

## The oxidation potential of adenine rich single strand oligonucleotides

– Electronic Supplementary Information –

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**TABLE S1.** Hydrogen model: sum of the Mulliken spin densities<sup>(a)</sup> [B97D/SV(P)] for the singly ionized hexamers.

	T <sub>3</sub> AT <sub>2</sub>	T <sub>2</sub> A <sub>2</sub> T <sub>2</sub>	T <sub>2</sub> A <sub>3</sub> T	TA <sub>4</sub> T
B <sup>(1)</sup>	0.10	0.05	0.02	0.00
B <sup>(2)</sup>	0.14	0.16	0.08	0.20
B <sup>(3)</sup>	0.21	0.41	0.32	0.33
B <sup>(4)</sup>	0.32	0.32	0.36	0.32
B <sup>(5)</sup>	0.09	0.02	0.21	0.15
B <sup>(6)</sup>	0.12	0.02	0.01	0.00

<sup>(a)</sup>The sum has been carried out only for the atoms belonging to each nucleobase B<sup>(i)</sup>, (i = 1, ... 6) without including ribose and phosphate atoms.

**TABLE S2.** Hydrogen model: sum of the Mulliken spin densities [B97D/6-31+G\*\*] for the singly ionized hexamers.

	T <sub>3</sub> AT <sub>2</sub>	T <sub>2</sub> A <sub>2</sub> T <sub>2</sub>	T <sub>2</sub> A <sub>3</sub> T	TA <sub>4</sub> T
B <sup>(1)</sup>	0.09	0.04	0.01	0.00
B <sup>(2)</sup>	0.12	0.16	0.07	0.19
B <sup>(3)</sup>	0.23	0.43	0.32	0.34
B <sup>(4)</sup>	0.33	0.33	0.36	0.32
B <sup>(5)</sup>	0.10	0.03	0.22	0.15
B <sup>(6)</sup>	0.11	0.01	0.01	0.00

**TABLE S3.** Hydrogen model: sum of the Mulliken spin densities [M06-2X/SV(P)] for the singly ionized hexamers.

	T <sub>3</sub> AT <sub>2</sub>	T <sub>2</sub> A <sub>2</sub> T <sub>2</sub>	T <sub>2</sub> A <sub>3</sub> T	TA <sub>4</sub> T
B <sup>(1)</sup>	0.00	0.00	0.00	0.00
B <sup>(2)</sup>	0.00	0.03	0.00	0.08
B <sup>(3)</sup>	0.13	0.67	0.30	0.61
B <sup>(4)</sup>	0.85	0.30	0.63	0.30
B <sup>(5)</sup>	0.01	0.00	0.07	0.01
B <sup>(6)</sup>	0.00	0.00	0.00	0.00

**TABLE S4.** Hydrogen model: sum of the Mulliken spin densities [M06-2X/6-31+G\*\*] for the singly ionized hexamers.

	T <sub>3</sub> AT <sub>2</sub>	T <sub>2</sub> A <sub>2</sub> T <sub>2</sub>	T <sub>2</sub> A <sub>3</sub> T	TA <sub>4</sub> T
B <sup>(1)</sup>	0.00	0.00	0.00	0.00
B <sup>(2)</sup>	0.00	0.02	0.00	0.09
B <sup>(3)</sup>	0.09	0.65	0.24	0.60
B <sup>(4)</sup>	0.85	0.29	0.64	0.28
B <sup>(5)</sup>	0.03	0.02	0.11	0.02
B <sup>(6)</sup>	0.00	0.00	0.00	0.00

**TABLE S5.** Hydrogen model: sum of the Mulliken spin densities [B3LYP-D/SV(P)] for the singly ionized hexamers.

	T <sub>3</sub> AT <sub>2</sub>	T <sub>2</sub> A <sub>2</sub> T <sub>2</sub>	T <sub>2</sub> A <sub>3</sub> T	TA <sub>4</sub> T
B <sup>(1)</sup>	0.01	0.00	0.00	0.00
B <sup>(2)</sup>	0.10	0.09	0.03	0.16
B <sup>(3)</sup>	0.31	0.53	0.35	0.41
B <sup>(4)</sup>	0.53	0.37	0.47	0.35
B <sup>(5)</sup>	0.03	0.00	0.17	0.08
B <sup>(6)</sup>	0.01	0.00	0.00	0.00

**TABLE S6.** Hydrogen model: sum of the Mulliken spin densities [B3LYP-D/6-31+G\*\*] for the singly ionized hexamers.

	T <sub>3</sub> AT <sub>2</sub>	T <sub>2</sub> A <sub>2</sub> T <sub>2</sub>	T <sub>2</sub> A <sub>3</sub> T	TA <sub>4</sub> T
B <sup>(1)</sup>	0.01	0.00	0.00	0.00
B <sup>(2)</sup>	0.07	0.09	0.03	0.12
B <sup>(3)</sup>	0.32	0.53	0.34	0.42
B <sup>(4)</sup>	0.54	0.37	0.46	0.37
B <sup>(5)</sup>	0.04	0.01	0.17	0.09
B <sup>(6)</sup>	0.01	0.00	0.00	0.00

## Hydrogen model [B97D/SV(P)]: local base step and conformational parameters

### T<sub>3</sub>AT<sub>2</sub> neutral

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Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 T/T	-0.22	0.29	2.42	17.06	-12.68	31.98
2 T/T	0.29	0.70	2.58	11.17	-1.24	35.42
3 T/A	1.55	1.23	2.78	11.04	-1.14	43.39
4 A/T	0.30	0.28	2.63	10.82	-2.80	34.83
5 T/T	0.42	0.26	2.59	11.27	-4.24	37.77
~~~~~						
ave.	0.47	0.55	2.60	12.27	-4.42	36.68
s.d.	0.65	0.42	0.13	2.68	4.79	4.28

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Sugar conformational parameters:

Note: v0: C4'-O4'-C1'-C2';      v1: O4'-C1'-C2'-C3'  
 v2: C1'-C2'-C3'-C4';      v3: C2'-C3'-C4'-O4';      v4: C3'-C4'-O4'-C1';

tm: the amplitude of pucker  
 P: the phase angle of pseudorotation

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 T	-16.2	32.9	-36.1	27.7	-7.3	36.4	172.8	C2'-endo
2 T	-43.5	45.3	-30.1	5.7	23.4	45.8	131.0	C1'-exo
3 T	-43.3	45.4	-30.3	6.1	23.0	45.8	131.5	C1'-exo
4 A	-42.4	45.1	-30.9	7.2	21.7	45.3	133.0	C1'-exo
5 T	-42.4	45.8	-31.7	7.9	21.3	45.7	133.8	C1'-exo
6 T	-44.0	43.6	-26.8	2.1	25.9	45.0	126.6	C1'-exo

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### T<sub>3</sub>AT<sub>2</sub> singly ionized

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Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 T/T	-0.22	0.17	2.47	15.42	-15.44	32.93
2 T/T	0.43	0.28	2.70	7.90	-5.27	38.48
3 T/A	0.13	2.32	2.46	18.19	6.43	24.68
4 A/T	0.22	0.26	2.81	6.41	-1.93	32.60
5 T/T	-0.08	-0.25	2.53	11.41	-8.55	32.95
~~~~~						
ave.	0.10	0.56	2.59	11.87	-4.95	32.33
s.d.	0.26	1.01	0.15	4.96	8.09	4.93

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Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 T	-15.9	33.3	-36.9	28.8	-8.2	37.1	173.9	C2'-endo
2 T	-43.1	46.1	-31.5	7.6	22.0	46.1	133.1	C1'-exo
3 T	-40.1	21.3	3.7	-27.5	42.4	42.8	85.0	O4'-endo
4 A	-37.3	43.7	-33.6	13.3	14.7	43.0	141.4	C1'-exo
5 T	-42.7	46.0	-31.7	7.9	21.6	45.9	133.6	C1'-exo
6 T	-44.2	44.2	-27.2	2.5	25.7	45.3	126.9	C1'-exo

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**T<sub>2</sub>A<sub>2</sub>T<sub>2</sub> neutral**

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## Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	T/T	-0.14	0.05	2.49	14.92	-14.41	32.44
2	T/A	0.33	2.48	2.51	17.98	9.03	23.71
3	A/A	0.46	0.85	3.12	1.95	9.89	33.05
4	A/T	0.37	0.27	2.59	12.28	-2.83	35.93
5	T/T	0.27	0.24	2.67	9.69	-4.18	36.26

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ave.      0.26      0.78      2.68      11.37      -0.50      32.28
s.d.      0.23      1.00      0.26      6.09      10.14      5.08

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## Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	T	-16.7	33.4	-36.3	27.7	-7.0	36.7	172.2	C2'-endo
2	T	-40.1	21.2	3.8	-27.7	42.5	42.9	85.0	O4'-endo
3	A	-37.8	43.3	-32.6	11.7	16.1	42.9	139.6	C1'-exo
4	A	-39.9	44.8	-32.6	10.5	18.2	44.4	137.4	C1'-exo
5	T	-42.7	45.6	-31.3	7.4	21.8	45.7	133.2	C1'-exo
6	T	-44.6	41.0	-22.2	-3.1	29.6	44.4	120.0	C1'-exo

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**T<sub>2</sub>A<sub>2</sub>T<sub>2</sub> singly ionized**

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## Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	T/T	-0.11	0.00	2.53	13.52	-15.30	33.62
2	T/A	0.24	2.60	2.38	20.26	6.74	27.14
3	A/A	1.30	1.26	2.98	3.30	4.22	38.21
4	A/T	0.50	0.20	2.52	12.66	-0.51	36.11
5	T/T	0.29	0.10	2.64	9.97	-5.61	36.65

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~~~~~
ave.      0.44      0.83      2.61      11.94      -2.09      34.34
s.d.      0.53      1.11      0.23      6.14      8.77      4.35

