Supplementary Material (ESI) for PCCP

Ab initio investigation of the methylation and hydration effects on the electronic spectrum of uracil and thymine

Electronic Supplementary Information

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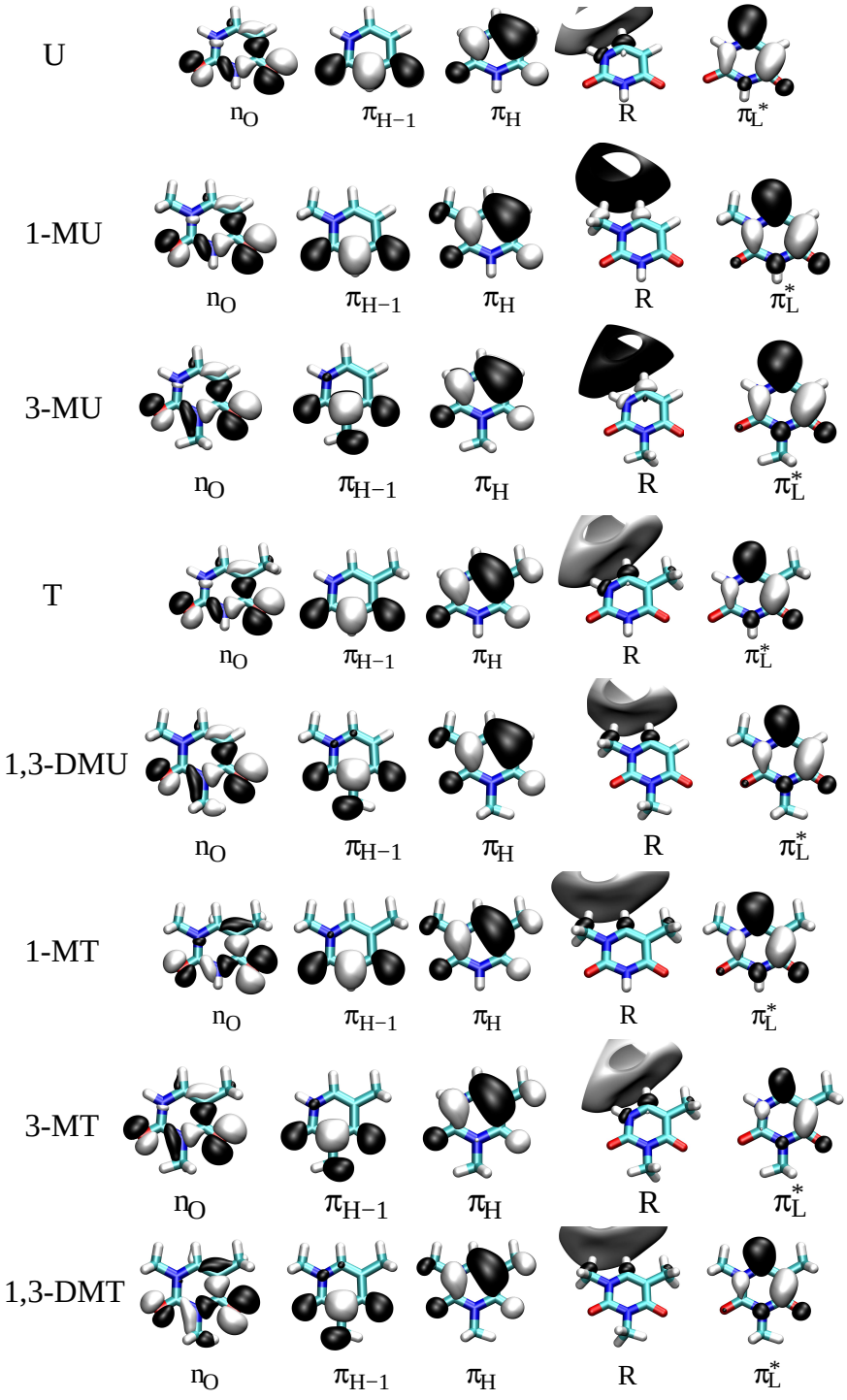

