Duplex DNA Retains the Conformational Features of Single-Strands: Perspectives from MD Simulations and Quantum Chemical Computations

– Supplementary Materials –

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Rigid coordinates

Shift, slide and Rise are expressed in Å; tilt, roll and twist in degrees. Please note that the same order as in the following ds-5′-C T G G G G A C T T T C C A G G-3′ has been considered for all the double helices (both experimental and predicted geometries), when the analysis has been carried out in terms of the rigid coordinates of the individual single strands composing the duplex.

Rigid coordinates extracted from experimental structures

Table S1: Local base-step parameters for the individual single strands composing the ds-5′-C T G G G G A C T T T C C A G G-3′ sequence, as stored in the 1kbd PDB file, method: NMR (solution).

step	Shift	Slide	Rise	Tilt	Roll	Twist
5′-C/T	-1.90	-0.79	3.03	12.60	-35.95	30.45
T/G	1.98	-0.27	3.24	9.10	0.11	36.16
G/G	-0.14	-0.71	3.46	-1.29	0.99	35.31
G/G	0.02	-1.63	4.01	-6.33	-12.33	34.40
G/G	0.03	-1.69	3.84	-2.74	-13.28	34.96
G/A	0.29	-1.18	3.37	2.38	-5.99	36.44
A/C	0.15	-1.39	3.64	-4.91	-4.40	35.93
C/T	-0.75	-1.92	3.72	-4.20	-14.21	30.80
T/T	-0.22	-0.81	2.98	7.93	-13.52	36.36
T/T	0.39	-0.31	2.93	8.14	-5.49	38.87
T/C	1.17	-0.86	3.24	1.21	5.82	36.29
C/C	-0.33	-1.82	3.79	-11.49	5.67	32.67
C/A	-0.55	-2.01	3.21	9.86	-14.04	26.65
A/G	0.41	-1.28	3.29	4.34	2.71	30.11
G/G	0.49	-1.27	3.52	0.28	-2.34	36.92
C/C	-0.82	-1.50	3.42	-1.10	-17.10	35.59
C/T	-0.57	-1.35	3.05	5.12	-5.77	28.44
T/G	0.25	-1.95	3.42	-0.27	2.87	28.26
G/G	0.14	-1.77	3.59	-3.38	-0.07	32.77
G/A	-0.32	-0.87	3.30	3.50	-4.73	35.93
A/A	0.03	-0.07	3.19	5.48	-4.04	38.94
A/A	0.52	-0.19	3.23	5.56	-3.03	37.30
A/G	0.55	-1.61	3.86	-5.69	-0.06	33.05
G/T	0.14	-1.30	3.41	2.03	-6.21	36.18
T/C	0.15	-1.19	3.44	-4.93	0.30	36.55
C/C	-0.31	-1.71	3.87	-8.76	-11.31	33.73
C/C	-0.74	-2.15	3.83	-8.38	-15.70	30.94
C/C	-0.46	-1.20	3.26	1.42	-13.13	35.18
C/A	-1.86	0.01	3.43	11.02	-24.41	31.51
A/G-3′	1.44	-0.21	3.38	3.15	-0.75	38.16

Table S2: Local base-step parameters for the individual single strands composing the ds-5′-C G C G A A A A A A C G-3′ sequence, as stored in the 1d89 PDB file, Method: X-ray diffraction.

step	Shift	Slide	Rise	Tilt	Roll	Twist
C/G	-0.14	1.58	3.81	6.53	9.14	34.01
G/C	2.52	0.86	3.33	6.87	-11.64	46.17
C/G	-0.74	0.66	2.86	11.91	10.99	24.82
G/A	1.00	-0.09	3.32	2.69	1.62	44.61
A/A	0.22	-0.08	3.25	4.21	-1.30	31.44
A/A	0.72	-0.42	3.20	4.10	-2.79	37.36
A/A	0.79	-0.22	3.07	6.41	2.16	39.12
A/A	0.17	-0.20	3.19	3.32	-0.60	29.76
A/A	0.81	-0.13	3.33	1.02	-0.26	36.72
A/C	0.90	-0.33	2.76	11.73	6.61	31.00
C/G	0.89	-0.77	3.75	-4.62	11.30	29.79
C/G	-0.88	-0.77	3.93	-11.10	-1.34	33.04
G/T	0.86	-0.61	3.20	7.69	8.16	39.08
T/T	0.02	0.02	2.37	18.74	-2.63	28.76
T/T	0.74	0.20	3.40	3.75	2.70	35.82
T/T	0.47	-0.32	3.79	-1.84	4.31	35.97
T/T	0.71	-0.73	3.40	0.74	-3.46	37.02
T/T	0.67	-0.46	3.44	0.96	-9.21	34.00
T/C	0.26	-0.69	2.82	9.51	-1.35	36.84
C/G	0.73	0.66	3.00	10.74	4.61	31.09
G/C	-0.12	1.20	2.89	10.56	-3.39	42.44
C/G	0.26	2.29	3.69	1.09	4.36	33.94

Table S3: Local base-step parameters for the individual single strands composing the 5′-G G C A A A A A A C G G- 3′ sequence, as stored in the 1fzx PDB file, method: NMR (solution).

step	Shift	Slide	Rise	Tilt	Roll	Twist
G/G	-0.02	-0.97	3.09	2.41	1.47	32.54
G/C	0.31	-0.85	2.69	8.71	0.85	33.51
C/A	0.47	-0.56	3.29	4.39	6.32	31.87
A/A	0.44	-0.52	3.04	4.42	0.35	38.06
A/A	0.39	-0.38	3.07	4.72	-0.92	32.97
A/A	0.64	-0.82	3.13	1.30	1.50	39.89
A/A	0.52	-0.84	3.01	2.43	-1.08	38.99
A/A	0.27	-0.90	3.26	-0.99	-3.31	37.68
A/C	0.11	-1.34	3.12	-1.85	-0.19	35.70
C/G	-0.52	-0.99	2.09	13.13	4.94	30.67
G/G	-0.18	-0.70	3.11	-1.15	7.21	33.49
C/C	0.91	-0.40	2.80	11.33	9.82	30.96
C/G	0.34	-0.67	3.25	4.91	9.71	28.03
G/T	1.62	-0.68	2.77	8.16	-3.83	39.54
T/T	0.83	-0.76	2.98	4.27	5.79	38.67
T/T	0.24	-1.16	2.98	4.46	-0.58	31.86
T/T	0.29	-1.37	2.95	4.55	-5.12	33.64
T/T	0.94	-1.04	3.16	2.55	-3.17	36.41
T/T	0.18	-0.99	2.70	8.60	-0.13	34.50
T/G	-0.07	-0.89	2.72	4.21	9.03	35.69
G/C	0.75	-0.49	2.97	4.90	-4.37	34.47
C/C	1.61	-0.02	2.76	10.42	6.42	38.23

Rigid coordinates extracted from optimized (DFT/PCM) geometries

Table S4: Local base-step parameters for ss-T6 [B3LYP-D3/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
T/T	-0.71	-0.26	2.35	16.80	-15.52	27.06
T/T	0.16	0.29	2.54	12.23	-4.34	34.50
T/T	0.24	0.42	2.56	12.02	-1.55	34.31
T/T	0.33	0.38	2.59	11.19	-1.30	34.93
T/T	0.36	0.19	2.70	9.38	-3.54	35.42
ave.	0.08	0.20	2.55	12.32	-5.25	33.24

Table S5: Local base-step parameters for ss-A6 [B3LYP-D3/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
A/A	0.33	1.11	3.11	3.07	10.40	30.71
A/A	0.57	0.75	3.07	5.20	7.30	37.15
A/A	0.68	0.73	3.12	4.46	3.51	39.02
A/A	0.68	0.61	3.16	3.35	2.82	39.54
A/A	0.65	0.36	3.24	0.53	3.55	41.12
ave.	0.58	0.71	3.14	3.32	5.51	37.51

Table S6: Local base-step parameters for the individual single strands composing the ds-A4 sequence optimized at the B3LYP-D3/6-31G(d,p) level

step	Shift	Slide	Rise	Tilt	Roll	Twist
A/A	0.89	1.53	2.89	15.87	-0.47	36.94
A/A	0.96	1.49	3.14	3.84	1.07	42.02
A/A	0.14	1.72	3.20	2.17	-5.36	47.22
T/T	1.15	1.56	3.13	9.91	-18.53	48.15
T/T	0.72	0.65	3.42	-0.11	-11.43	42.01
T/T	0.42	0.19	3.05	5.09	-7.97	39.66

Table S7: Local base-step parameters for ds-A4 [B3LYP-D3/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
AA/TT	-0.22	0.87	3.11	-5.38	-4.10	39.68
AA/TT	0.50	1.63	3.24	3.85	-12.05	48.31
AA/TT	-0.13	1.07	3.41	-1.97	-5.20	42.68
ave.	0.05	1.19	3.25	-1.17	-7.12	43.56

Table S8: Local base-step parameters for ss-C6 [B3LYP-D3/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
C/C	-0.46	0.31	2.45	16.39	-10.72	29.23
C/C	0.19	0.54	2.81	8.12	-0.29	33.90
C/C	0.11	0.44	2.70	10.24	-1.52	33.49
C/C	0.14	0.45	2.76	9.32	-0.31	33.77
C/C	0.16	0.31	2.97	5.49	-0.53	35.21
ave.	0.03	0.41	2.74	9.91	-2.67	33.12

Table S9: Local base-step parameters for ss-G6 [B3LYP-D3/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
G/G	1.06	0.82	3.12	11.77	-8.73	40.46
G/G	1.06	0.89	3.09	7.09	-4.10	41.29
G/G	1.12	0.76	3.03	9.15	-4.47	41.18
G/G	1.36	0.50	3.05	8.29	-6.45	41.36
G/G	1.48	0.24	2.98	8.88	-3.53	55.91
ave.	1.22	0.64	3.05	9.04	-5.46	44.04

Table S10: Local base-step parameters for the individual single strands composing the ds-G4 sequence optimized at the B3LYP-D3/6-31G(d,p) level

step	Shift	Slide	Rise	Tilt	Roll	Twist
G/G	1.53	1.40	3.23	12.56	-10.29	42.76
G/G	1.20	0.87	3.29	4.19	-7.28	41.39
G/G	0.36	-0.10	3.26	2.19	-3.24	40.20
C/C	0.13	0.51	3.14	5.62	-14.49	40.02
C/C	0.11	0.85	3.58	-2.38	-6.24	41.43
C/C	-0.35	0.81	3.79	-6.75	-15.13	43.97

Table S11: Local base-step parameters for ds-G4 [B3LYP-D3/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
GG/CC	0.97	1.11	3.58	9.74	-12.75	43.67
GG/CC	0.56	0.85	3.50	3.33	-6.78	41.48
GG/CC	0.11	0.21	3.23	-1.65	-8.91	40.05
ave.	0.55	0.72	3.43	3.81	-9.48	41.74

Table S12: Local base-step parameters for ss-AACCAA [B3LYP-D3/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
A/A	0.28	1.09	3.12	2.51	10.97	28.48
A/C	0.58	0.08	2.66	9.90	4.45	35.14
C/C	0.35	0.50	2.63	11.91	-0.53	35.61
C/A	1.32	1.22	2.94	9.47	1.16	41.30
A/A	0.73	0.38	3.23	0.77	6.55	40.63
ave.	0.65	0.65	2.92	6.91	4.52	36.23

Table S13: Local base-step parameters for ss-T6 (B3LYP-D3/TZVP)

step	Shift	Slide	Rise	Tilt	Roll	Twist
T/T	0.19	0.48	2.78	8.65	-2.32	33.07
T/T	-0.22	-0.05	2.63	11.70	-6.99	31.09
T/T	-0.33	-0.14	2.59	12.40	-8.49	30.63
T/T	-0.13	0.00	2.59	12.74	-6.31	31.94
T/T	-0.01	0.01	2.71	10.53	-6.55	33.30
ave.	-0.10	0.06	2.66	11.20	-6.13	32.01

Table S14: Local base-step parameters for ss-A6 (B3LYP-D3/TZVP)

step	Shift	Slide	Rise	Tilt	Roll	Twist
A/A	0.24	1.49	3.28	1.78	-0.78	40.77
A/A	1.00	-0.15	3.51	-7.15	10.82	51.17
A/A	1.63	1.47	3.18	4.98	13.34	34.29
A/A	0.32	1.77	3.16	3.77	0.89	43.20
A/A	0.80	0.16	3.35	-1.91	8.20	46.64
ave.	0.80	0.94	3.30	0.29	6.49	43.21

Table S15: Local base-step parameters for the individual single strands composing the ds-A4 sequence optimized at the B3LYP-D3/TZVP level

step	Shift	Slide	Rise	Tilt	Roll	Twist
A/A	0.34	1.98	2.97	8.04	-0.55	45.40
A/A	0.30	1.86	3.11	5.13	-3.86	45.68
A/A	0.50	1.52	3.31	0.50	-5.63	48.16
T/T	0.71	1.32	3.12	9.34	-18.23	44.95
T/T	1.06	0.94	3.43	1.49	-10.58	44.01
T/T	0.62	0.76	3.08	8.11	-13.77	46.12

Table S16: Local base-step parameters for ds-A4 (B3LYP-D3/TZVP)

AA/TT	0.14	1.36	3.12	0.10	-7.31	46.94
AA/TT	0.35	1.40	3.38	-1.82	-7.32	45.40
AA/TT	0.12	1.41	3.28	4.46	-12.00	47.10
ave.	0.21	1.39	3.26	0.91	-8.88	46.48

Table S17: Local base-step parameters for ss-C6 (B3LYP-D3/TZVP)

step	Shift	Slide	Rise	Tilt	Roll	Twist
C/C	-0.43	0.33	2.82	11.05	-8.68	29.66
C/C	-0.17	0.30	3.04	5.70	-2.42	32.33
C/C	-0.22	0.21	2.95	7.23	-3.93	32.23
C/C	-0.32	-0.02	3.18	3.05	-4.14	32.07
C/C	0.92	-0.64	4.20	-12.56	13.83	46.36
ave.	-0.04	0.04	3.24	2.89	-1.07	34.53

Table S18: Local base-step parameters for ss-G6 (B3LYP-D3/TZVP)

step	Shift	Slide	Rise	Tilt	Roll	Twist
G/G	1.28	1.05	3.14	8.14	-4.12	40.81
G/G	1.30	0.89	3.11	8.11	-3.61	41.87
G/G	1.29	0.82	3.08	10.26	-4.16	41.77
G/G	1.16	0.87	3.21	5.94	-7.40	47.54
G/G	1.52	0.40	3.17	6.07	-5.09	57.26
ave.	1.31	0.81	3.14	7.70	-4.88	45.85

Table S19: Local base-step parameters for the individual single strands composing the ds-G4 sequence optimized at the B3LYP-D3/TZVP level

step	Shift	Slide	Rise	Tilt	Roll	Twist
G/G	0.96	0.99	3.30	5.31	-5.72	39.24
G/G	0.17	1.96	3.39	3.96	-9.59	48.29
G/G	0.37	1.45	3.61	-3.27	-10.36	49.37
C/C	0.91	2.09	3.21	10.27	-6.19	51.13
C/C	1.12	1.66	3.69	-5.00	-5.04	48.58
C/C	-0.45	0.02	3.77	-7.46	-5.53	37.54

Table S20: Local base-step parameters for ds-G4 (B3LYP-D3/TZVP)

step	Shift	Slide	Rise	Tilt	Roll	Twist
GG/CC	0.72	0.53	3.58	6.37	-5.66	38.35
GG/CC	-0.45	1.82	3.61	4.49	-7.30	48.31
GG/CC	-0.29	1.77	3.49	-6.87	-8.31	50.64
ave.	-0.01	1.37	3.56	1.33	-7.09	45.76

Table S21: Local base-step parameters for ss-AACCAA (B3LYP-D3/TZVP)

step	Shift	Slide	Rise	Tilt	Roll	Twist
A/A	0.18	1.67	3.17	3.72	0.92	37.34
A/C	0.19	-0.01	3.00	6.09	-1.08	33.33
C/C	-0.25	0.22	2.94	7.77	-3.29	32.26
C/A	0.69	0.98	3.14	4.07	-2.41	46.58
A/A	0.78	0.07	3.36	-2.00	8.71	47.45
ave.	0.31	0.59	3.12	3.93	0.57	39.39

Table S22: Local base-step parameters for ss-T6 [M06-2X/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
T/T	-0.70	-0.39	2.19	16.52	-14.97	27.47
T/T	0.08	0.22	2.35	13.19	-8.96	35.67
T/T	0.03	0.07	2.40	12.26	-8.92	34.78
T/T	-0.25	-0.16	2.36	13.35	-11.37	31.51
T/T	-0.01	0.03	2.33	14.27	-13.80	38.69
ave.	-0.17	-0.05	2.33	13.92	-11.60	33.62

Table S23: Local base-step parameters for ss-A6 [M06-2X/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
A/A	0.11	1.56	2.85	6.03	9.17	28.20
A/A	0.37	1.44	2.75	10.38	8.75	32.18
A/A	0.46	1.10	2.94	6.39	6.30	32.85
A/A	0.70	0.22	3.12	0.16	4.80	41.07
A/A	1.08	-0.10	3.14	-1.97	6.80	51.75
ave.	0.54	0.84	2.96	4.20	7.16	37.21

Table S24: Local base-step parameters for the individual single strands composing the ds-A4 sequence optimized at the M06-2X/6-31G(d,p) level

step	Shift	Slide	Rise	Tilt	Roll	Twist
A/A	1.12	1.10	2.97	4.92	6.00	33.70
A/A	1.03	0.32	2.95	5.81	3.38	42.06
A/A	0.59	0.07	3.04	0.51	2.29	46.93
T/T	-0.04	0.06	2.62	9.43	-14.94	36.93
T/T	0.08	0.17	3.00	2.93	-9.22	39.06
T/T	0.39	0.16	2.91	3.83	-4.75	39.22

Table S25: Local base-step parameters for ds-A4 [M06-2X/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
AA/TT	-0.35	0.60	3.07	-0.68	0.56	37.34
AA/TT	-0.47	0.23	3.03	-1.62	-3.03	41.12
AA/TT	-0.30	0.07	2.84	4.72	-6.19	42.19
ave.	-0.37	0.30	2.98	0.81	-2.89	40.22

Table S26: Local base-step parameters for ss-C6 [M06-2X/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
C/C	-0.94	-0.25	2.44	13.05	-17.59	25.91
C/C	-0.48	-0.06	2.40	12.35	-8.40	31.28
C/C	-0.14	0.10	2.46	11.69	-5.18	33.32
C/C	-0.09	0.22	2.53	10.42	-4.91	33.63
C/C	0.13	0.21	2.83	4.56	-8.30	42.16
ave.	-0.31	0.04	2.53	10.41	-8.88	33.26

Table S27: Local base-step parameters for ss-G6 [M06-2X/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
G/G	1.01	1.25	2.94	7.51	-2.47	41.83
G/G	1.14	1.13	2.94	7.58	-2.30	42.24
G/G	1.15	0.98	2.93	9.12	-3.08	41.71
G/G	1.29	0.46	3.03	6.18	-5.69	41.26
G/G	1.42	0.04	2.85	7.96	-1.73	54.28
ave.	1.20	0.77	2.94	7.67	-3.05	44.26

Table S28: Local base-step parameters for the individual single strands composing the ds-G4 sequence optimized at the M06-2X/6-31G(d,p) level

step	Shift	Slide	Rise	Tilt	Roll	Twist
G/G	0.75	1.18	2.99	6.89	-3.35	40.38
G/G	1.02	1.46	3.06	5.66	-4.94	47.08
G/G	-0.56	1.54	3.35	-1.37	-11.70	43.60
C/C	1.48	2.08	2.62	15.92	-12.52	46.65
C/C	0.24	1.00	3.77	-9.06	-0.65	47.80
C/C	-0.04	0.13	3.35	-3.86	-5.20	39.92

Table S29: Local base-step parameters for ds-G4 [M06-2X/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
GG/CC	0.41	0.67	3.23	5.37	-4.32	40.28
GG/CC	0.44	1.25	3.48	7.47	-2.74	47.19
GG/CC	-1.06	1.81	3.04	-8.73	-12.22	45.78
ave.	-0.07	1.24	3.25	1.37	-6.43	44.42

Table S30: Local base-step parameters for ss-AACCAA [M06-2X/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
A/A	0.17	1.38	2.90	4.46	10.83	24.71
A/C	0.55	-0.03	2.57	9.53	4.03	34.06
C/C	-0.59	-0.17	2.34	13.48	-6.93	29.25
C/A	0.72	0.74	2.84	6.26	-2.90	47.92
A/A	0.86	-0.01	3.12	-0.72	4.55	48.60
ave.	0.34	0.38	2.75	6.60	1.92	36.91

Table S31: Local base-step parameters for ss-T6 (M06-2X/TZVP)

step	Shift	Slide	Rise	Tilt	Roll	Twist
T/T	-0.74	-0.20	2.55	12.31	-19.36	27.76
T/T	-0.47	-0.20	2.33	14.23	-12.72	30.45
T/T	-0.43	-0.18	2.31	14.55	-10.94	30.76
T/T	-0.40	-0.18	2.32	14.38	-11.19	31.01
T/T	-0.17	0.04	2.49	13.16	-16.43	38.04
ave.	-0.44	-0.15	2.40	13.73	-14.13	31.60

Table S32: Local base-step parameters for ss-A6 (M06-2X/TZVP)

step	Shift	Slide	Rise	Tilt	Roll	Twist
A/A	0.20	1.84	3.14	1.88	0.25	41.49
A/A	0.92	-0.01	3.16	-0.73	6.50	46.26
A/A	0.69	0.11	3.17	-0.13	4.49	41.81
A/A	0.72	0.07	3.18	-0.87	5.25	43.94
A/A	0.76	0.04	3.24	-2.62	5.46	45.97
ave.	0.66	0.41	3.18	-0.49	4.39	43.90

Table S33: Local base-step parameters for the individual single strands composing the ds-A4 sequence optimized at the M06-2X/TZVP level

step	Shift	Slide	Rise	Tilt	Roll	Twist
A/A	0.20	1.72	2.90	5.88	1.38	42.41
A/A	0.42	2.03	2.78	10.54	-1.32	47.36
A/A	0.33	1.90	3.14	0.74	-7.59	47.96
T/T	0.70	0.87	3.20	4.90	-22.25	49.82
T/T	0.53	0.65	3.18	3.61	-18.55	44.66
T/T	0.43	0.31	2.90	5.30	-8.77	40.89

Table S34: Local base-step parameters for the ds-A4 sequence (M06-2X/TZVP)

step	Shift	Slide	Rise	Tilt	Roll	Twist
AA/TT	0.13	1.00	3.00	-0.22	-3.74	42.48
AA/TT	0.18	1.37	3.26	2.11	-15.20	49.69
AA/TT	0.05	1.36	3.09	-3.31	-10.08	47.49
ave.	0.12	1.24	3.12	-0.47	-9.67	46.56

Table S35: Local base-step parameters for ss-C6 (M06-2X/TZVP)

step	Shift	Slide	Rise	Tilt	Roll	Twist
C/C	-0.03	-0.27	2.93	3.89	-5.98	38.19
C/C	0.16	-0.30	3.55	-4.67	4.77	39.57
C/C	0.02	-0.14	3.32	-2.23	-1.10	38.99
C/C	-0.03	-0.14	3.25	-0.98	-2.02	37.55
C/C	0.09	-0.68	4.04	-12.81	8.38	39.16
ave.	0.04	-0.31	3.42	-3.36	0.81	38.69

Table S36: Local base-step parameters for ss-G6 (M06-2X/TZVP)

step	Shift	Slide	Rise	Tilt	Roll	Twist
G/G	1.38	1.01	2.95	6.85	-0.22	40.02
G/G	1.27	0.66	3.04	5.99	-4.01	47.52
G/G	1.42	0.09	2.94	7.52	-4.01	54.70
G/G	1.03	1.20	3.08	4.52	-4.58	44.88
G/G	1.32	0.74	3.08	3.83	-3.08	48.92
ave.	1.28	0.74	3.02	5.74	-3.18	47.21

Table S37: Local base-step parameters for the individual single strands composing the ds-G4 sequence optimized at the M06-2X/TZVP level

step	Shift	Slide	Rise	Tilt	Roll	Twist
G/G	0.48	1.73	3.10	3.02	-3.70	45.30
G/G	1.03	1.31	3.03	11.44	-4.91	41.53
G/G	0.50	1.77	3.25	-0.36	-7.43	50.53
C/C	0.63	1.86	3.08	10.74	-9.22	51.83
C/C	0.14	0.71	3.89	-10.65	-6.09	41.77
C/C	0.09	0.49	3.71	-8.94	-9.93	43.23

Table S38: Local base-step parameters for the ds-G4 sequence (M06-2X/TZVP)

step	Shift	Slide	Rise	Tilt	Roll	Twist
GG/CC	0.21	1.15	3.47	5.98	-6.89	44.49
GG/CC	0.50	1.05	3.52	11.14	-5.44	41.71
GG/CC	-0.08	1.81	3.22	-5.64	-8.38	51.65
ave.	0.21	1.33	3.40	3.83	-6.90	45.95

Table S39: Local base-step parameters for ss-AACCAA (M06-2X/TZVP)

step	Shift	Slide	Rise	Tilt	Roll	Twist
A/A	0.25	1.85	3.08	2.47	2.24	41.54
A/C	0.82	-0.30	3.04	2.03	5.77	40.32
C/C	0.25	-0.35	3.52	-4.61	8.64	39.45
C/A	0.75	0.86	2.98	5.70	-1.04	46.30
A/A	0.77	0.10	3.28	-3.19	5.98	43.72
ave.	0.57	0.43	3.18	0.48	4.32	42.27

Table S40: Local base-step parameters for ss-C4 [ONIOM-EE /B3LYP-D3/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
C/C	0.45	-0.77	3.37	-1.36	1.64	32.04
C/C	0.37	-0.70	3.04	3.03	-2.10	40.81
C/C	0.72	0.27	2.90	11.14	1.37	37.66
ave.	0.51	-0.40	3.10	4.27	0.30	36.84

Table S41: Local base-step parameters for ss-C4 [ONIOM-ME /B3LYP-D3/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
C/C	-0.54	-0.17	2.65	9.83	3.55	17.22
C/C	0.78	0.46	2.85	5.33	3.72	40.61
C/C	1.18	0.69	1.95	24.53	3.95	30.68
ave.	0.47	0.33	2.49	13.23	3.74	29.50

Table S42: Local base-step parameters for ss-C4 [ONIOM-EE /B3LYP-D3/TZVP]

step	Shift	Slide	Rise	Tilt	Roll	Twist
C/C	0.41	-0.68	3.43	-1.84	4.50	29.26
C/C	0.60	-0.65	3.18	1.21	1.54	42.70
C/C	0.68	0.21	2.91	11.54	0.66	37.66
ave.	0.56	-0.37	3.17	3.64	2.23	36.54