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## Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	T	-16.8	33.8	-37.0	28.4	-7.3	37.3	172.5	C2'-endo
2	T	-40.4	22.1	2.7	-26.7	42.0	42.7	86.4	O4'-endo
3	A	-36.7	43.7	-34.1	13.9	14.1	43.0	142.4	C1'-exo
4	A	-40.5	45.3	-32.7	10.4	18.5	44.7	137.0	C1'-exo
5	T	-42.2	46.1	-32.5	9.0	20.5	45.9	135.0	C1'-exo
6	T	-44.2	42.5	-24.9	-0.0	27.4	44.7	123.8	C1'-exo

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**T<sub>2</sub>A<sub>3</sub>T neutral**

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*****
Local base step parameters
  step      Shift      Slide      Rise      Tilt      Roll      Twist
  1  T/T      -0.12      0.00      2.47      15.23     -14.97     32.77
  2  T/A       0.14      2.38      2.45      19.34      8.22      23.05
  3  A/A       0.34      1.28      2.96      5.84      11.06     29.14
  4  A/A       0.67      0.55      3.08      3.47      7.64      38.22
  5  A/T       0.37      0.18      2.81      8.57      -4.65     36.61
  ~~~~~
  ave.       0.28      0.88      2.75      10.49      1.46      31.96
  s.d.       0.29      0.97      0.28      6.62      10.99      6.10
*****
Sugar conformational parameters:
base      v0      v1      v2      v3      v4      tm      P      Puckering
  1  T     -16.8    33.5   -36.3    27.7    -6.9    36.7   172.0    C2'-endo
  2  T     -39.6    20.3     4.6   -28.2    42.5    42.7    83.9    O4'-endo
  3  A     -38.3    42.0   -30.1     8.7    18.3    41.9   135.9    C1'-exo
  4  A     -41.0    45.7   -33.1    10.3    18.9    45.3   136.9    C1'-exo
  5  A     -40.2    45.0   -32.7    10.3    18.6    44.7   137.1    C1'-exo
  6  T     -44.8    41.7   -23.1    -2.3    29.2    44.8   121.1    C1'-exo
*****

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**T<sub>2</sub>A<sub>3</sub>T singly ionized**

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*****
Local base step parameters
  step      Shift      Slide      Rise      Tilt      Roll      Twist
  1  T/T      -0.17     -0.05     2.48     14.14    -15.15     32.85
  2  T/A       0.12      2.43      2.41     19.88      7.67     26.19
  3  A/A       1.00      1.79      2.78      8.36      3.62     36.47
  4  A/A       1.15      0.66      2.97      5.02      5.34     38.94
  5  A/T       0.34      0.04      2.70     10.58     -3.79     36.13
  ~~~~~
  ave.       0.49      0.97      2.67     11.60     -0.46     34.11
  s.d.       0.57      1.10      0.23      5.70      9.26      4.93
*****
Sugar conformational parameters:
base      v0      v1      v2      v3      v4      tm      P      Puckering
  1  T     -16.8    33.7   -36.7    28.1    -7.1    37.1   172.3    C2'-endo
  2  T     -40.4    22.0     2.8   -26.7    42.0    42.7    86.3    O4'-endo
  3  A     -38.2    42.2   -30.5     9.4    17.7    42.0   136.6    C1'-exo
  4  A     -39.3    45.6   -34.3    12.7    16.3    44.8   140.0    C1'-exo
  5  A     -41.0    45.1   -32.0     9.2    19.6    44.8   135.6    C1'-exo
  6  T     -44.2    43.3   -25.9     1.1    26.7    45.0   125.2    C1'-exo
*****

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**TA<sub>4</sub>T neutral**

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*****
Local base step parameters
  step      Shift      Slide      Rise      Tilt      Roll      Twist
  1  T/A      0.29      1.39      2.25      25.67     -4.19     32.06
  2  A/A      0.30      1.41      2.92      6.19      7.75      30.64
  3  A/A      0.30      1.34      2.82      9.98      8.83      30.00
  4  A/A      0.55      0.60      3.07      3.40      7.03      36.61
  5  A/T      0.29      0.13      2.82      8.50      -4.99     35.85
  ~~~~~
  ave.      0.35      0.97      2.77      10.75     2.89      33.03
  s.d.      0.11      0.58      0.31      8.70      6.86      3.03
*****
Sugar conformational parameters:
base      v0      v1      v2      v3      v4      tm      P      Puckering
  1  T     -12.8    25.8   -28.2   21.5    -5.6    28.5    172.5   C2'-endo
  2  A     -42.4    43.2   -28.0    4.3     23.5    44.1    129.5   C1'-exo
  3  A     -43.0    41.8   -25.1    0.8     26.1    43.7    125.1   C1'-exo
  4  A     -41.6    45.5   -32.3    9.2     20.0    45.3    135.4   C1'-exo
  5  A     -40.7    44.9   -32.0    9.3     19.4    44.6    135.8   C1'-exo
  6  T     -44.8    41.7   -23.0   -2.4     29.3    44.7    120.9   C1'-exo
*****

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**TA<sub>4</sub>T singly ionized**

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*****
Local base step parameters
  step      Shift      Slide      Rise      Tilt      Roll      Twist
  1  T/A      0.27      1.22      2.26      24.24     -6.38     35.66
  2  A/A      1.02      1.86      2.88      7.04      2.43      41.67
  3  A/A      1.04      2.11      2.67      12.71     2.37      41.08
  4  A/A      1.37      1.34      3.00      4.94      2.11      40.88
  5  A/T      0.36      0.15      2.79      8.40      -3.53     36.04
  ~~~~~
  ave.      0.81      1.34      2.72      11.47     -0.60     39.07
  s.d.      0.48      0.76      0.28      7.69      4.10      2.95
*****
Sugar conformational parameters:
base      v0      v1      v2      v3      v4      tm      P      Puckering
  1  T     -14.0    28.8   -31.6   24.4    -6.6    31.9    173.1   C2'-endo
  2  A     -42.5    44.8   -30.3    6.7     22.1    45.1    132.2   C1'-exo
  3  A     -41.4    43.3   -29.0    6.0     21.8    43.6    131.6   C1'-exo
  4  A     -39.5    45.0   -33.4   11.6     17.2    44.4    138.8   C1'-exo
  5  A     -40.5    45.0   -32.4   10.0     18.8    44.6    136.7   C1'-exo
  6  T     -43.9    44.3   -27.9    3.3     25.1    45.3    127.9   C1'-exo
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## Na model [B3LYP-D/SV(P)]: local base step and conformational parameters

### T<sub>3</sub>AT<sub>2</sub> neutral

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#### Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 T/T	-0.78	-0.23	2.40	13.96	-16.08	27.47
2 T/T	0.01	0.12	2.42	12.00	-6.16	34.11
3 T/A	0.31	0.81	2.39	15.15	-4.66	38.90
4 A/T	0.27	0.24	2.77	7.38	-4.49	34.61
5 T/T	-0.09	-0.13	2.53	10.24	-8.80	33.47
~~~~~						
ave.	-0.06	0.16	2.50	11.74	-8.04	33.71
s.d.	0.44	0.41	0.16	3.08	4.82	4.09

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#### Sugar conformational parameters:

Note: v0: C4'-O4'-C1'-C2';      v1: O4'-C1'-C2'-C3';      v2: C1'-C2'-C3'-C4'  
 v3: C2'-C3'-C4'-O4';      v4: C3'-C4'-O4'-C1'

tm: the amplitude of pucker  
 P: the phase angle of pseudorotation

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 T	-16.4	34.2	-37.9	29.6	-8.5	38.1	173.9	C2'-endo
2 T	-39.6	46.5	-35.6	13.8	15.9	45.7	141.1	C1'-exo
3 T	-39.3	45.9	-35.0	13.5	15.9	45.1	140.8	C1'-exo
4 A	-32.9	44.1	-38.2	20.4	7.6	43.5	151.3	C2'-endo
5 T	-39.6	46.3	-35.4	13.7	16.0	45.5	141.0	C1'-exo
6 T	-41.6	45.3	-31.6	8.5	20.5	45.1	134.5	C1'-exo

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### T<sub>3</sub>AT<sub>2</sub> singly ionized

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#### Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 T/T	-0.42	-0.04	2.38	14.30	-14.57	31.26
2 T/T	0.32	0.36	2.45	10.70	-4.63	38.25
3 T/A	0.99	1.65	2.56	12.94	-1.16	45.55
4 A/T	0.26	0.43	2.91	3.88	-4.89	35.29
5 T/T	0.23	0.03	2.53	10.04	-6.20	36.08
~~~~~						
ave.	0.27	0.49	2.56	10.37	-6.29	37.29
s.d.	0.50	0.68	0.20	4.01	4.99	5.27

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#### Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 T	-16.6	34.6	-38.4	30.0	-8.6	38.6	173.9	C2'-endo
2 T	-39.5	47.0	-36.5	14.9	15.1	46.1	142.3	C1'-exo
3 T	-40.1	46.4	-34.6	12.8	16.8	45.4	139.7	C1'-exo
4 A	-32.8	44.2	-38.5	21.0	7.0	43.6	152.0	C2'-endo
5 T	-39.8	46.3	-34.9	13.1	16.5	45.4	140.2	C1'-exo
6 T	-39.9	24.9	-2.0	-21.5	38.8	40.7	92.8	O4'-endo

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**T<sub>2</sub>A<sub>2</sub>T<sub>2</sub> neutral**