Figure 1: Hartree-Fock orbitals in aug-cc-pVDZ basis

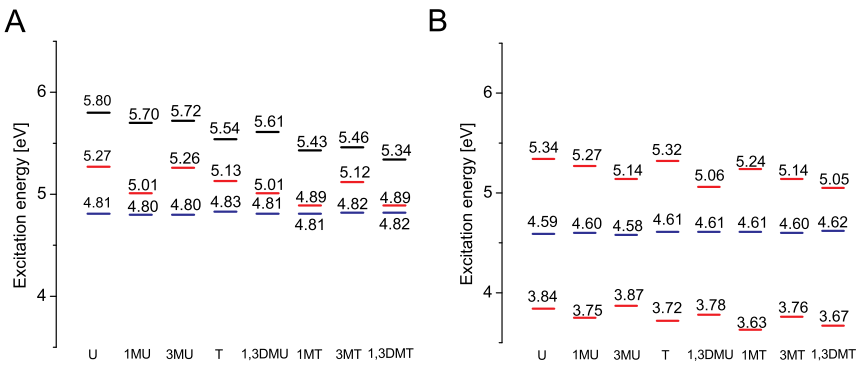

Figure 2: Vertical excitation spectra of the bare chromophores computed at the RI-CC2/aug-cc-pVDZ level. The ground-state geometries were optimized at the RI-CC2/cc-pVDZ level. (n $\rightarrow \pi^*$ blue; $\pi \rightarrow \pi^*$ red; $\pi \rightarrow$R black): A singlet states, B triplet states. For the denomination of the compounds see Figure 1 of the main paper.

For obtaining the results shown in Figure 2 we used ground-state geometries optimized at the RI-CC2/cc-pVDZ level whereas the excitation energies relating to B3-LYP/TZVP optimized coordinates are presented in Figure 3 of the main paper. Similar trends are observed for these two sets of calculations. The $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ state excitation energies are somewhat higher at the DFT-optimized geometries. The main reason for the increase of the computed excitation energy when using DFT-optimized structures is the contraction of the C-O bond lengths. This phenomenon has been discussed in detail in a recent paper.[1] In the Rydberg states, the C-O bond length is of less importance.

References

[1] M. Etinski, T. Fleig and C. M. Marian, *J. Phys. Chem. A*, 2009, **113**, 11809–11816.

Table 1: Excited states of uracil and their character, RI-CC2/aug-cc-pVDZ level. The ground state dipole moment is 4.16 D.

state	transition	energy [eV]	$f(L)$	dipole moment [D]
S_1	$n_O \rightarrow \pi_L^\star$	4.81	$4 \cdot 10^{-6}$	1.53
S_2	$\pi_H \rightarrow \pi_L^\star$	5.27	0.1808	5.36
S_3	$\pi_H \rightarrow$R	5.80	0.0026	5.25
T_1	$\pi_H \rightarrow \pi_L^\star$	3.84		3.60
T_2	$n_O \rightarrow \pi_L^\star$	4.59		1.78
T_3	$\pi_{H-1} \rightarrow \pi_L^\star$	5.34		5.06

Table 2: Excited states of 1-methyluracil and their character, RI-CC2/aug-cc-pVDZ level. The ground state dipole moment is 4.61 D.

state	transition	energy [eV]	$f(L)$	dipole moment [D]
S_1	$n_O \rightarrow \pi_L^\star$	4.80	$1 \cdot 10^{-5}$	1.14
S_2	$\pi_H \rightarrow \pi_L^\star$	5.01	0.2283	6.02
S_3	$\pi_H \rightarrow$R	5.70	0.0217	3.50
T_1	$\pi_H \rightarrow \pi_L^\star$	3.75		4.00
T_2	$n_O \rightarrow \pi_L^\star$	4.60		1.39
T_3	$\pi_{H-1} \rightarrow \pi_L^\star$	5.27		3.24

Table 3: Excited states of 3-methyluracil and their character, RI-CC2/aug-cc-pVDZ level. The ground state dipole moment is 3.46 D.

state	transition	energy [eV]	$f(L)$	dipole moment [D]
S_1	$n_O \rightarrow \pi_L^\star$	4.80	$1 \cdot 10^{-5}$	1.44
S_2	$\pi_H \rightarrow \pi_L^\star$	5.26	0.1291	4.80
S_3	$\pi_H \rightarrow$R	5.72	0.00030	6.35
T_1	$\pi_H \rightarrow \pi_L^\star$	3.87		2.95
T_2	$n_O \rightarrow \pi_L^\star$	4.58		1.63
T_3	$\pi_{H-1} \rightarrow \pi_L^\star$	5.14		2.15