Table S43: Local base-step parameters for ss-C4 [ONIOM-ME /B3LYP-D3/TZVP]

step	Shift	Slide	Rise	Tilt	Roll	Twist
C/C	0.15	0.18	2.71	11.61	-5.64	33.27
C/C	-1.58	0.11	3.37	-2.12	-1.46	25.47
C/C	0.90	0.13	2.18	20.22	0.56	39.05
ave.	-0.18	0.14	2.75	9.90	-2.18	32.60

Table S44: Local base-step parameters for ss-C4 [ONIOM-EE /M06-2X/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
C/C	0.31	-0.63	3.18	0.89	-0.48	32.12
C/C	0.46	-0.78	3.21	-1.15	-0.01	41.21
C/C	0.58	0.23	2.71	12.94	0.50	38.23
ave.	0.45	-0.39	3.03	4.23	0.00	37.19

Table S45: Local base-step parameters for ss-C4 [ONIOM-ME /M06-2X/6-31G(d,p)]

step	Shift	Slide	Rise	Tilt	Roll	Twist
C/C	-0.65	-1.05	1.87	20.72	-12.28	24.75
C/C	-1.29	0.31	2.86	5.36	-9.92	24.89
C/C	1.32	-0.18	2.49	12.41	2.74	41.01
ave.	-0.21	-0.31	2.41	12.83	-6.49	30.22

Table S46: Local base-step parameters for ss-C4 [ONIOM-EE/M06-2X/TZVP]

step	Shift	Slide	Rise	Tilt	Roll	Twist
C/C	0.50	-0.72	3.20	2.00	-2.76	32.88
C/C	0.57	-0.93	3.46	-5.04	2.40	43.43
C/C	0.21	0.24	2.64	14.16	-5.19	38.35
ave.	0.43	-0.47	3.10	3.71	-1.85	38.22

Table S47: Local base-step parameters for ss-C4 [ONIOM-ME/M06-2X/TZVP]

step	Shift	Slide	Rise	Tilt	Roll	Twist
C/C	-1.61	0.30	2.97	6.11	-13.02	29.25
C/C	-0.34	-0.16	2.97	2.35	-2.50	27.91
C/C	0.67	0.21	2.38	14.15	-0.27	41.89
ave.	-0.43	0.12	2.77	7.54	-5.26	33.02

Predicted sugar conformational parameters of double strands

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; angles are given in degrees

ds-G4 M06-2X/6-31G(d,p)

Strand I

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 G	-11.9	31.6	-38.4	32.7	-13.2	38.4	181.2	C3'-exo
2 G	-36.5	46.0	-38.1	18.1	11.3	45.3	147.1	C2'-endo
3 G	-33.7	43.2	-36.3	18.0	9.6	42.6	148.5	C2'-endo
4 G	-10.1	28.2	-34.5	29.5	-12.3	34.5	181.9	C3'-exo

Strand II

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-22.6	35.7	-34.5	22.6	-0.1	36.4	161.5	C2'-endo
2 C	-16.7	31.0	-33.0	24.0	-4.7	33.5	169.4	C2'-endo
3 C	-42.3	48.9	-37.1	13.9	17.4	48.2	140.4	C1'-exo
4 C	-16.1	29.9	-31.6	23.0	-4.5	32.2	169.2	C2'-endo

ds-A4 M06-2X/6-31G(d,p)

Strand I

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 T	-20.5	37.5	-39.5	29.0	-5.4	40.3	169.0	C2'-endo
2 T	-41.4	47.9	-36.2	13.5	17.2	47.2	140.2	C1'-exo
3 T	-39.3	47.3	-37.2	15.7	14.6	46.5	143.3	C1'-exo
4 T	-43.6	32.9	-10.7	-14.7	36.5	42.9	104.5	O4'-endo

Strand II

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-14.4	31.1	-35.0	27.8	-8.6	35.1	175.2	C2'-endo
2 A	-36.6	45.2	-36.3	16.1	12.7	44.3	144.9	C2'-endo
3 A	-38.5	46.8	-37.2	16.1	13.7	45.9	144.1	C2'-endo
4 A	-25.7	39.9	-38.5	24.9	0.3	40.7	160.9	C2'-endo

ds-G4 M06-2X/TZVP

Strand I

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 G	-22.4	37.9	-38.6	26.8	-3.0	39.8	165.6	C2'-endo
2 G	-13.5	31.1	-36.0	29.2	-10.0	36.1	177.2	C2'-endo
3 G	-36.9	45.6	-37.1	16.9	12.2	44.9	145.7	C2'-endo
4 G	-10.8	27.9	-33.6	28.1	-11.0	33.6	180.2	C3'-exo

Strand II

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-16.3	31.0	-33.2	24.8	-5.5	33.7	170.6	C2'-endo
2 C	-11.3	27.3	-32.0	26.1	-9.5	32.0	178.3	C2'-endo
3 C	3.5	14.7	-25.8	28.3	-20.3	28.5	205.1	C3'-exo
4 C	-17.1	30.2	-31.3	22.1	-3.3	32.1	167.1	C2'-endo

ds-A4 M06-2X/TZVP

Strand I

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 T	-13.9	28.8	-31.9	24.4	-6.8	32.1	173.3	C2'-endo
2 T	-10.7	23.7	-26.8	21.1	-6.7	26.9	175.5	C2'-endo
3 T	-12.0	26.2	-29.6	23.3	-7.3	29.7	175.2	C2'-endo
4 T	-21.2	33.6	-32.7	21.5	-0.3	34.4	161.8	C2'-endo

Strand II

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-10.9	28.1	-33.7	28.2	-11.0	33.7	180.2	C3'-exo
2 A	-7.9	28.5	-37.2	33.8	-16.3	37.5	186.8	C3'-exo
3 A	-13.8	31.9	-37.0	30.1	-10.3	37.0	177.3	C2'-endo
4 A	-22.8	38.0	-38.4	26.5	-2.5	39.8	164.9	C2'-endo

ds-G4 B3LYP-D3/6-31G(d,p)

Strand I

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 G	-8.8	25.1	-30.6	26.2	-11.0	30.6	182.0	C3'-exo
2 G	-38.4	45.0	-34.5	13.0	15.7	44.4	141.0	C1'-exo
3 G	-38.2	46.0	-36.3	15.0	14.3	45.3	143.2	C1'-exo
4 G	-38.8	44.2	-32.7	11.1	17.1	43.6	138.5	C1'-exo

Strand II

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-16.9	31.3	-33.1	24.1	-4.6	33.7	169.1	C2'-endo
2 C	-36.9	45.7	-37.2	16.8	12.3	45.0	145.7	C2'-endo
3 C	-38.5	45.9	-36.0	14.6	14.7	45.3	142.7	C1'-exo
4 C	-15.9	34.1	-38.5	30.3	-9.1	38.6	174.8	C2'-endo

ds-A4 B3LYP-D3/6-31G(d,p)

Strand I

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 T	-13.5	30.8	-35.5	28.5	-9.5	35.6	176.7	C2'-endo
2 T	-39.1	45.9	-35.5	13.8	15.6	45.3	141.5	C1'-exo
3 T	-39.7	46.0	-34.7	12.5	16.8	45.4	139.9	C1'-exo
4 T	-42.7	44.4	-29.2	5.3	23.1	44.9	130.5	C1'-exo

Strand II

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-10.7	26.4	-31.1	25.5	-9.5	31.1	178.8	C2'-endo
2 A	-36.5	44.4	-35.3	15.1	13.1	43.6	144.0	C2'-endo
3 A	-37.3	44.4	-34.7	14.0	14.3	43.8	142.5	C1'-exo
4 A	-6.8	21.0	-26.2	22.8	-10.2	26.3	183.6	C3'-exo

ds-G4 B3LYP-3D/TZVP

Strand I

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 G	-17.5	34.4	-37.6	28.3	-7.0	38.0	171.9	C2'-endo
2 G	-37.2	44.7	-35.1	14.4	14.0	43.9	143.0	C1'-exo
3 G	-14.2	32.2	-37.2	29.8	-9.9	37.3	176.7	C2'-endo
4 G	-8.1	25.9	-32.8	28.8	-13.2	32.9	184.6	C3'-exo

Strand II

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-13.1	29.0	-33.1	26.2	-8.4	33.2	175.8	C2'-endo
2 C	-11.3	26.9	-31.4	25.5	-9.1	31.4	177.9	C2'-endo
3 C	-1.3	20.5	-30.6	30.4	-18.4	31.8	196.0	C3'-exo
4 C	-12.2	26.4	-29.8	23.2	-7.1	29.9	174.8	C2'-endo

ds-A4 B3LYP-3D/TZVP

Strand I

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 T	-14.8	32.1	-36.5	28.7	-8.8	36.6	175.2	C2'-endo
2 T	-38.6	44.7	-33.9	12.3	16.2	44.2	140.2	C1'-exo
3 T	-39.8	44.9	-32.9	10.6	18.0	44.5	137.7	C1'-exo
4 T	-20.9	33.2	-32.2	20.9	-0.1	33.9	161.5	C2'-endo

Strand II

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-7.8	25.2	-32.1	28.2	-12.9	32.2	184.7	C3'-exo
2 A	-11.6	30.0	-36.0	30.1	-11.7	36.0	180.1	C3'-exo
3 A	-13.4	31.7	-37.2	30.3	-10.7	37.2	178.0	C2'-endo
4 A	-26.5	40.1	-38.1	23.8	1.5	40.7	159.3	C2'-endo

Predicted (ONIOM) sugar conformational parameters of ss-C4

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; angles are given in degrees

ONIOM-EE B3LYP-D3/6-31G(d,p)

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-21.4	34.8	-33.5	22.6	-1.0	35.2	162.5	C2'-endo
2 C	-38.7	41.8	-28.4	6.8	20.1	41.7	133.0	C1'-exo
3 C	-22.4	32.8	-29.3	17.3	3.0	32.2	155.6	C2'-endo
4 C	-28.4	40.2	-35.5	21.0	4.4	39.3	154.6	C2'-endo

ONIOM-ME B3LYP-D3/6-31G(d,p)

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-12.1	31.0	-36.4	30.3	-12.0	36.4	179.6	C2'-endo
2 C	-26.7	42.1	-39.9	26.3	-0.2	42.2	161.0	C2'-endo
3 C	-39.6	29.8	-9.4	-13.5	33.3	38.9	104.0	O4'-endo
4 C	-31.7	44.8	-40.0	23.1	5.2	44.3	154.5	C2'-endo

ONIOM-EE B3LYP-D3/TZVP

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-21.2	34.5	-33.3	22.5	-1.0	34.9	162.6	C2'-endo
2 C	-39.8	43.3	-29.5	7.3	20.4	43.0	133.4	C1'-exo
3 C	-22.0	33.0	-30.0	18.4	2.1	32.5	157.2	C2'-endo
4 C	-28.0	40.0	-35.7	21.5	3.8	39.3	155.4	C2'-endo

ONIOM-ME B3LYP-D3/TZVP

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-7.9	26.2	-33.1	29.4	-13.9	33.2	185.2	C3'-exo
2 C	-21.7	38.2	-39.1	28.0	-4.3	40.1	167.1	C2'-endo
3 C	-30.4	39.2	-32.4	15.6	9.0	38.3	147.8	C2'-endo
4 C	-11.0	28.5	-33.6	28.3	-11.1	33.6	179.9	C2'-endo

ONIOM-EE M06-2X/6-31G(d,p)

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-27.4	36.4	-30.7	15.9	7.1	35.5	149.9	C2'-endo
2 C	-38.5	42.2	-29.2	7.7	19.4	41.9	134.2	C1'-exo
3 C	-22.8	33.3	-29.9	17.6	3.1	32.8	155.7	C2'-endo
4 C	-26.6	39.2	-35.7	22.4	2.4	38.7	157.4	C2'-endo

ONIOM-ME M06-2X/6-31G(d,p)

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-18.0	33.2	-34.5	25.0	-4.8	35.2	168.6	C2'-endo
2 C	-27.2	39.5	-35.3	21.3	3.4	38.7	155.8	C2'-endo
3 C	-41.2	43.3	-28.1	5.0	22.5	43.4	130.3	C1'-exo
4 C	-14.2	33.5	-38.3	31.9	-11.2	38.4	177.8	C2'-endo

ONIOM-EE M06-2X/TZVP

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-24.6	36.1	-32.6	19.6	3.0	35.6	156.3	C2'-endo
2 C	-37.6	43.8	-32.2	11.5	16.3	42.7	139.0	C1'-exo
3 C	-21.0	32.9	-30.7	19.5	0.8	32.8	159.6	C2'-endo
4 C	-21.3	35.9	-35.3	25.1	-2.6	36.6	164.8	C2'-endo

ONIOM-ME M06-2X/TZVP

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-11.7	26.3	-29.8	23.8	-8.0	29.9	176.1	C2'-endo
2 C	1.2	18.8	-30.0	31.7	-21.0	32.1	200.8	C3'-exo
3 C	-27.4	39.0	-34.7	20.1	4.3	38.4	154.6	C2'-endo
4 C	1.5	19.2	-30.9	32.8	-21.7	33.2	201.1	C3'-exo

DFT optimized geometries

ss-A6 B3LYP-D3/6-31G(d,p)

O	11.99417	-4.55600	-0.15851
C	12.51285	-3.37469	-0.75914
C	11.44401	-2.29521	-0.75350
O	10.37420	-2.65337	-1.65135
C	10.78212	-2.06780	0.61403
O	10.44335	-0.66947	0.68287
C	9.52789	-2.92934	0.52489
C	9.13971	-2.71221	-0.93219
N	8.31196	-3.75675	-1.50193
C	8.00098	-5.00592	-0.99742
N	7.20478	-5.70476	-1.77702
C	6.98258	-4.87663	-2.86870
C	6.19097	-5.01030	-4.02587
N	5.40107	-6.09485	-4.24231
N	6.17107	-3.99939	-4.91540
C	6.86834	-2.88662	-4.63329
N	7.62771	-2.62353	-3.56324
C	7.65388	-3.65985	-2.71396
P	9.91397	-0.04900	2.09978
O	10.99241	-0.11781	3.16173
O	8.59509	-0.67522	2.52984
O	9.71674	1.49998	1.64807
C	9.57045	1.99241	0.30619
C	8.12279	2.11145	-0.13996
O	7.62042	0.83201	-0.56918
C	7.15922	2.60992	0.96014
O	6.30066	3.59996	0.35368
C	6.37683	1.35307	1.32360
C	6.29362	0.68877	-0.04236

N	5.92156	-0.70122	-0.06163
C	6.20247	-1.69213	0.86414
N	5.72265	-2.87027	0.52098
C	5.09581	-2.65170	-0.70144
C	4.38713	-3.48598	-1.58671
N	4.14706	-4.80606	-1.32650
N	3.88148	-2.94973	-2.71303
C	4.05732	-1.63923	-2.93854
N	4.70327	-0.74452	-2.18179
C	5.20789	-1.30834	-1.07831
P	5.36246	4.51531	1.33092
O	6.19989	5.45274	2.17684
O	4.40149	3.65881	2.14404
O	4.58009	5.39110	0.20794
C	4.38196	5.05235	-1.17437
C	3.04668	4.37785	-1.44746
O	3.13199	2.96666	-1.17383
C	1.87613	4.91474	-0.59470
O	0.73851	5.05086	-1.47463
C	1.65455	3.79573	0.41617
C	1.94234	2.58855	-0.46318
N	2.16962	1.33703	0.20719
C	2.84729	1.09706	1.38995
N	2.93802	-0.18476	1.68195
C	2.28643	-0.82910	0.63546
C	2.04236	-2.18305	0.33711
N	2.45634	-3.20401	1.14458
N	1.34379	-2.48344	-0.77380
C	0.91815	-1.48233	-1.55759
N	1.10506	-0.16652	-1.40146
C	1.79895	0.10162	-0.28898
P	-0.58138	5.84350	-0.92211
O	-0.30187	7.32296	-0.75461
O	-1.14254	5.18541	0.33090
O	-1.56757	5.64361	-2.19779
C	-1.50366	4.60609	-3.19050
C	-2.41106	3.42134	-2.89590
O	-1.76042	2.50113	-1.99885
C	-3.75635	3.79409	-2.23429
O	-4.77843	3.00338	-2.88194
C	-3.55522	3.34887	-0.79078
C	-2.72944	2.09235	-1.01980
N	-2.04931	1.54535	0.12271
C	-1.41239	2.21404	1.15358
N	-0.81948	1.40297	2.00639
C	-1.07618	0.12838	1.51276
C	-0.71226	-1.16302	1.93814
N	0.05251	-1.38599	3.04729
N	-1.16226	-2.22319	1.24189
C	-1.92017	-2.00623	0.15693
N	-2.29825	-0.83727	-0.37249
C	-1.84546	0.19693	0.34601
P	-6.34826	3.33515	-2.56159
O	-6.76388	4.66023	-3.16649
O	-6.64740	3.22645	-1.07236
O	-7.05667	2.13778	-3.39992
C	-6.47595	0.88383	-3.79488
C	-6.81310	-0.26856	-2.85948
O	-5.90107	-0.29885	-1.74463
C	-8.23112	-0.20827	-2.25222
O	-8.74356	-1.55848	-2.25722
C	-7.96126	0.26355	-0.82859
C	-6.67361	-0.49946	-0.54889
N	-5.90076	-0.07989	0.58881
C	-5.67042	1.20391	1.04852
N	-4.86637	1.24293	2.09261
C	-4.54843	-0.08840	2.33728
C	-3.72900	-0.72431	3.28846
N	-3.01588	-0.03359	4.22777
N	-3.66907	-2.06867	3.29448
C	-4.36406	-2.74702	2.36890
N	-5.12962	-2.26277	1.38480
C	-5.18894	-0.92641	1.41764
P	-10.31041	-1.82479	-1.86732
O	-11.23776	-1.24577	-2.91596
O	-10.62677	-1.36230	-0.45149
O	-10.33832	-3.44419	-1.98863
C	-9.22494	-4.33465	-1.81477

C	-9.06625	-4.86197	-0.39917
O	-8.37778	-3.90052	0.42090
C	-10.38470	-5.21120	0.33265
O	-10.22178	-6.52836	0.86152
C	-10.45240	-4.14886	1.43406
C	-8.96820	-3.94481	1.72372
N	-8.60763	-2.74744	2.44007
C	-8.91708	-1.44329	2.09097
N	-8.31587	-0.54890	2.84705
C	-7.57084	-1.29926	3.74841
C	-6.66673	-0.95158	4.77063
N	-6.34339	0.34152	5.05982
N	-6.10485	-1.93737	5.49890
C	-6.38508	-3.20988	5.17870
N	-7.16739	-3.67049	4.19517
C	-7.73769	-2.66975	3.51131
H	13.38781	-2.99531	-0.21145
H	12.81709	-3.55382	-1.79956
H	11.89636	-1.35838	-1.09698
H	11.43378	-2.33156	1.45030
H	9.82649	-3.96489	0.69022
H	8.59795	-1.77008	-1.06571
H	8.37451	-5.33986	-0.04235
H	6.80384	-2.09498	-5.37626
H	5.61048	-6.94121	-3.73358
H	5.01736	-6.20493	-5.16999
H	8.75978	-2.62994	1.23266
H	10.01429	2.99160	0.31203
H	10.12272	1.36207	-0.39266
H	8.08708	2.81372	-0.98240
H	7.68925	3.05363	1.80498
H	6.98045	0.73780	1.99415
H	5.57445	1.20336	-0.68924
H	6.80004	-1.47367	1.73857
H	3.61865	-1.25857	-3.85761
H	4.83773	-5.26497	-0.74552
H	3.88773	-5.34398	-2.14569
H	5.41323	1.58368	1.76545
H	4.40869	6.00271	-1.71436
H	5.19507	4.41761	-1.53072
H	2.80631	4.52447	-2.50798
H	2.10285	5.87990	-0.13790
H	2.40969	3.86757	1.20202
H	1.12244	2.40734	-1.16649
H	3.26871	1.91765	1.95564
H	0.35270	-1.78229	-2.43623
H	3.25992	-2.99816	1.72441
H	2.51408	-4.10016	0.67405
H	0.65331	3.81306	0.83250
H	-1.83452	5.07428	-4.12139
H	-0.47581	4.25997	-3.31285
H	-2.61561	2.91161	-3.84577
H	-3.99254	4.85471	-2.33898
H	-2.95491	4.09430	-0.26491
H	-3.34791	1.28100	-1.41791
H	-1.41037	3.29553	1.18589
H	-2.26289	-2.89768	-0.36191
H	0.66790	-0.62787	3.31234
H	0.49062	-2.29879	3.07109
H	-4.49699	3.17417	-0.28250
H	-6.89719	0.66557	-4.78003
H	-5.39241	0.97778	-3.88589
H	-6.71126	-1.20069	-3.42892
H	-8.90325	0.44226	-2.81494
H	-7.76242	1.33734	-0.83492
H	-6.87303	-1.56574	-0.40054
H	-6.11376	2.05268	0.54391
H	-4.28463	-3.82965	2.42286
H	-2.77261	0.91574	3.97519
H	-2.24831	-0.55868	4.62900
H	-8.77732	0.02313	-0.15588
H	-9.42600	-5.18251	-2.47529
H	-8.30013	-3.85053	-2.13444
H	-8.46264	-5.77788	-0.45679
H	-11.24504	-5.16319	-0.34207
H	-10.87258	-3.22374	1.03104
H	-8.56114	-4.78059	2.30359
H	-9.58711	-1.25002	1.26121

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H         -5.89934       -3.96457        5.79323
H         -6.48137        1.00493        4.30808
H         -5.46350        0.45205        5.54870
H        -11.02290       -4.47556        2.30609
H        -11.04168       -6.75955        1.31963
H         12.68982       -5.22565       -0.17213

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ss-C6 B3LYP-D3/6-31G(d,p)
O         11.95513       -4.96098       -0.58174
C         12.52073       -3.93052       -1.39014
C         11.53995       -2.77352       -1.50277
O         10.39730       -3.16572       -2.28372
C         10.98124       -2.28839       -0.15777
O         10.70880       -0.87662       -0.29566
C          9.68658       -3.07584       -0.03166
C          9.20808       -3.11717       -1.48262
N          8.35702       -4.25211       -1.81171
C          7.16682       -4.02793       -2.56995
O          6.93788       -2.89975       -3.01000
N          6.33258       -5.08975       -2.76051
C          6.67947       -6.30065       -2.34095
N          5.77530       -7.29430       -2.49383
C          7.94559       -6.58220       -1.72837
C          8.75072       -5.51754       -1.48754
P         10.37056       -0.01427        1.05332
O         11.60197        0.15905        1.91865
O          9.18044       -0.59885        1.80212
O         10.01943        1.41907        0.37500
C          9.51222        1.64772       -0.95020
C          7.99454        1.69829       -1.02918
O          7.45441        0.37154       -1.12615
C          7.30522        2.36333        0.18665
O          6.33858        3.30034       -0.33396
C          6.62233        1.18706        0.87882
C          6.25101        0.34548       -0.33630
N          5.85773       -1.02998       -0.11879
C          4.85696       -1.58737       -0.97995
O          4.32909       -0.86808       -1.82872
N          4.52716       -2.89725       -0.80167
C          5.15126       -3.63209        0.10491
N          4.76003       -4.92837        0.23854
C          6.17233       -3.11141        0.96229
C          6.49945       -1.80336        0.80096
P          5.63113        4.34808        0.70143
O          6.64792        5.30225        1.29645
O          4.79420        3.62560        1.74904
O          4.69868        5.17106       -0.34458
C          4.23025        4.71219       -1.62288
C          2.88695        4.00490       -1.56529
O          3.05836        2.63921       -1.15873
C          1.86708        4.63058       -0.58321
O          0.62231        4.76940       -1.30033
C          1.75870        3.57943        0.51785
C          1.94625        2.31118       -0.30680
N          2.23081        1.08043        0.39962
C          1.65110       -0.13094       -0.09698
O          0.91909       -0.08465       -1.08651
N          1.93123       -1.28547        0.57054
C          2.75276       -1.28259        1.60844
N          2.95765       -2.46683        2.24705
C          3.38690       -0.09606        2.09638
C          3.10135        1.06260        1.44783
P         -0.57883        5.64595       -0.62230
O         -0.17992        7.10156       -0.48170
O         -1.06559        5.02338        0.67982
O         -1.69605        5.51976       -1.79501
C         -1.76427        4.50960       -2.81472
C         -2.62998        3.32045       -2.43392
O         -1.89200        2.40796       -1.60643
C         -3.91050        3.68726       -1.64746
O         -5.00432        2.96880       -2.25734
C         -3.61688        3.15917       -0.24680
C         -2.79742        1.92305       -0.59838
N         -2.04219        1.28781        0.46038
C         -1.95216       -0.14154        0.45920
O         -2.52849       -0.77880       -0.42348
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N	-1.23821	-0.73087	1.45914
C	-0.61179	0.00439	2.36424
N	0.04891	-0.65341	3.35565
C	-0.64105	1.43510	2.36153
C	-1.36345	2.03188	1.37815
P	-6.52797	3.38489	-1.83904
O	-6.84618	4.80259	-2.27121
O	-6.79490	3.12980	-0.36115
O	-7.35978	2.35414	-2.77879
C	-6.87873	1.13445	-3.36614
C	-7.14872	-0.09458	-2.51458
O	-6.14990	-0.22094	-1.49094
C	-8.51629	-0.08653	-1.79192
O	-9.10886	-1.38525	-1.99521
C	-8.13009	0.11914	-0.33013
C	-6.81794	-0.65807	-0.29391
N	-5.93932	-0.45896	0.83964
C	-5.21530	-1.58971	1.33811
O	-5.36534	-2.68674	0.79838
N	-4.39648	-1.39420	2.41017
C	-4.23885	-0.18541	2.92676
N	-3.43081	-0.06966	4.01552
C	-4.90880	0.97220	2.41758
C	-5.74323	0.78378	1.36201
P	-10.68221	-1.60074	-1.60901
O	-11.56880	-0.68528	-2.43034
O	-10.92177	-1.49359	-0.10901
O	-10.87667	-3.12743	-2.13276
C	-9.83552	-4.10232	-2.29479
C	-9.52569	-4.89334	-1.03841
O	-8.72562	-4.11412	-0.13904
C	-10.75766	-5.38586	-0.23558
O	-10.64223	-6.80638	-0.14127
C	-10.58893	-4.68840	1.11990
C	-9.07033	-4.53898	1.18532
N	-8.54183	-3.58946	2.14451
C	-7.50997	-4.01035	3.03897
O	-7.14041	-5.18743	3.02407
N	-6.98775	-3.07933	3.88730
C	-7.40887	-1.82166	3.84905
N	-6.84133	-0.94261	4.71592
C	-8.44033	-1.37337	2.96479
C	-8.96815	-2.29499	2.11885
H	13.45696	-3.55544	-0.95261
H	12.73901	-4.29478	-2.40221
H	12.04548	-1.94465	-2.01026
H	11.67931	-2.44936	0.66785
H	9.91649	-4.07452	0.33922
H	8.62576	-2.23312	-1.73918
H	9.74157	-5.60992	-1.05587
H	8.24723	-7.58803	-1.46853
H	4.94996	-7.10673	-3.04297
H	6.03441	-8.25567	-2.34024
H	8.98093	-2.59162	0.63386
H	12.54661	-5.72390	-0.61255
H	9.90816	2.62307	-1.24507
H	9.89160	0.88848	-1.63696
H	7.72616	2.26696	-1.92945
H	8.01311	2.89225	0.82724
H	7.36408	0.67103	1.49088
H	5.43031	0.80342	-0.89061
H	7.29898	-1.32812	1.35836
H	6.68448	-3.73157	1.68598
H	4.24535	-5.31700	-0.53933
H	5.37393	-5.56838	0.72020
H	5.77475	1.50434	1.47830
H	4.12243	5.61345	-2.23226
H	4.97149	4.05765	-2.08494
H	2.45188	4.03320	-2.57335
H	2.18607	5.60930	-0.22005
H	2.59122	3.71315	1.21129
H	1.06187	2.10452	-0.91118
H	3.56914	2.00803	1.70305
H	4.08366	-0.11710	2.92380
H	2.70595	-3.29880	1.73089
H	3.76610	-2.55439	2.84498
H	0.80758	3.63449	1.03870
H	-2.21191	5.00178	-3.68230