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*****
Local base step parameters
  step      Shift      Slide      Rise      Tilt      Roll      Twist
  1  T/T      -0.54      -0.31      2.28      15.27     -14.85     28.66
  2  T/A       0.20       0.93       2.27      18.90     -5.59      37.47
  3  A/A       0.54       0.48       3.11       0.52       4.56      38.63
  4  A/T       0.16       0.17       2.69       9.51      -4.90      35.05
  5  T/T       0.21       0.09       2.60       9.01      -7.08      35.86
  ~~~~~
  ave.       0.11       0.27       2.59      10.64     -5.57      35.13
  s.d.       0.40       0.46       0.35       7.00       6.92       3.88
*****
Sugar conformational parameters:
  base      v0       v1       v2       v3       v4       tm       P       Puckering
  1  T      -17.8     35.4    -38.4     29.4     -7.4     38.8     172.2     C2'-endo
  2  T      -41.2     45.6    -32.6     9.9      19.3     45.2     136.2     C1'-exo
  3  A      -34.0     45.1    -38.7     20.3      8.3     44.5     150.6     C1'-endo
  4  A      -34.9     44.7    -37.2     18.1     10.3     43.9     147.9     C2'-endo
  5  T      -38.6     46.2    -36.1     14.9     14.6     45.3     142.7     C1'-exo
  6  T      -42.2     44.6    -29.9      6.5     22.1     44.8     131.9     C1'-exo
*****

```

**T<sub>2</sub>A<sub>2</sub>T<sub>2</sub> singly ionized**

```

*****
Local base step parameters
  step      Shift      Slide      Rise      Tilt      Roll      Twist
  1  T/T      -0.50      -0.28      2.32      14.68     -15.56     29.13
  2  T/A       0.04       1.11       2.19      20.42     -7.79      40.21
  3  A/A       1.29       1.56       2.87       4.79     -0.52      44.55
  4  A/T       0.19       0.23       2.74       7.35     -4.11      33.86
  5  T/T       0.04      -0.06       2.51      10.36     -7.62      34.67
  ~~~~~
  ave.       0.21       0.51       2.53      11.52     -7.12      36.48
  s.d.       0.66       0.79       0.28       6.19       5.58       5.98
*****
Sugar conformational parameters:
  base      v0       v1       v2       v3       v4       tm       P       Puckering
  1  T      -17.3     35.0    -38.4     29.6     -7.9     38.7     172.9     C2'-endo
  2  T      -41.7     46.1    -33.0     10.1     19.5     45.6     136.2     C1'-exo
  3  A      -33.0     44.7    -39.0     21.3      7.1     44.1     152.1     C2'-endo
  4  A      -33.5     44.4    -38.0     19.9      8.2     43.6     150.5     C2'-endo
  5  T      -40.1     46.5    -35.1     13.1     16.6     45.7     140.2     C1'-exo
  6  T      -42.1     44.6    -30.0      6.7     21.9     44.7     132.2     C1'-exo
*****

```



**T<sub>2</sub>A<sub>3</sub>T neutral**

```

*****
Local base step parameters
  step      Shift      Slide      Rise      Tilt      Roll      Twist
  1  T/T      -0.53      -0.26      2.34      14.27     -14.69     28.91
  2  T/A       0.27       0.99      2.28      18.91      -4.39     38.22
  3  A/A       0.52       0.68      3.06       2.08       5.19     37.25
  4  A/A       0.53       0.33      3.06       1.66       3.14     41.30
  5  A/T       0.05       0.07      2.96       5.27      -8.49     34.45
  ~~~~~
  ave.       0.17       0.36       2.74       8.44      -3.85     36.03
  s.d.       0.44       0.50       0.40       7.75       8.21      4.67
*****
Sugar conformational parameters:
base      v0      v1      v2      v3      v4      tm      P      Puckering
  1  T     -17.6    35.2   -38.4    29.4    -7.5    38.7    172.3    C2'-endo
  2  T     -41.2    45.3   -32.2     9.5    19.6    45.0    135.7    C1'-exo
  3  A     -34.0    44.8   -38.3    19.8     8.7    44.2    150.1    C2'-endo
  4  A     -34.2    45.6   -39.1    20.6     8.3    44.9    150.8    C2'-endo
  5  A     -33.1    43.9   -37.7    19.6     8.3    43.3    150.5    C2'-endo
  6  T     -42.8    44.3   -29.0     5.3    23.2    44.8    130.4    C1'-exo
*****