Table 4: Excited states of thymine and their character, RI-CC2/aug-cc-pVDZ level. The ground state dipole moment is 4.09 D.

state	transition	energy [eV]	$f(L)$	dipole moment [D]
S_1	$n_O \rightarrow \pi^\star_L$	4.83	$2 \cdot 10^{-5}$	1.92
S_2	$\pi_H \rightarrow \pi^\star_L$	5.13	0.1814	5.15
S_3	$\pi_H \rightarrow$R	5.54	0.0003	6.31
T_1	$\pi_H \rightarrow \pi^\star_L$	3.72		3.82
T_2	$n_O \rightarrow \pi^\star_L$	4.61		2.21
T_3	$\pi_{H-1} \rightarrow \pi^\star_L$	5.32		6.25

Table 5: Excited states of 1,3-dimethyluracil and their character, RI-CC2/aug-cc-pVDZ level. The ground state dipole moment is 3.97 D.

state	transition	energy [eV]	$f(L)$	dipole moment [D]
S_1	$n_O \rightarrow \pi^\star_L$	4.81	$2 \cdot 10^{-5}$	1.00
S_2	$\pi_H \rightarrow \pi^\star_L$	5.01	0.1873	5.29
S_3	$\pi_H \rightarrow$R	5.61	0.0208	4.29
T_1	$\pi_H \rightarrow \pi^\star_L$	3.78		3.38
T_2	$n_O \rightarrow \pi^\star_L$	4.61		1.18
T_3	$\pi_{H-1} \rightarrow \pi^\star_L$	5.06		4.01

Table 6: Excited states of 1-methylthymine and their character, RI-CC2/aug-cc-pVDZ level. The ground state dipole moment is 4.43 D.

state	transition	energy [eV]	$f(L)$	dipole moment [D]
S_1	$n_O \rightarrow \pi^\star_L$	4.81	$3 \cdot 10^{-5}$	1.53
S_2	$\pi_H \rightarrow \pi^\star_L$	4.89	0.2339	5.70
S_3	$\pi_H \rightarrow$R	5.43	0.0094	2.22
T_1	$\pi_H \rightarrow \pi^\star_L$	3.63		4.05
T_2	$n_O \rightarrow \pi^\star_L$	4.61		1.82
T_3	$\pi_{H-1} \rightarrow \pi^\star_L$	5.24		3.36

Table 7: Excited states of 3-methylthymine and their character, RI-CC2/aug-cc-pVDZ level. The ground state dipole moment is 3.37 D.

state	transition	energy [eV]	$f(L)$	dipole moment [D]
S_1	$n_O \rightarrow \pi^\star_L$	4.82	$4 \cdot 10^{-6}$	1.70
S_2	$\pi_H \rightarrow \pi^\star_L$	5.12	0.1360	4.51
S_3	$\pi_H \rightarrow$R	5.46	0.0005	6.99
T_1	$\pi_H \rightarrow \pi^\star_L$	3.76		3.14
T_2	$n_O \rightarrow \pi^\star_L$	4.60		1.94
T_3	$\pi_{H-1} \rightarrow \pi^\star_L$	5.14		6.90

Table 8: Excited states of 1,3-dimethylthymine and their character, RI-CC2/aug-cc-pVDZ level. The ground state dipole moment is 3.76 D.

state	transition	energy [eV]	$f(L)$	dipole moment [D]
S_1	$n_O \rightarrow \pi_L^\star$	4.82	$2 \cdot 10^{-6}$	1.22
S_2	$\pi_H \rightarrow \pi_L^\star$	4.89	0.1984	5.00
S_3	$\pi_H \rightarrow$R	5.34	0.0091	2.85
T_1	$\pi_H \rightarrow \pi_L^\star$	3.67		3.40
T_2	$n_O \rightarrow \pi_L^\star$	4.62		1.49
T_3	$\pi_{H-1} \rightarrow \pi_L^\star$	5.05		2.50