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H         -0.76175        4.16756       -3.07728
H         -2.92793        2.81283       -3.36102
H         -4.12174        4.75777       -1.67323
H         -3.00306        3.89150        0.28105
H         -3.43376        1.14027       -1.01374
H         -1.40766        3.10968        1.25666
H         -0.09636        2.02147        3.08951
H          0.26103       -1.62585        3.17873
H          0.74064       -0.14764        3.88903
H         -4.52750        2.94701        0.30481
H         -7.42212        1.03130       -4.30927
H         -5.81072        1.20977       -3.57803
H         -7.11082       -0.97342       -3.17182
H         -9.18709        0.68347       -2.17688
H         -7.95450        1.18304       -0.16031
H         -7.00227       -1.73246       -0.33686
H         -6.26058        1.60253        0.87138
H         -4.74218        1.95858        2.82962
H         -2.78924       -0.83401        4.17694
H         -3.08338        0.84650        4.25806
H         -8.89133       -0.25903        0.34509
H        -10.20417       -4.79747       -3.05392
H         -8.92663       -3.62463       -2.66569
H         -8.96066       -5.78521       -1.34605
H        -11.69432       -5.10317       -0.72657
H        -11.05974       -3.70296        1.08705
H         -8.59221       -5.49212        1.41804
H         -9.72107       -2.05086        1.37281
H         -8.76608       -0.34189        2.94272
H         -5.96484       -1.22509        5.13202
H         -6.93728        0.04457        4.52955
H        -11.00110       -5.27069        1.94699
H        -11.42595       -7.12970        0.32401

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ss-G6 B3LYP-D3/6-31G(d,p)
O         10.70709       -5.39826       -0.40572
C         11.70497       -4.40232       -0.61677
C         11.07820       -3.01762       -0.54921
O         10.19771       -2.80511       -1.66921
C         10.22178       -2.76401        0.69861
O         10.27749       -1.34478        0.95618
C          8.83616       -3.18014        0.23236
C          8.84124       -2.71730       -1.22314
N          7.98134       -3.50577       -2.08509
C          7.83429       -4.88605       -2.12590
N          6.90484       -5.27557       -2.96730
C          6.41640       -4.09985       -3.52193
C          5.36025       -3.87780       -4.46306
O          4.59969       -4.67995       -5.00326
N          5.23867       -2.49027       -4.74845
C          5.96826       -1.47554       -4.17807
N          5.70466       -0.20716       -4.60937
N          6.91413       -1.68599       -3.28550
C          7.08806       -2.99482       -2.99679
P          9.63320       -0.72884        2.32891
O         10.59084       -0.85360        3.49567
O          8.25464       -1.30842        2.60458
O          9.56794        0.83989        1.90317
C          9.41217        1.35257        0.57001
C          7.97154        1.64407        0.18226
O          7.31453        0.44720       -0.27179
C          7.09532        2.21551        1.31949
O          6.35164        3.31320        0.75233
C          6.17524        1.04790        1.66096
C          5.98503        0.44774        0.27492
N          5.44288       -0.88511        0.21376
C          5.70026       -1.96552        1.04804
N          5.10201       -3.06585        0.65099
C          4.41348       -2.70253       -0.49812
C          3.56084       -3.46859       -1.35648
O          3.24104       -4.65396       -1.30096
N          3.04267       -2.64727       -2.39662
C          3.27879       -1.30669       -2.56238
N          2.68766       -0.69611       -3.64273
N          4.07678       -0.61466       -1.77987
C          4.61227       -1.35176       -0.78004
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P	5.52518	4.32263	1.73651
O	6.46721	5.15772	2.58026
O	4.47372	3.58378	2.55082
O	4.84361	5.27911	0.61092
C	4.64030	4.95731	-0.77404
C	3.27242	4.36501	-1.06576
O	3.24204	2.96680	-0.72655
C	2.10903	5.02607	-0.29224
O	1.04164	5.22559	-1.24169
C	1.73643	3.96349	0.73548
C	1.98412	2.70488	-0.08455
N	2.06302	1.46711	0.64675
C	2.64789	1.22537	1.88400
N	2.55324	-0.03355	2.24896
C	1.87726	-0.65770	1.20930
C	1.44937	-2.01500	1.05578
O	1.56865	-2.97441	1.81445
N	0.78121	-2.18238	-0.18977
C	0.51611	-1.19688	-1.10554
N	-0.12282	-1.57326	-2.26023
N	0.90227	0.05099	-0.95139
C	1.56954	0.26070	0.20645
P	-0.23439	6.15996	-0.82790
O	0.17150	7.61388	-0.69591
O	-0.95315	5.61791	0.39866
O	-1.13401	5.98342	-2.17079
C	-1.03054	4.92741	-3.13940
C	-1.98559	3.77408	-2.88511
O	-1.46437	2.89945	-1.86733
C	-3.39564	4.19861	-2.41409
O	-4.33386	3.38917	-3.14958
C	-3.38424	3.81883	-0.93871
C	-2.55735	2.54113	-1.00479
N	-2.04897	2.04655	0.24910
C	-1.57416	2.77293	1.33437
N	-1.20227	2.00384	2.33304
C	-1.44079	0.70876	1.89401
C	-1.27565	-0.54551	2.56319
O	-0.87171	-0.79097	3.69781
N	-1.67953	-1.61237	1.71388
C	-2.18964	-1.49087	0.44720
N	-2.47071	-2.65648	-0.22269
N	-2.34425	-0.33448	-0.15945
C	-1.96294	0.71842	0.60088
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O	-6.27966	5.00586	-3.74299
O	-6.47445	3.58234	-1.64822
O	-6.46957	2.47049	-4.00347
C	-5.76220	1.24698	-4.25226
C	-6.02968	0.16511	-3.22408
O	-5.33995	0.45602	-1.99818
C	-7.52765	-0.04730	-2.86463
O	-7.84289	-1.42707	-3.17452
C	-7.57801	0.35424	-1.39171
C	-6.17306	-0.01439	-0.93365
N	-5.74468	0.53881	0.32359
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N	-5.30097	1.98778	1.98470
C	-4.95731	0.69975	2.37810
C	-4.42230	0.20220	3.60867
O	-4.12902	0.79883	4.64397
N	-4.25702	-1.21105	3.54283
C	-4.57477	-2.01692	2.47814
N	-4.30718	-3.35765	2.57488
N	-5.06387	-1.54669	1.35041
C	-5.23123	-0.20808	1.35678
P	-8.64864	-2.49243	-2.24079
O	-8.88139	-3.72279	-3.08894
O	-9.86245	-1.88260	-1.56566
O	-7.59721	-2.81247	-1.02649
C	-6.57378	-3.80677	-1.14998
C	-6.80389	-4.92215	-0.14401
O	-6.69163	-4.43048	1.20535
C	-8.18109	-5.58855	-0.20848
O	-7.99761	-6.93656	0.22189
C	-9.01122	-4.77215	0.79081
C	-7.97915	-4.26251	1.80754
N	-8.19109	-2.87885	2.21490

C	-8.79513	-1.82653	1.53054
N	-8.71654	-0.68794	2.17938
C	-8.01655	-0.98421	3.34002
C	-7.59349	-0.13409	4.41151
O	-7.77523	1.06870	4.58465
N	-6.84557	-0.88026	5.36615
C	-6.53887	-2.21459	5.28470
N	-5.66770	-2.71082	6.21342
N	-6.96730	-2.99992	4.31613
C	-7.67819	-2.33546	3.37328
H	12.49457	-4.46475	0.14597
H	12.17539	-4.51445	-1.60244
H	11.88416	-2.27806	-0.60146
H	10.57739	-3.31742	1.57188
H	8.75570	-4.26472	0.29331
H	8.48912	-1.68694	-1.31804
H	8.47199	-5.52620	-1.53371
H	4.49827	-2.25773	-5.39999
H	6.07322	0.50048	-3.98754
H	4.74916	-0.02825	-4.89493
H	8.04950	-2.71836	0.81680
H	9.96873	2.29367	0.55486
H	9.85683	0.66700	-0.15406
H	7.99191	2.37368	-0.63742
H	7.68663	2.56981	2.16609
H	6.71439	0.34058	2.29538
H	5.32485	1.07167	-0.33609
H	6.36861	-1.86151	1.89048
H	2.42596	-3.12694	-3.04173
H	2.62395	0.30675	-3.51223
H	1.79798	-1.09437	-3.92348
H	5.25333	1.37518	2.13099
H	4.72623	5.90578	-1.31160
H	5.41992	4.27905	-1.12473
H	3.08339	4.47934	-2.14090
H	2.39340	5.98342	0.14920
H	2.44359	4.00265	1.56736
H	1.19805	2.56335	-0.83347
H	3.15077	2.02095	2.41663
H	0.44265	-3.12191	-0.36107
H	-0.56870	-0.78809	-2.71907
H	-0.74437	-2.36924	-2.17196
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H	-3.13501	1.72284	-1.44501
H	-1.50313	3.85081	1.28331
H	-1.59131	-2.53408	2.12542
H	-3.10592	-2.50221	-0.99617
H	-2.76211	-3.43230	0.36259
H	-4.38483	3.67833	-0.54314
H	-6.11896	0.89137	-5.22295
H	-4.68972	1.43792	-4.31823
H	-5.65318	-0.78033	-3.63728
H	-8.18464	0.57012	-3.47847
H	-7.68733	1.44117	-1.34513
H	-6.07770	-1.09527	-0.82078
H	-6.13082	2.63891	0.10865
H	-3.89021	-1.62733	4.39188
H	-4.96835	-3.89913	2.01486
H	-4.23011	-3.71801	3.51780
H	-8.37018	-0.12761	-0.82392
H	-6.55260	-4.22116	-2.16137
H	-5.61905	-3.32322	-0.92850
H	-6.02164	-5.67545	-0.28140
H	-8.60102	-5.54216	-1.21932
H	-9.50050	-3.94670	0.27833
H	-7.97557	-4.84342	2.73125
H	-9.25749	-1.95391	0.56292
H	-6.40716	-0.31380	6.08314
H	-5.63644	-3.72049	6.25430
H	-5.61509	-2.25530	7.11422
H	-9.77930	-5.37991	1.27319
H	-8.86717	-7.35930	0.23381
H	11.11630	-6.26302	-0.53799

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ss-T6 B3LYP-D3/6-31G(d,p)
C          -8.66480       -2.48534        2.07449
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N          -6.65231       -3.00815        3.76113
C          -7.20648       -1.72626        3.84498
C          -8.29778       -1.48788        2.91486
C          -8.50543       -4.74265        1.12257
O          -8.23627       -4.30355       -0.21097
C          -8.96053       -5.19094       -1.07810
C         -10.11725       -5.79637       -0.24078
C          -9.99919       -5.05757        1.09806
C          -9.37955       -4.47675       -2.34839
O         -10.51899       -3.61694       -2.19061
P         -10.46856       -2.06893       -1.69622
O         -10.65289       -1.95837       -0.18882
O          -9.84899       -7.19373       -0.12380
O          -6.42633       -5.11958        2.92434
O          -6.76002       -0.91108        4.65100
C          -8.95607       -0.13957        2.93043
O          -8.94235       -1.70675       -2.15889
C          -8.44562       -0.36678       -1.97817
C          -7.07274       -0.29690       -2.68909
O          -6.07733       -0.32762       -1.65226
C          -6.72723       -0.78985       -0.45931
C          -8.08889       -0.10740       -0.51782
C          -6.87518        0.92105       -3.57464
O          -7.44206        2.12512       -3.03400
P          -6.68719        3.22370       -2.10521
O          -6.92993        2.96239       -0.62409
N          -5.88446       -0.50774        0.68686
C          -5.13596       -1.56203        1.20840
N          -4.36377       -1.21280        2.29743
C          -4.23240        0.04093        2.90258
C          -5.02053        1.08771        2.27277
C          -5.78599        0.77093        1.20181
O          -5.16908       -2.70576        0.77342
O          -3.47965        0.18791        3.86317
C          -4.93875        2.47332        2.84033
O          -5.13917        2.91271       -2.52907
C          -4.07998        3.67419       -1.91256
C          -2.77447        3.32623       -2.66755
O          -2.02015        2.46377       -1.79864
C          -2.93356        1.96951       -0.80706
C          -3.80061        3.18284       -0.49611
C          -1.94126        4.52759       -3.07806
O          -1.90232        5.56799       -2.08818
P          -0.80770        5.73038       -0.89866
O          -1.30370        5.11325        0.40270
N          -2.18663        1.38017        0.28750
C          -2.08453       -0.01046        0.32066
N          -1.34241       -0.49050        1.38020
C          -0.68685        0.23477        2.37983
C          -0.82127        1.67641        2.25066
C          -1.54096        2.17363        1.21806
O          -2.62138       -0.75516       -0.48922
O          -0.04617       -0.35062        3.25005
C          -0.13925        2.54219        3.26730
O           0.42081        4.86779       -1.54808
C           1.64786        4.74510       -0.79947
C           2.69885        4.11706       -1.74674
O           2.88228        2.76011       -1.30975
C           1.74758        2.43128       -0.49456
C           1.51507        3.70524        0.30849
C           4.03042        4.84611       -1.79125
O           4.46945        5.33356       -0.51296
P           5.38047        4.52701        0.56481
O           4.52147        3.79463        1.58776
N           2.01948        1.21503        0.24693
C           1.44087        0.03343       -0.21479
N           1.75690       -1.07515        0.54322
C           2.59087       -1.15238        1.66318
C           3.18347        0.11807        2.04910
C           2.88533        1.22179        1.32474
O           0.69372       -0.03000       -1.18277
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O	2.78767	-2.23259	2.21513
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O	6.13028	3.48779	-0.44966
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C	7.80649	1.89333	-1.10770
O	7.30212	0.54895	-1.18488
C	6.07624	0.52853	-0.43699
C	6.40071	1.38705	0.77929
C	9.32380	1.89533	-1.02753
O	9.84125	1.71167	0.30088
P	10.20760	0.29223	1.00035
O	9.00475	-0.33053	1.69648
N	5.67470	-0.84297	-0.19884
C	4.63185	-1.35538	-0.97023
N	4.31292	-2.66492	-0.67968
C	4.96053	-3.53760	0.19789
C	6.07763	-2.94014	0.91383
C	6.38015	-1.64107	0.68067
O	4.01489	-0.70378	-1.80323
O	4.58590	-4.70380	0.30171
C	6.84841	-3.80726	1.86445
O	10.63171	-0.55022	-0.33743
C	10.94911	-1.95270	-0.21695
C	11.47947	-2.40563	-1.58458
O	10.31801	-2.80365	-2.33915
C	9.15943	-2.79273	-1.50134
C	9.68025	-2.77573	-0.06559
C	12.48551	-3.54414	-1.52611
O	11.96721	-4.60307	-0.72284
N	8.32775	-3.94944	-1.81740
C	7.07212	-3.73133	-2.37181
N	6.32587	-4.88184	-2.52496
C	6.69184	-6.19728	-2.22009
C	8.06142	-6.34235	-1.74296
C	8.80577	-5.22506	-1.57785
O	6.64537	-2.62647	-2.68751
O	5.89257	-7.11529	-2.38540
C	8.57586	-7.72438	-1.47104
O	11.39412	0.50413	1.91639
O	6.36604	5.49416	1.18852
O	-0.43724	7.19360	-0.76784
O	-7.11170	4.60882	-2.54839
O	-11.47909	-1.26480	-2.48888
H	13.42640	-3.15790	-1.10927
H	12.68006	-3.88253	-2.55176
H	11.95132	-1.55859	-2.09363
H	11.67384	-2.10074	0.58778
H	9.94298	-3.77854	0.27003
H	8.54578	-1.91743	-1.71598
H	9.84300	-5.26084	-1.26052
H	5.39086	-4.74591	-2.88921
H	8.98391	-2.32185	0.62986
H	12.57198	-5.35335	-0.78876
H	9.68285	2.87904	-1.34082
H	9.73155	1.13888	-1.70084
H	7.52106	2.43657	-2.01819
H	7.78693	3.09624	0.74360
H	7.12104	0.88053	1.42372
H	5.26901	0.97847	-1.01860
H	7.22141	-1.15219	1.16190
H	3.54957	-3.05022	-1.22176
H	5.53030	1.70816	1.34082
H	3.91590	5.73571	-2.41613
H	4.79130	4.19885	-2.23103
H	2.28453	4.11633	-2.76369
H	1.95147	5.72874	-0.43667
H	2.31831	3.85492	1.03166
H	0.88338	2.20799	-1.12325
H	3.33983	2.18403	1.53775
H	1.34036	-1.94277	0.22880
H	0.54462	3.75569	0.78971
H	-2.40131	4.98214	-3.95947
H	-0.92940	4.20659	-3.33117
H	-3.04137	2.77713	-3.58009
H	-4.31935	4.73798	-1.96350
H	-3.22340	3.94332	0.03214
H	-3.53864	1.16044	-1.22075
H	-1.62531	3.24158	1.04502

H	-1.26257	-1.49879	1.42663
H	-4.71757	2.94965	0.03413
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H	-5.81165	1.06013	-3.77647
H	-6.96618	-1.18973	-3.31893
H	-9.16403	0.34775	-2.38422
H	-7.98967	0.96840	-0.36555
H	-6.84058	-1.87557	-0.48518
H	-6.35097	1.52513	0.66335
H	-3.82438	-1.96886	2.70046
H	-8.82570	-0.53109	0.15626
H	-9.68447	-5.23208	-3.07748
H	-8.53673	-3.91389	-2.75389
H	-8.30309	-6.02163	-1.37207
H	-11.08743	-5.62392	-0.71705
H	-10.57436	-4.13013	1.05683
H	-7.92429	-5.63797	1.35339
H	-9.44589	-2.35113	1.33001
H	-5.88451	-3.21091	4.38983
H	-10.32603	-5.66412	1.94519
H	-10.59036	-7.59206	0.35271
H	9.61111	-7.69459	-1.12456
H	7.96789	-8.22180	-0.70829
H	8.52752	-8.34586	-2.37128
H	7.62494	-3.23448	2.37559
H	6.18386	-4.24282	2.61722
H	7.32349	-4.64092	1.33572
H	4.47339	1.14646	3.42394
H	3.59688	-0.22877	4.12544
H	4.96950	-0.52050	3.06197
H	-0.31056	3.59999	3.05691
H	-0.51202	2.32214	4.27298
H	0.94012	2.35708	3.27758
H	-5.57137	3.16298	2.27754
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H	-9.33950	0.09262	3.92910
H	-8.24132	0.64926	2.67238

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ss-A2C2A2 B3LYP-D3/6-31G(d,p)

O	11.96435	-4.60221	-0.75714
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O	9.97652	-2.90944	-2.03389
C	10.77734	-2.13825	0.07145
O	10.42375	-0.74380	0.14483
C	9.55117	-3.02225	0.26866
C	8.89483	-2.89986	-1.10102
N	7.97702	-3.97271	-1.42953
C	7.68366	-5.11871	-0.71322
N	6.74812	-5.85988	-1.26505
C	6.40196	-5.16932	-2.41828
C	5.43734	-5.40104	-3.41797
N	4.57794	-6.45282	-3.36700
N	5.32293	-4.51268	-4.42368
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C	7.14348	-3.98897	-2.53302
P	10.18722	-0.06991	1.61539
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O	8.95558	-0.63774	2.30777
O	9.93266	1.47176	1.16881
C	9.66286	1.95348	-0.15671
C	8.17847	2.07764	-0.45431
O	7.62135	0.78805	-0.77191
C	7.33886	2.63635	0.71610
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C	6.61767	1.39893	1.23623
C	6.37213	0.66936	-0.07681
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C	4.98481	-2.65293	-0.29726
C	4.08279	-3.49831	-0.96970

N	3.78197	-4.75556	-0.52410
N	3.44892	-3.03250	-2.06109
C	3.68158	-1.76960	-2.44914
N	4.49201	-0.86408	-1.88963
C	5.11753	-1.36065	-0.81618
P	5.47162	4.48355	1.13545
O	6.30359	5.47064	1.92849
O	4.56469	3.61981	2.00207
O	4.63271	5.30661	0.01376
C	4.33703	4.87038	-1.32299
C	3.02728	4.11112	-1.44478
O	3.20935	2.73244	-1.08365
C	1.88268	4.65156	-0.55210
O	0.72273	4.80770	-1.39725
C	1.68128	3.53310	0.46569
C	2.00973	2.32465	-0.40258
N	2.23461	1.05782	0.25959
C	1.69262	-0.12306	-0.34112
O	1.07221	-0.03015	-1.40161
N	1.89001	-1.30580	0.30462
C	2.60967	-1.35952	1.41377
N	2.72128	-2.57290	2.02560
C	3.22461	-0.20607	1.99872
C	3.00990	0.98394	1.37914
P	-0.55545	5.64222	-0.81210
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O	-1.14429	4.97645	0.42458
O	-1.55503	5.53135	-2.08825
C	-1.54059	4.52100	-3.11020
C	-2.42959	3.32659	-2.80551
O	-1.74819	2.40618	-1.93972
C	-3.76726	3.67661	-2.10921
O	-4.81346	2.98697	-2.82672
C	-3.58423	3.10629	-0.70741
C	-2.72586	1.88761	-1.01968
N	-2.04811	1.24049	0.08427
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O	-2.38779	-0.81246	-0.89528
N	-1.26074	-0.78254	1.08852
C	-0.72202	-0.05670	2.05574
N	-0.10754	-0.71866	3.07324
C	-0.79588	1.37189	2.08829
C	-1.46382	1.97554	1.07167
P	-6.36906	3.38242	-2.51524
O	-6.72526	4.72836	-3.11431
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O	-7.11935	2.22273	-3.37424
C	-6.56121	0.96633	-3.78977
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O	-5.93341	-0.14140	-1.72102
C	-8.26713	-0.16719	-2.21855
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C	-4.58492	0.05225	2.37048
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N	-3.14119	0.12394	4.32546
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C	-4.10428	-2.56230	2.20782
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C	-5.12697	-0.77976	1.38534
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O	-11.22774	-1.28724	-2.88529
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O	-10.24924	-3.48495	-2.02650
C	-9.09101	-4.33061	-1.93965
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C	-6.15268	-3.30730	5.03451
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H	5.95608	-2.72560	-5.22646
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H	8.92188	-2.69411	1.09194
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H	10.13570	1.30958	-0.89985
H	8.06327	2.74407	-1.31847
H	7.95111	3.13685	1.46898
H	7.30256	0.81852	1.85791
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H	5.71037	1.64917	1.77828
H	4.26260	5.78630	-1.91508
H	5.15532	4.26184	-1.71249
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H	-0.32514	1.95237	2.87061
H	0.12400	-1.68751	2.90153
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ds-A4 B3LYP-D3/6-31G(d,p)

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C	0.28040	6.90831	2.50302
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C	2.13490	3.52462	4.43017

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C	-5.52476	-1.49426	0.46821
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H	-0.44263	-3.48969	-1.64611
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H	-3.47774	8.40494	-0.93487
H	-3.62361	6.67861	-0.52232
H	-1.38202	7.54911	-0.06660
H	-1.42175	8.97777	-2.44851
H	-1.36652	7.11669	-3.91701

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H          0.58050        5.53993       -2.18272
H         -2.75624        5.39278       -4.10292
H          2.03988        1.29908       -2.70524
H         -2.42783        0.76703       -5.41167
H         -1.28093       -0.52418       -5.15573
H          0.38020        7.36399       -3.74830
H          0.89458        9.00703       -2.03996
H          0.33186       -6.05811       -5.59069
H         -0.99452       -5.21306       -4.76835
H         -0.60005       -4.80158       -6.43250
H          4.42628       -6.07335        0.09668
H          2.83082       -6.06467        0.88130
H          2.94646       -6.28538       -0.86195
H          6.25236       -1.64076        3.50060
H          4.97378       -2.43870        4.43843
H          5.31778       -2.97911        2.79966
H          4.55654        3.40739        5.50339
H          4.08282        2.14818        6.66073
H          4.68686        1.68967        5.07350
H          3.62485       -7.48973       -6.02711
H         -4.01825       -8.34317        4.51097