```

**T<sub>2</sub>A<sub>3</sub>T singly ionized**

```

*****
Local base step parameters
  step      Shift      Slide      Rise      Tilt      Roll      Twist
  1  T/T      -0.57      -0.30      2.33      14.43     -15.87     28.57
  2  T/A       0.10       1.07      2.22      19.39      -5.87     40.60
  3  A/A       1.13       1.89      2.79       6.80       0.01     46.74
  4  A/A       1.39       1.43      2.95       4.37      -0.67     43.89
  5  A/T       0.28       0.09      2.85       5.80      -4.81     34.74
  ~~~~~
  ave.       0.47       0.84       2.63      10.16     -5.44     38.91
  s.d.       0.79       0.92       0.33       6.47       6.36      7.30
*****
Sugar conformational parameters:
base      v0      v1      v2      v3      v4      tm      P      Puckering
  1  T     -17.0    34.8   -38.3    29.7    -8.1    38.6    173.2    C2'-endo
  2  T     -41.6    46.0   -32.9     9.9    19.6    45.6    136.1    C1'-exo
  3  A     -32.9    44.3   -38.7    21.0     7.3    43.8    151.9    C2'-endo
  4  A     -31.7    44.1   -39.3    22.3     5.6    43.7    154.0    C2'-endo
  5  A     -35.3    44.9   -37.1    17.9    10.7    44.0    147.4    C2'-endo
  6  T     -42.6    45.1   -30.3     6.6    22.3    45.2    132.1    C1'-exo
*****

```

**T<sub>2</sub>A<sub>4</sub>T neutral**

\*\*\*\*\*

## Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	T/A	-0.02	0.97	2.04	25.61	-9.33	33.96
2	A/A	0.28	0.99	3.02	2.29	5.81	34.65
3	A/A	0.61	0.51	3.02	3.22	4.99	39.27
4	A/A	0.49	0.32	3.08	1.26	2.70	41.25
5	A/T	-0.01	0.07	2.99	4.87	-8.93	34.14

ave.		0.27	0.57	2.83	7.45	-0.95	36.65
s.d.		0.29	0.40	0.44	10.24	7.55	3.38

\*\*\*\*\*

## Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	T	-15.1	31.7	-35.1	27.5	-7.9	35.3	173.9	C2'-endo
2	A	-35.9	45.1	-37.0	17.4	11.3	44.3	146.7	C2'-endo
3	A	-34.1	45.1	-38.6	20.1	8.5	44.4	150.4	C2'-endo
4	A	-33.9	45.5	-39.4	21.1	7.8	44.9	151.4	C2'-endo
5	A	-33.0	43.8	-37.7	19.6	8.3	43.3	150.6	C2'-endo
6	T	-42.3	45.1	-30.7	7.3	21.7	45.1	132.9	C1'-exo

\*\*\*\*\*

**T<sub>2</sub>A<sub>4</sub>T singly ionized**

\*\*\*\*\*

## Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	T/A	-0.00	1.03	2.10	24.27	-9.41	37.26
2	A/A	1.12	1.96	2.86	4.62	0.12	47.18
3	A/A	1.38	1.62	2.86	6.49	-0.73	43.22
4	A/A	0.72	0.48	3.09	0.90	3.69	41.10
5	A/T	0.11	0.03	2.83	7.30	-6.96	34.70

ave.		0.67	1.02	2.75	8.72	-2.66	40.69
s.d.		0.61	0.80	0.38	9.04	5.38	4.91

\*\*\*\*\*

## Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	T	-15.6	32.6	-36.2	28.3	-8.1	36.4	173.9	C2'-endo
2	A	-34.9	45.2	-38.3	19.5	9.4	44.5	149.3	C2'-endo
3	A	-32.3	44.0	-38.5	21.1	6.8	43.4	152.4	C2'-endo
4	A	-35.0	46.0	-39.2	20.3	8.9	45.2	150.0	C2'-endo
5	A	-34.1	44.4	-37.4	18.7	9.5	43.6	149.0	C2'-endo
6	T	-42.2	45.1	-30.7	7.4	21.5	45.1	133.0	C1'-exo

\*\*\*\*\*

**Hydrogen model [B97D/SV(P)]. Optimized geometries (Å)**

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T3AT2 neut. E(RB97D)=-7711.74787683 Hartree

C	0.029264859001	4.376423047307	-15.809417930081
N	1.075235406012	3.642290640266	-15.278386904414
C	1.015845853438	2.235748934149	-15.176030923611
N	-0.169961389169	1.701339294274	-15.666207285654
C	-1.293974430717	2.370293496007	-16.195980447086
C	-1.135204056158	3.823448229168	-16.265278622325
C	2.233585192369	4.332254803124	-14.732596049873
C	2.969566545387	5.316413513679	-15.652104131674
C	3.814323381702	6.096164710048	-14.621432744163
C	2.967926011619	5.965665661377	-13.312928785613
O	1.831104248735	5.153714315183	-13.628494119190
O	5.080065654047	5.493227886605	-14.367140787612
C	2.529407616666	7.276356885799	-12.678404626143
O	1.941989505849	8.205304027086	-13.619634283578
P	0.428659141369	8.187458842307	-14.178441129531
O	0.051465109565	9.763924063314	-14.258463871323
O	1.914847250236	1.541085512246	-14.725137165628
O	-2.286431023927	1.734727779710	-16.549675618115
C	-2.267383948759	4.642577758110	-16.827290163733
O	-0.364701661802	7.582288810160	-12.893004610119
C	-1.801219544045	7.373597728295	-12.886644620172

C	-2.202879531008	6.171125578745	-13.742260120236
C	-1.951311795052	5.035828556757	-12.742877469763
C	-2.555373281713	5.535181192676	-11.536312229952
O	-2.186076323204	6.917577245570	-11.442087141661
N	-2.486324583142	3.725402553325	-13.061429899763
C	-1.647482929962	2.604086243884	-12.893562350510
N	-2.260864488603	1.403269630912	-13.212599264656
C	-3.576820644860	1.170902327758	-13.665422069673
C	-4.381611552651	2.390314186753	-13.777936126237
C	-3.805395113208	3.587745275348	-13.466788127902
C	-3.299198866045	7.732545441108	-10.7972419866289
O	-4.415699831445	7.966533318425	-11.686055702762
P	-5.666995984079	6.984154972713	-11.963937371380
O	-6.941043326616	7.987767443421	-11.981049239630
O	-0.483906031340	2.670050053357	-12.520835625586
O	-3.956142433147	0.029364239346	-13.911411797337
C	-5.809697649458	2.267674893718	-14.236874315955
O	-5.727372979375	6.169714344331	-10.561016337835
C	-6.708562138549	5.141050363212	-10.268278949100
C	-6.446324804186	3.859823711386	-11.063479209490
C	-5.386029336686	3.200805886147	-10.176700324458
O	-5.928122675736	3.365171312893	-8.856275180062
C	-6.451473612812	4.696618561942	-8.791799286189
N	-5.103057515959	1.813532112617	-10.427486978299
C	-3.846850631579	1.230534145798	-10.340299140923
N	-4.060607233796	-0.130586940693	-10.622585449675
C	-5.395537418933	-0.387777616149	-10.868032187587
C	-5.981164939415	0.786574646634	-10.750370370238
C	-2.895146942220	-0.944703813101	-10.656802703713
N	-1.695477897082	-0.364088780266	-10.418053089885
C	-1.657034858544	0.950545405773	-10.132539593448
N	-2.674926104711	1.822858153824	-10.073795760388
C	-7.668128504708	4.747689880253	-7.877612398975
O	-8.852900013096	4.168509499508	-8.467242479373
O	-9.232179175823	2.599439345102	-8.548856063417
O	-10.831900183712	2.601213619770	-8.277522280928
N	-2.947521727055	-2.269527369862	-10.928386198165
O	-8.529953327479	2.038758619936	-7.191612696553
C	-8.476490158976	0.618629733316	-6.889402946497
C	-7.441525707606	-0.106326162006	-7.754469845125
C	-6.173656873127	0.157509626023	-6.935236476858
O	-6.599209639858	-0.124523856012	-5.589935566422
C	-7.889732981661	0.478315188797	-5.445999793533
N	-4.981932872799	-0.608895861883	-7.245823263373
C	-3.736489354157	0.059181607497	-7.184221096105
N	-2.654593574751	-0.774207391532	-7.433433708744
C	-2.639358853635	-2.164197707575	-7.666518827768
C	-3.970240120117	-2.770810332092	-7.686401630774
C	-5.057188058193	-1.972276838259	-7.475115713774
C	-8.747146179959	-0.325644942040	-4.477138214836
O	-9.265260782257	-1.547603645137	-5.050156966759
P	-8.499726816530	-2.959831106588	-5.212475180643
O	-9.656076885344	-4.044246853472	-4.866467112830
O	-3.611014939408	1.250386719158	-6.950232104847
O	-1.573808318869	-2.757653098067	-7.824384907504
C	-4.079359410494	-4.253944622353	-7.915066273231
O	-7.493844838184	-2.923122746154	-3.933600059044
C	-6.571763390448	-4.015576688468	-3.671222767409
C	-5.378036899725	-3.992778171337	-4.631182160557
C	-4.462998253645	-3.002667389975	-3.900695809591
O	-4.534016771027	-3.454183666709	-2.535770110316
C	-5.913341723057	-3.736940745330	-2.280445320354
N	-3.075902637416	-2.914296160951	-4.314834418643
C	-2.479595995755	-1.634175146677	-4.368052345661
N	-1.128257776630	-1.669586419209	-4.679238911797
C	-0.290945716810	-2.788850594646	-4.873101933516
C	-0.993063191592	-4.070197432396	-4.779443081243
C	-2.328920830764	-4.065666906947	-4.504451687447
C	-6.049868069966	-4.863915176111	-1.263485300867
O	-5.827830579269	-6.176717300664	-1.825441970488
P	-4.408209053319	-6.901900288782	-2.086040506604
O	-4.752593707186	-8.461149167559	-1.801695224979
O	-3.088741084138	-0.590122700329	-4.188100895611
O	0.910220082882	-2.638454077869	-5.084836245906
C	-0.208356664065	-5.337333398293	-4.984670792846
C	-3.545052016768	-6.372313567766	-0.813670470849
C	-2.119990619460	-6.657563636251	-0.688242308443
C	-1.303900052568	-5.780739063498	-1.631648086328
O	-1.290964782576	-4.442877269826	-0.875193309809
C	-1.289436070808	-4.779710177679	0.513476925580
C	-1.675447819210	-6.152991912612	0.701635826164
N	-0.140442103450	-3.585998953489	-1.175496183877
C	-0.368215804474	-2.240992758501	-1.519640098080
N	0.791517607993	-1.554367873420	-1.853132849384
C	2.127691834537	-2.011985986955	-1.836065325773
C	2.272145994469	-3.391071475045	-1.357656410548
C	1.143552099247	-4.093166950556	-1.044372802399
C	-0.537309646621	-6.960911665699	1.327916654158
O	0.527514732362	-7.122587119719	0.396998382206
O	-1.474435965161	-1.716296029183	-1.540359638388
O	3.043501089903	-1.267279265448	-2.177185656544
C	3.658558152597	-3.964017868940	-1.222978116339
O	-3.790183157125	-6.772432482615	-3.439598052866
O	-7.906791123218	-3.282680248023	-6.544641206880
O	-8.946537186085	1.877719122063	-9.823646725152
O	-5.646604689441	6.192026410633	-13.230691565223
O	0.179931548258	7.555010690786	-15.508945504279
H	1.285548367545	-7.517375046788	0.867452652174
H	-2.188081732203	-3.846656608581	-1.118695684872
H	-0.290113542760	-6.205847533281	-1.716015374947
H	-1.752690357229	-5.700903554698	-2.630152549334
H	-1.951031818024	-7.741605145630	-0.823405176183
H	-2.533610283493	-6.185940928226	1.402824575914
H	-0.948018450165	-7.948140398626	1.643783768264
H	-0.200564312330	-6.416797336068	2.238570375859
H	0.652586290341	-0.582275038333	-2.134986107813