Table 9: Vibrational spectrum of the uracil ground state at RI-CC2/cc-pVDZ level(unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
126.87	0.05
155.15	0.43
374.19	17.83
374.78	29.60
505.87	14.04
522.90	5.88
546.04	2.32
554.01	36.68
688.91	78.57
720.97	1.02
734.78	42.79
760.89	2.20
799.66	55.57
939.52	0.72
962.29	9.46
980.37	5.35
1083.63	5.43
1197.19	94.15
1226.45	0.37
1368.70	6.94
1389.57	45.73
1405.10	60.24
1499.65	100.95
1660.91	12.60
1744.15	386.69
1797.67	587.67
3247.13	3.42
3289.50	1.00
3593.91	63.74
3647.53	114.92

Table 10: Vibrational spectrum of the uracil S_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
44.64	4.16
157.51	1.45
288.28	10.75
302.84	5.31
313.56	50.47
344.23	68.84
472.65	8.89
503.74	3.67
533.81	12.48
548.88	36.69
591.99	38.48
690.98	46.30
718.30	2.33
743.43	44.76
909.93	12.32
970.89	19.03
1012.89	34.69
1105.26	8.82
1150.47	9.38
1276.98	6.88
1307.29	14.44
1405.87	3.40
1426.88	7.63
1451.21	6.33
1631.52	132.31
1777.05	470.40
3255.87	5.64
3275.17	1.24
3627.07	78.00
3629.45	126.46

Table 11: Vibrational spectrum of the uracil T_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
126.55	2.14
158.63	1.03
228.91	2.44
367.47	20.89
460.39	18.79
480.02	8.89
497.54	10.57
530.56	7.06
554.46	37.23
640.59	31.81
683.21	109.17
697.62	2.96
727.46	70.26
762.46	0.28
938.30	4.97
959.28	17.32
1014.62	8.53
1144.59	74.00
1226.79	32.13
1353.70	85.19
1361.39	55.81
1378.64	6.23
1404.58	61.11
1456.89	150.99
1609.48	82.20
1769.32	318.66
3240.73	10.54
3255.24	1.91
3599.47	101.11
3599.65	42.43

Table 12: Vibrational spectrum of the 1-methyluracil ground state at RI-CC2/cc-pVDZ level(unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
68.94	0.00
107.92	0.03
147.12	1.17
215.40	3.23
324.39	3.16
375.48	18.86
394.92	7.16
455.76	14.38
522.81	6.59
612.68	1.31
682.79	52.27
712.56	2.00
736.11	40.50
750.33	4.69
790.02	2.41
794.40	43.34
931.22	1.77
964.16	10.15
1037.25	5.54
1147.77	0.15
1153.76	28.34
1205.46	19.60
1234.55	17.77
1342.24	31.88
1369.91	36.96
1392.01	86.29
1448.41	26.93
1467.74	83.31
1469.20	7.76
1516.71	45.47
1659.04	28.11
1743.15	353.55
1769.16	608.71
3098.32	33.81
3196.58	7.88
3218.61	4.47
3236.85	5.25
3284.25	0.68
3589.34	65.08

Table 13: Vibrational spectrum of the 1-methyluracil S_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
65.32	2.08
111.12	0.37
119.73	0.92
237.54	2.55
294.75	2.94
297.69	8.56
332.59	42.29
352.39	11.76
385.95	82.98
433.22	15.42
521.76	9.51
571.73	0.65
577.80	0.98
682.41	27.64
709.96	3.10
737.19	39.62
756.61	5.87
956.75	0.74
1009.87	20.66
1095.01	5.15
1107.81	38.49
1146.63	0.50
1186.04	5.26
1241.11	31.87
1293.04	19.80
1358.50	6.58
1407.66	6.26
1430.62	10.97
1458.08	30.66
1494.05	8.78
1506.65	4.36
1640.43	129.66
1742.03	422.91
3079.37	47.83
3167.55	20.72
3228.63	0.07
3235.73	5.88
3273.02	2.33
3620.61	145.16

