.53531	-4.87871	1.22624
N	-4.47135	-3.52856	2.74031
C	-4.21843	-2.30245	3.34897
O	-3.36837	-2.16055	4.21492
C	-5.05809	-1.22728	2.80241
N	-5.92147	-1.40327	1.86210
H	10.40501	0.52062	-0.11605
H	10.25306	-0.77899	-1.32706
H	8.72616	1.19053	-1.61835
H	8.07159	0.96108	1.09346
H	6.92423	-1.10267	0.89480
H	5.65500	-0.27694	-1.74100
H	7.21849	-5.02710	-0.07365
H	4.38084	-4.32728	-3.13103
H	5.54222	0.01375	0.64081
H	4.16104	4.18564	-0.95979
H	4.86155	2.71607	-1.69250
H	2.45241	3.04245	-2.20986
H	1.99221	3.68758	0.47852
H	2.40301	1.41135	1.23604
H	0.86894	0.46571	-1.23312
H	4.04788	-2.08013	2.07775
H	1.71380	-3.92527	-0.92831
H	0.62273	1.40294	1.01279
H	-2.54286	3.51595	-3.10888
H	-1.06015	2.62766	-2.67656
H	-3.28643	1.35906	-2.85053
H	-4.00706	3.08762	-0.54569
H	-3.63852	1.44300	1.00745
H	-3.55761	-0.71324	-1.14489
H	-1.19658	-3.80586	0.95173
H	-5.00791	0.54788	0.28842
H	-7.85705	0.18747	-2.90771
H	-6.12983	-0.12310	-2.58524
H	-7.51205	-2.17688	-2.70056
H	-9.44819	-0.88133	-1.13184

H	-8.11609	-0.97433	0.87759
H	-7.21299	-3.77183	0.04143
H	-3.92259	-4.32725	3.04490
H	-9.05029	-2.49669	1.04386
H	-10.22920	-3.08132	-1.00548
H	0.04523	0.98983	3.21035
H	0.07409	-0.48265	4.21619
H	1.31913	-0.23303	2.98651
H	-1.54550	0.94359	1.37190
H	-4.93983	-0.22437	3.19788
H	10.30779	-1.59611	0.85245
Na	7.05464	4.63375	2.95489
Na	-0.95701	4.57613	2.75693
Na	-8.17074	4.70629	-0.65447

XTAX

O	9.79605	-0.01733	-0.02230
C	9.58065	1.04512	-0.94705
C	8.08883	1.20045	-1.18546
O	7.59979	0.05877	-1.92602
C	7.26367	1.26544	0.12219
O	6.20656	2.23406	-0.06660
C	6.69263	-0.13913	0.22104
C	6.44632	-0.43374	-1.25496
N	6.23021	-1.84381	-1.56269
C	5.29246	-2.19735	-2.54456
O	4.64781	-1.38957	-3.19074
N	5.15138	-3.57024	-2.69727
C	5.83332	-4.56438	-1.99612
O	5.66186	-5.75404	-2.20529
C	6.75116	-3.99869	-0.99644
N	6.93853	-2.73500	-0.82595
P	5.42697	2.78478	1.26923
O	6.36418	3.60793	2.13093
O	4.73146	1.65297	2.01508
O	4.33536	3.77521	0.57844
C	3.93015	3.82278	-0.79819
C	2.64194	3.06314	-1.07433
O	2.90649	1.65463	-1.18974
C	1.54597	3.21515	0.01333
O	0.30910	3.46090	-0.67611
C	1.53466	1.84287	0.68117
C	1.83932	0.96147	-0.52914
N	2.28291	-0.39862	-0.26144
C	1.75342	-1.44208	-1.03056
O	0.92649	-1.28296	-1.91943
N	2.23649	-2.68843	-0.68496
C	3.13048	-3.01210	0.34181
O	3.44318	-4.18701	0.53707
C	3.63779	-1.86577	1.08091
C	4.64391	-2.10839	2.16926
C	3.20802	-0.63048	0.73528
P	-1.01165	3.95791	0.16482
O	-0.76872	5.31598	0.79175
O	-1.50992	2.89116	1.12644
O	-2.01108	4.16403	-1.10749
C	-2.12639	3.23299	-2.19652
C	-2.90096	1.96174	-1.87896
O	-2.07200	0.99716	-1.22922
C	-4.14013	2.16276	-0.97714
O	-5.28861	2.10488	-1.83654
C	-4.02893	1.03690	0.07401
C	-2.95636	0.12549	-0.52036
N	-2.16672	-0.65549	0.40298
C	-1.34960	-0.18886	1.41445
N	-0.58613	-1.12032	1.94201
C	-0.89838	-2.26704	1.22557
C	-0.48564	-3.61076	1.31994
N	0.40575	-4.04057	2.25529
N	-1.02577	-4.50876	0.47267
C	-1.94155	-4.09007	-0.42266
N	-2.43086	-2.86193	-0.60435
C	-1.88319	-1.99737	0.26577
P	-6.79865	2.27185	-1.20841
O	-7.65657	2.90630	-2.28173
O	-6.76306	2.92972	0.15252
O	-7.22722	0.69948	-0.98095
C	-7.18027	-0.15604	-2.13284
C	-7.44273	-1.58732	-1.71551
O	-6.34372	-2.06288	-0.91306
C	-8.72384	-1.78282	-0.87805