H	1.192160033522	-5.112929317902	-0.640004365098
H	3.621790149936	-5.004843738861	-0.843950765439
H	4.274547591997	-3.351674758482	-0.529533172192
H	4.180624700022	-3.959203122214	-2.204169017910
H	-4.876802294821	-1.980203060652	-3.983011949359
H	-4.927768925277	-5.000134882015	-4.659426443085
H	-5.664881000186	-3.677095289323	-5.643563781841
H	-7.128488128484	-4.969546882257	-3.691083798102
H	-6.403089016375	-2.840024471462	-1.841924140119
H	-7.090916019428	-4.886001855367	-0.892589159668
H	-5.359949555025	-4.692931958274	-0.415270734377
H	-0.675701534337	-0.755446094437	-4.727399803880

H	-2.885411927080	-5.001926889224	-4.393111479592
H	-0.854880665641	-6.228693547817	-4.865246020363
H	0.629284597596	-5.402381149308	-4.258022410867
H	0.240749900328	-5.355348412978	-6.001110075017
H	-5.886245953218	1.221422947253	-7.023342811455
H	-7.689428640374	-1.182073115771	-7.767244163501
H	-7.406241915984	0.288266520777	-8.779108834316
H	-9.492025341716	0.192311559638	-6.975396136636
H	-7.781190885694	1.499063399417	-5.017994619117
H	-9.641797084336	0.267221001645	-4.212425622814
H	-8.170127257336	-0.552125309278	-3.56061632001
H	-1.745215175474	-0.31099627048	-7.428208684499
H	-6.066867054911	-2.394301102538	-7.445542659532
H	-5.137406999956	-4.581053549064	-7.903763685549
H	-3.523517357624	-4.812958285558	-7.132321504466
H	-3.628522518514	-4.531827039947	-8.891785415028
H	-4.415269872031	3.731984870580	-10.257404106881
H	-7.363631941127	3.244145479135	-11.057470478500
H	-6.118417741241	4.056360439006	-12.095290132136
H	-7.721382565385	5.555108817751	-10.421315579326
H	-5.689222456899	5.378064412160	-8.354615340622
H	-7.928430715416	5.805378189864	-7.688364983622
H	-7.438404011542	4.247043821537	-6.917993421543
H	-0.654878546070	1.365783620939	-9.942227819519
H	-2.111172250150	-2.835885687504	-10.798826384580
H	-3.851001210424	-2.727681396818	-11.016869325852
H	-7.050685964398	0.988005905220	-10.863736327597
H	-0.864349022644	4.898101178304	-12.594866076505
H	-3.278037063154	6.247727399325	-13.982919350971
H	-1.609911530863	6.098686091634	-14.663738146653
H	-2.302679207294	8.311982272606	-13.184185562763
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T3AT2 sing. ion. E(UB97D)=-7711.54417022 Hartree

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P	-8.046987968847	-2.151982263276	-5.166004563505
O	-9.36655425503	-3.082518271660	-5.061535226812
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H	-8.965757525420	2.709786487481	1.068944151451
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H	-3.146732896426	-3.685295675095	-2.152044819287
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H	4.688455291427	3.727988811929	-0.375258629546
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T2A3T neut. E(RB97D)=-7738.04860083 Hartree

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N	2.695981964911	0.237619531244	1.896689384460
C	2.454465782829	1.500472194165	1.610183523148
C	2.2713485356492	-1.831553712450	0.429694567286
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C	1.409163218827	-1.230114132079	-1.636995965068
N	1.358166366871	0.097221789881	-1.435445845372
N	2.608803123181	-2.796609897788	1.330268710505
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O	7.293188637755	0.413782076460	-1.237257352694
C	5.872806172289	0.225168918063	-1.314965986644
C	5.263949492331	1.247270149405	-0.325176798132
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O	9.234740996250	2.081643531971	0.622700229168
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N	5.559331713283	-1.166274189045	-1.029293909668
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C	4.637209918771	-3.235506060436	-1.582476237516
N	5.025474127407	-3.870066167124	-0.389040237971
C	5.775615264541	-3.009544886367	0.526712524022
C	5.984431046233	-1.708596792818	0.168971491592
O	4.408924261803	-1.467391419123	-3.026872550793
O	4.707365962638	-5.041344025070	-0.174287358326
C	6.248861159220	-3.587137544621	1.833305813524
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C	10.552295186681	-1.584273342147	0.856940951459
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TA4T neut. E(RB97D)=-7751.19490714 Hartree

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H	10.072084821590	0.690245330951	-3.051470940498
H	10.147568457826	-0.047439567268	-1.407176094845
H	8.897181135092	1.188306729172	-1.805730259331
H	11.217336751136	-2.295171270864	3.026251741181
H	7.602069077630	4.847453988485	3.642474732298
H	0.735394867974	8.147748042458	0.645177276634
H	-5.935128537844	6.065527538902	-2.676519905176
H	-11.590128177227	1.024095320651	-2.644329727488

## Na model [B3LYP-D/SV(P)]. Optimized geometries (Å)

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O	11.702263819034	-4.757232809197	-0.944390410862
C	12.151910405455	-3.707663752710	-1.787085363549
C	11.164777923518	-2.549482342407	-1.765057802984
O	9.932700733261	-2.920541283035	-2.394710732371
C	10.776174374918	-2.063405833581	-0.358303831579
O	10.461274257155	-0.671751916597	-0.461217487705
C	9.522902613421	-2.884172451801	-0.075219677601
C	8.863428960697	-2.894672975463	-1.456413540627
N	7.980745411578	-4.030323166114	-1.696777229523
C	6.705840536502	-3.796611731693	-2.208976180562
O	6.292301025265	-2.696360510944	-2.532963481033
N	5.928806629066	-4.935392729955	-2.308790579365
C	6.284824627350	-6.259207691049	-2.019700054397
O	5.468396920566	-7.161017933720	-2.138928992400
C	7.680764925004	-6.424631214321	-1.615857989349
C	8.192046084315	-7.815887469119	-1.376254415344
C	8.449756362645	-5.314651950470	-1.487097554675
P	10.164541241344	0.226305617235	0.885666982212
O	11.430450718596	0.435909619575	1.691182333443
O	8.999321125995	-0.342481304098	1.692313409443
O	9.767369570181	-1.631378729278	0.158871587403
C	9.237373417548	1.838880340466	-1.148284773291
C	7.716170158335	1.881583838215	-1.197390362179
O	7.167000973972	0.560111589666	-1.230138189885
C	7.061078425390	2.597586788077	0.012701642044
O	6.063058218947	3.496124143735	-0.484043782968
C	6.426302219648	1.436394017569	0.776432536980
C	6.003149952891	0.564430222825	-0.402646282956
N	5.594107852466	-0.796460639268	-0.123212350303
O	4.471051283494	-1.296121096072	-0.787461374718
C	3.804983105454	-0.651932057293	-1.578659665154
N	4.141697334581	-2.589706906177	-0.434140807803
C	4.844905375079	-3.467731322497	0.394867215819
O	4.451525933835	-4.615171731589	0.560658238640
C	6.046028846884	-2.888530654256	0.987144313417
C	6.886121384228	-3.765219941622	1.870625837593
C	6.357503620366	-1.597556847536	0.701765601889
F	5.396484310523	4.596185467123	0.541895452123
O	6.451167335757	5.557558002660	1.054376459719
O	4.589371989555	3.914230569974	1.644969826028
O	4.420133163917	5.374174773177	-0.506896837065
C	3.950266874012	4.938800093225	-1.779609335593
C	2.614732375020	4.213660037188	-1.716580814166
O	2.792424307453	2.862522403655	-1.285172270043
C	1.586618683663	4.852098922091	-0.745090033213
O	0.328339854920	4.935386581963	-1.421018867811
C	1.530882924492	3.834386375319	0.394214219952
C	1.710626953938	2.547658957881	-0.411290070103
N	2.008727972508	1.329694255702	0.315535461774
C	1.359651851518	0.154581735239	-0.072197403593
O	0.554716574522	0.086663036286	-0.982786381301
N	1.683005582509	-0.943222624418	0.704720017782
C	2.569723769602	-1.014671267654	1.779497317453
O	2.704031140565	-2.062676537812	2.404321552459
C	3.272551036568	0.231413297076	2.052453993221
C	4.303276494898	0.239063714448	3.144435165069
C	2.957819280824	1.330281226943	1.316525500856
P	-0.832023360338	5.944810622354	-0.837864880639
O	-0.357333099272	7.383968413257	-0.888194302684
O	-1.327698669275	5.497998936463	0.534757508075
O	-1.988008772765	5.692512257243	-1.960777072111
C	-2.022976992592	4.749288270647	-3.027860331534
C	-2.896169426450	3.542480928194	-2.712384765275
O	-2.209440169215	2.623621463284	-1.854379553595



C	-4.213892569076	3.900994014192	-1.988323355061
O	-5.241243279569	3.055703343827	-2.512961440617
C	-3.896614094085	3.531512407039	-0.541467450210
C	-3.076574713330	2.267315413551	-0.777299426066
N	-2.299052462927	1.800698570107	0.336503309341
C	-1.601825479254	2.551750863945	1.263447545070
N	-0.949497524353	1.821462470924	2.137610360627
C	-1.225157858707	0.520974196207	1.770745870775
C	-0.813487146056	-0.727304563158	2.283550402111
N	-0.034572036242	-0.823598620324	3.388677579563
N	-1.204794573163	-1.844319783864	1.639907277716
C	-1.987426830272	-1.726522625377	0.554821625867
N	-2.459046975213	-0.613864626146	-0.004016182273
C	-2.046366859914	0.481587961684	0.638383537831
P	-6.817372813496	3.323714192412	-2.134507293355
O	-7.280514707510	4.663201034988	-2.673458296308
O	-7.083970674081	3.128186108410	-0.643530625091
O	-7.490276775835	2.125436167147	-3.013801979731
C	-6.859293981692	0.971523046998	-3.561995403557
C	-6.925552984074	-0.241876313319	-2.649123623200
O	-5.956918362672	-0.150120608714	-1.599935613185
C	-8.300521663014	-0.439691984539	-1.958565198036
O	-8.661153202875	-1.815547316862	-2.093306491555
C	-7.992606513010	-0.090767451708	-0.502469053218
C	-6.572282316460	-0.644513074693	-0.410441284027
N	-5.778583000039	-0.272402968898	0.742669695931
C	-5.040157751012	-1.268740996276	1.382021412418
O	-5.014415636415	-2.435148565475	1.027588011361
N	-4.339282608564	-0.825809971151	2.485547236626
C	-4.264460668486	0.470864236036	3.006320972701