Table 14: Vibrational spectrum of the 1-methyluracil T_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
98.46	0.31
108.69	0.09
136.57	2.80
207.74	3.07
261.49	4.44
343.42	0.15
378.64	22.38
438.67	8.37
474.49	10.57
502.67	16.18
568.03	4.29
607.69	15.23
688.02	57.40
700.09	15.59
723.10	69.68
749.53	3.55
784.39	11.41
941.85	2.29
1013.60	12.13
1080.88	20.15
1137.02	2.16
1186.22	23.26
1213.49	88.34
1302.77	73.97
1353.79	31.21
1373.81	93.05
1397.36	2.34
1424.12	114.47
1440.11	67.36
1490.34	14.23
1503.63	32.40
1609.79	81.61
1739.28	268.37
3082.52	35.68
3174.82	14.32
3226.13	10.33
3233.34	0.01
3250.77	3.02
3588.62	69.01

Table 15: Vibrational spectrum of the 3-methyluracil ground state at RI-CC2/cc-pVDZ level(unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
84.27	1.42
123.93	4.93
150.14	0.65
208.36	6.07
340.58	5.87
391.57	23.63
397.84	15.60
487.67	4.21
531.29	7.70
565.91	57.93
576.53	8.66
698.65	1.05
717.78	5.98
728.17	21.04
795.68	47.27
854.20	0.41
933.31	0.79
973.45	14.85
1082.59	6.08
1127.84	54.74
1150.52	0.28
1173.08	0.88
1233.91	21.66
1281.22	33.54
1387.02	36.84
1404.46	35.26
1434.13	76.41
1488.77	8.30
1499.71	39.19
1506.27	83.06
1658.82	3.97
1719.25	488.23
1767.61	363.02
3105.52	21.58
3198.82	10.27
3245.75	0.23
3247.40	3.48
3287.69	0.93
3644.52	112.71

Table 16: Vibrational spectrum of the 3-methyluracil S_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
30.23	0.49
92.58	2.31
154.79	0.78
184.33	4.85
299.02	3.91
311.95	4.36
359.30	6.71
371.64	95.63
462.35	3.47
507.38	1.91
549.93	28.52
563.23	17.00
593.08	28.45
687.17	42.43
689.08	1.44
725.10	25.31
777.81	8.70
928.47	1.40
978.18	32.80
1069.41	13.46
1113.32	3.52
1139.61	0.26
1226.56	13.87
1248.31	17.38
1302.00	11.85
1360.41	50.73
1403.20	5.17
1424.53	20.65
1449.13	7.65
1490.11	9.18
1501.99	24.73
1632.38	157.30
1747.21	393.54
3085.06	37.05
3177.45	11.02
3224.41	1.70
3239.73	9.40
3268.78	1.34
3619.81	61.81

Table 17: Vibrational spectrum of the 3-methyluracil T_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
75.24	1.09
109.96	4.43
152.51	1.47
190.91	3.29
243.67	1.39
331.78	6.23
371.97	26.61
451.33	12.34
482.74	2.26
500.06	13.92
557.51	46.47
586.06	65.68
649.75	12.62
690.27	0.89
702.98	3.22
728.88	23.07
835.46	15.67
957.80	9.55
991.78	13.02
1098.45	87.80
1148.53	2.88
1174.17	4.66
1223.96	6.31
1274.33	41.75
1359.98	138.16
1379.97	5.31
1404.94	56.71
1428.16	12.68
1465.93	210.60
1486.57	24.85
1503.25	7.06
1585.63	84.15
1738.29	244.11
3101.50	26.16
3199.33	11.47
3237.42	12.47
3241.59	0.15
3254.11	2.13
3594.13	72.73

Table 18: Vibrational spectrum of the thymine ground state at RI-CC2/cc-pVDZ level(unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
102.95	0.00
135.28	0.28
146.84	0.04
270.27	2.82
286.59	0.00
373.67	23.95
377.23	16.65
450.82	14.46
529.10	6.17
554.74	51.59
591.78	1.02
686.47	78.05
732.00	38.07
736.60	3.65
749.66	5.57
792.18	1.68
884.25	16.62
960.48	11.10
1012.80	1.21
1057.52	1.03
1157.52	4.75
1199.75	106.57
1257.74	18.64
1366.62	8.79
1372.94	5.40
1409.02	18.06
1419.17	45.47
1465.17	6.28
1482.45	10.22
1501.72	103.91
1686.84	3.24
1725.42	338.46
1796.72	639.58
3079.24	24.55
3169.09	8.08
3183.30	11.29
3234.65	5.36
3593.93	63.24
3646.27	111.24