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ds-G4 B3LYP-D3/6-31G(d,p)
O          4.73390       -6.29000       -5.71095
C          5.98091       -5.95139       -6.31513
C          6.63600       -4.82189       -5.53554
O          5.93957       -3.58036       -5.75200
C          6.65059       -5.04432       -4.01687
O          7.86429       -4.45425       -3.50719
C          5.42442       -4.28076       -3.54408
C          5.30256       -3.13884       -4.55173
N          3.92618       -2.77292       -4.83371
C          2.90753       -3.61706       -5.25850
N          1.75931       -2.99837       -5.40445
C          2.02587       -1.67874       -5.05962
C          1.17738       -0.53414       -5.01949
O         -0.03354       -0.47395       -5.30586
N          1.86829        0.61136       -4.60436
C          3.20005        0.65864       -4.27266
N          3.68997        1.87023       -3.91218
N          4.00640       -0.39324       -4.33133
C          3.37059       -1.51897       -4.71190
P          8.30503       -4.74870       -1.95627
O          9.29741       -5.89032       -1.87243
O          7.08464       -4.92338       -1.06809
O          9.12276       -3.37685       -1.63949
C          8.86492       -2.09178       -2.22517
C          7.91390       -1.22370       -1.42031
O          6.54735       -1.56811       -1.69682
C          8.08592       -1.31873        0.11451
O          8.10412        0.03667        0.59475
C          6.82128       -2.04883        0.55617
C          5.82423       -1.49054       -0.45117
N          4.57509       -2.18617       -0.58489
C          4.33255       -3.55469       -0.50488
N          3.09256       -3.86827       -0.79382
C          2.47445       -2.65382       -1.07571
C          1.13561       -2.35138       -1.45960
O          0.20725       -3.15180       -1.68687
N          0.92812       -0.97359       -1.57935
C          1.88664       -0.00389       -1.39497
N          1.47899        1.26279       -1.55507
N          3.15522       -0.27964       -1.10536
C          3.37920       -1.59653       -0.94802
P          8.47336        0.39439        2.14228
O          9.93727        0.11877        2.42871
O          7.52797       -0.26858        3.13211
O          8.22618        2.00336        2.08500
C          7.53777        2.69732        1.03325
C          6.06216        2.89936        1.31508
O          5.33481        1.66532        1.19835
C          5.74753        3.45588        2.72184
O          4.76660        4.49147        2.51749
C          5.13878        2.25210        3.43269
C          4.37299        1.63334        2.27050
N          3.86777        0.30213        2.45101
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C	4.51824	-0.82882	2.93415
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C	1.30053	-2.13927	2.17462
O	1.05793	-3.35628	2.29504
N	0.30744	-1.27259	1.70093
C	0.47215	0.07052	1.44737
N	-0.58602	0.72027	0.94935
N	1.61619	0.71201	1.65806
C	2.58144	-0.08621	2.13948
P	4.33005	5.49468	3.72983
O	5.48278	6.38857	4.14304
O	3.70538	4.73270	4.88988
O	3.24684	6.39862	2.92463
C	2.45761	5.97972	1.79373
C	1.09698	5.42755	2.17132
O	1.20786	4.05799	2.59814
C	0.38323	6.19278	3.31163
O	-0.94626	6.47036	2.85668
C	0.39689	5.17919	4.45987
C	0.28668	3.87496	3.67604
N	0.60818	2.65630	4.37042
C	1.82096	2.29605	4.94659
N	1.85025	1.03595	5.31621
C	0.60050	0.53060	4.96661
C	0.05720	-0.78640	5.04467
O	0.60735	-1.82257	5.46376
N	-1.25658	-0.83697	4.54879
C	-1.95052	0.22600	4.01806
N	-3.22484	-0.00439	3.62507
N	-1.44202	1.44758	3.91893
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C	-7.17843	-7.66922	4.31264
C	-7.39101	-6.29599	3.69404
O	-6.38783	-5.37251	4.15566
C	-7.30366	-6.25420	2.16236
O	-8.13880	-5.15048	1.75119
C	-5.83375	-5.93595	1.92927
C	-5.56894	-4.94159	3.05771
N	-4.18523	-4.86076	3.51866
C	-3.59227	-3.58689	3.66879
O	-4.23451	-2.58339	3.32037
N	-2.34466	-3.50883	4.19156
C	-1.68638	-4.61259	4.57347
N	-0.46608	-4.45600	5.09230
C	-2.28305	-5.91423	4.46411
C	-3.53832	-5.98242	3.95630
P	-8.45025	-4.84073	0.17673
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O	-7.17765	-4.83051	-0.65810
O	-9.08289	-3.35036	0.32834
C	-8.84083	-2.42214	1.39759
C	-7.80117	-1.36745	1.06117
O	-6.47581	-1.89206	1.22933
C	-7.87035	-0.82455	-0.38371
O	-7.73414	0.61017	-0.28764
C	-6.63760	-1.44312	-1.03781
C	-5.67313	-1.39337	0.14337
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O	-7.26157	1.21573	-2.78359
O	-7.73229	3.00542	-0.96015
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C	-5.47530	3.69686	-0.23357
O	-4.67665	2.53783	-0.52420
C	-5.39924	4.59518	-1.48780
O	-4.40994	5.60903	-1.21730
C	-4.88594	3.63713	-2.55778
C	-3.91522	2.81972	-1.71227

N	-3.42481	1.56446	-2.24726
C	-2.08041	1.19752	-1.99556
O	-1.29103	2.05708	-1.56267
N	-1.70534	-0.08071	-2.23927
C	-2.57508	-0.97817	-2.72366
N	-2.17717	-2.24947	-2.83683
C	-3.90313	-0.59633	-3.09325
C	-4.29616	0.66503	-2.79186
P	-4.35468	6.94648	-2.16421
O	-5.42688	7.92911	-1.73967
O	-4.33204	6.59175	-3.63714
O	-2.85062	7.45567	-1.78269
C	-2.40004	7.51345	-0.41926
C	-0.90894	7.24895	-0.35316
O	-0.63002	5.91148	-0.82593
C	-0.00769	8.18704	-1.16650
O	1.17667	8.37659	-0.38797
C	0.26351	7.38872	-2.43882
C	0.28043	5.94544	-1.92768
N	-0.13988	4.95372	-2.92017
C	0.72988	3.90692	-3.29018
O	1.89545	3.89962	-2.84638
N	0.25971	2.94511	-4.12224
C	-0.99866	2.98485	-4.58292
N	-1.44219	1.94630	-5.30060
C	-1.84871	4.10615	-4.32542
C	-1.38996	5.04240	-3.46311
H	6.66267	-6.81378	-6.31626
H	5.84500	-5.62184	-7.35330
H	7.66056	-4.70434	-5.90353
H	6.61716	-6.10569	-3.75909
H	4.54882	-4.92836	-3.58775
H	5.78304	-2.22778	-4.18750
H	3.11253	-4.65928	-5.46092
H	1.29651	1.46848	-4.45206
H	4.58987	1.83279	-3.45601
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H	5.55387	-3.91478	-2.53350
H	9.83627	-1.59085	-2.26361
H	8.48839	-2.20779	-3.24364
H	8.08960	-0.18152	-1.71788
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H	6.95269	-3.11976	0.38495
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H	5.13498	-4.24441	-0.29009
H	-0.03657	-0.65810	-1.81278
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H	8.00882	3.68229	0.96352
H	7.66766	2.17550	0.08495
H	5.68497	3.61674	0.57408
H	6.62552	3.87176	3.22123
H	5.93328	1.57016	3.74729
H	3.50243	2.24345	2.01233
H	5.55884	-0.77561	3.22671
H	-0.60113	-1.69796	1.43079
H	-0.45503	1.66285	0.62263
H	-1.50273	0.28168	0.82487
H	4.51336	2.53982	4.27287
H	2.30389	6.87566	1.18702
H	3.00651	5.24109	1.20659
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H	1.36076	5.20936	4.97501
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H	-5.24816	-6.84711	2.05376
H	-5.83735	-3.92853	2.76217

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H         -1.76818       -6.80150        4.80761
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H          0.07512       -5.26172        5.36184
H         -5.66336       -5.51526        0.94597
H         -9.79626       -1.92066        1.57618
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H         -8.80816       -1.07395       -0.88359
H         -6.85591       -2.47906       -1.30927
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H         -6.31468       -0.87452       -1.90311
H         -7.35419        4.12183        0.69034
H         -6.84065        2.42555        0.83468
H         -5.03296        4.23793        0.61270
H         -6.35946        5.05565       -1.72920
H         -5.71195        3.01630       -2.91210
H         -3.02853        3.40453       -1.46682
H         -5.32108        0.99833       -2.92548
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H         -1.28123       -2.56132       -2.43148
H         -2.84701       -2.94873       -3.11605
H         -4.42470        4.17679       -3.37890
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H         -1.99073        5.88772       -3.15976
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H         -2.40989        1.92623       -5.58228
H          1.19976        7.66417       -2.92922
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H         -5.81579       -9.07074        4.29108

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B3LYP-D3/TZVP
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ss-A6 B3LYP-D3/TZVP
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O         10.75315       -1.78306       -1.19460
C         10.27207       -2.62281        0.97972
O          9.59768       -1.56308        1.67947
C          9.33199       -3.24495       -0.04294
C          9.37962       -2.18799       -1.13396
N          8.95000       -2.60949       -2.44411
C          8.88705       -3.87996       -2.98339
N          8.47707       -3.89317       -4.22732
C          8.26710       -2.56021       -4.54119
C          7.81168       -1.91031       -5.70255
N          7.43856       -2.58046       -6.80995
N          7.72663       -0.56804       -5.68981
C          8.04213        0.08821       -4.56687
N          8.46119       -0.41556       -3.40653
C          8.55763       -1.74738       -3.44802
P          8.86342       -1.87755        3.11790
O          9.91025       -2.04651        4.20986
O          7.84236       -3.00005        2.99685
O          8.01911       -0.48784        3.25861
C          8.63260        0.80192        3.12089
C          7.68291        1.74142        2.40276
O          7.47179        1.30603        1.04329
C          6.28419        1.85436        3.02230
O          5.84930        3.20576        2.78266
C          5.50510        0.80397        2.24663
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O	3.73679	3.52023	1.34989
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C	3.09175	4.56004	-0.74475
O	2.91521	3.36116	-1.52519
C	1.71251	4.88689	-0.17569
O	1.04366	5.73928	-1.12713
C	1.05286	3.51914	-0.06502
C	1.68107	2.71587	-1.20452
N	1.92715	1.32444	-0.86739
C	2.61259	0.86392	0.23808
N	2.83229	-0.42552	0.21323
C	2.26749	-0.85376	-0.97693
C	2.19623	-2.11059	-1.59631
N	2.71768	-3.22954	-1.04125
N	1.56288	-2.20083	-2.77945
C	1.05397	-1.09030	-3.32671
N	1.08800	0.15560	-2.85158
C	1.70677	0.22268	-1.66939
P	-0.29826	6.57161	-0.66090
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O	-0.18771	7.02771	0.78330
O	-1.47193	5.41923	-0.69346
C	-1.89618	4.88952	-1.95626
C	-2.82493	3.72307	-1.71206
O	-2.07441	2.58947	-1.22363
C	-3.91361	3.99521	-0.65870
O	-5.11611	3.34285	-1.09380
C	-3.37546	3.29332	0.58187
C	-2.74007	2.07444	-0.06403
N	-1.78956	1.33994	0.73400
C	-1.05490	1.74403	1.82300
N	-0.24670	0.81173	2.27266
C	-0.45618	-0.27969	1.43722
C	0.04333	-1.59516	1.40603
N	0.91744	-2.08386	2.31589
N	-0.40998	-2.42272	0.45008
C	-1.31131	-1.97661	-0.42793
N	-1.86340	-0.76518	-0.49126
C	-1.40864	0.03793	0.47023
P	-6.57375	4.03104	-0.76837
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O	-7.52241	2.82466	-1.32157
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C	-7.61362	0.78083	-2.59357
O	-6.55287	0.12166	-1.87190
C	-8.91225	0.35429	-1.90037
O	-9.36362	-0.83244	-2.58156
C	-8.45515	0.10460	-0.47137
C	-7.05445	-0.46046	-0.66357
N	-6.14949	-0.19994	0.43606
C	-6.04696	0.92615	1.22990
N	-5.13186	0.81244	2.16347
C	-4.59509	-0.45211	1.98378
C	-3.60499	-1.17593	2.66662
N	-2.94723	-0.68000	3.73874
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C	-4.01422	-2.92944	1.22201
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C	-5.21760	-1.09840	0.91676
P	-10.54155	-1.81694	-1.98204
O	-11.27417	-2.39863	-3.18077
O	-11.35196	-1.13952	-0.89593
O	-9.65270	-2.99437	-1.24459
C	-8.86743	-3.87999	-2.05706
C	-8.57550	-5.16207	-1.30690
O	-7.66577	-4.93666	-0.21325

C	-9.80019	-5.84272	-0.69424
O	-9.56255	-7.25388	-0.75135
C	-9.80697	-5.31330	0.73722
C	-8.32129	-5.10521	1.04348
N	-8.04861	-3.96163	1.89466
C	-8.55698	-2.68304	1.77411
N	-8.03038	-1.83394	2.62079
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H	13.26308	-2.32732	-0.78606
H	11.61642	-1.00181	0.52067
H	10.68628	-3.34508	1.68142
H	9.76841	-4.17842	-0.39293
H	8.76338	-1.32671	-0.87117
H	9.14488	-4.75285	-2.40857
H	7.94202	1.16671	-4.61095
H	7.60429	-3.57007	-6.88046
H	7.22336	-2.06500	-7.64724
H	8.33475	-3.41415	0.34747
H	8.86171	1.19992	4.11226
H	9.55475	0.72604	2.54550
H	8.14678	2.72892	2.37684
H	6.28436	1.66449	4.09490
H	5.72790	-0.16804	2.67779
H	5.60218	1.68123	0.26010
H	6.50585	-1.87129	1.45860
H	4.66791	1.03018	-3.98479
H	5.61051	-4.00437	-2.84526
H	5.05967	-3.40969	-4.35921
H	4.43521	0.95981	2.26934
H	4.39466	5.38776	0.73053
H	5.07756	4.00554	-0.15288
H	3.40930	5.34858	-1.42851
H	1.77023	5.39802	0.78330
H	1.31345	3.08441	0.89528
H	1.05145	2.69477	-2.09267
H	2.94357	1.55530	0.99115
H	0.55745	-1.22344	-4.28136
H	3.43120	-3.11009	-0.33747
H	2.84740	-4.01381	-1.66191
H	-0.02541	3.56694	-0.15917
H	-2.42239	5.66104	-2.52242
H	-1.03615	4.55323	-2.53993
H	-3.30071	3.45375	-2.65703
H	-4.08218	5.06031	-0.51233
H	-2.61561	3.92317	1.04129
H	-3.50010	1.35436	-0.37158
H	-1.15493	2.72852	2.24633
H	-1.63109	-2.68900	-1.17920
H	1.48852	-1.42871	2.82417
H	1.36885	-2.95192	2.07016
H	-4.14994	3.04262	1.29817
H	-8.11513	2.74289	-3.30244
H	-6.37982	2.46815	-3.02888
H	-7.60905	0.40847	-3.61930
H	-9.68806	1.11594	-1.95995
H	-8.41692	1.06145	0.04124
H	-7.06735	-1.54451	-0.77476
H	-6.63993	1.81170	1.06580
H	-3.75672	-3.94336	0.93924
H	-2.98247	0.31068	3.91425
H	-2.12791	-1.17350	4.05479
H	-9.11211	-0.55834	0.07612
H	-9.41074	-4.12020	-2.97340
H	-7.92622	-3.39304	-2.32215
H	-8.08876	-5.84681	-2.00411
H	-10.71569	-5.58638	-1.23072
H	-10.34450	-4.36918	0.76747
H	-7.88218	-5.96068	1.55484
H	-9.29752	-2.45334	1.02743
H	-4.88743	-5.21137	4.80105
H	-6.47125	-0.24710	4.33936

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H         -5.28910       -0.81712        5.42903
H        -10.27231       -6.00419        1.43805
H        -10.30073       -7.70160       -0.32079
H         13.12074       -4.62359       -0.50357

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ss-C6 B3LYP-D3/TZVP
O         12.50861       -4.70658       -0.83341
C         12.97675       -3.58686       -1.59156
C         11.91704       -2.50349       -1.62018
O         10.77381       -2.92919       -2.38729
C         11.37232       -2.11301       -0.24267
O         11.03055       -0.71364       -0.30169
C         10.12820       -2.97622       -0.11571
C          9.60803       -2.98712       -1.54809
N          8.80851       -4.14659       -1.91093
C          7.64220       -3.95782       -2.70716
O          7.36608       -2.83120       -3.11484
N          6.87972       -5.04961       -2.97161
C          7.25996       -6.25614       -2.57986
N          6.43189       -7.28575       -2.83161
C          8.50241       -6.49031       -1.91087
C          9.23756       -5.40095       -1.60014
P         10.66656        0.08574        1.08825
O         11.90583        0.28273        1.94970
O          9.50448       -0.57865        1.82556
O         10.25072        1.53034        0.45656
C          9.68671        1.78005       -0.84123
C          8.17204        1.74340       -0.88606
O          7.70224        0.39249       -1.03225
C          7.46000        2.32323        0.35744
O          6.48111        3.26773       -0.12091
C          6.80389        1.09831        0.98428
C          6.49223        0.28547       -0.26191
N          6.15927       -1.11145       -0.09226
C          5.14181       -1.67481       -0.91917
O          4.53669       -0.95050       -1.70705
N          4.88586       -3.00012       -0.78557
C          5.58506       -3.74755        0.05125
N          5.27623       -5.05948        0.12813
C          6.62037       -3.21438        0.87581
C          6.87583       -1.89206        0.75972
P          5.71788        4.25221        0.94887
O          6.69328        5.22138        1.60265
O          4.88495        3.45111        1.94956
O          4.77690        5.08707       -0.08936
C          4.31667        4.66206       -1.38217
C          2.97799        3.95190       -1.36282
O          3.14550        2.56330       -1.02932
C          1.94752        4.52189       -0.36231
O          0.71864        4.71699       -1.09037
C          1.81771        3.41087        0.67243
C          2.02517        2.18859       -0.20824
N          2.31054        0.93080        0.44658
C          1.69497       -0.25568       -0.05101
O          0.92722       -0.18101       -1.00858
N          1.98548       -1.42407        0.57453
C          2.85400       -1.46475        1.57028
N          3.08440       -2.66120        2.15369
C          3.52378       -0.30118        2.05314
C          3.22067        0.87282        1.45542
P         -0.50006        5.57487       -0.40278
O         -0.09688        7.02721       -0.18659
O         -1.02717        4.88931        0.85826
O         -1.58307        5.50957       -1.62036
C         -1.65039        4.53281       -2.67204
C         -2.55432        3.35584       -2.36505
O         -1.86037        2.37404       -1.57526
C         -3.84294        3.70921       -1.59069
O         -4.93798        3.07820       -2.28487
C         -3.60622        3.08025       -0.22304
C         -2.80387        1.85154       -0.62365
N         -2.09283        1.14494        0.41896
C         -2.10211       -0.28121        0.41005
O         -2.71929       -0.87610       -0.47205
N         -1.42978       -0.91999        1.39992
C         -0.74026       -0.24249        2.30167
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N	-0.10746	-0.94532	3.26612
C	-0.66975	1.18223	2.30172
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P	-6.47897	3.48254	-1.88961
O	-6.74532	4.95844	-2.14839
O	-6.82736	3.03151	-0.47058
O	-7.27696	2.60960	-3.01233
C	-6.84024	1.39229	-3.63602
C	-7.19994	0.12991	-2.87797
O	-6.23203	-0.13138	-1.84590
C	-8.58853	0.13656	-2.19512
O	-9.31461	-1.00110	-2.70306
C	-8.24603	0.02671	-0.71446
C	-6.93439	-0.74361	-0.75753
N	-6.11503	-0.69059	0.43689
C	-5.62158	-1.90047	1.00137
O	-5.87153	-2.97247	0.45112
N	-4.90001	-1.81239	2.14772
C	-4.60164	-0.63559	2.67501
N	-3.87694	-0.62073	3.81124
C	-5.04554	0.59427	2.10252
C	-5.80090	0.51364	0.98437
P	-10.81246	-1.37721	-2.12850
O	-11.59916	-1.97508	-3.28262
O	-11.43245	-0.21392	-1.37580
O	-10.47108	-2.54045	-1.00945
C	-9.98453	-3.81028	-1.47494
C	-10.14966	-4.85910	-0.39780
O	-9.23569	-4.61456	0.68774
C	-11.54941	-4.93267	0.22403
O	-11.82971	-6.31859	0.45670
C	-11.39268	-4.14757	1.52227
C	-9.94287	-4.43096	1.91536
N	-9.29105	-3.36246	2.66599
C	-8.68028	-3.64181	3.91772
O	-8.76962	-4.77262	4.39723
N	-8.02013	-2.62720	4.53557
C	-7.95413	-1.42257	3.98720
N	-7.30228	-0.45776	4.66425
C	-8.55724	-1.11752	2.72845
C	-9.19851	-2.12757	2.10399
H	13.88650	-3.17017	-1.14557
H	13.19904	-3.88160	-2.62124
H	12.34835	-1.62407	-2.10219
H	12.09793	-2.28290	0.55239
H	10.42419	-3.96810	0.21394
H	8.97999	-2.12377	-1.74687
H	10.20238	-5.46746	-1.11757
H	8.83845	-7.48452	-1.65977
H	5.57882	-7.11964	-3.33979
H	6.68437	-8.23184	-2.60457
H	9.41726	-2.55870	0.58394
H	13.16254	-5.41109	-0.89780
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H	7.85545	2.32495	-1.75734
H	8.15206	2.82606	1.02994
H	7.54125	0.58658	1.60005
H	5.66237	0.72231	-0.81244
H	7.67668	-1.40243	1.29938
H	7.19322	-3.83789	1.54487
H	4.66764	-5.44441	-0.57628
H	5.88417	-5.69588	0.61534
H	5.93124	1.36324	1.56780
H	4.21085	5.57836	-1.96309
H	5.06124	4.02542	-1.85768
H	2.55110	4.02632	-2.36769
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H	1.15335	2.00581	-0.83213
H	3.70353	1.80548	1.72182
H	4.25250	-0.35207	2.84754
H	2.74138	-3.48642	1.68840
H	3.86600	-2.77461	2.77706
H	0.85795	3.43523	1.17369
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H	-0.65255	4.17315	-2.91776
H	-2.84292	2.90413	-3.31894

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H         -0.08246        1.72313        3.02771
H         -0.02121       -1.94145        3.14230
H          0.57548       -0.49389        3.85104
H         -4.53566        2.85533        0.28555
H         -7.35053        1.36884       -4.59882
H         -5.76477        1.42112       -3.80745
H         -7.18244       -0.69730       -3.59430
H         -9.15000        1.03994       -2.41670
H         -8.07601        1.02956       -0.32515
H         -7.09794       -1.80042       -0.95811
H         -6.17710        1.38918        0.46571
H         -4.78304        1.54871        2.53253
H         -3.44652       -1.47910        4.11504
H         -3.49062        0.24163        4.15590
H         -9.02613       -0.46206       -0.14443
H        -10.54402       -4.11662       -2.36111
H         -8.92762       -3.72241       -1.73646
H         -9.90462       -5.82792       -0.83908
H        -12.30400       -4.49650       -0.43275
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H         -9.85637       -5.31974        2.53302
H         -9.65140       -2.02501        1.12829
H         -8.48914       -0.13590        2.28823
H         -6.75787       -0.71973        5.47022
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ss-G6 B3LYP-D3/TZVP
O         10.78930       -5.54665       -0.29819
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C         10.95266       -3.16738       -0.66127
O          9.93693       -3.10969       -1.68446
C         10.22870       -2.86684        0.65540
O         10.25794       -1.43695        0.82868
C          8.81678       -3.35513        0.37792
C          8.64261       -2.96364       -1.08149
N          7.67411       -3.75357       -1.80796
C          7.36344       -5.09791       -1.67185
N          6.43896       -5.48992       -2.50807
C          6.12322       -4.36265       -3.24852
C          5.15655       -4.16333       -4.27601
O          4.35036       -4.95382       -4.75940
N          5.19310       -2.82575       -4.73913
C          6.00536       -1.82778       -4.26433
N          5.90599       -0.61268       -4.85994
N          6.88020       -2.01941       -3.30332
C          6.89138       -3.27990       -2.83213
P          9.74976       -0.74920        2.23232
O         10.79828       -0.89120        3.32670
O          8.36299       -1.24415        2.63593
O          9.72975        0.81250        1.75358
C          9.52129        1.29925        0.41910
C          8.07209        1.56615        0.06679
O          7.40813        0.34657       -0.31551
C          7.22142        2.19063        1.19371
O          6.50622        3.29562        0.60886
C          6.27341        1.06246        1.57674
C          6.07898        0.39857        0.22500
N          5.51023       -0.92197        0.23359
C          5.72320       -1.94978        1.14079
N          5.06927       -3.03751        0.82495
C          4.38805       -2.72689       -0.34153
C          3.48316       -3.49897       -1.12568
O          3.08466       -4.64804       -0.96165
N          3.01112       -2.74394       -2.22782
C          3.32272       -1.43831       -2.50326
N          2.77364       -0.89217       -3.62318
N          4.15591       -0.73683       -1.77278
C          4.65399       -1.41562       -0.72154
P          5.71924        4.37396        1.56385
O          6.70609        5.24528        2.32942
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O	4.67782	3.69805	2.45309
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C	3.39782	4.28866	-1.19104
O	3.36917	2.90708	-0.78219
C	2.24798	4.99079	-0.43763
O	1.18278	5.18076	-1.38883
C	1.86311	3.97277	0.62585
C	2.11302	2.67806	-0.12819
N	2.18720	1.48378	0.67082
C	2.76275	1.31930	1.92293
N	2.63140	0.09844	2.37471
C	1.93816	-0.58333	1.38681
C	1.46203	-1.92533	1.33925
O	1.54832	-2.82091	2.17404
N	0.78475	-2.16960	0.11912
C	0.55553	-1.25359	-0.87284
N	-0.09432	-1.69323	-1.98660
N	0.98577	-0.01628	-0.81194
C	1.65967	0.26476	0.31986
P	-0.07531	6.17433	-1.03697
O	0.35268	7.63507	-1.05658
O	-0.78369	5.75672	0.24983
O	-1.00465	5.88198	-2.34883
C	-0.94252	4.74198	-3.21935
C	-1.92316	3.64225	-2.86511
O	-1.41484	2.83167	-1.78567
C	-3.31628	4.12895	-2.41712
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C	-3.29141	3.88642	-0.91528
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C	-2.14726	-1.31241	0.87696
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O	-6.06186	4.55224	-4.42730
O	-6.39998	4.29084	-1.88524
O	-6.52135	2.21351	-3.32886
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O	-5.36032	-0.14897	-2.19465
C	-7.52555	-0.57007	-3.07284
O	-7.57244	-2.01136	-3.20522
C	-7.65079	-0.06021	-1.64686
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N	-4.49033	-0.64856	3.56428
C	-4.76583	-1.63854	2.65542
N	-4.49799	-2.92932	2.99835
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O	-8.53431	-4.35611	-3.07465
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C	-6.78669	-5.05774	0.40828
O	-6.76942	-4.30391	1.63726
C	-8.13370	-5.77843	0.40762
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C	-9.04593	-4.82668	1.18324
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N	-6.29207	-1.64491	6.37478
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H	10.69616	-3.35739	1.50886
H	8.79267	-4.43438	0.50068
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H	7.86043	-5.72214	-0.94953
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H	6.35099	0.14270	-4.36187
H	5.04085	-0.36976	-5.31745
H	8.08848	-2.88851	1.02750
H	10.06323	2.24397	0.37063
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H	7.83040	2.54214	2.02465
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H	5.43597	1.00105	-0.41907
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H	2.81542	0.11558	-3.65303
H	1.90089	-1.27762	-3.95226
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H	4.84345	5.80549	-1.54554
H	5.53453	4.19002	-1.30008
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H	0.83997	4.09402	0.95925
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H	-2.04321	3.01247	-3.75094
H	-3.49891	5.16693	-2.68860
H	-2.72432	4.67854	-0.42693
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H	-1.54515	-2.22794	2.62459
H	-3.05979	-2.42503	-0.49626
H	-2.71320	-3.26108	0.92340
H	-4.28448	3.80875	-0.48969
H	-6.47045	1.14391	-5.10213
H	-4.89417	1.37201	-4.31418
H	-5.65850	-0.92028	-4.08860
H	-8.26954	-0.14405	-3.74383
H	-7.82953	1.01235	-1.68635
H	-6.19240	-1.37095	-0.74785
H	-6.25094	2.51159	-0.55050
H	-4.15674	-0.89990	4.48662
H	-5.09529	-3.58793	2.50135
H	-4.41228	-3.13439	3.98277
H	-8.43726	-0.53704	-1.07517
H	-6.45254	-4.78855	-1.68914
H	-5.60703	-3.61860	-0.64486
H	-5.97617	-5.78592	0.46642
H	-8.49665	-5.95144	-0.60730
H	-9.52867	-4.14409	0.49141
H	-8.12609	-4.48246	3.14373
H	-9.34230	-2.11743	0.39672
H	-7.07767	0.64686	5.73019
H	-6.20780	-2.62140	6.61032
H	-6.29011	-1.00627	7.15436
H	-9.81928	-5.35948	1.73343
H	-8.78751	-7.47816	1.13412
H	11.24505	-6.38769	-0.41177