O	-3.595710574062	0.699815174273	4.004206558225
C	-5.017814781546	1.458729621243	2.240090336483
C	-4.954889378699	2.892763545100	2.679722781742
C	-5.721579343149	1.045823102064	1.154952469248
P	-10.167680040566	-2.325100635159	-1.676407321066
O	-11.221435450811	-1.603075023632	-2.493352488738
O	-10.391694341835	-2.254718040767	-0.167741051227
O	-10.052271436385	-3.871320745508	-2.185525323269
C	-8.860784559017	-4.617518568083	-2.414929754227
C	-8.329129884625	-5.316404112340	-1.176126605885
O	-7.693388503214	-4.389201869841	-0.291772626084
C	-9.403892032373	-6.067449713410	-0.344212370610
C	-8.954704146348	-7.406460271145	-0.178794570379
O	-9.406058169133	-5.287918549448	0.975677626608
O	-7.941056074533	-4.852306073907	1.030287634593
N	-7.598689873955	-3.826506608278	1.996142607486
C	-6.570248365324	-4.081140381476	2.906598556888
O	-5.937124126165	-5.121021032364	2.951134784696
N	-6.348167419755	-3.045525890553	3.797727923698
C	-6.978223377833	-1.797055108923	3.855603769834
O	-6.648121125725	-0.974652052353	4.701478175789
C	-8.009357697796	-1.605500266233	2.842542355199
C	-8.731783191242	-0.288535144689	2.813396900629
C	-8.265281184476	-2.618448881954	1.972814219852
H	13.139036555662	-3.326880869342	-1.454185137753
H	12.248357245616	-4.051626169474	-2.835726430008
H	11.613276670961	-1.714697622710	-2.330199543182
H	11.581165402002	-2.217452253442	0.379449469647
H	9.818362867944	-3.895685068059	0.232402906400
H	8.253061454207	-1.992221052660	-1.604195053609
H	9.511138366235	-5.373953784191	-1.229153236127
H	4.975383452038	-4.784551540801	-2.630719730867
H	8.895327070205	-2.425136075446	0.693097573463
H	9.615725449335	2.823157392426	-1.4773207025227
H	9.605210926002	1.067381552501	-1.844506219555
H	7.425650942305	2.418148418910	-2.119887093027
H	7.799422072423	3.155563609712	0.608917226084
H	7.203177188552	0.928020568631	1.366239350095
H	5.161095203609	1.035823761565	-0.931979917892
H	7.258932378581	-1.120541495226	1.104192373418
H	3.309223548560	-2.960244862688	-0.885444374226
H	5.598619771691	1.771092105418	1.408235728940
H	3.815488892645	5.852452790687	-2.383571199426
H	4.695588989867	4.291974907690	-2.270432964501
H	2.181036527926	4.2190720232505	-2.734199247638
H	1.902263845611	5.854504725562	-0.416138219484
H	2.396181556897	3.992740284738	1.055850387047
H	0.800184958609	2.341978010012	-0.994117634650
H	3.470078072840	2.287623225089	1.473260047163
H	1.137259234986	-1.7810447956149	0.512864085068
O	0.588419001875	3.885938975126	0.951332804288
H	-2.459901440906	5.272376225776	-3.896508507056
H	-1.007486650290	4.409437637519	-3.287142451683
H	-3.135445776249	3.040537099239	-3.667704504191
H	-4.490804535723	4.95873498420	-2.122544034379
H	-3.259496057082	4.309416199113	-0.092240353269
H	-3.727160426278	1.426142078405	-1.073053681096
H	-1.589753355457	3.644912494187	1.187403602788
H	-2.285697735877	-2.669775161412	0.082350757184
H	0.391711919655	0.021041038473	3.742496436972
H	0.480646331484	-1.695333221907	3.526382912384
H	-4.803228436764	3.369094584662	0.050818513366
H	-7.411328419186	0.730801529090	-4.486791224090
H	-5.808804889936	1.184496697219	-3.817632703777
H	-6.713219158515	-1.136266985118	-3.264318335954
H	-9.083512255965	0.196101299292	-2.400380723157
H	-7.985041019015	1.003436371594	-0.384906138360
H	-6.600786675161	-1.744804468550	-0.422484054493
H	-6.274818509874	1.755903581907	0.527164520553
H	-3.789929878620	-1.538375253477	2.959878393013
H	-8.700254334957	-0.561600144278	0.187323974717
H	-9.125590482888	-5.395842569771	-3.150864975973
H	-8.075518892705	-3.973844891177	-2.843394058280
H	-7.586474946555	-6.065799279703	-1.512107596347
H	-10.388777700942	-6.041644004853	-0.841857204705
H	-10.051533725158	-4.399588885492	0.883200779062
H	-7.300324846828	-5.717844325102	1.256900556822
H	-9.024046992412	-2.523837916088	1.183895451981
H	-5.611176034883	-3.212910063459	4.479112532669
H	-9.711203093749	-5.908390175816	1.834431628394
H	-9.623674542097	-7.882313684578	0.341818174810
H	12.290472680785	-5.521624893931	-1.058825878143
H	9.257457526243	-7.798964149420	-1.088053255555
H	7.614181732473	-8.311874735960	-0.573369607891
H	8.078125169267	-8.439600308396	-2.283268581017
H	7.679946450377	-3.183162228224	2.367025405952
H	6.259991019648	-4.249424474713	2.642609057808
H	7.360399807821	-4.575532252415	1.283268328626

H	4.650406598573	1.264901571478	3.351497945323
H	3.885138224504	-0.193405476286	4.072134754725
H	5.178541850649	-0.378119906090	2.864229441133
H	-5.665819419272	3.511115527880	2.106650063540
H	-5.190392032383	2.978245491538	3.756708940402
H	-3.936738851022	3.303347942940	2.536478195937
H	-9.608819637615	-0.334592302827	2.146928046801
H	-9.066937654776	-0.010552413688	3.829421611445
H	-8.063856955334	0.520890489239	2.460207802532
Na	10.418510694313	-0.337001358276	3.736873578011
Na	5.976794642907	5.025689900678	3.358403838033
Na	-0.719757332762	7.688420680380	1.497344658305
Na	-8.107304773720	5.391344055548	-0.540266948770
Na	-12.360834114674	-0.795924800474	-0.520426320700

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O	11.479871547147	-4.816314205756	-0.965276116615
C	12.063508685141	-3.697944632329	-1.615182193789
C	11.130204111576	-2.497523075668	-1.547194072079
O	9.954035466268	-2.725742177387	-2.332601880856
C	10.618702997534	-2.157869222346	-0.136950083530
O	10.356052040342	-0.752143977119	-0.108478967027
C	9.315915353758	-2.946425542163	-0.075978978753
C	8.798123415234	-2.753482698103	-1.503008158964
N	7.893771814737	-3.798737344026	-1.968571939924
C	6.691756720027	-3.429972080386	-2.569105954237
O	6.356843799946	-2.274616804370	-2.770819473528
N	5.886477897586	-4.500584083680	-2.908355982317
C	6.150271395190	-5.869080008852	-2.759690565388
O	5.316705139419	-6.700166548540	-3.087881605558
C	7.481383385285	-6.163253969100	-2.229583050809
C	7.899308291022	-7.600573399459	-2.113731453039
C	8.279819919907	-5.124195970984	-1.879260017080
P	9.953298154412	0.012753574419	1.292339725335
O	11.153679551476	0.132252956462	2.208043135424
O	8.729753861100	-0.625477310402	1.948000167763
O	9.607407828733	1.481753969214	0.674402239437
C	9.217882997543	1.815623834150	-0.655805433478
C	7.710687188713	1.903871691504	-0.843157728526
O	7.135384774312	0.603631703187	-1.021450590958
C	6.963635744302	2.548648209941	0.3517471133982
O	6.014753467233	3.481696430121	-0.173298748700
C	6.258519607555	1.347549232544	0.981300746605
C	5.911151107028	0.578387867439	-0.290530937695
N	5.452866732294	-0.791742942778	-0.151296437127
C	4.399467774860	-1.217780767597	-0.969579368931
C	3.773688780735	-0.477010782295	-1.706860505647
N	4.082196552196	-2.553063600672	-0.826551155923
O	4.721097192694	-3.516822873791	-0.039334588055
C	4.352955502850	-4.682095893132	-0.061045678103
C	5.833443582775	-2.994526217975	0.750502803115
C	6.585435490630	-3.957931586870	1.619026893269
C	6.151365662313	-1.676840170764	0.643766623770
P	5.211528484243	4.497927838748	0.838728900467
O	6.167777200206	5.451608955829	1.523303718269
O	4.309512327072	3.726122185264	1.803044703192
O	4.335390447260	5.308984318456	-0.271935734732
C	3.983362017896	4.892486216737	-1.589253615290
C	2.653174443917	4.159481973471	-1.654697000456
O	2.798936688379	2.798341388477	-1.224094773767
C	1.545101816797	4.781401858011	-0.766137198869
O	0.349157606217	4.889678275055	-1.540476004618
C	1.384611166862	3.741722113059	0.343243972187
C	1.640571154706	2.473704683167	-0.471162910600
N	1.884788488536	1.231724880737	0.263580056835
O	1.301121134883	0.041368346401	-0.232067833921
C	0.513474913520	0.014247513993	-1.153042977550
N	1.677192179367	-1.094610419990	0.455954814906
C	2.528694723600	-1.204260788588	1.554737730383
O	2.756184485489	-2.287580427889	2.07008831504
C	3.095031877060	0.070813737688	1.992850636887
C	4.058365667555	0.054892231923	3.134456501439
C	2.767921269587	1.215215428702	1.300964066800
P	-0.819451912897	5.944926105818	-1.056453168726
O	-0.331807863141	7.372829947527	-1.192280566008
O	-1.344339757724	5.592080397529	0.332966606812
O	-1.951117597749	5.624229334578	-2.184932341019
C	-1.965262105571	4.604192867571	-3.178513090409
O	-2.849807023219	3.429669911630	-2.791909727121
C	-2.201666425033	2.605314312349	-1.810607095919
O	-4.205913687292	3.834586970473	-2.171957683639
C	-5.181181668614	2.912360420957	-2.654915874283
C	-3.956214453267	3.625814050485	-0.677103379376
C	-3.114886326646	2.358185313565	-0.751288723009
N	-2.361442486899	2.019176587953	0.435939781921
C	-1.767030131107	2.852033347812	1.342816264725
N	-1.017200355024	2.214285127134	2.238284859437
C	-1.320425084757	0.910362865090	1.894550136296
C	-0.550732205946	-0.287495844466	2.408510685395
N	0.358714674627	-0.271355303642	3.389755275295
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T2A2T2 neut. E(RB3LYP-D)=-8537.96786176 Hartree

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H	3.386179046619	2.408807505463	-10.236499735081
H	1.667336183712	2.441794846336	-10.279044143654
H	5.942302003050	-4.195927544305	-11.844786351439
H	2.776490842111	-8.875577437688	-10.641595945017
H	3.387642764171	-7.317511256248	-9.992427432096
H	1.079149092277	-7.356408276258	-11.114085486033
H	2.395175110398	-8.511724115776	-13.357271966716
H	3.487217678840	-6.406051678570	-13.895837000853
H	0.799549295462	-5.164898144145	-13.050822151243
H	4.392575425537	-4.64857774862	-13.324657554891