O	-9.33372	-2.99511	-1.32587
C	-8.17529	-1.91142	0.54366
C	-6.87232	-2.65650	0.27066
N	-5.87202	-2.57235	1.32723
C	-5.04899	-3.68443	1.56509
O	-5.12047	-4.72700	0.93858
N	-4.15065	-3.49807	2.60709
C	-3.93470	-2.31191	3.29558
O	-3.07587	-2.19108	4.15391
C	-4.87221	-1.24952	2.89042
N	-5.75639	-1.38520	1.96315
H	9.96470	1.99943	-0.55561
H	10.07392	0.84413	-1.90951
H	7.91721	2.11069	-1.77239
H	7.88083	1.55168	0.97789
H	7.45625	-0.81522	0.60734
H	5.55032	0.08637	-1.60470
H	7.32776	-4.67985	-0.37984
H	4.48163	-3.86604	-3.40137
H	5.79382	-0.17709	0.82820
H	3.75761	4.88092	-1.02028
H	4.72529	3.44615	-1.44683
H	2.24079	3.43255	-2.02767
H	1.75698	4.03488	0.70509
H	2.34879	1.79968	1.40886
H	0.96508	0.88643	-1.17877
H	3.61255	0.25343	1.22025
H	1.85047	-3.46409	-1.21277
H	0.57761	1.62413	1.14999
H	-2.67742	3.77411	-2.97107
H	-1.13295	2.97675	-2.57723
H	-3.24820	1.54478	-2.83685
H	-4.12138	3.13609	-0.48728
H	-3.66972	1.46086	1.01429
H	-3.40860	-0.59843	-1.21029
H	-1.36639	0.86356	1.66948
H	-2.33270	-4.86328	-1.08066
H	0.96960	-3.33235	2.70809
H	0.87729	-4.91574	2.06309
H	-4.97060	0.50858	0.23231
H	-7.94156	0.15471	-2.85921
H	-6.19205	-0.09150	-2.60244
H	-7.51515	-2.19643	-2.62566
H	-9.41111	-0.93503	-0.98498
H	-7.95728	-0.92195	0.94966
H	-7.05581	-3.72025	0.10892
H	-3.52973	-4.27915	2.79794
H	-8.84462	-2.45862	1.21405
H	-10.10621	-3.15101	-0.75906
H	10.74914	-0.06374	0.14691
H	4.90402	-1.16801	2.66516
H	4.24599	-2.80846	2.91437
H	5.55980	-2.55410	1.76008
H	-4.80010	-0.28504	3.38125
Na	5.95364	2.19684	4.05623
Na	-1.34075	4.42233	3.00448
Na	-8.20664	4.72981	-0.70407

XTCX

O	9.78304	-0.08264	-0.00766
C	9.56128	0.97076	-0.94131
C	8.06845	1.11536	-1.18040
O	7.58612	-0.03564	-1.90934
C	7.24384	1.18765	0.12678
O	6.18397	2.15027	-0.06719
C	6.67737	-0.21984	0.23865
C	6.43248	-0.52540	-1.23472
N	6.22031	-1.93433	-1.54322
C	5.26832	-2.29446	-2.51090
O	4.60025	-1.49222	-3.13960
N	5.15455	-3.66902	-2.67873
C	5.85325	-4.66042	-1.98703
O	5.71489	-5.84951	-2.22068
C	6.73495	-4.08776	-0.95913
N	6.90946	-2.82257	-0.78547
P	5.38493	2.69204	1.26113
O	6.31027	3.50878	2.14151
O	4.67457	1.55844	1.98969
O	4.31131	3.69225	0.55549
C	3.90559	3.70833	-0.82169
C	2.62827	2.92953	-1.08898

H	1.12811	3.70254	0.93941
H	4.77819	-0.76149	0.58063
H	7.66643	0.82240	-3.78013
H	6.06860	0.59533	-3.02718
H	7.54391	2.67093	-2.46988
H	9.29853	0.67571	-1.28822
H	8.04055	0.65113	0.73040
H	7.25082	3.53526	0.08753
H	3.90458	4.16376	3.00817
H	9.03663	2.11738	1.06533
H	10.43905	2.63009	-0.92620
H	-10.76319	0.36288	0.05665
H	-7.17643	4.96013	-0.16143
H	4.94706	0.07768	3.31600
H	-0.16642	-1.08089	3.19541
H	-0.18097	0.39531	4.19566
H	-1.42993	0.15441	2.97097
H	-4.83757	1.23243	2.72212
H	-4.13904	2.83784	3.06236
H	-5.45071	2.68136	1.88717
Na	-6.02320	-2.21863	3.80177
Na	0.95946	-4.78321	2.75398
Na	7.87249	-3.66621	0.41668