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ss-T6 B3LYP-D3/TZVP

O	12.15368	-4.72965	-2.21787
C	12.00965	-3.55474	-3.01352
C	10.84383	-2.68971	-2.57619
O	9.62306	-3.44301	-2.74673
C	10.87415	-2.25109	-1.09777
O	10.49952	-0.86536	-1.07586
C	9.80959	-3.12716	-0.44580
C	8.80918	-3.22748	-1.58444
N	7.80188	-4.26973	-1.50837
C	6.60247	-4.02930	-2.17263
O	6.35590	-2.99193	-2.76428
N	5.69770	-5.06235	-2.09126
C	5.84949	-6.29258	-1.45090
O	4.93865	-7.10987	-1.46645
C	7.14197	-6.47978	-0.81386
C	7.40649	-7.76326	-0.09260
C	8.03908	-5.47893	-0.88557
P	10.59694	0.01029	0.31071
O	12.02975	0.08164	0.81492
O	9.59815	-0.48369	1.35752
O	10.15438	1.46395	-0.28415
C	9.45061	1.70412	-1.51322
C	7.94527	1.72876	-1.36282
O	7.41508	0.39173	-1.27497
C	7.42565	2.48918	-0.12186
O	6.41680	3.40261	-0.59019
C	6.83013	1.38198	0.73919
C	6.32776	0.43847	-0.34174
N	5.97904	-0.90771	0.06932
C	4.81920	-1.46921	-0.45288
O	4.07916	-0.90345	-1.23925
N	4.55434	-2.73627	0.01691
C	5.30281	-3.49912	0.91346
O	4.92248	-4.62048	1.22978
C	6.52067	-2.85715	1.36858
C	7.41314	-3.59567	2.31702
C	6.79821	-1.61401	0.92477
P	5.76328	4.51604	0.42398
O	6.80980	5.50990	0.90598
O	4.97883	3.85301	1.55615
O	4.77184	5.26671	-0.63185
C	4.22164	4.71248	-1.83687
C	2.88447	4.02671	-1.65101
O	3.06101	2.69123	-1.14282
C	1.90833	4.73701	-0.68611
O	0.65269	4.86051	-1.38010
C	1.81067	3.76674	0.48497
C	1.97358	2.44216	-0.24400
N	2.26657	1.27703	0.56751
C	1.57017	0.10378	0.30403
O	0.73814	-0.01418	-0.58013
N	1.87591	-0.93012	1.15996
C	2.81182	-0.94476	2.19273
O	2.96733	-1.95746	2.86632
C	3.54775	0.29476	2.34757
C	4.60313	0.37399	3.40670
C	3.24438	1.33010	1.53714
P	-0.56651	5.74572	-0.72636
O	-0.18306	7.21304	-0.60539
O	-1.06475	5.12980	0.58169
O	-1.66586	5.58241	-1.92022
C	-1.73007	4.52718	-2.89255
C	-2.59737	3.35772	-2.47647
O	-1.87440	2.47146	-1.60037
C	-3.89847	3.74112	-1.73656
O	-4.97664	3.04640	-2.39186
C	-3.66589	3.21171	-0.32795
C	-2.81335	1.99006	-0.62990
N	-2.10541	1.39464	0.48712
C	-2.14130	0.01236	0.62543
O	-2.71550	-0.73841	-0.14614
N	-1.49173	-0.45282	1.74657
C	-0.78595	0.27953	2.69953
O	-0.25889	-0.29259	3.64712
C	-0.73627	1.70474	2.43819
C	0.02519	2.57906	3.38565

C	-1.38872	2.18565	1.35959
P	-6.53026	3.41767	-2.00795
O	-6.87079	4.84680	-2.40267
O	-6.83453	3.09646	-0.54439
O	-7.29549	2.39199	-3.01897
C	-6.77365	1.16704	-3.55855
C	-7.05802	-0.05625	-2.71192
O	-6.10445	-0.16697	-1.63830
C	-8.45816	-0.09349	-2.05909
O	-9.02986	-1.37803	-2.36619
C	-8.15202	0.04160	-0.57335
C	-6.81456	-0.67783	-0.50274
N	-6.02264	-0.48075	0.69680
C	-5.40609	-1.58925	1.26500
O	-5.48388	-2.72111	0.81707
N	-4.71079	-1.30948	2.42026
C	-4.52407	-0.07260	3.03579
O	-3.86876	0.00654	4.06869
C	-5.14119	1.03860	2.33865
C	-4.97754	2.41624	2.90174
C	-5.84986	0.78327	1.21940
P	-10.60745	-1.67930	-2.02204
O	-11.52712	-0.75958	-2.81288
O	-10.87268	-1.66776	-0.51697
O	-10.71323	-3.18312	-2.64693
C	-9.64030	-4.12994	-2.75557
C	-9.38654	-4.94397	-1.50585
O	-8.63969	-4.18094	-0.54573
C	-10.64331	-5.47604	-0.77745
O	-10.59101	-6.90602	-0.84426
C	-10.48856	-4.93293	0.64617
C	-8.98265	-4.70985	0.73463
N	-8.53049	-3.79373	1.76664
C	-7.55984	-4.22478	2.66051
O	-7.05910	-5.33792	2.64579
N	-7.21475	-3.27999	3.60277
C	-7.69074	-1.97503	3.72931
O	-7.26841	-1.25251	4.62621
C	-8.67228	-1.59713	2.73121
C	-9.23885	-0.21160	2.77577
C	-9.03880	-2.51339	1.81008
H	12.93414	-2.98635	-2.90834
H	11.88559	-3.81365	-4.06962
H	10.80869	-1.79367	-3.20088
H	11.85809	-2.37530	-0.64749
H	10.25720	-4.09054	-0.21027
H	8.26693	-2.28907	-1.68891
H	9.01008	-5.57683	-0.42873
H	4.81470	-4.90159	-2.55918
H	9.40175	-2.67993	0.45292
H	11.37373	-5.27646	-2.37338
H	9.77544	2.69009	-1.84636
H	9.73378	0.96622	-2.26147
H	7.53385	2.21413	-2.25287
H	8.21439	3.04337	0.38318
H	7.62736	0.91409	1.31391
H	5.43837	0.84246	-0.82187
H	7.71777	-1.10892	1.19701
H	3.70598	-3.15875	-0.33703
H	6.05182	1.75098	1.39501
H	4.07884	5.56180	-2.50517
H	4.92865	4.02017	-2.29091
H	2.40597	3.96951	-2.63334
H	2.26155	5.72370	-0.39354
H	2.65014	3.93627	1.15710
H	1.07268	2.19498	-0.80260
H	3.78149	2.27089	1.58934
H	1.35865	-1.78552	1.00490
H	0.87063	3.86589	1.01223
H	-2.17101	4.98002	-3.78071
H	-0.72889	4.17467	-3.13436
H	-2.87135	2.81059	-3.38346
H	-4.08573	4.81261	-1.76250
H	-3.09438	3.94477	0.23843
H	-3.41844	1.19237	-1.05682
H	-1.36436	3.23924	1.10342
H	-1.52578	-1.45500	1.87973
H	-4.59731	2.98273	0.17273

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H         -7.27398        1.04092       -4.51870
H         -5.70151        1.25517       -3.72680
H         -6.96321       -0.93344       -3.35898
H         -9.10788        0.69541       -2.43235
H         -8.03244        1.09575       -0.33035
H         -6.95128       -1.75376       -0.59628
H         -6.30996        1.57803        0.64353
H         -4.27597       -2.10706        2.86555
H         -8.92436       -0.40750        0.03636
H         -9.94240       -4.81392       -3.54855
H         -8.72345       -3.62450       -3.05641
H         -8.79148       -5.81519       -1.80349
H        -11.55695       -5.11243       -1.24663
H        -11.01000       -3.98085        0.73263
H         -8.45624       -5.64639        0.91265
H         -9.74526       -2.28099        1.01923
H         -6.52062       -3.57625        4.27676
H        -10.86034       -5.62512        1.39975
H        -11.41639       -7.25267       -0.48498
H          8.41426       -7.77474        0.32061
H          6.69491       -7.89903        0.72481
H          7.29494       -8.61826       -0.76225
H          8.29446       -3.00228        2.55665
H          6.88689       -3.82276        3.24669
H          7.73714       -4.54880        1.89401
H          5.03226        1.37380        3.44914
H          4.18577        0.13504        4.38684
H          5.40655       -0.34179        3.21744
H         -0.07262        3.62697        3.10703
H         -0.34411        2.45616        4.40568
H          1.08644        2.31936        3.39533
H         -5.53964        3.14166        2.31586
H         -5.33130        2.45565        3.93389
H         -3.92701        2.71645        2.91108
H        -10.00896       -0.08423        2.01682
H         -9.67929       -0.00572        3.75322
H         -8.46107        0.53769        2.61097

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ss-A2C2A2 B3LYP-D3/TZVP
O         12.07931       -4.82353       -1.25535
C         12.21194       -3.59782       -1.97735
C         11.03280       -2.70001       -1.67266
O          9.83025       -3.23986       -2.26132
C         10.73194       -2.53353       -0.17505
O         10.29637       -1.17942        0.03310
C          9.57228       -3.49363        0.05156
C          8.81440       -3.32580       -1.25553
N          7.90257       -4.39022       -1.59760
C          7.82062       -5.67595       -1.09896
N          6.87939       -6.39027       -1.66419
C          6.30953       -5.54174       -2.59932
C          5.24976       -5.69495       -3.51145
N          4.55583       -6.84347       -3.63153
N          4.93598       -4.65494       -4.30441
C          5.62022       -3.51271       -4.17154
N          6.62451       -3.24389       -3.33779
C          6.93037       -4.29488       -2.57260
P         10.52103       -0.48943        1.50826
O         12.01010       -0.33163        1.78608
O          9.73092       -1.21037        2.59437
O          9.76709        0.92889        1.23767
C          9.82389        1.67033        0.01103
C          8.42031        2.07696       -0.39876
O          7.66178        0.92492       -0.81860
C          7.59953        2.72492        0.72218
O          6.70916        3.66427        0.09028
C          6.83356        1.54364        1.29723
C          6.52003        0.75546        0.03486
N          6.26122       -0.64853        0.24908
C          6.81197       -1.49842        1.19199
N          6.29938       -2.70529        1.15077
C          5.36488       -2.66161        0.12863
C          4.46655       -3.60928       -0.38644
N          4.33505       -4.84912        0.14195
N          3.67694       -3.24998       -1.41054
C          3.75725       -1.99953       -1.87928
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N	4.54509	-1.01153	-1.45737
C	5.33098	-1.39376	-0.44944
P	5.75325	4.65215	0.99109
O	6.57350	5.72181	1.69650
O	4.84258	3.85643	1.92491
O	4.92437	5.36369	-0.22036
C	4.56250	4.76865	-1.47780
C	3.23581	4.03472	-1.47196
O	3.39991	2.68643	-0.99827
C	2.13093	4.67566	-0.60104
O	0.96231	4.82283	-1.43473
C	1.90881	3.64123	0.49554
C	2.20304	2.36100	-0.26983
N	2.41914	1.15632	0.50053
C	1.78718	-0.05152	0.08195
O	1.05767	-0.04077	-0.90748
N	2.02373	-1.16865	0.81448
C	2.84341	-1.14373	1.85131
N	3.01299	-2.29290	2.54242
C	3.51873	0.04277	2.26774
C	3.27476	1.16715	1.55741
P	-0.27743	5.75778	-0.89988
O	0.12977	7.22315	-0.82989
O	-0.85825	5.21881	0.40769
O	-1.31714	5.56122	-2.14019
C	-1.35162	4.49462	-3.10279
C	-2.32424	3.38288	-2.75648
O	-1.71459	2.43488	-1.85985
C	-3.62566	3.84763	-2.07105
O	-4.70965	3.11358	-2.67504
C	-3.42550	3.40514	-0.62833
C	-2.69579	2.09230	-0.86271
N	-2.03721	1.46776	0.26216
C	-2.06745	0.04610	0.36176
O	-2.65659	-0.60771	-0.49786
N	-1.44556	-0.52301	1.42454
C	-0.78052	0.21349	2.29748
N	-0.20872	-0.41918	3.34579
C	-0.68018	1.63196	2.18571
C	-1.32490	2.21246	1.14867
P	-6.25439	3.65913	-2.53037
O	-6.57713	4.61087	-3.67349
O	-6.54248	4.18110	-1.12929
O	-7.04211	2.23447	-2.66194
C	-6.75377	1.26422	-3.67569
C	-7.11169	-0.11340	-3.15296
O	-6.22464	-0.48834	-2.07853
C	-8.52831	-0.23330	-2.58116
O	-8.96607	-1.57975	-2.85522
C	-8.30738	0.03086	-1.10081
C	-6.95757	-0.62789	-0.85465
N	-6.20387	-0.06487	0.24106
C	-6.00042	1.26502	0.55164
N	-5.26493	1.43211	1.62555
C	-4.96370	0.14875	2.05376
C	-4.21595	-0.35034	3.13057
N	-3.60758	0.45650	4.03356
N	-4.14364	-1.68187	3.29556
C	-4.76188	-2.47543	2.41381
N	-5.46783	-2.11934	1.34036
C	-5.54073	-0.79483	1.20489
P	-10.34068	-2.20674	-2.19816
O	-10.89232	-3.20701	-3.19974
O	-11.27052	-1.11737	-1.69664
O	-9.76777	-2.99269	-0.86676
C	-9.02538	-4.21054	-1.04054
C	-9.13723	-5.08393	0.19201
O	-8.40471	-4.53138	1.30191
C	-10.56227	-5.30025	0.70298
O	-10.61131	-6.62418	1.24696
C	-10.70905	-4.22565	1.77737
C	-9.28743	-4.07931	2.32789
N	-8.93736	-2.72293	2.70858
C	-9.16838	-1.56457	1.99349
N	-8.61318	-0.50544	2.52637
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N	-6.91531	0.97110	4.63190

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N         -6.67279       -1.11824        5.62513
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H         12.24494       -3.77981       -3.05586
H         11.22850       -1.71721       -2.10645
H         11.60013       -2.75344        0.44381
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H          8.47071       -6.02183       -0.31387
H          5.31426       -2.70497       -4.82671
H          4.69890       -7.59033       -2.97319
H          3.73551       -6.86319       -4.21437
H          8.98409       -3.24370        0.92761
H         10.42987        2.56456        0.17148
H         10.26899        1.07230       -0.78263
H          8.49892        2.76816       -1.24043
H          8.22232        3.23747        1.45488
H          7.49485        0.98304        1.95148
H          5.63729        1.15089       -0.46842
H          7.61541       -1.19520        1.84751
H          3.09282       -1.76316       -2.70155
H          5.06692       -5.19311        0.74245
H          3.83629       -5.53513       -0.40227
H          5.94682        1.85446        1.83399
H          4.48741        5.60430       -2.17332
H          5.34996        4.09689       -1.81712
H          2.87381        4.00297       -2.50430
H          2.42747        5.64894       -0.21581
H          2.64948        3.79246        1.27885
H          1.39813        2.12630       -0.96239
H          3.75790        2.11422        1.76706
H          4.20304        0.04559        3.10217
H          2.67491       -3.14419        2.12085
H          3.78492       -2.37817        3.18272
H          0.90708        3.69383        0.90145
H         -1.67510        4.95829       -4.03496
H         -0.35590        4.07663       -3.24110
H         -2.58452        2.87104       -3.68724
H         -3.78668        4.91840       -2.17707
H         -2.77944        4.12126       -0.12274
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H         -5.69345        1.28245       -3.92729
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H         -9.22527        0.46968       -3.03406
H         -8.24155        1.10424       -0.94735
H         -7.06384       -1.68661       -0.61932
H         -6.39901        2.06641       -0.05207
H         -4.67352       -3.54025        2.59669
H         -3.46169        1.42063        3.77959
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H         -9.41544       -4.75972       -1.89958
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H         -6.12676        1.26851        5.18702
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H         12.81342       -5.39839       -1.49749

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ds-A4 B3LYP-D3/TZVP
O         -3.09665       -6.89812        6.10368
C         -4.23031       -6.36297        6.79317
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H	7.73723	-4.09701	-5.58999
H	7.13002	-6.24238	-3.99221
H	4.74268	-5.94629	-4.18642
H	5.14463	-2.95678	-3.70424
H	2.88080	-5.64911	-5.19963
H	0.53506	0.35870	-5.05030
H	3.74001	1.14632	-3.94525
H	2.16163	1.76404	-4.33141
H	5.08300	-5.13017	-2.64170
H	9.31421	-1.49272	-1.70088
H	8.17600	-2.14332	-2.89589
H	7.43251	-0.16855	-1.48995
H	8.12055	-1.70468	0.77531
H	6.18321	-3.14379	0.49589
H	4.73705	-0.58942	-0.35126
H	4.61503	-4.40679	-0.59508
H	-0.72270	-1.11438	-2.15729
H	1.32072	1.63917	-1.57965
H	-0.29062	1.09920	-1.90043
H	5.53775	-1.87971	1.59956
H	8.01739	3.74251	0.52059
H	7.18160	2.34842	-0.19651
H	5.79690	4.39039	-0.09090
H	6.63856	4.94647	2.45296
H	5.74869	2.90858	3.41083
H	3.14878	3.36469	1.88341
H	5.55904	0.67842	3.23878
H	-0.32426	-1.24994	1.39713
H	-0.77828	2.12801	0.69737
H	-1.54999	0.56650	0.80774
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H	2.66118	8.21479	0.63545
H	2.90082	6.46374	0.44350
H	0.59615	7.15618	0.05122
H	0.65770	8.87621	2.18505
H	0.91703	7.23143	3.88733
H	-1.07141	5.32667	2.60081
H	2.43887	5.62844	4.13433
H	-0.51863	-0.05486	4.79435
H	-2.98963	1.39478	2.87253
H	-2.54846	0.02787	3.82940
H	-0.84875	7.35017	3.87506
H	-1.68148	8.64024	2.00381
H	-3.71612	-8.59964	5.75831
H	-2.87957	-7.50403	6.87996
H	-5.03443	-6.64771	5.97951
H	-4.22959	-7.44941	3.43925
H	-2.52099	-5.85745	3.14513
H	-4.02989	-3.63590	4.54669
H	-1.10227	-5.69483	4.91366
H	1.16546	-4.72782	5.31199
H	1.61674	-1.06215	5.55785

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H         -8.08797       -3.86544        2.95630
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H         -7.65102       -1.49983        2.70019
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H         -4.80462       -4.29969       -0.11858
H         -2.62896       -5.41384        0.07353
H          0.28631       -3.59538        1.48816
H         -0.32805       -5.12745        0.90411
H         -6.69754       -1.98793       -1.23361
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H         -7.42403        1.31890        0.89577
H         -6.38079        3.47010        0.53672
H         -7.63145        3.76736       -1.90741
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H         -3.81089        2.77581       -1.70788
H         -6.19939        0.20017       -2.61080
H         -5.48180       -2.07093       -3.28471
H         -1.98216       -3.14184       -2.75221
H         -3.59435       -3.62070       -3.23031
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H         -1.30767        6.46531       -0.56628
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H         -2.25531        6.28077       -4.29738
H          0.29874        4.98109       -3.26959
H         -3.20980        4.44652       -3.92270
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H         -3.39826        0.16806       -5.78531
H         -0.58372        6.79377       -4.56953
H          0.18529        8.37034       -2.86973
H          5.51258       -7.11028       -7.13749
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M06-2X/6-31G(d,p)
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ss-A6 M06-2X/6-31G(d,p)
O         11.21183       -4.69655       -0.47239
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O          9.71258       -2.65103       -1.78533
C         10.38631       -2.04180        0.37477
O         10.03075       -0.65542        0.34097
C          9.13703       -2.90311        0.49703
C          8.59915       -2.84540       -0.93107
N          7.89142       -4.04956       -1.33621
C          7.64983       -5.20988       -0.63916
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C          6.62692       -5.43750       -2.47880
C          5.81477       -5.78234       -3.57571
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N          5.73534       -4.93590       -4.61054
C          6.38263       -3.76406       -4.52340
N          7.13335       -3.29589       -3.53027
C          7.22524       -4.18269       -2.53104
P          9.69372        0.08651        1.74704
O         10.89990        0.08857        2.65194
O          8.44757       -0.47308        2.39875
O          9.42964        1.58518        1.20108
C          9.24911        1.98763       -0.15569
C          7.78268        2.04464       -0.53610
O          7.29458        0.72181       -0.77392
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O          6.00635        3.59752       -0.04854
C          6.11492        1.43971        1.08309
C          5.99579        0.63311       -0.19997
N          5.64680       -0.75464       -0.04586
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O	4.39291	3.92365	1.95305
O	4.40216	5.49669	-0.09598
C	4.09635	5.16001	-1.44810
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C	-4.00203	4.20116	-1.99763
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C	-2.83435	2.56376	-0.86884
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C	-1.08059	0.54864	1.52625
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O	-6.99202	4.94494	-2.74211
O	-6.83263	3.43472	-0.71757
O	-7.25241	2.40875	-3.02048
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C	-6.72034	0.03952	-3.02025
O	-5.73750	-0.01798	-1.97871
C	-8.08690	-0.18540	-2.33825
O	-8.43408	-1.55741	-2.56577
C	-7.76228	0.09286	-0.87656
C	-6.36632	-0.50575	-0.79917
N	-5.58098	-0.13007	0.34549
C	-5.40930	1.13357	0.85544
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C	-4.32612	-0.15931	2.14603
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C	-8.42813	-4.34757	-1.33068
C	-8.19768	-5.32586	-0.19676
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C	-9.46875	-5.78703	0.52192
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C	-9.56546	-4.80451	1.68464

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N	-7.82736	-3.23562	2.54277
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C	-7.06290	-2.91947	3.63888
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H	12.06068	-3.78120	-2.13756
H	11.40194	-1.52532	-1.45985
H	11.12825	-2.22172	1.15933
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H	7.90394	-2.00673	-1.07183
H	8.04797	-5.36826	0.35213
H	6.27107	-3.10814	-5.38455
H	5.30998	-7.64535	-2.93053
H	4.65161	-7.19033	-4.45655
H	8.43379	-2.51591	1.23219
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H	6.74143	0.89468	1.79552
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H	6.47823	-1.24949	1.86691
H	3.63611	-1.93674	-3.85067
H	4.61752	-5.36131	-0.03915
H	3.73085	-5.68314	-1.45487
H	5.16130	1.71898	1.52696
H	4.08726	6.10332	-2.00066
H	4.86355	4.50484	-1.86684
H	2.39628	4.58212	-2.61186
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H	0.84750	2.57890	-1.00514
H	2.90247	2.29339	2.16530
H	0.76413	-1.70705	-2.37654
H	3.14360	-2.62308	2.17047
H	2.52380	-3.79732	1.10884
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H	-0.83482	4.84225	-3.30143
H	-2.90747	3.39854	-3.68386
H	-4.31837	5.24260	-2.10732
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H	-3.45781	1.74393	-1.25072
H	-1.62399	3.68864	1.45297
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H	0.56298	-0.28873	3.38381
H	0.46712	-1.94183	2.99863
H	-4.57547	3.58605	0.01894
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H	-5.57519	1.60054	-3.95687
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H	-8.86664	0.46727	-2.73676
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H	-8.96457	-4.84543	-2.14605
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H	-7.67636	-6.20098	-0.60086
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H	-7.71816	-5.25864	2.77452
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H	-10.11910	-5.20621	2.53545
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H	11.77932	-5.46587	-0.59443

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ss-C6 M06-2X/6-31G(d,p)

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C	10.97974	-2.30518	-0.66641
O	10.56431	-0.93373	-0.73609
C	9.81504	-3.18315	-0.23537
C	9.00068	-3.22426	-1.52625
N	8.13463	-4.38176	-1.66116
C	6.78969	-4.19454	-2.07335
O	6.41265	-3.07454	-2.40213
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C	6.46715	-6.48637	-1.81188
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C	7.86304	-6.72665	-1.56835
C	8.65308	-5.63170	-1.50223
P	10.48199	-0.07482	0.64092
O	11.85042	0.10298	1.24718
O	9.46531	-0.65358	1.60226
O	9.97939	1.34163	0.04735
C	9.38295	1.58068	-1.22731
C	7.86837	1.58479	-1.16727
O	7.37218	0.24609	-1.14312
C	7.29106	2.28572	0.08551
O	6.24624	3.16367	-0.35860
C	6.71223	1.12245	0.88290
C	6.24086	0.24410	-0.27069
N	5.86810	-1.11667	0.03487
C	4.66630	-1.63813	-0.51758
O	3.99540	-0.93732	-1.26745
N	4.29803	-2.89806	-0.15025
C	5.09523	-3.63435	0.59663
N	4.65090	-4.86175	0.96444
C	6.36561	-3.17533	1.07849
C	6.69860	-1.89693	0.77580
P	5.69664	4.28029	0.68630
O	6.79814	5.23151	1.08227
O	4.99256	3.64433	1.86654
O	4.62318	5.03871	-0.25127
C	4.20427	4.68555	-1.56901
C	2.83365	4.03701	-1.55171
O	2.94773	2.67335	-1.14556
C	1.85296	4.69946	-0.56063
O	0.57809	4.77647	-1.21338
C	1.80702	3.69155	0.58288
C	1.88751	2.40241	-0.22757
N	2.17441	1.17816	0.48674
C	1.45098	0.00256	0.14128
O	0.63369	0.04738	-0.77162
N	1.68306	-1.12205	0.87653
C	2.61121	-1.12926	1.80946
N	2.74646	-2.25961	2.55273
C	3.42923	0.00848	2.11021
C	3.16654	1.14280	1.41565
P	-0.55161	5.74482	-0.56203
O	-0.09585	7.18232	-0.56940
O	-0.98644	5.25490	0.80322
O	-1.74108	5.54594	-1.63605
C	-1.81284	4.59718	-2.70047
C	-2.70241	3.42250	-2.34014
O	-1.98740	2.50622	-1.51128
C	-3.96268	3.83016	-1.54589
O	-5.06525	3.08401	-2.07970
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C	-2.12412	0.02807	0.65956
O	-2.78508	-0.61439	-0.14913
N	-1.41586	-0.55386	1.66863
C	-0.68613	0.18044	2.48252
N	-0.03963	-0.45590	3.49430
C	-0.59198	1.60676	2.37914
C	-1.32120	2.19167	1.39714