H	1.530032641737	-0.816571853436	-13.129270640950
H	1.984767205607	-6.318773420700	-14.907420430651
H	-3.270206914289	-8.329422712092	-13.219384888829
H	-1.769853177959	-7.584211947306	-12.576094921040
H	-3.598197026673	-6.008090131192	-13.313455098357
H	-3.582648344650	-7.493406695893	-15.794639589330
H	-1.738818681111	-6.226302637865	-16.650861165582
H	-2.828914963532	-3.905817017825	-14.956416448531
H	0.209062606506	-5.599275208754	-15.991785887183
H	0.236464103091	-0.814582228901	-15.721975758598
H	-3.087777313391	-5.105483751480	-17.114319346253
H	-5.236985618838	-5.921308646113	-16.167865018088
H	-0.825648576632	7.788767969554	1.427643596275
H	-3.447308272651	5.647685298565	-0.475684809916
H	-4.090010459787	4.823443357448	-1.936723911315
H	-4.197381616468	4.018872047674	-0.356386485518
H	0.866655258466	6.457492979262	-4.385843031026
H	-0.371420754094	5.668106722898	-5.423410169656
H	-0.540657823552	5.623362278399	-3.652921769736
H	6.346982862635	-3.274424156280	-13.829012533616
H	6.011852088281	-1.692898866023	-14.615790511780
H	6.266875617147	-1.769627887557	-12.855755408530
H	2.484155143789	-5.634233132849	-16.917929087302
H	3.082541928445	-4.109917602251	-17.658102488257
H	3.469657831590	-4.479710105433	-15.962273474053
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Na	9.173282503413	5.392906730197	-6.673761415959
Na	10.855855192161	-1.353419623099	-10.526294596821
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Na	1.402945378765	-9.402206707377	-17.100085323034

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T2A2T2 sing. ion. E(UB3LYP-D)=-8537.76112996 Hartree

O	-0.352848372816	6.918396670293	0.947549406349
C	0.817428310713	6.648726820647	1.703148010255
C	1.850993435771	5.936811797802	0.842262174471
O	1.395527033029	4.624595033621	0.491935448275
C	2.164778968846	6.632988625755	-0.493468067989
C	3.511742131327	6.302685044111	-0.841529412709
O	1.182610002332	5.953899946248	-1.440374010905
C	1.228158998927	4.515841959824	-0.917036296111
N	0.039004251166	3.726132537608	-1.208662593575
C	0.194769669893	2.452724780355	-1.753075142141
O	1.272967401304	1.905550879050	-1.908815904792
N	-0.996420735842	1.857494537188	-2.125529300477
C	-2.301018884489	2.339182821373	-1.948833860851
O	-3.258960445837	1.694230721774	-2.348620665961
C	-2.372298480035	3.615075212633	-1.236813747577
C	-3.727685118198	4.171919526265	-0.909322928943
C	-1.211295515470	4.229671508673	-0.898594853031
P	4.247020792237	6.992472356080	-2.143950405149
O	4.519908598235	8.461498879965	-1.893909183617
O	3.484516050592	6.709474454914	-3.436331627801
O	5.657962310231	6.175598453363	-2.083682563538
C	5.900335136210	4.892474788586	-1.514602068496
C	5.7151177813	3.744331598875	-2.492351414068
O	4.330694827541	3.429645618569	-2.664620771410
C	6.284773970344	4.008721478509	-3.913254547150
O	7.102036427101	2.89206510818	-4.271249755404
C	5.025962968574	4.057664712734	-4.779046008697
C	4.164133746532	3.044486103756	-4.025782277341
N	2.753709885940	2.998161276179	-4.351705683247
C	2.173773431773	1.760520289443	-4.624866765570
O	2.794257145682	0.711296135663	-4.678971463957
N	0.820647643726	1.823580689506	-4.892511786349
C	0.002425138196	2.953788890583	-4.950529967326
O	-1.166516805176	2.849896799705	-5.306211955661
C	0.671802785559	4.193672640958	-4.577102773774
C	-0.146649142796	5.451955926394	-4.527562050777
C	2.003318986545	4.155088265715	-4.305994821703
P	8.246916749322	3.065921266683	-5.435471083336
O	9.254528909239	4.126817433200	-5.040621021080
O	7.620493945639	3.281979672382	-6.811829440871
O	8.924619171342	1.584670241004	-5.345166584871
C	8.473218199255	0.432406300502	-4.638225420384
C	7.778462591072	-0.573928066488	-5.54390044080
O	6.430234019636	-0.166448284314	-5.830128420788
C	8.465429571123	-0.748786629397	-6.914830214556
O	8.376763562705	-2.128243651954	-7.273117471562
C	7.581027229384	0.100232475769	-7.827055625779
C	6.218170962011	-0.246934425483	-7.233005570435
N	5.114562167285	0.625943114451	-7.579613871513
C	5.139005173050	1.975488160071	-7.784237219123
N	3.924473496913	2.513560309756	-7.922626445608
C	3.076604357243	1.470926413355	-7.787014650467
N	1.651643602108	1.383846479236	-7.740353923538
N	0.881529363204	2.457189800031	-7.916044529542

N	1.094783108358	0.185857290970	-7.467768014093
C	1.888341026983	-0.868531783426	-7.300498584716
N	3.240039644326	-0.919177204579	-7.334889278755
C	3.779068619272	0.259175078956	-7.561799745137
P	9.304713195652	-2.745459254978	-8.481068917457
O	10.770673990242	-2.723927993143	-8.098152960372
O	8.998020169474	-2.085869086005	-9.823587179653
O	8.743222100063	-4.277764339491	-8.469296062626
C	7.652448377953	-4.826138586297	-7.735566376929
C	6.389016144924	-4.950966865689	-8.572845830843
O	5.752670276369	-3.673087585961	-8.735605789591
C	6.636115066110	-5.488005430581	-10.001215377656
O	5.562159389739	-6.372312098441	-10.320584788694
C	6.562670252112	-4.215227623573	-10.843816247539
C	5.433747097437	-3.501561729290	-10.110541455472
N	5.291043508428	-2.093032439810	-10.391307221853
C	6.274520840244	-1.167631805334	-10.629155543632
N	5.810145057761	0.061735730812	-10.796526887296
C	4.463322147666	-0.066025678783	-10.658893408146
C	3.387543852214	0.859063301786	-10.743132409096
N	3.589368013064	2.154625934254	-10.983066070961
N	2.125569391637	0.401632228839	-10.551780960200
C	1.938425949366	-0.890451350824	-10.301901530971
C	2.872231701318	-1.858797227037	-10.206752842470
N	4.099276045729	-1.401656501649	-10.395132174254
P	5.606363118360	-7.283653445810	-11.689379274012
O	6.776090790052	-8.246073775931	-11.652069375894
O	5.555863187531	-6.414092704435	-12.943938087419
O	4.211874960433	-8.102178180669	-11.479028727838
C	3.116225130101	-7.762647544222	-10.631893106577
C	2.05944420043	-6.914175362038	-11.319230027179
O	2.474309399603	-5.547213626308	-11.422660121302
C	1.717582596156	-7.377413658639	-12.759422058944
O	0.295022050222	-7.418591855906	-12.877416550370
C	2.309183605508	-6.259288009787	-13.617236928226
C	2.037066833097	-5.072637530780	-12.695490441235
N	2.697068883032	-3.817796970791	-13.001391243095
C	1.941972555608	-2.646527637576	-12.948939268728
O	0.761408246541	-2.603093606318	-12.648073765668
N	2.650674518199	-1.507360631471	-13.278965091984
O	4.005251773270	-1.389915513925	-13.611758107818
O	4.489554116616	-0.292058250620	-13.848298101380
C	4.726597828731	-2.657766584165	-13.599839066325
C	6.194159311031	-2.643847480001	-13.914427051417
O	4.047957544959	-3.793214694962	-13.290483172031
P	-0.410639281632	-8.091878444272	-14.202296118401
O	-0.015398810911	-9.549758152000	-14.331813660923
O	-0.164351568285	-7.265059066438	-15.462439519450
O	-1.967333762985	-7.993785997754	-13.722537924324
C	-2.520898310708	-7.091159955699	-12.770126226358
C	-2.909760359826	-5.742196313485	-13.349216327140
O	-1.758787874251	-4.925291686728	-13.572196021864
C	-3.686131133018	-5.804108247772	-14.693073419613
O	-4.906856185768	-5.098343157382	-14.511327732931
C	-2.736589275400	-5.088913815879	-15.662358758235
C	-2.049451029031	-4.115070227607	-14.703606120726
N	-0.839326798894	-3.472865647977	-15.180065029932
C	-0.757157584247	-2.079198513756	-15.134538804298
O	-1.650913508856	-1.352681716429	-14.738623326114
N	0.439948657692	-1.577996656376	-15.616903858053
C	1.554341028076	-2.283757782129	-16.085378129411
C	2.556351926576	-1.684106917689	-16.455903244239
1	1.388975463680	-3.732161443571	-16.06788288136
C	2.536814152056	-4.577492372267	-16.542160532494
C	0.214325241778	-4.248874899830	-15.618446917038
H	1.270108355290	7.586887415498	2.084291607900
H	0.590944013040	5.996611581586	2.569672533817
H	2.777671782496	5.84540548268	1.434336251623
H	2.043365159325	7.727717641676	-0.4389294220129
H	0.187430909503	6.397090640571	-1.306443979876
H	2.077679565042	3.970042391225	-1.354382392361
H	-1.195210625969	5.164307874391	-0.330540944421
H	-0.906341743821	0.947541736403	-2.572023581657
H	1.495247127203	6.039765290378	-2.483635985915
H	6.956553538103	4.896774652629	-1.195748735431
H	5.261290630055	4.730030024028	-0.631435689526
H	6.237208273470	2.863281404810	-2.074159794957
H	6.875943302010	4.936523975584	-3.950813479487
H	4.571555071019	5.058013142166	-4.706265739333
H	4.553455257998	2.027451945827	-4.187865197103
H	2.564182023656	5.055854432443	-4.024960305826
H	0.400279235680	0.945294975404	-5.191777931545
H	5.227051158314	3.785925380974	-5.823878740434
H	9.372312776337	-0.050312919052	-4.217465793879
H	7.798011907172	0.713114198202	-3.814429790810
H	7.756571665802	-1.545873879144	-5.020145789858
H	9.517262539725	-0.422685038504	-6.899100553591
H	7.795457079150	1.166936653097	-7.659473706401
H	5.903576097590	-1.265346058001	-7.521512682999
H	6.082099063912	2.534621385285	-7.733734634194
H	1.385814804098	-1.821772167992	-7.101415195425
H	1.304604305271	3.365382925890	-8.085477146368
H	-0.125439784976	2.388625565687	-7.782114325833
H	7.706506943024	-0.163335289028	-8.881198198973
H	7.959024408941	-5.840613505578	-7.426175941454
H	7.439656489449	-4.226812122767	-6.836218015325
H	5.698753091877	-5.633637876095	-8.045908775475
H	7.599789825473	-6.014021687397	-10.090074805655
H	7.497675753425	-3.645272297906	-10.727891007570
H	4.456277612721	-3.959689544375	-10.342018173437
H	7.331500436666	-1.460642762315	-10.596481433321
H	0.901941751564	-1.211600517502	-10.166071828135
H	4.530757240827	2.507318693096	-11.129061737012
H	2.802909315315	2.799641100217	-10.983163426742
H	6.347195804157	-4.423774510791	-11.897524322792
H	2.645922879609	-8.718705642263	-10.345208588048
H	3.469390502397	-7.251295144506	-9.721989245608
H	1.138867416890	-6.969044185104	-10.708793957683
H	2.139834945455	-8.368212720311	-12.988805793513
H	3.392561117872	-6.418386987409	-13.725591338975
H	0.957645165763	-4.855469391476	-12.676660025633
H	4.555183853240	-4.764902434465	-13.229580472237
H	2.109017497092	-0.646380677757	-13.267315586233
H	1.814237098841	-6.192451214315	-14.590633480390
H	-3.840730223132	-7.572120260682	-12.396203029994
H	-1.827062709556	-6.943762529762	-11.926406148905
H	-3.569427833148	-5.245314109883	-12.611471145865
H	-3.876933727908	-6.847414329655	-14.998463237640

H	-1.995407852137	-5.803343780629	-16.054294428662
H	-2.742880897782	-3.306495833833	-14.426237670227
H	0.042883000914	-5.332902296133	-15.563766976642
H	0.518806893080	-0.563497110250	-15.605902093139
H	-3.272066152088	-4.587881354973	-16.485530017787
H	-5.405747665811	-5.148350502229	-15.344139580302
H	-1.034095777125	7.268679874594	1.544626090911
H	-3.638727322076	5.131276719414	-0.370756307744
H	-4.315482002838	4.335739927816	-1.832449203896
H	-4.305154240687	3.464450164534	-0.284237450009
H	0.498142884518	6.340782013540	-4.429020072950
H	-0.757313581843	5.549117573893	-5.443651908604
H	-0.848260480962	5.432243029784	-3.670722568229
H	6.588826890180	-3.670834495512	-13.990570489125
H	6.379771864371	-2.116043817810	-14.868166115795
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H	2.917359033195	-4.201356075067	-17.509414631819
H	3.380177941811	-4.538754056922	-15.826058557121
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O	-0.022219834644	7.450699635530	0.954922274331
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C	2.155731465492	6.408337652450	0.946559542697
C	1.663934824003	5.082649672522	0.717213723226
C	2.487989387428	6.970468211381	-0.446521807346
O	3.827065624071	6.577171633678	-0.760084402506
C	1.489727059875	6.231742922901	-1.330384398242
N	1.501338729859	4.847903387193	-0.676798773945
N	0.295325011536	4.061094482825	-0.901083324475
C	0.425800156635	2.738391533822	-1.320789124662
O	1.492258248027	2.159014242222	-1.426675992124
N	-0.778571357780	2.131457102805	-1.628488166980
C	-2.072795307306	2.653232906632	-1.499404923708
O	-3.044483202663	1.991087625315	-1.832625978867
C	-2.117587312139	3.994329102051	-0.916666907273
C	-3.460865305911	4.607524721225	-0.644618717489
C	-0.944146990428	4.617099223729	-0.642137461427
P	4.572431073464	7.153123224253	-2.111381966174
O	4.851060231875	8.636429263824	-1.978896200237
O	3.811253083791	6.770894260451	-3.378508139282
C	5.978484355636	6.337177786196	-1.981322755931
C	6.210486933735	5.081670641417	-1.347894670212
C	6.006117227514	3.879513096818	-2.257186132362
O	4.619568682868	3.551177284656	-2.370021476566
C	6.534908059412	4.066603973378	-3.706419072988
C	7.37273221118	2.95383917216	-4.022821265265
O	5.253874492418	4.044218760149	-4.539653190593
C	4.412845198429	3.083389213487	-3.700815791249
N	2.993467826944	3.02264942208	-3.985573640594
C	2.393422974795	1.769092386257	-4.130570860755
O	2.992935897770	0.711596338707	-4.061619656340
N	1.040135540107	1.828446491616	-4.408706498482
C	0.230341135074	2.955589776067	-4.535478510118
O	-0.951493179526	2.837347951256	-4.846988899848
O	0.918702290779	4.215283456019	-4.284839174280
C	0.115954510301	5.483415556470	-4.337646746329
C	2.254879085242	4.185420130234	-4.035316427547
P	8.422219225118	3.095417346914	-5.286780098926
O	9.491369753867	4.127504746780	-4.981850593804
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T2A3T sing. ion. E(UB3LYP-D)=-8550.93507205 Hartree

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H	3.124807165799	6.003406194064	1.523470021163
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H	0.257640529161	6.408724899477	-0.955406825188
H	2.222927350786	4.050692256289	-1.156202087623

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H	-0.751383949172	0.898205293046	-2.014480079109
H	1.457058709454	6.077204337956	-2.250846385276
H	7.073471183713	5.191589832185	-1.490180100764
H	5.452515728872	4.961023053359	-0.755183950462
H	6.365003933107	3.112768536059	-2.261696677860
H	6.708640082153	5.176089456143	-4.225999469094
H	4.339035257288	5.171090911108	-4.749515163380
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H	2.413955580010	5.092520075546	-3.866356969467
H	0.344481648592	0.870666421283	-4.77522372751
H	4.941573357118	3.904168489357	-5.901234804859
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H	7.798287405380	0.993729137966	-4.135826050885
H	7.675857552866	-1.281569403733	-5.289940538496
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H	7.389406597536	1.357076322557	-7.997815652628
H	5.580950883721	-1.107287936672	-7.594268068933
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H	-0.546667998946	2.310876705406	-7.244401947169
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TA4T neut. E(RB3LYP-D)=-8564.31247536 Hartree

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C	1.516032890063	5.809687143653	-1.591445099765
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O	1.585321195453	1.823952039096	-1.064298417897
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C	-2.085037767606	3.613169037352	-1.005099159816
C	-3.452224164454	4.230119203395	-0.935056482406
C	-0.942791235730	4.295440263394	-0.735445555241
P	4.545558790405	7.153496678011	-2.191127502419
O	4.837226329351	8.626819747434	-1.984535004455
O	3.823405382753	6.832004656588	-3.494607775468
O	5.941615156965	6.323724383531	-2.040707937936
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C	2.434968777781	2.062106081577	-4.085439813745
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C	7.980287962607	-0.480115259875	-5.381549167815

O	6.616189183259	-0.045458615282	-5.453255123458
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C	8.328785310432	-2.021334383550	-7.201669209221
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C	6.188662542709	-0.125844124742	-6.813746476172
N	5.045542732569	0.719308797165	-7.013611904916
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C	2.969219917454	1.444385888653	-7.184205427942
C	1.569617140745	1.262053097255	-7.167214597080
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C	1.944449587617	-0.983411692977	-6.768676710464
N	3.276815362067	-0.941691988514	-6.756565090859
C	3.736253551746	0.294435277317	-6.959570813685
P	9.007473437661	-2.563552298659	-8.598128657013
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O	8.509350422519	-4.116331331381	-8.546335416749
C	7.488919368836	-4.725451294899	-7.760205508311
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O	5.398446894008	-3.738962916683	-8.531865354011
C	6.379694461933	-5.332708485157	-10.003268815420
O	5.372486423008	-6.297451022034	-10.338145914624
C	6.122479605983	-4.007302137296	-10.717027166355
C	4.961683061481	-3.496727980529	-9.870615977865
N	4.607410131560	-2.114746188317	-10.017699668314
C	5.444899445566	-1.031627540578	-10.170442544552
N	4.804829433262	0.113962755037	-10.250396387811
C	3.471599442255	-0.230955425554	-10.147305014337
C	2.276345919199	0.518844231869	-10.147121040622
N	2.271827308501	1.880567522409	-10.242802114578
N	1.108629234802	-0.136567667649	-10.072291508044
C	1.117940993141	-1.470699314055	-9.965062066147
N	2.172984835646	-2.283571229831	-9.906773891739
C	3.324076372511	-1.615756109137	-10.007386808940
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O	5.440751066454	-6.175257037471	-12.955317477099
O	4.099258635799	-7.990191181603	-11.657602245973
C	2.948403032728	-7.790490723608	-10.840405341921
C	1.780904575036	-7.143792010559	-11.580019015323
O	1.906570426857	-5.716654828390	-11.591058253701
C	1.654084473710	-7.574976209549	-13.059269909091
O	0.264492212382	-7.745080037848	-13.350107039573
C	2.221059241394	-6.363962847699	-13.794397566884
C	1.674405734615	-5.240410360982	-12.917855133278
N	2.292974617955	-3.951416003822	-13.073073770339
C	3.645664454895	-3.681131165006	-13.117853422459
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C	2.685189095789	-1.783661344575	-13.162053120643
C	2.283525291419	-0.429727620258	-13.180347283731
N	3.178536972940	0.595417720661	-13.169186099585
N	0.967446274637	-0.152423665623	-13.206449577382
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N	0.344810238368	-2.469277416452	-13.048971050817
C	1.654160350682	-2.730270105995	-13.091489489528
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O	0.183623756540	-7.560278041871	-15.972134319314
O	-1.824033623999	-8.399173075169	-14.519601457381
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O	-1.827798487126	-5.306777639943	-14.426906112468
C	-3.489570382893	-6.344479890779	-15.805734431337
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C	-2.441046863790	-5.594694363472	-16.637531309097
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N	-0.771351031995	-3.819093193093	-15.910096298065
C	-0.799961197435	-2.424591641494	-15.864886079778
O	-1.800214174162	-1.766896344331	-15.632151666105
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C	1.594394614314	-3.910854016058	-16.372308994824
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