P	-6.56516	3.56619	-1.68260
O	-6.82969	4.96106	-2.19213
O	-6.83307	3.40167	-0.20116
O	-7.43857	2.50281	-2.52857
C	-6.96976	1.35787	-3.23835
C	-7.18574	0.08679	-2.44201
O	-6.18722	-0.02019	-1.42704
C	-8.54717	0.03205	-1.71157
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O	-5.48726	-2.56030	0.91535
N	-4.47504	-1.26989	2.49430
C	-4.26959	-0.05970	2.97357
N	-3.47466	0.05692	4.06651
C	-4.88042	1.11526	2.42408
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O	-11.47744	-1.32863	-2.74602
O	-11.05716	-0.91560	-0.26141
O	-10.51009	-3.18261	-1.20977
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C	-9.22518	-5.18609	-1.31112
O	-8.26268	-4.63677	-0.40965
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C	-8.38189	-1.75988	2.56937
C	-8.70365	-2.75691	1.71333
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H	12.26526	-4.20378	-3.28581
H	11.52822	-1.90313	-2.71687
H	11.87124	-2.39577	-0.03758
H	10.19114	-4.17265	0.02826
H	8.35127	-2.35030	-1.61714
H	9.72778	-5.67854	-1.34439
H	8.25990	-7.72420	-1.44077
H	4.63989	-7.35260	-2.01007
H	5.92478	-8.46584	-1.65622
H	9.26795	-2.75452	0.60088
H	12.56329	-5.63424	-1.50594
H	9.72363	2.57252	-1.53653
H	9.72414	0.84273	-1.95674
H	7.48819	2.10200	-2.05883
H	8.04910	2.86097	0.62432
H	7.51966	0.62520	1.42934
H	5.37461	0.68939	-0.76706
H	7.63147	-1.43302	1.09506
H	7.01802	-3.80633	1.66803
H	3.88261	-5.23384	0.42461
H	5.31563	-5.53440	1.31550
H	5.91982	1.44440	1.55680
H	4.15250	5.61743	-2.13899
H	4.92643	4.01491	-2.03910
H	2.40589	4.08948	-2.56143
H	2.17565	5.70052	-0.26061
H	2.70184	3.81293	1.20183
H	0.94965	2.22591	-0.76118
H	3.72918	2.06450	1.56261
H	4.21586	-0.03150	2.85279
H	2.37397	-3.10046	2.13264
H	3.60144	-2.38276	3.07558
H	0.90045	3.79112	1.17741
H	-2.24956	5.12498	-3.55280
H	-0.81654	4.23996	-2.96938
H	-3.01392	2.92015	-3.26539
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H	-2.96038	4.09150	0.33375
H	-3.56473	1.31841	-0.84316

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H          0.10531       -1.44846        3.36401
H          0.71460        0.03171        3.95603
H         -4.52442        3.20846        0.46581
H         -7.55530        1.30555       -4.16045
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H         -7.98636        1.33044       -0.08814
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H         -6.20568        1.75161        0.85634
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H         -2.87233       -0.73057        4.26379
H         -3.10065        0.96564        4.29662
H         -8.91320       -0.12867        0.41620
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H         -9.04670       -3.52301       -2.64579
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H        -11.25109       -5.87714       -0.83253
H        -10.62641       -4.44638        1.00879
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H         -8.81885       -0.77405        2.48792
H         -6.20843       -1.28292        4.99615
H         -7.26698       -0.14768        4.25608
H        -10.31975       -6.04556        1.73558
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ss-G6 M06-2X/6-31G(d,p)
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C         11.25915       -4.29660       -1.08922
C         10.56782       -2.97056       -0.83077
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O          9.82827       -1.42686        0.79601
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N          7.33785       -3.66343       -1.89493
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N          5.58655       -0.40843       -4.82622
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P          9.40762       -0.87345        2.26380
O         10.53735       -1.03628        3.24801
O          8.10008       -1.46932        2.73587
O          9.21693        0.69293        1.90802
C          9.21537        1.29676        0.61534
C          7.81580        1.68925        0.18143
O          7.10982        0.54320       -0.30579
C          6.95179        2.26503        1.31882
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C          5.54085       -1.87449        1.04828
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C          3.22909       -1.27755       -2.61580
N          2.65781       -0.70314       -3.72206
N          3.98127       -0.56235       -1.81991
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O          4.65917        5.27925        0.65342
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H	1.11389	2.63896	-0.81872
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H	0.63115	-3.08861	-0.34892
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ss-T6 M06-2X/6-31G(d,p)

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C	-8.19119	-2.05560	2.58981
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C	-8.22199	-5.42115	-1.57931
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C	-9.17117	-5.74784	0.59164
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P	-10.07583	-2.10152	-1.76345
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O	-8.51121	-7.63770	-0.79145
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O	-6.94777	-1.36503	4.49918
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O	-8.53049	-1.66203	-2.04163
C	-8.16554	-0.28652	-1.88613
C	-6.78107	-0.09808	-2.55139
O	-5.82838	-0.04399	-1.48528
C	-6.47514	-0.59864	-0.34220
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O	-7.29770	2.27002	-2.76035
P	-6.55446	3.41465	-1.89581
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C	-4.79799	2.69846	2.96259
O	-5.00936	3.05602	-2.24764
C	-3.97725	3.90998	-1.74155
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C	2.73120	4.13457	-1.80733
O	2.86394	2.84283	-1.20938
C	1.81440	2.72427	-0.25150
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C	4.09721	4.75532	-2.01471
O	4.63800	5.25217	-0.79124
P	5.70702	4.51041	0.16858
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C	3.08566	1.62270	1.53620
O	0.43286	0.34920	-0.44427
O	2.79737	-1.66065	2.87401
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O	6.10109	3.25424	-0.78289
C	7.10405	2.34046	-0.32147

C	7.52463	1.47377	-1.53231
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O	3.99458	-4.52945	1.08490
C	6.62534	-3.86158	2.02886
O	10.17275	-1.16577	-0.99212
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N	7.33325	-4.33869	-1.60619
C	6.03153	-3.99694	-1.92727
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C	6.82405	-6.66397	-1.27268
C	7.70436	-5.64743	-1.35660
O	5.68252	-2.87659	-2.26180
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C	7.20763	-8.08527	-0.99863
O	11.50069	0.00180	0.89249
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O	-10.93540	-1.73293	-2.94543
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H	11.45195	-4.85627	-3.19266
H	11.01430	-2.43684	-2.85911
H	11.28905	-2.70323	-0.13673
H	9.38897	-4.24457	0.06739
H	7.81773	-2.35220	-1.76059
H	8.77768	-5.79249	-1.25144
H	4.17300	-4.81026	-2.01247
H	8.66034	-2.66620	0.49017
H	11.57468	-6.13153	-1.28064
H	9.41762	2.22852	-2.15898
H	9.24234	0.46610	-2.33789
H	7.12535	1.93789	-2.44402
H	7.94297	2.89574	0.10676
H	7.28212	0.79650	1.16898
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H	7.11711	-1.28834	1.08390
H	2.83980	-2.86889	-0.34002
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H	3.99577	5.61754	-2.67953
H	4.77254	4.02830	-2.46997
H	2.23629	4.04110	-2.78300
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H	1.06394	-1.43465	1.12332
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H	-2.32995	5.15773	-3.78128
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H	-5.64119	1.36485	-3.63861

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H	-8.92709	0.36391	-2.32686
H	-7.84281	1.07757	-0.24425
H	-6.52335	-1.68873	-0.42144
H	-6.09894	1.72749	0.71566
H	-3.92270	-1.79362	3.09601
H	-8.59990	-0.49099	0.22350
H	-9.51336	-4.95338	-3.23512
H	-8.23285	-3.75128	-2.92223
H	-7.55347	-6.02403	-2.20583
H	-10.14466	-6.42933	-1.25501
H	-9.89011	-4.92518	0.62144
H	-7.04782	-6.02328	0.93694
H	-9.02845	-2.96506	0.85827
H	-5.73207	-3.51013	4.27222
H	-9.40295	-6.46781	1.37916
H	-9.06018	-8.24694	-0.28216
H	8.28697	-8.17761	-0.86658
H	6.71103	-8.44990	-0.09501
H	6.89758	-8.73532	-1.82182
H	7.52338	-3.34888	2.37956
H	6.06905	-4.22956	2.89517
H	6.92849	-4.73711	1.44178
H	4.91490	1.62097	3.43969
H	4.08752	0.34559	4.35942
H	5.26582	-0.09413	3.12542
H	-0.01418	4.25089	3.06871
H	-0.09614	3.07556	4.39953
H	1.24267	3.00620	3.25663
H	-5.45225	3.37418	2.40745
H	-5.06651	2.73870	4.02161
H	-3.76598	3.05953	2.87534
H	-9.83933	-0.89749	1.86573
H	-9.56623	-0.79021	3.62369
H	-8.49493	0.07196	2.52514

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ss-A2C2A2 M06-2X/6-31G(d,p)

O	10.87859	-5.35159	-1.76882
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C	10.14827	-3.15908	-2.32457
O	8.79008	-3.55358	-2.55496
C	10.23020	-2.76449	-0.84252
O	10.03792	-1.34892	-0.76696
C	9.04420	-3.50254	-0.23509
C	8.03496	-3.38736	-1.36839
N	6.99844	-4.40090	-1.33037
C	6.79008	-5.38213	-0.38875
N	5.71370	-6.09610	-0.59403
C	5.17340	-5.55430	-1.74324
C	3.98478	-5.81457	-2.44856
N	3.08465	-6.73186	-2.01378
N	3.70763	-5.08722	-3.53788
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N	5.67250	-3.71793	-3.26649
C	5.94309	-4.49230	-2.20887
P	10.34251	-0.61277	0.64978
O	11.77805	-0.82768	1.06031
O	9.34093	-0.99848	1.71710
O	10.11750	0.92888	0.21560
C	9.64851	1.39857	-1.04656
C	8.15218	1.63201	-1.02468
O	7.47196	0.37433	-1.04358
C	7.65694	2.37017	0.23830
O	6.67686	3.31887	-0.19668
C	7.00110	1.25357	1.04226
C	6.40689	0.44936	-0.10376
N	5.95193	-0.87534	0.22030
C	6.37000	-1.71620	1.22853
N	5.65841	-2.81289	1.32177
C	4.71587	-2.69165	0.31584
C	3.61752	-3.47848	-0.07785
N	3.24555	-4.60133	0.60331
N	2.87266	-3.07692	-1.11398
C	3.16607	-1.90801	-1.69955
N	4.13487	-1.04877	-1.39347

C	4.88178	-1.49754	-0.38057
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O	7.19166	5.30066	1.37694
O	5.28100	3.74962	1.95691
O	5.14704	5.25279	-0.13994
C	4.64997	4.81433	-1.40370
C	3.31404	4.11013	-1.29441
O	3.48922	2.77596	-0.81718
C	2.31629	4.79315	-0.32712
O	1.08108	4.94534	-1.03759
C	2.17477	3.76838	0.79417
C	2.34225	2.48979	-0.01702
N	2.54935	1.26092	0.71469
C	1.77795	0.12074	0.35727
O	1.00788	0.18880	-0.59493
N	1.93010	-1.00379	1.11191
C	2.80748	-1.03914	2.09681
N	2.87106	-2.17589	2.83538
C	3.65267	0.07021	2.43233
C	3.47809	1.20348	1.70845
P	-0.05646	5.91272	-0.40000
O	0.45253	7.32508	-0.26009
O	-0.61820	5.34317	0.88573
O	-1.16134	5.84551	-1.57660
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C	-2.11560	3.78989	-2.47405
O	-1.48553	2.81148	-1.64382
C	-3.43300	4.17334	-1.76333
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C	-3.22103	3.62505	-0.35812
C	-2.47096	2.34929	-0.71738
N	-1.82576	1.61708	0.34914
C	-1.92613	0.19949	0.34948
O	-2.53018	-0.36283	-0.55799
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C	-0.69205	0.17109	2.32131
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C	-0.48644	1.58947	2.29485
C	-1.08101	2.26829	1.28179
P	-6.02909	3.94081	-2.21616
O	-6.44431	4.85926	-3.33531
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O	-6.76673	2.49907	-2.32782
C	-6.59879	1.68873	-3.48857
C	-6.95851	0.25908	-3.12778
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C	-5.64823	1.27703	0.56795
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C	-4.64365	0.06673	1.99232
C	-3.91793	-0.51348	3.04667
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C	-4.48448	-2.57290	2.19179
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C	-5.22816	-0.81603	1.08954
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O	-10.83252	-2.67351	-3.27441
O	-10.93959	-0.84260	-1.47416
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C	-8.76116	-4.01264	-1.52477
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O	-9.70786	-6.76946	0.71638
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C	-8.56734	-4.26172	1.84284
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C	-8.59894	-1.74696	1.77785
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H         10.38386       -2.28722       -2.94532
H         11.18858       -3.03645       -0.38977
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H          7.54070       -2.40522       -1.37588
H          7.46399       -5.51403        0.44543
H          4.26557       -3.52318       -4.75067
H          3.40834       -7.44270       -1.37402
H          2.35501       -6.99799       -2.65901
H          8.70849       -3.06351        0.70424
H         10.15526        2.34978       -1.23088
H          9.90341        0.69488       -1.84180
H          7.87326        2.21990       -1.90853
H          8.46396        2.88473        0.76773
H          7.77469        0.66051        1.53898
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H          2.51967       -1.62380       -2.52634
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H          2.64256       -5.22270        0.07437
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H          2.85587        4.08488       -2.29292
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H          3.01015        3.88073        1.49153
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H          4.38989        0.01066        3.22263
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H          3.71977       -2.34240        3.35774
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H         -1.55304        5.55237       -3.54300
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H         -0.99281        3.34794        1.16319
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H         -0.14706       -1.54406        3.21606
H          0.52243       -0.14781        3.92588
H         -4.15784        3.45985        0.16928
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H         -9.07024        0.82906       -2.85940
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H         -3.13180        1.20232        3.75084
H         -2.55956       -0.21516        4.49640
H         -8.81567       -0.23950       -0.39293
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H         -7.77161       -3.68600       -1.86542
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H         -8.23360       -4.97123        2.60648
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H         -6.59978        1.19868        3.73494
H         -5.64385        0.93943        5.11925
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ds-A4 M06-2X/6-31G(d,p)
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C	5.34029	4.68104	3.19719
N	3.90274	4.65188	3.40492
C	3.26740	3.41746	3.38072
O	3.85326	2.36939	3.14336
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O	-0.01554	4.43378	4.29100
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C	1.16625	7.05260	4.47933
C	3.23023	5.79502	3.79008
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O	9.08091	2.99942	0.86017
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C	7.71032	1.04773	1.38545
O	6.41182	1.63450	1.48130
C	7.87294	0.60244	-0.08570
O	7.66172	-0.81512	-0.11259
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O	3.15357	0.16152	0.70051
N	2.17690	2.20581	0.57873
C	2.18880	3.57483	0.43486
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C	4.54469	3.34648	0.00388
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O	7.20565	-1.22141	-2.64343
O	7.57459	-3.13161	-0.96448
C	6.84722	-3.46819	0.21736
C	5.39861	-3.78463	-0.09579
O	4.66005	-2.57825	-0.30504
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O	4.22122	-5.61126	-1.09593
C	4.69208	-3.59967	-2.37195
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O	1.15092	-2.05427	-1.30156
N	1.58759	0.05793	-2.01713
C	2.41618	1.06107	-2.47749
O	1.99392	2.21204	-2.62826
C	3.78503	0.66778	-2.76177
C	4.67996	1.67939	-3.40920
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O	3.39273	-6.38579	-3.44450
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C	1.86963	-7.16640	-0.53381
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O	0.98194	-5.33266	-1.84657
C	0.39939	-7.49190	-2.65331
O	-0.72403	-8.29053	-2.32983
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C	0.06582	-5.12753	-2.90936
N	0.44509	-3.92278	-3.62281
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C	3.56170	-2.59431	-5.33267
C	1.71991	-3.83030	-4.13420
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H	-0.94012	-4.95093	-2.51698
H	2.31622	-4.73464	-4.00742
H	-0.63047	-0.96620	-4.44171
H	-0.79719	-6.61432	-4.26830
H	-0.85151	-8.92898	-3.04133
H	-8.44333	5.84577	-6.25533
H	-7.23690	4.88187	-7.13856
H	-8.35915	3.66901	-5.27449
H	-8.05823	5.88347	-3.64325
H	-5.63246	5.74235	-3.72037
H	-5.97273	2.72798	-3.25122
H	-3.51891	5.47038	-3.58921
H	-3.45134	-0.76934	-5.09885
H	0.39327	2.70333	-4.32391
H	0.63380	1.07462	-4.88116
H	-6.01064	4.93913	-2.15268
H	-10.39974	1.22570	-1.55338
H	-9.25718	1.88410	-2.75029
H	-8.54169	-0.22767	-1.51241
H	-9.21424	1.13401	0.86063
H	-7.28952	2.64077	0.59000
H	-5.85059	0.09105	-0.32015
H	-5.54523	3.88114	-0.12745
H	-1.96855	-1.10775	-2.03919
H	-0.72761	3.91985	-1.10799
H	0.37178	2.71342	-1.74153
H	-6.64320	1.36645	1.69044
H	-7.95613	-4.27440	1.07879
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H	-5.65005	-4.41320	0.62156
H	-6.43336	-4.31835	3.33286
H	-5.66874	-2.02077	3.53860
H	-3.30374	-2.90873	1.79086
H	-5.41086	0.08052	2.85295
H	0.53784	-0.94587	0.63468
H	-2.00477	3.44074	2.00302
H	-0.35089	3.39726	1.43861
H	-4.24409	-2.93543	4.12714
H	-2.15125	-7.47177	2.47631
H	-2.50987	-5.93667	1.63676
H	-0.12470	-6.53456	1.48892
H	-0.11316	-7.41211	4.08628
H	-0.56959	-5.24647	5.06896
H	1.39818	-3.90546	3.15984
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H          1.21113       -5.26901        5.14860
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H          0.35673        7.27105        3.77671
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H          4.49049        5.94504       -0.55177
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H          4.20298        2.07668       -4.31002
H          4.87118        2.52753       -2.74176
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ds-G4 M06-2X/6-31G(d,p)
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N          3.36111       -1.53967       -4.18825
C          2.75626       -2.73563       -4.33304
P          7.90598       -4.97419       -1.39827
O          8.93605       -6.07473       -1.35674
O          6.75314       -5.18794       -0.44317
O          8.62804       -3.55384       -1.11840
C          8.54140       -2.37078       -1.91239
C          7.59884       -1.34892       -1.30752
O          6.23975       -1.70681       -1.56699
C          7.71678       -1.22314        0.22424
O          7.58199        0.16817        0.53196
C          6.48749       -1.97826        0.71616
C          5.49712       -1.54105       -0.35538
N          4.26943       -2.27681       -0.46796
C          4.07490       -3.64092       -0.36123
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C          3.07900       -1.74809       -0.90110
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C          7.20831        2.91666        0.60396
C          5.76234        3.28703        0.87095
O          4.95461        2.10959        0.91526
C          5.55753        3.99663        2.22438
O          4.57587        5.02077        2.02865
C          4.97992        2.89331        3.10165
C          4.12093        2.16991        2.07380
N          3.70345        0.83566        2.41047
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P	4.72025	6.40405	2.87642
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O	1.05378	5.83553	1.12898
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O	-0.57045	8.33974	1.02974
C	0.28010	7.12032	2.95448
C	0.20353	5.75563	2.26495
N	0.61993	4.65931	3.11705
C	1.78835	4.59056	3.85502
N	1.94156	3.44857	4.46649
C	0.82064	2.72458	4.12028
C	0.46588	1.38234	4.43451
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C	-7.37809	-1.96251	1.75174
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C	-5.51716	-2.12818	0.42618
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C	-2.98031	-1.25468	-2.47024
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O	-3.44261	6.32815	-2.31488
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C	-0.69640	7.28012	-2.64180
O	0.64565	7.62605	-2.33590
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O	1.19040	2.96311	-4.14285
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M06-2X/TZVP
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ss-A6 M06-2X/TZVP
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C	-3.45824	-1.19533	2.95171
N	-2.65308	-0.51333	3.80363
N	-3.53502	-2.52670	3.04785
C	-4.34925	-3.18562	2.21678
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C	-9.16745	-4.97316	0.13390
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C	-7.32354	-2.83442	3.82193
H	12.71119	-3.71880	-0.62718
H	12.30597	-3.53299	-2.34888
H	11.34178	-1.78374	-0.86584
H	10.61819	-3.73243	0.94536
H	9.04901	-4.77415	-0.58505
H	8.10988	-1.93685	-1.26783
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H	6.67395	-0.03867	-5.18348
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H	8.96965	2.66869	1.17474
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H	6.50980	0.22672	2.72432
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H	5.52350	4.08017	-0.51810
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H	-8.54950	-4.99993	3.09665
H	-9.10673	-1.64194	1.42745
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ss-C6 M06-2X/TZVP
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O          2.93868        3.02268       -1.42292
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ss-T6 M06-2X/TZVP
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ds-A4_M06-2X/TZVP
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ds-G4 M06-2X/TZVP
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C	3.22850	-4.43312	-0.21137
C	4.35176	-3.69616	-0.09573
P	8.71040	0.39779	0.85579
O	9.82462	1.38266	0.59937
O	8.75322	-0.37079	2.15392
O	7.25627	1.14624	0.80010
C	6.93295	1.87668	-0.38533
C	5.82826	2.86179	-0.08515
O	4.61891	2.17677	0.24326
C	6.11156	3.80243	1.08984
O	5.52696	5.05756	0.72971
C	5.41730	3.10982	2.25609
C	4.22767	2.42485	1.58918
N	3.80418	1.15573	2.18288
C	2.42725	0.87290	2.25354
O	1.62045	1.79141	2.10776
N	2.03333	-0.40344	2.47230
C	2.92645	-1.37119	2.65327
N	2.49210	-2.62712	2.72733
C	4.32755	-1.08555	2.73076

C	4.71072	0.17157	2.43211
P	5.24973	6.29038	1.76208
O	5.50711	7.57716	1.01542
O	5.95380	6.10252	3.08348
O	3.64733	6.11158	2.03556
C	2.77172	6.17884	0.90641
C	1.33776	6.18141	1.37779
O	1.02597	4.93731	2.00848
C	1.00227	7.27100	2.39862
O	-0.33643	7.67730	2.13545
C	1.11460	6.54057	3.73175
C	0.64929	5.13384	3.36311
N	1.23456	4.06033	4.15883
C	0.41879	3.02244	4.63151
O	-0.80793	3.13356	4.56352
N	1.01025	1.92342	5.15899
C	2.33443	1.82242	5.20775
N	2.86726	0.67747	5.63652
C	3.18628	2.89709	4.80335
C	2.58946	3.96334	4.24029
H	-6.73460	-6.51328	6.50223
H	-5.66812	-5.43155	7.42580
H	-6.82154	-4.35222	5.51372
H	-6.26687	-6.51232	3.91437
H	-3.85511	-6.19727	4.06714
H	-4.38589	-3.22312	3.56519
H	-1.79692	-5.77325	4.65755
H	-0.17148	0.41966	5.26246
H	-3.49521	0.93958	4.41584
H	-1.97740	1.67895	4.75623
H	-4.24397	-5.40612	2.50351
H	-9.45801	-2.78566	1.56965
H	-8.25036	-2.83470	2.87800
H	-8.46367	-0.59271	1.90183
H	-8.69066	-1.61304	-0.62177
H	-6.48406	-2.61669	-0.66377
H	-5.31050	-0.07576	0.54500
H	-5.14293	-3.91561	0.44439
H	0.21372	-0.77283	2.13909
H	-1.83469	2.02190	2.04469
H	-0.19949	1.42699	2.19027
H	-6.17979	-1.05319	-1.46171
H	-7.62872	3.92932	-0.01854
H	-7.11276	2.29779	0.46198
H	-5.29706	4.01474	-0.06289
H	-6.60851	4.42245	-2.50864
H	-5.95972	2.19702	-3.31171
H	-3.29607	2.83376	-1.94550
H	-5.40281	-0.00290	-3.38570
H	0.40829	-1.54608	-1.06390
H	0.51975	1.79406	-0.16690
H	1.41272	0.30758	-0.32564
H	-4.64957	3.24544	-3.97323
H	-3.11997	8.23217	-0.97686
H	-3.43825	6.51952	-0.61504
H	-1.13616	7.17361	-0.11327
H	-1.00051	8.68727	-2.39206
H	-1.18997	6.87497	-3.94390
H	0.67653	5.11328	-2.30488
H	-2.66278	5.26119	-4.18711
H	0.44645	-0.36329	-4.30276
H	2.69691	1.18729	-2.21595
H	2.37895	-0.18191	-3.21652
H	0.57836	6.98062	-3.81709
H	1.30441	8.41920	-2.00973
H	4.66373	-8.38026	-5.93086
H	3.70510	-7.33006	-6.99989
H	5.67286	-6.21475	-5.95968
H	4.96441	-7.39227	-3.54001
H	2.99251	-6.11966	-3.18965
H	4.26476	-3.59015	-4.30063
H	1.59903	-5.90408	-4.94813
H	-0.77432	-5.16330	-5.26383
H	-1.61422	-1.56460	-5.12665
H	-2.21182	-3.18888	-5.36751
H	4.16813	-5.05368	-2.39552
H	8.30411	-3.40867	-2.90001
H	6.72330	-3.03008	-3.62658

H	7.74891	-1.05502	-2.60155
H	8.69282	-2.59962	-0.52094
H	6.74253	-3.12198	0.55267
H	5.25930	-0.53966	0.02024
H	5.29639	-4.17106	0.10919
H	3.25663	-5.50495	-0.08813
H	0.14418	-3.95513	-1.37852
H	0.96485	-5.44474	-0.96006
H	6.93460	-1.56224	1.33396
H	7.81250	2.41955	-0.74248
H	6.60003	1.18055	-1.16055
H	5.65506	3.45552	-0.98494
H	7.17882	3.93947	1.26729
H	6.11107	2.39168	2.68914
H	3.34319	3.06120	1.60577
H	5.75416	0.44450	2.33817
H	5.05106	-1.86311	2.92550
H	1.51641	-2.84563	2.50999
H	3.14992	-3.38331	2.82317
H	5.12018	3.81597	3.02422
H	2.96705	7.08990	0.33451
H	2.94130	5.31004	0.26389
H	0.70549	6.30200	0.49659
H	1.68641	8.11895	2.32553
H	2.15088	6.54642	4.06551
H	-0.42722	5.02937	3.46879
H	3.14708	4.77916	3.79575
H	4.25980	2.81577	4.87736
H	2.27056	-0.14700	5.74107
H	3.86631	0.55371	5.61079
H	0.48919	6.98534	4.50435
H	-0.59498	8.33104	2.79455
H	-4.59319	-7.41078	6.95386
H	2.36458	-8.50874	-5.50071

ONIOM Optimized geometries

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ss-C4 B3LYP-D3/6-31G(d,p) mechanical embedding

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H	17.05919	27.28177	30.47253
O	16.79772	26.78585	29.66032
C	16.97805	25.39629	29.96666
H	16.16707	24.85809	29.46846
H	16.87195	25.23663	31.05109
C	18.30829	24.79786	29.50005
H	18.49197	23.90095	30.10292
O	18.23345	24.38136	28.12928
C	19.08533	25.19031	27.31635
H	19.94132	24.60136	26.98812
N	18.32212	25.53609	26.09312
C	17.90451	26.77255	25.76887
H	18.20923	27.59188	26.40709
C	17.12779	26.99792	24.66761
H	16.79664	28.00140	24.41322
C	16.72513	25.85630	23.91484
N	15.90090	26.02824	22.81067
H	15.35002	25.20832	22.54435
H	15.29185	26.84324	22.85503
N	17.15834	24.63733	24.17319
C	18.02562	24.42468	25.22331
O	18.52476	23.33583	25.45235
C	19.51342	25.75915	29.59707
H	19.32598	26.55467	30.34000
C	19.50234	26.36823	28.18137
H	18.72265	27.13572	28.20171
H	20.46904	26.79671	27.91980
O	20.64935	25.01049	29.97093
P	22.21746	25.37357	29.45503
O	23.13478	24.84169	30.51472
O	22.28002	26.79364	28.96716
O	22.29067	24.42142	28.12010
C	22.56063	23.02144	28.25041
H	21.61974	22.48957	28.44908
H	23.24962	22.84700	29.08097

C	23.15905	22.51772	26.95274
H	23.43351	21.46537	27.06120
O	22.16447	22.66106	25.91015
C	22.71145	23.45431	24.87756
H	23.17891	22.81333	24.13057
N	21.62830	24.14628	24.16623
C	21.42911	25.47562	24.17834
H	22.05546	26.08071	24.82591
C	20.48561	26.04694	23.37001
H	20.34177	27.12458	23.35193
C	19.77576	25.18536	22.48125
N	18.97176	25.72543	21.49298
H	18.14596	25.19618	21.23934
H	18.73270	26.71754	21.61550
N	19.91496	23.87605	22.48300
C	20.84296	23.29688	23.31306
O	21.04565	22.09562	23.32936
C	24.39968	23.30721	26.46282
H	24.95231	23.77060	27.28584
C	23.75858	24.34062	25.53705
H	23.29755	25.11920	26.14678
H	24.47566	24.76788	24.83170
O	25.23988	22.50412	25.64622
P	26.39761	21.53413	26.37094
O	25.71345	20.68810	27.41353
O	27.63603	22.31752	26.67544
O	26.72733	20.61906	25.03612
C	25.90631	19.50576	24.73053
H	25.02988	19.46736	25.38380
H	26.48242	18.58077	24.88516
C	25.48548	19.53182	23.27610
H	25.03908	18.55603	23.01577
O	24.52312	20.57184	23.05561
C	24.56899	20.85481	21.66531
H	23.97854	20.13703	21.08806
N	23.94752	22.15789	21.42536
C	24.42813	23.26126	22.04301
H	25.24290	23.11529	22.74408
C	23.87913	24.48664	21.80531
H	24.26510	25.38311	22.28386
C	22.75645	24.53503	20.92710
N	22.20960	25.76321	20.56813
H	21.21974	25.75853	20.32762
H	22.35335	26.49926	21.27617
N	22.24236	23.47167	20.35303
C	22.83804	22.24201	20.52306
O	22.45942	21.25942	19.90658
C	26.63707	19.76690	22.27080
H	27.51784	20.17328	22.76756
C	26.05142	20.79078	21.28070
H	26.52365	21.76618	21.43106
H	26.19000	20.49934	20.24144
O	26.95259	18.49232	21.70838
P	28.12966	18.38204	20.56432
O	28.55583	16.94508	20.51308
O	29.10546	19.51278	20.64826
O	27.23399	18.71905	19.19622
C	26.08378	17.97138	18.88273
H	25.34050	18.02326	19.68799
H	26.32466	16.91139	18.71202
C	25.51112	18.57018	17.61230
H	24.71907	17.92872	17.20291
O	24.96429	19.87342	17.90393
C	25.54502	20.81238	17.01410
H	24.98994	20.83234	16.06735
N	25.44221	22.14576	17.57242
C	26.46439	22.77611	18.20353
H	27.40862	22.25118	18.27287
C	26.30264	24.02639	18.70829
H	27.11881	24.53402	19.21142
C	25.02139	24.64262	18.53659
N	24.83577	25.93440	18.92960
H	23.90814	26.24797	19.20549
H	25.59409	26.38027	19.45050
N	23.99242	24.02750	17.97245
C	24.13268	22.74564	17.50817
O	23.20414	22.09110	17.05431
C	26.59432	18.80015	16.53793

H	27.45327	18.13329	16.66238
C	26.94678	20.26599	16.75715
H	27.58781	20.33090	17.63616
H	27.44462	20.71428	15.89127
O	25.97707	18.59646	15.25944
H	26.41773	19.19321	14.60766

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ss-C4 B3LYP-D3/6-31G(d,p) electrical embedding
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H	15.76203	28.23439	29.03443
O	16.72577	28.09639	29.18278
C	16.88722	27.13347	30.22495
H	15.93374	26.63040	30.39843
H	17.16544	27.64363	31.14818
C	17.94646	26.05318	29.92831
H	18.00242	25.38740	30.79191
O	17.53152	25.30562	28.78977
C	18.55296	25.35106	27.80605
H	19.20228	24.47344	27.92830
N	17.88519	25.35712	26.46552
C	17.18120	26.44515	26.04398
H	17.15065	27.30081	26.70309
C	16.52137	26.43263	24.85798
H	15.95945	27.29433	24.52165
C	16.51922	25.19720	24.12925
N	15.83795	25.11927	22.96942
H	15.67254	24.20983	22.53560
H	15.18801	25.85486	22.73349
N	17.17886	24.12068	24.55316
C	17.89741	24.15701	25.70956
O	18.54438	23.18948	26.13270
C	19.35606	26.59813	29.65302
H	19.47235	27.61207	30.04271
C	19.40625	26.58320	28.12740
H	18.96732	27.50598	27.75668
H	20.41972	26.48546	27.74506
O	20.31046	25.72862	30.25176
P	21.88852	25.98887	30.16206
O	22.56242	25.41762	31.34587
O	22.10838	27.41187	29.84581
O	22.32501	25.10592	28.90486
C	22.30374	23.68920	29.00342
H	21.30490	23.36441	29.29671
H	23.00757	23.36858	29.77249
C	22.66637	23.00089	27.68892
H	22.71998	21.92664	27.87429
O	21.64080	23.23720	26.73593
C	22.25691	23.35900	25.47643
H	22.53290	22.36542	25.10420
N	21.34706	24.05946	24.52883
C	20.92024	25.32458	24.79405
H	21.23989	25.76439	25.72956
C	20.10870	25.98134	23.92537
H	19.75743	26.98339	24.12963
C	19.72864	25.26324	22.74898
N	18.96822	25.85370	21.79290
H	18.58542	25.19783	21.11519
H	18.38042	26.63227	22.04902
N	20.12116	24.02143	22.50754
C	20.89873	23.35079	23.39187
O	21.21427	22.16012	23.23544
C	24.00398	23.46964	27.08097
H	24.49873	24.20274	27.72283
C	23.53454	24.13281	25.78519
H	23.32581	25.18075	25.99622
H	24.25086	24.05737	24.97234
O	24.84440	22.33606	26.88456
P	26.24648	22.39196	26.09891
O	27.19083	21.49943	26.80660
O	26.61656	23.80418	25.85731
O	25.83763	21.71192	24.71257
C	25.41240	20.35421	24.67874
H	24.49565	20.24337	25.26019
H	26.18315	19.72766	25.12907
C	25.16104	19.83566	23.26009
H	24.87391	18.78974	23.33917
O	24.08969	20.54865	22.65564

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C         24.51818       21.05513       21.40082
H         24.24142       20.34750       20.61233
N         23.89732       22.39216       21.17981
C         24.11146       23.38204       22.09433
H         24.72982       23.12749       22.94578
C         23.56359       24.61000       21.93347
H         23.73178       25.40711       22.64323
C         22.70203       24.77498       20.80448
N         22.09007       25.95858       20.60418
H         21.33487       25.99970       19.93659
H         22.14326       26.68429       21.31062
N         22.47330       23.80146       19.92726
C         23.07392       22.58442       20.04771
O         22.93674       21.67908       19.21252
C         26.40373       19.94346       22.36564
H         27.29523       20.16464       22.95924
C         26.04588       21.12372       21.47126
H         26.39067       22.03802       21.95285
H         26.48664       21.04132       20.48314
O         26.58752       18.73472       21.64122
P         27.83102       18.51605       20.65492
O         28.17703       17.08152       20.65539
O         28.89952       19.48429       20.96775
O         27.27044       18.90428       19.22428
C         26.22264       18.17727       18.60010
H         25.33671       18.17681       19.23781
H         26.53095       17.14430       18.43704
C         25.86186       18.81068       17.25051
H         25.09111       18.20065       16.77812
O         25.35364       20.11832       17.48172
C         26.08296       21.02635       16.67984
H         25.62180       21.05171       15.68777
N         26.00960       22.37461       17.30963
C         26.79568       22.70765       18.37075
H         27.54181       21.99662       18.69606
C         26.61932       23.88704       19.01963
H         27.22579       24.15633       19.87323
C         25.59142       24.74889       18.52498
N         25.34136       25.91897       19.15384
H         24.72494       26.56877       18.67616
H         26.09232       26.31914       19.70358
N         24.84233       24.43031       17.47403
C         24.98787       23.22939       16.85663
O         24.26109       22.89276       15.90860
C         27.07143       18.95336       16.30256
H         27.88220       18.27653       16.58179
C         27.47120       20.40890       16.49310
H         28.09295       20.49012       17.38072
H         27.98807       20.81644       15.62533
O         26.68944       18.75955       14.94906
H         27.39080       19.11275       14.35792

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ss-C4 B3LYP-D3/TZVP mechanical embedding
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H         16.34919       27.82630       30.07009
O         16.88697       27.19776       29.54592
C         17.05975       26.01387       30.34269
H         16.15473       25.39632       30.29641
H         17.23702       26.29118       31.38974
C         18.25013       25.20376       29.86234
H         18.43070       24.42835       30.61127
O         17.98621       24.56078       28.60780
C         18.79018       25.14916       27.56837
H         19.51358       24.41606       27.23291
N         17.93206       25.40880       26.40788
C         17.11260       26.47782       26.33801
H         17.14595       27.18726       27.15430
C         16.25498       26.63914       25.29934
H         15.61725       27.51269       25.23855
C         16.21745       25.60625       24.31794
N         15.29902       25.67983       23.30077
H         15.41283       25.05483       22.51327
H         14.97237       26.59962       23.03450
N         16.94913       24.51852       24.39486
C         17.84601       24.36341       25.42057
O         18.54113       23.37228       25.53073
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C	19.53668	26.02519	29.66736
H	19.51791	26.93727	30.27332
C	19.47079	26.36771	28.17441
H	18.86916	27.26883	28.06547
H	20.45584	26.55233	27.76040
O	20.61990	25.20111	30.05091
P	22.20755	25.51440	29.59725
O	23.06906	24.91045	30.67632
O	22.34814	26.94574	29.14275
O	22.29792	24.60565	28.22114
C	22.26096	23.18119	28.30645
H	21.23069	22.84634	28.47343
H	22.87875	22.83824	29.13997
C	22.77811	22.58687	27.01483
H	22.84885	21.50317	27.13253
O	21.86194	22.87294	25.93544
C	22.53707	23.62786	24.94058
H	22.87080	22.97209	24.14422
N	21.57718	24.53903	24.30416
C	21.38664	25.80405	24.70844
H	22.00802	26.17960	25.50666
C	20.44608	26.58994	24.12251
H	20.29199	27.61598	24.43096
C	19.69664	26.02320	23.05120
N	18.72298	26.81625	22.46599
H	18.30694	26.46798	21.60320
H	19.02151	27.78377	22.33976
N	19.82376	24.77470	22.67360
C	20.74314	23.96073	23.28577
O	20.86930	22.78386	23.01295
C	24.14018	23.14166	26.56180
H	24.73777	23.49280	27.40084
C	23.72578	24.27710	25.63088
H	23.42981	25.12740	26.23738
H	24.52819	24.54982	24.94822
O	24.81947	22.16411	25.79490
P	26.39203	21.75941	26.20472
O	26.33952	20.84448	27.40567
O	27.28201	22.97641	26.15631
O	26.68070	20.87872	24.83485
C	26.04700	19.61418	24.70281
H	25.09423	19.58716	25.23497
H	26.69207	18.83238	25.12163
C	25.81377	19.32511	23.23877
H	25.56048	18.26579	23.12043
O	24.71484	20.12651	22.75238
C	25.09584	20.72523	21.51893
H	24.83972	20.09099	20.67340
N	24.33077	21.95673	21.31803
C	24.56430	23.03831	22.08901
H	25.27103	22.92551	22.89911
C	23.93010	24.21288	21.85147
H	24.12990	25.09485	22.44712
C	22.99233	24.24191	20.78105
N	22.44504	25.44681	20.40721
H	21.58435	25.46799	19.86749
H	22.52764	26.22547	21.06518
N	22.66727	23.17808	20.08638
C	23.34603	21.99950	20.27449
O	23.15179	21.02985	19.56553
C	27.02760	19.63218	22.33584
H	27.93081	19.78678	22.92463
C	26.60071	20.91412	21.62752
H	26.83984	21.74517	22.29123
H	27.09561	21.05853	20.67360
O	27.21369	18.49590	21.48725
P	27.89706	18.53597	19.98891
O	28.32103	17.10699	19.74447
O	28.84138	19.70704	19.83614
O	26.57858	18.91777	19.04576
C	25.75305	17.92376	18.46675
H	24.78686	17.90503	18.97782
H	26.21876	16.93654	18.54165
C	25.52605	18.28530	17.00822
H	24.88014	17.53606	16.54104
O	24.84952	19.54749	16.92690
C	25.70575	20.53203	16.38973
H	25.38472	20.76577	15.36742

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N         25.58089       21.78653       17.13036
C         26.51144       22.27017       17.98531
H         27.39200       21.67507       18.16974
C         26.34421       23.47836       18.57826
H         27.09266       23.87055       19.25355
C         25.18072       24.21990       18.22859
N         25.05506       25.53814       18.60825
H         24.11499       25.85096       18.85027
H         25.70125       25.81715       19.35647
N         24.21338       23.71795       17.49850
C         24.33571       22.46993       16.95737
O         23.42699       21.91829       16.36316
C         26.83000       18.44619       16.21380
H         27.63065       17.83326       16.62687
C         27.11046       19.93199       16.36097
H         27.66014       20.07724       17.28454
H         27.68924       20.33910       15.52907
O         26.60078       18.06769       14.83634
H         27.19157       18.63326       14.28228

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ss-C4 B3LYP-D3/TZVP electrical embedding
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H         15.65489       28.11814       29.06418
O         16.63274       28.02660       29.16832
C         16.85160       27.08237       30.22043
H         15.91351       26.56208       30.42567
H         17.13793       27.61047       31.13131
C         17.92137       26.01290       29.92284
H         17.96045       25.33107       30.77562
O         17.53518       25.28478       28.76194
C         18.57993       25.34752       27.80413
H         19.22871       24.46861       27.92191
N         17.92513       25.35867       26.45907
C         17.30334       26.47620       25.99126
H         17.32497       27.35089       26.61527
C         16.64982       26.47023       24.81151
H         16.14973       27.35489       24.44689
C         16.54500       25.21446       24.13248
N         15.84102       25.14575       23.00086
H         15.66436       24.25060       22.54738
H         15.39835       25.97589       22.62649
N         17.11823       24.10925       24.60710
C         17.83421       24.13469       25.75432
O         18.39937       23.13628       26.22168
C         19.33623       26.56154       29.69042
H         19.44412       27.56811       30.10102
C         19.42930       26.57086       28.16671
H         19.00893       27.50382       27.80612
H         20.45169       26.47351       27.80668
O         20.27009       25.67876       30.29961
P         21.84962       25.93304       30.25009
O         22.49957       25.34372       31.43778
O         22.08123       27.35885       29.95690
O         22.29647       25.06567       28.98818
C         22.27937       23.64801       29.06724
H         21.28258       23.31017       29.35828
H         22.98767       23.31916       29.82884
C         22.64776       22.99271       27.73735
H         22.71420       21.91536       27.90024
O         21.61830       23.23856       26.78818
C         22.24438       23.38469       25.53627
H         22.55912       22.40001       25.17107
N         21.32363       24.04117       24.56689
C         20.92423       25.32691       24.74644
H         21.25790       25.82700       25.64293
C         20.11646       25.93397       23.84671
H         19.79441       26.95422       23.98384
C         19.70569       25.15280       22.72646
N         18.92914       25.68200       21.76077
H         18.54807       25.02306       21.08675
H         18.43745       26.54396       21.92016
N         20.08255       23.89577       22.56686
C         20.86156       23.27757       23.47744
O         21.17183       22.07999       23.38505
C         23.98116       23.48928       27.13714
H         24.47538       24.20682       27.79711
C         23.50024       24.18594       25.86313
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H	23.26768	25.22095	26.10969
H	24.21832	24.15228	25.04830
O	24.82619	22.36571	26.90152
P	26.23222	22.45162	26.12421
O	27.19343	21.58319	26.83909
O	26.57541	23.86900	25.87902
O	25.85292	21.75937	24.73563
C	25.47987	20.38661	24.69799
H	24.56737	20.24008	25.27829
H	26.27329	19.78851	25.14756
C	25.24971	19.86143	23.27814
H	24.99529	18.80749	23.35627
O	24.15616	20.53985	22.67456
C	24.57818	21.07862	21.43177
H	24.33142	20.37395	20.63091
N	23.91298	22.39504	21.22733
C	24.10179	23.38309	22.14586
H	24.71845	23.13848	22.99847
C	23.53015	24.59491	21.99029
H	23.68302	25.39076	22.70110
C	22.67888	24.75380	20.85835
N	22.04987	25.92130	20.65973
H	21.34952	25.98204	19.93869
H	22.11026	26.66286	21.34650
N	22.47378	23.77906	19.98171
C	23.08954	22.57616	20.09871
O	22.96682	21.67548	19.26074
C	26.48972	20.01099	22.38410
H	27.37732	20.24098	22.98003
C	26.10269	21.19765	21.51112
H	26.41591	22.11206	22.01352
H	26.55229	21.15012	20.52424
O	26.69910	18.82054	21.63630
P	27.94188	18.64743	20.63761
O	28.33244	17.22360	20.63072
O	28.98055	19.65033	20.94386
O	27.35063	19.02340	19.21458
C	26.33204	18.25405	18.59206
H	25.44729	18.22045	19.23055
H	26.68084	17.23352	18.43215
C	25.94478	18.86617	17.23962
H	25.19058	18.22884	16.77671
O	25.39662	20.15864	17.46462
C	26.09996	21.08478	16.66011
H	25.63300	21.09919	15.67064
N	25.99787	22.43051	17.28879
C	26.78118	22.77968	18.34274
H	27.53436	22.08094	18.66986
C	26.59084	23.95437	18.98587
H	27.19474	24.23218	19.83529
C	25.54817	24.79588	18.50022
N	25.27620	25.95623	19.12931
H	24.63082	26.59056	18.67079
H	26.02068	26.37370	19.67347
N	24.80407	24.45849	17.45710
C	24.96131	23.26373	16.84406
O	24.22490	22.91318	15.91215
C	27.14307	19.03957	16.28197
H	27.97378	18.38480	16.55526
C	27.50468	20.50517	16.46738
H	28.13073	20.60269	17.35086
H	28.00625	20.92594	15.59665
O	26.75687	18.83605	14.93112
H	27.42679	19.23728	14.33475

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ss-C4 M06-2X/6-31G(d,p) mechanical embedding

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H	16.77931	27.71398	30.36377
O	17.21435	27.05995	29.77988
C	17.35991	25.85883	30.52754
H	16.40513	25.31407	30.57054
H	17.67039	26.08383	31.55886
C	18.42219	24.98400	29.89066
H	18.61054	24.13877	30.56299
O	17.96186	24.49076	28.63426
C	18.81846	24.93251	27.58194

H	19.47725	24.13149	27.24851
N	17.97479	25.27760	26.43281
C	17.02583	26.23041	26.56041
H	16.93063	26.69985	27.53916
C	16.23262	26.56811	25.51243
H	15.47627	27.34135	25.60344
C	16.43454	25.85218	24.28903
N	15.63442	26.13878	23.21329
H	16.00906	25.94320	22.29076
H	15.14441	27.02816	23.23466
N	17.28963	24.86173	24.15888
C	18.11259	24.53474	25.21826
O	18.92415	23.63228	25.14395
C	19.75571	25.71469	29.62758
H	19.84383	26.60879	30.26241
C	19.60098	26.10611	28.15335
H	18.99865	27.02027	28.10505
H	20.56143	26.27073	27.66933
O	20.78510	24.79813	29.90427
P	22.29480	24.95614	29.20890
O	23.24712	24.18443	30.05027
O	22.51935	26.38345	28.82962
O	22.00157	24.14710	27.81385
C	22.16168	22.73159	27.78622
H	21.17454	22.25376	27.86217
H	22.79886	22.40524	28.61290
C	22.81075	22.38051	26.46930
H	23.06183	21.31629	26.43395
O	21.89314	22.70794	25.41523
C	22.52056	23.58819	24.52472
H	22.98873	23.03009	23.71310
N	21.50856	24.42637	23.87158
C	21.15010	25.64186	24.31271
H	21.67380	26.04490	25.17133
C	20.18634	26.36381	23.67638
H	19.91039	27.36334	23.99889
C	19.63697	25.78574	22.49550
N	18.71249	26.52263	21.75804
H	18.65207	26.23482	20.78512
H	18.94068	27.52484	21.78196
N	19.88509	24.56242	22.10449
C	20.78332	23.79592	22.81728
O	20.97497	22.62329	22.57163
C	24.08578	23.21602	26.21457
H	24.50914	23.59495	27.15129
C	23.56488	24.34329	25.33310
H	23.11572	25.09532	25.98232
H	24.35177	24.78534	24.71591
O	25.03762	22.48380	25.46769
P	26.14748	21.68088	26.40708
O	25.39354	20.83850	27.39019
O	27.23054	22.61263	26.82309
O	26.74079	20.72478	25.21221
C	26.01995	19.55863	24.87486
H	25.06141	19.51565	25.40069
H	26.60756	18.67766	25.17182
C	25.81097	19.50291	23.37838
H	25.51076	18.48599	23.07943
O	24.79282	20.43668	23.00440
C	25.16708	20.94093	21.73608
H	24.93517	20.23481	20.93608
N	24.41067	22.14853	21.41570
C	24.67345	23.31256	22.04572
H	25.36643	23.27645	22.88193
C	24.06343	24.46682	21.66933
H	24.27387	25.40614	22.17117
C	23.06675	24.36852	20.64857
N	22.43500	25.51863	20.21700
H	21.50736	25.42114	19.80902
H	22.46231	26.30023	20.88340
N	22.74194	23.24157	20.06829
C	23.45809	22.09585	20.34806
O	23.29850	21.07531	19.70770
C	27.09582	19.86250	22.57722
H	27.93117	20.05427	23.25523
C	26.67183	21.14375	21.85965
H	26.87672	21.96862	22.54960
H	27.18853	21.30965	20.91628

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O         27.44310       18.74946       21.76215
P         27.82294       18.80516       20.18071
O         28.25923       17.41605       19.85025
O         28.67610       19.99616       19.85293
O         26.34916       19.12951       19.51466
C         25.54467       18.10396       18.97124
H         24.56733       18.12119       19.46778
H         26.01235       17.12233       19.11047
C         25.33576       18.39167       17.49025
H         24.66808       17.63716       17.05259
O         24.72333       19.67178       17.36024
C         25.62136       20.58214       16.78248
H         25.33592       20.74850       15.72861
N         25.50562       21.88817       17.40943
C         26.37382       22.35714       18.33992
H         27.18521       21.70597       18.65094
C         26.23523       23.61536       18.83169
H         26.93467       24.02264       19.55298
C         25.18258       24.40901       18.27568
N         25.15398       25.76448       18.51688
H         24.22058       26.17981       18.54874
H         25.69615       26.06472       19.33450
N         24.26168       23.92894       17.47747
C         24.31993       22.61365       17.09225
O         23.41245       22.06590       16.49530
C         26.63733       18.47704       16.67701
H         27.40064       17.79250       17.05362
C         27.01288       19.93911       16.84985
H         27.52287       20.07678       17.80108
H         27.67686       20.28358       16.05071
O         26.38009       18.17945       15.29968
H         26.48238       19.02315       14.79146


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ss-C4 M06-2X/6-31G(d,p) electrical embedding
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H         15.85734       28.42158       29.06989
O         16.83150       28.28351       29.15605
C         17.02464       27.32374       30.19889
H         16.05885       26.88702       30.46130
H         17.41399       27.82104       31.08872
C         17.97643       26.17046       29.83210
H         17.99991       25.46702       30.66728
O         17.46945       25.50688       28.68163
C         18.51792       25.34290       27.74224
H         19.04564       24.40344       27.94658
N         17.90542       25.35679       26.37726
C         17.17939       26.43054       25.96412
H         17.13903       27.27530       26.63850
C         16.51868       26.41981       24.78511
H         15.93929       27.27138       24.45570
C         16.51805       25.17565       24.06653
N         15.76167       25.06539       22.96487
H         15.61572       24.15484       22.52908
H         15.07419       25.77687       22.76730
N         17.22878       24.12802       24.46083
C         17.98655       24.19274       25.58790
O         18.72002       23.27191       25.95428
C         19.41833       26.60964       29.54022
H         19.58836       27.63944       29.86271
C         19.48979       26.49145       28.01986
H         19.15008       27.42294       27.57527
H         20.49426       26.26380       27.67500
O         20.31574       25.72768       30.20676
P         21.90414       25.94885       30.19265
O         22.50883       25.35150       31.40039
O         22.17434       27.36951       29.90745
O         22.38566       25.06771       28.95158
C         22.35031       23.65072       29.04174
H         21.34388       23.33226       29.31725
H         23.04010       23.32034       29.81936
C         22.72750       22.96902       27.72775
H         22.78439       21.89414       27.90807
O         21.70719       23.20623       26.76942
C         22.33075       23.35304       25.51593
H         22.62112       22.36713       25.13499
N         21.42199       24.05191       24.56467
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C	21.01674	25.32574	24.80904
H	21.36163	25.78233	25.72669
C	20.20299	25.98097	23.94810
H	19.86718	26.99148	24.13736
C	19.77915	25.24038	22.79682
N	18.97227	25.79835	21.88608
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H	18.71074	26.77808	21.89632
N	20.15228	23.98874	22.57792
C	20.95533	23.33754	23.44773
O	21.29509	22.15774	23.28144
C	24.06675	23.44728	27.13123
H	24.56133	24.16866	27.78625
C	23.59866	24.13358	25.84731
H	23.38185	25.17431	26.08228
H	24.31851	24.08471	25.03592
O	24.90610	22.31646	26.91795
P	26.29663	22.37917	26.11402
O	27.24732	21.47473	26.79719
O	26.66763	23.79365	25.88819
O	25.86085	21.71912	24.72543
C	25.42600	20.36443	24.68120
H	24.51117	20.25394	25.26574
H	26.19462	19.72939	25.12341
C	25.16689	19.85813	23.25901
H	24.89121	18.80861	23.32939
O	24.08352	20.56480	22.66792
C	24.49712	21.08681	21.41356
H	24.22785	20.38141	20.62054
N	23.86249	22.41949	21.20429
C	24.03193	23.38411	22.15149
H	24.62467	23.10746	23.01508
C	23.48449	24.60931	22.00454
H	23.61495	25.39098	22.73954
C	22.66788	24.79581	20.84338
N	22.05865	25.97730	20.66302
H	21.39951	26.08559	19.90681
H	22.12108	26.70167	21.37089
N	22.48490	23.85029	19.93289
C	23.08946	22.63554	20.05093
O	22.99199	21.75306	19.19336
C	26.40102	19.98836	22.35651
H	27.29583	20.20911	22.94521
C	26.02305	21.17787	21.48345
H	26.35161	22.09052	21.98009
H	26.46456	21.11758	20.49473
O	26.58858	18.79227	21.61208
P	27.82381	18.60068	20.60981
O	28.19680	17.17277	20.60049
O	28.87752	19.58776	20.91429
O	27.24034	18.98339	19.18618
C	26.20613	18.23269	18.56666
H	25.31796	18.22820	19.20129
H	26.52937	17.20193	18.42064
C	25.83956	18.83662	17.20471
H	25.07958	18.20594	16.74274
O	25.30824	20.13762	17.41300
C	26.04829	21.05420	16.63066
H	25.59551	21.09425	15.63539
N	25.96442	22.38974	17.28459
C	26.73751	22.70276	18.35840
H	27.48900	21.99052	18.66923
C	26.54626	23.85862	19.03619
H	27.14321	24.11557	19.89987
C	25.50706	24.71693	18.55687
N	25.24440	25.86617	19.21104
H	24.62863	26.51803	18.73548
H	25.99753	26.26583	19.76044
N	24.77081	24.41643	17.49936
C	24.94187	23.23864	16.84955
O	24.23248	22.92549	15.88682
C	27.04644	18.98602	16.25464
H	27.86009	18.31182	16.53076
C	27.43980	20.44292	16.44482
H	28.06328	20.52664	17.33045
H	27.95502	20.85299	15.57731
O	26.66310	18.79396	14.90151
H	27.34681	19.17923	14.30995

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ss-C4 M06-2X/TZVP mechanical embedding
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H         16.68567       27.80557       30.10660
O         16.77895       27.10477       29.43708
C         17.11253       25.90272       30.13885
H         16.25178       25.22961       30.12021
H         17.35330       26.12899       31.18310
C         18.30814       25.22086       29.51381
H         18.62698       24.41671       30.17963
O         17.95733       24.65463       28.25544
C         18.69038       25.25957       27.19447
H         19.41927       24.55725       26.80090
N         17.75161       25.51525       26.09625
C         16.82449       26.49002       26.19279
H         16.87717       27.13783       27.06039
C         15.84676       26.63288       25.26749
H         15.11384       27.42527       25.33941
C         15.78542       25.64130       24.24088
N         14.81691       25.73323       23.27499
H         14.56698       24.89081       22.76631
H         14.01985       26.34275       23.42481
N         16.62336       24.64237       24.16475
C         17.65849       24.52584       25.06386
O         18.43817       23.60193       25.03231
C         19.51093       26.14937       29.26804
H         19.43615       27.05919       29.87615
C         19.36383       26.49144       27.77997
H         18.72373       27.37152       27.70798
H         20.32055       26.70744       27.31243
O         20.65637       25.42335       29.63806
P         22.18456       25.65580       29.02991
O         23.12671       25.18514       30.09796
O         22.29418       27.00724       28.38542
O         22.14178       24.54971       27.81169
C         21.97430       23.18686       28.19450
H         20.91978       22.90961       28.08599
H         22.27094       23.06033       29.23733
C         22.82351       22.28080       27.33471
H         22.80436       21.28014       27.77468
O         22.31049       22.17633       26.00878
C         23.08586       22.94358       25.10775
H         23.47166       22.28203       24.33380
N         22.17973       23.87278       24.39914
C         21.90908       25.12365       24.80281
H         22.44500       25.51451       25.65574
C         20.97524       25.88207       24.16775
H         20.77297       26.90066       24.47550
C         20.28012       25.27352       23.08415
N         19.24087       25.94651       22.48700
H         18.89397       25.57280       21.60800
H         19.27039       26.95820       22.51548
N         20.50426       24.05030       22.68686
C         21.46947       23.29723       23.29776
O         21.70972       22.15771       22.96491
C         24.27964       22.73060       27.17326
H         24.63162       23.31295       28.02703
C         24.22155       23.58472       25.90233
H         24.01498       24.60970       26.19490
H         25.16773       23.55680       25.36575
O         25.02732       21.54275       27.03733
P         26.59221       21.46102       26.51068
O         27.13161       20.23801       27.18737
O         27.24883       22.80594       26.56816
O         26.32584       21.12137       24.91149
C         25.79321       19.83728       24.63468
H         24.78952       19.74295       25.06390
H         26.43489       19.06609       25.07287
C         25.71719       19.62817       23.14288
H         25.46362       18.58088       22.94990
O         24.69948       20.46806       22.58316
C         25.24561       21.19231       21.49662
H         25.10216       20.65804       20.55890
N         24.51170       22.44327       21.33580
C         24.73763       23.51379       22.12062
H         25.49380       23.41273       22.88940
C         24.05293       24.67185       21.94830
```

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H         24.23721       25.54399       22.56408
C         23.07724       24.68261       20.90722
N         22.44559       25.85831       20.57019
H         21.58106       25.78270       20.04873
H         22.38986       26.58878       21.28259
N         22.78211       23.63463       20.19160
C         23.46038       22.45729       20.37128
O         23.21303       21.46230       19.72862
C         27.02690       19.94626       22.39036
H         27.87844       19.98041       23.07129
C         26.72983       21.32091       21.79797
H         26.91923       22.04228       22.59372
H         27.33146       21.55003       20.92148
O         27.23870       18.89122       21.45494
P         27.80075       18.97359       19.92389
O         28.23320       17.56921       19.60874
O         28.70215       20.15756       19.70420
O         26.42207       19.34553       19.08437
C         25.48533       18.34840       18.72539
H         24.55104       18.52051       19.26706
H         25.87250       17.35135       18.95656
C         25.21274       18.45521       17.23578
H         24.53104       17.65490       16.93014
O         24.59263       19.69930       16.92236
C         25.51986       20.60592       16.37574
H         25.17420       20.87249       15.36890
N         25.50862       21.87074       17.11299
C         26.44496       22.26778       18.00923
H         27.27601       21.60648       18.21759
C         26.34432       23.47333       18.62005
H         27.10754       23.81276       19.30711
C         25.24426       24.30290       18.24334
N         25.20314       25.61238       18.64981
H         24.28618       26.04238       18.72742
H         25.79938       25.86834       19.42851
N         24.26591       23.88260       17.48673
C         24.31304       22.62901       16.94306
O         23.38384       22.14052       16.33860
C         26.46901       18.41639       16.36624
H         27.24256       17.79380       16.80561
C         26.87421       19.88405       16.28780
H         27.54726       20.11242       17.10721
H         27.38028       20.10509       15.34436
O         26.17346       17.86289       15.08143
H         25.96731       18.58288       14.44559

*****************************************************************************
ss-C4 M06-2X/TZVP electrical embedding
*****************************************************************************
H         15.66605       28.31330       29.01810
O         16.64312       28.22740       29.13276
C         16.85442       27.31617       30.21505
H         15.90047       26.85430       30.47841
H         17.20710       27.86252       31.09054
C         17.85648       26.18506       29.91678
H         17.89908       25.52987       30.78902
O         17.38616       25.44081       28.80057
C         18.42282       25.34735       27.83843
H         19.01208       24.44038       28.02942
N         17.78757       25.32517       26.48419
C         17.03689       26.37361       26.06085
H         16.96586       27.21852       26.72745
C         16.37965       26.32764       24.88411
H         15.77629       27.15475       24.54204
C         16.46490       25.09695       24.16092
N         15.72347       24.95948       23.02489
H         15.57350       24.00854       22.67607
H         14.90516       25.54938       22.96435
N         17.21438       24.09252       24.54382
C         17.88738       24.15016       25.72005
O         18.54725       23.21055       26.16084
C         19.28378       26.66180       29.61144
H         19.43352       27.69373       29.93684
C         19.33598       26.54875       28.09110
H         18.93900       27.46112       27.65513
H         20.34359       26.37535       27.72311
O         20.21009       25.79789       30.26134
P         21.79487       26.02678       30.18720
```

O	22.44799	25.45976	31.38384
O	22.04746	27.44554	29.87242
O	22.25560	25.13852	28.94500
C	22.28810	23.72412	29.07330
H	21.30821	23.37496	29.40092
H	23.02333	23.44657	29.83015
C	22.63816	23.00881	27.76968
H	22.67334	21.93788	27.97567
O	21.60996	23.25144	26.81983
C	22.23004	23.42361	25.56847
H	22.52395	22.44281	25.17756
N	21.31725	24.12052	24.61784
C	20.91481	25.39403	24.84626
H	21.25108	25.85514	25.76307
C	20.12023	26.04214	23.96602
H	19.79070	27.05552	24.13786
C	19.74261	25.31358	22.79364
N	18.98345	25.89716	21.85265
H	18.85359	25.38490	20.98485
H	18.83803	26.90102	21.82364
N	20.10313	24.05938	22.59822
C	20.86024	23.39270	23.50296
O	21.16381	22.21157	23.37479
C	23.98283	23.43839	27.14693
H	24.53769	24.10440	27.81296
C	23.50292	24.19346	25.90690
H	23.28721	25.22249	26.19213
H	24.21415	24.17642	25.08581
O	24.74858	22.26920	26.85208
P	26.15168	22.29586	26.06334
O	27.07955	21.36276	26.74084
O	26.56557	23.69682	25.84644
O	25.73088	21.66279	24.65891
C	25.29885	20.31004	24.57601
H	24.36749	20.18885	25.13174
H	26.05475	19.66538	25.02552
C	25.08383	19.83813	23.13397
H	24.80797	18.78663	23.17010
O	24.01740	20.56329	22.53274
C	24.47761	21.16491	21.33004
H	24.22804	20.51248	20.48659
N	23.86249	22.51576	21.17000
C	23.96333	23.41582	22.18438
H	24.49062	23.08393	23.06775
C	23.42721	24.64651	22.07515
H	23.50384	25.37831	22.86410
C	22.70067	24.91521	20.87470
N	22.08875	26.09824	20.73926
H	21.58245	26.31606	19.89406
H	22.20919	26.82149	21.43968
N	22.59782	24.03746	19.89127
C	23.19591	22.82045	19.97193
O	23.18825	22.00668	19.04991
C	26.34276	19.99124	22.26889
H	27.22651	20.16467	22.88918
C	26.00124	21.23371	21.45668
H	26.31526	22.11505	22.01621
H	26.47899	21.22352	20.48411
O	26.52862	18.83061	21.46594
P	27.78651	18.65672	20.48411
O	28.19195	17.23628	20.49196
O	28.81390	19.67164	20.78853
O	27.21455	19.01040	19.04650
C	26.24917	18.19366	18.39896
H	25.33931	18.15298	19.00042
H	26.62976	17.17841	18.29123
C	25.90392	18.73886	17.00583
H	25.17872	18.06462	16.54857
O	25.32457	20.02860	17.15670
C	26.12009	20.96599	16.45019
H	25.70699	21.06005	15.44159
N	26.04286	22.27963	17.15001
C	26.81133	22.55285	18.23594
H	27.51900	21.80478	18.55833
C	26.65908	23.70803	18.91717
H	27.25025	23.93080	19.79177
C	25.66571	24.61084	18.43452
N	25.44341	25.76908	19.08443

H	24.84849	26.43858	18.60636
H	26.21296	26.15286	19.62302
N	24.93329	24.34192	17.37101
C	25.05700	23.16517	16.72152
O	24.33337	22.88700	15.75922
C	27.12468	18.89248	16.07653
H	27.93389	18.21736	16.36268
C	27.51217	20.34808	16.27649
H	28.13201	20.42688	17.16442
H	28.03730	20.76217	15.41668
O	26.76209	18.70411	14.71746
H	27.44084	19.11403	14.13715

Structures from the MD simulation of ss-C_6

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*****************************************************************************
Starting structure of ss-C6 used in MD simulation, Figure 2 in the main text
*****************************************************************************

 H    -3.360000    -8.979000    -3.256000
 O    -3.152000    -8.520000    -2.439000
 C    -3.142000    -9.254000    -1.217000
 H    -2.370000   -10.013000    -1.348000
 H    -4.103000    -9.740000    -1.047000
 C    -2.795000    -8.387000    -0.006000
 H    -3.048000    -8.979000     0.874000
 O    -1.362000    -8.199000     0.083000
 C    -1.136000    -6.940000     0.748000
 H    -0.479000    -7.229000     1.568000
 N    -0.303000    -6.068000    -0.070000
 C    -0.395000    -6.077000    -1.444000
 H    -0.997000    -6.824000    -1.940000
 C     0.249000    -5.176000    -2.180000
 H     0.193000    -5.198000    -3.268000
 C     0.999000    -4.151000    -1.433000
 N     1.574000    -3.111000    -2.118000
 H     2.083000    -2.421000    -1.584000
 H     1.483000    -3.051000    -3.122000
 N     1.128000    -4.159000    -0.142000
 C     0.474000    -5.116000     0.599000
 O     0.572000    -5.122000     1.827000
 C    -3.400000    -6.987000     0.040000
 H    -3.351000    -6.429000    -0.895000
 C    -2.498000    -6.334000     1.065000
 H    -2.877000    -5.340000     1.303000
 H    -2.477000    -6.941000     1.970000
 O    -4.733000    -7.008000     0.494000
 P    -5.919000    -6.869000    -0.606000
 O    -5.468000    -7.568000    -1.874000
 O    -7.204000    -7.266000     0.063000
 O    -5.879000    -5.277000    -0.889000
 C    -6.286000    -4.402000     0.155000
 H    -6.077000    -4.929000     1.086000
 H    -7.343000    -4.163000     0.038000
 C    -5.482000    -3.098000     0.123000
 H    -5.518000    -2.681000     1.129000
 O    -4.078000    -3.395000    -0.097000
 C    -3.490000    -2.274000    -0.772000
 H    -2.703000    -2.054000    -0.050000
 N    -2.758000    -2.687000    -1.965000
 C    -3.308000    -3.587000    -2.850000
 H    -4.200000    -4.132000    -2.579000
 C    -2.758000    -3.801000    -4.044000
 H    -3.187000    -4.526000    -4.736000
 C    -1.551000    -3.014000    -4.349000
 N    -0.948000    -3.132000    -5.574000
 H    -0.122000    -2.576000    -5.746000
 H    -1.328000    -3.757000    -6.270000
 N    -0.997000    -2.197000    -3.507000
 C    -1.611000    -1.960000    -2.294000
 O    -1.125000    -1.126000    -1.532000
 C    -5.877000    -2.076000    -0.940000
 H    -6.156000    -2.505000    -1.902000
```

C	-4.593000	-1.283000	-1.093000
H	-4.730000	-0.511000	-1.850000
H	-4.338000	-0.817000	-0.141000
O	-6.856000	-1.162000	-0.483000
P	-8.325000	-1.110000	-1.163000
O	-8.926000	-2.487000	-1.061000
O	-9.040000	0.096000	-0.607000
O	-7.959000	-0.841000	-2.717000
C	-7.282000	0.348000	-3.089000
H	-6.470000	0.501000	-2.378000
H	-7.981000	1.184000	-3.075000
C	-6.694000	0.210000	-4.506000
H	-5.917000	0.958000	-4.662000
O	-5.997000	-1.070000	-4.617000
C	-6.662000	-1.830000	-5.645000
H	-6.180000	-1.775000	-6.621000
N	-6.619000	-3.254000	-5.318000
C	-7.317000	-3.750000	-4.237000
H	-7.957000	-3.090000	-3.670000
C	-7.222000	-5.027000	-3.873000
H	-7.775000	-5.407000	-3.014000
C	-6.327000	-5.865000	-4.687000
N	-6.161000	-7.188000	-4.376000
H	-5.539000	-7.732000	-4.957000
H	-6.650000	-7.592000	-3.590000
N	-5.659000	-5.410000	-5.704000
C	-5.757000	-4.079000	-6.039000
O	-5.053000	-3.650000	-6.955000
C	-7.753000	0.240000	-5.618000
H	-8.677000	0.760000	-5.367000
C	-8.045000	-1.226000	-5.843000
H	-9.057000	-1.451000	-5.507000
H	-7.956000	-1.456000	-6.905000
O	-7.195000	0.752000	-6.834000
P	-7.330000	2.360000	-7.053000
O	-8.778000	2.681000	-7.311000
O	-6.559000	3.034000	-5.946000
O	-6.503000	2.508000	-8.447000
C	-6.206000	3.843000	-8.843000
H	-5.821000	4.335000	-7.950000
H	-7.112000	4.323000	-9.213000
C	-5.149000	3.921000	-9.959000
H	-4.844000	4.961000	-10.077000
O	-3.938000	3.232000	-9.532000
C	-3.747000	2.092000	-10.393000
H	-2.839000	2.374000	-10.927000
N	-3.348000	0.904000	-9.635000
C	-3.757000	0.737000	-8.329000
H	-4.261000	1.546000	-7.821000
C	-3.545000	-0.403000	-7.676000
H	-3.865000	-0.530000	-6.642000
C	-2.887000	-1.468000	-8.450000
N	-2.723000	-2.715000	-7.893000
H	-2.267000	-3.422000	-8.452000
H	-3.052000	-2.902000	-6.957000
N	-2.460000	-1.315000	-9.665000
C	-2.688000	-0.121000	-10.316000
O	-2.316000	0.000000	-11.484000
C	-5.570000	3.293000	-11.286000
H	-6.640000	3.264000	-11.492000
C	-5.042000	1.885000	-11.171000
H	-5.877000	1.189000	-11.092000
H	-4.451000	1.645000	-12.055000
O	-4.868000	3.937000	-12.359000
P	-5.782000	4.797000	-13.395000
O	-6.557000	3.814000	-14.235000
O	-6.456000	5.902000	-12.623000
O	-4.612000	5.436000	-14.329000
C	-3.938000	6.580000	-13.832000
H	-3.747000	6.373000	-12.779000
H	-4.565000	7.461000	-13.972000
C	-2.601000	6.831000	-14.549000
H	-2.160000	7.739000	-14.138000
O	-1.667000	5.778000	-14.189000
C	-2.284000	5.459000	-16.477000
H	-1.441000	6.051000	-16.834000
N	-1.199000	3.646000	-15.101000
C	-2.295000	2.999000	-14.574000

H	-3.219000	3.544000	-14.448000
C	-2.247000	1.722000	-14.216000
H	-3.129000	1.208000	-13.834000
C	-0.933000	1.076000	-14.340000
N	-0.774000	-0.190000	-13.838000
H	0.135000	-0.621000	-13.931000
H	-1.548000	-0.662000	-13.394000
N	0.099000	1.652000	-14.878000
C	-0.006000	2.956000	-15.320000
O	0.959000	3.470000	-15.890000
C	-2.666000	6.868000	-16.079000
H	-3.362000	6.517000	-16.841000
C	-1.287000	5.078000	-15.388000
H	-0.319000	5.466000	-15.071000
H	-1.759000	4.556000	-14.556000
O	-1.644000	7.752000	-16.558000
P	-2.050000	8.777000	-17.749000
O	-3.046000	9.780000	-17.231000
O	-2.276000	7.986000	-19.010000
O	-0.627000	9.542000	-17.924000
C	-0.246000	10.443000	-16.899000
H	-0.342000	9.919000	-15.948000
H	-0.888000	11.323000	-16.931000
C	1.211000	10.882000	-17.087000
H	1.446000	11.695000	-16.401000
O	2.090000	9.805000	-16.687000
C	2.847000	9.375000	-17.831000
H	3.872000	9.693000	-17.642000
N	2.934000	7.922000	-17.845000
C	1.784000	7.171000	-17.764000
H	0.828000	7.667000	-17.678000
C	1.821000	5.845000	-17.789000
H	0.905000	5.255000	-17.790000
C	3.163000	5.244000	-17.782000
N	3.267000	3.889000	-17.602000
H	4.193000	3.486000	-17.599000
H	2.437000	3.327000	-17.478000
N	4.256000	5.936000	-17.911000
C	4.176000	7.310000	-18.018000
O	5.189000	7.972000	-18.254000
C	1.567000	11.232000	-18.534000
H	0.711000	11.506000	-19.151000
C	2.192000	9.967000	-19.073000
H	1.586000	9.583000	-19.894000
H	3.198000	10.183000	-19.434000
O	2.555000	12.276000	-18.565000
H	2.829000	12.549000	-19.444000

****
Representative structure of ss-C6 form MD simulations, Figure 2 in the main text
****

H	14.724	13.365	26.322
O	14.569	13.280	25.379
C	13.246	12.782	25.189
H	12.937	12.059	25.944
H	13.136	12.326	24.205
C	12.247	13.919	25.314
H	11.362	13.571	24.782
O	11.875	14.234	26.597
C	11.086	15.387	26.480
H	10.066	15.089	26.239
N	11.028	16.156	27.759
C	12.176	16.384	28.491
H	12.967	15.649	28.458
C	12.177	17.376	29.404
H	13.015	17.426	30.083
C	11.009	18.160	29.573
N	10.958	19.009	30.574
H	10.090	19.478	30.795
H	11.720	18.982	31.236
N	9.943	18.043	28.814
C	9.981	17.086	27.841
O	9.116	17.153	26.915
C	12.608	15.231	24.653
H	13.653	15.453	24.872
C	11.706	16.246	25.364
H	12.279	17.102	25.720

H	10.932	16.534	24.653
O	12.388	15.216	23.274
P	13.358	15.992	22.322
O	14.755	15.902	22.818
O	13.025	15.516	20.940
O	13.016	17.545	22.497
C	11.746	18.084	22.056
H	10.957	17.543	22.579
H	11.677	17.863	20.991
C	11.465	19.573	22.316
H	10.585	19.833	21.728
O	11.164	19.835	23.675
C	11.968	20.857	24.162
H	11.521	21.808	23.870
N	12.349	20.901	25.578
C	13.177	19.925	26.078
H	13.625	19.136	25.492
C	13.344	19.904	27.402
H	13.903	19.086	27.833
C	12.751	20.846	28.227
N	13.153	20.835	29.409
H	12.769	21.562	29.996
H	13.918	20.240	29.694
N	11.980	21.878	27.768
C	11.688	21.816	26.428
O	10.851	22.600	26.053
C	12.622	20.501	21.937
H	13.285	20.023	21.215
C	13.305	20.633	23.279
H	13.911	19.755	23.502
H	13.943	21.493	23.482
O	12.056	21.725	21.445
P	12.861	22.977	21.102
O	14.228	22.596	20.587
O	12.051	23.939	20.309
O	13.116	23.592	22.527
C	12.271	24.566	23.122
H	11.418	24.046	23.557
H	11.782	25.201	22.383
C	12.998	25.360	24.169
H	12.303	26.137	24.489
O	13.316	24.549	25.317
C	14.726	24.585	25.473
H	14.897	25.363	26.218
N	15.329	23.355	26.050
C	16.030	22.411	25.312
H	16.056	22.520	24.238
C	16.543	21.333	25.879
H	16.863	20.487	25.289
C	16.448	21.257	27.279
N	16.921	20.132	27.850
H	16.654	19.976	28.812
H	17.528	19.564	27.276
N	15.785	22.030	28.028
C	15.265	23.138	27.443
O	14.817	24.003	28.239
C	14.249	26.138	23.661
H	14.326	26.127	22.574
C	15.264	25.157	24.144
H	15.338	24.359	23.405
H	16.235	25.635	24.265
O	14.370	27.423	24.342
P	15.645	28.387	24.209
O	16.176	28.182	22.877
O	15.135	29.746	24.547
O	16.628	27.906	25.305
C	16.236	27.994	26.607
H	15.305	27.501	26.886
H	16.136	29.047	26.871
C	17.314	27.274	27.446
H	17.098	27.426	28.503
O	17.356	25.940	27.261
C	18.730	25.648	27.293
H	19.041	25.754	28.332
N	18.998	24.305	26.784
C	18.928	23.979	25.407
H	18.622	24.756	24.723
C	19.263	22.799	24.952

H	19.210	22.578	23.896
C	19.597	21.844	25.938
N	19.886	20.573	25.700
H	20.120	20.002	26.499
H	19.920	20.231	24.751
N	19.704	22.009	27.208
C	19.385	23.252	27.665
O	19.472	23.412	28.881
C	18.694	27.870	27.337
H	18.618	28.775	26.734
C	19.360	26.786	26.558
H	19.000	26.886	25.534
H	20.448	26.744	26.601
O	19.231	28.134	28.604
P	20.619	28.896	28.944
O	20.726	30.104	28.109
O	20.695	28.952	30.402
O	21.691	27.832	28.541
C	23.072	28.127	28.404
H	23.626	28.294	29.328
H	23.200	28.999	27.764
C	23.946	27.051	27.772
H	24.985	27.344	27.622
O	23.984	25.932	28.600
C	22.992	25.015	28.142
H	22.030	25.413	28.466
N	23.148	23.725	28.725
C	22.418	23.439	29.846
H	21.482	23.890	30.140
C	22.767	22.398	30.679
H	22.118	22.065	31.475
C	23.846	21.555	30.182
N	24.203	20.480	30.850
H	25.120	20.060	30.791
H	23.672	20.243	31.676
N	24.457	21.727	29.110
C	24.150	22.835	28.384
O	24.897	23.015	27.440
C	23.265	26.582	26.459
H	22.392	27.221	26.329
C	22.854	25.082	26.622
H	21.837	24.899	26.276
H	23.636	24.474	26.165
O	24.239	26.645	25.389
P	24.746	28.080	24.763
O	23.498	28.872	24.808
O	25.483	27.871	23.540
O	25.728	28.672	25.894
C	25.822	30.048	26.263
H	24.868	30.392	26.662
H	26.173	30.715	25.475
C	26.829	30.262	27.411
H	26.843	31.333	27.611
O	26.357	29.553	28.537
C	27.487	28.929	29.096
H	27.993	29.704	29.672
N	26.973	27.791	29.908
C	27.280	26.488	29.656
H	28.031	26.300	28.903
C	26.719	25.437	30.331
H	26.939	24.412	30.070
C	25.941	25.858	31.438
N	25.286	25.044	32.159
H	24.530	25.507	32.643
H	25.140	24.082	31.888
N	25.582	27.078	31.703
C	26.151	28.065	30.996
O	25.869	29.206	31.269
C	28.278	29.719	27.119
H	28.343	29.432	26.069
C	28.334	28.508	27.950
H	27.740	27.809	27.362
H	29.358	28.254	28.225
O	29.388	30.610	27.492
H	29.297	31.342	26.878