Table 19: Vibrational spectrum of the thymine S_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
49.57	2.94
93.00	0.06
153.64	0.35
189.10	7.48
236.51	2.34
303.40	6.95
314.78	0.76
344.20	54.89
368.55	71.18
454.45	7.92
485.18	6.31
550.65	43.21
553.11	12.50
588.70	47.27
692.96	23.90
714.60	3.18
775.58	4.69
908.67	14.46
967.30	6.69
1050.45	2.60
1079.94	1.62
1140.97	31.66
1212.83	43.16
1236.34	1.16
1295.52	10.51
1405.36	0.15
1407.88	10.39
1422.27	3.66
1455.91	14.14
1475.16	6.29
1492.06	6.87
1677.13	99.56
1776.72	516.19
3061.55	42.15
3149.68	18.47
3157.11	15.84
3235.92	5.77
3624.26	68.09
3627.27	130.97

Table 20: Vibrational spectrum of the thymine T_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
74.66	0.54
139.86	1.44
151.53	0.77
180.35	0.65
274.63	5.69
308.52	9.37
376.35	15.57
436.72	19.19
484.44	8.69
546.67	23.84
574.76	5.84
633.49	36.75
678.75	82.78
691.14	4.35
720.99	83.17
738.45	7.80
780.76	5.78
947.21	4.30
972.21	10.12
980.33	0.84
1147.93	61.77
1150.68	69.34
1243.09	7.10
1348.23	116.76
1354.84	13.91
1379.47	26.98
1405.27	56.38
1422.93	1.28
1453.02	47.14
1466.04	13.48
1491.05	85.13
1601.99	89.85
1769.29	346.00
3041.38	13.82
3110.82	10.29
3197.19	1.90
3223.70	11.68
3594.31	71.74
3602.05	71.27

Table 21: Vibrational spectrum of the 1,3-dimethyluracil ground state at RI-CC2/cc-pVDZ level(unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
80.55	0.62
106.07	1.17
108.10	1.36
131.49	6.37
188.90	2.05
242.86	0.01
309.76	1.44
355.88	11.52
394.56	20.59
416.45	0.90
469.71	8.16
501.07	11.48
615.16	1.99
676.76	3.55
702.06	0.93
733.21	22.28
790.25	34.67
795.45	1.02
925.17	1.67
933.93	8.57
1010.00	14.95
1081.90	2.48
1144.19	43.25
1147.15	0.30
1150.63	0.23
1177.95	0.16
1265.87	16.50
1279.01	10.48
1350.88	30.91
1386.37	93.63
1420.70	64.35
1451.25	22.20
1468.07	7.99
1472.29	99.04
1492.78	7.94
1498.41	14.88
1518.80	61.79
1656.05	6.00
1719.95	643.33
1738.86	204.90
3097.46	36.67
3101.76	24.86
3195.91	6.37
3196.60	13.34
3217.25	4.79
3235.33	5.38
3239.77	0.48
3282.67	0.65

Table 22: Vibrational spectrum of the 1,3-dimethyluracil S_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
73.04	0.42
87.71	0.31
98.61	0.84
117.59	6.88
158.23	1.79
250.02	0.13
305.99	3.66
314.19	0.10
329.03	4.76
387.50	22.92
405.15	66.34
448.66	11.57
506.45	5.70
561.41	4.84
571.57	3.38
680.08	14.06
687.09	10.58
710.30	6.10
724.25	22.27
921.90	1.27
949.87	0.18
1054.94	21.98
1076.13	5.21
1109.86	13.94
1137.26	15.33
1145.75	0.39
1223.25	41.12
1251.76	7.76
1279.47	13.81
1358.50	18.48
1377.41	55.29
1407.92	14.10
1422.53	10.79
1456.51	31.98
1477.07	12.60
1493.96	8.50
1504.11	8.98
1507.04	1.24
1638.04	127.96
1712.19	372.54
3078.58	68.41
3081.15	19.13
3166.65	21.32
3175.96	12.20
3221.05	10.58
3226.96	0.50
3229.85	0.00
3266.22	1.97

Table 23: Vibrational spectrum of the 1,3-dimethyluracil T_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
72.71	1.26
86.22	0.10
102.39	0.19
112.63	5.18
191.71	3.58
207.18	4.21
275.30	1.84
316.03	2.10
366.74	3.99
382.92	29.83
453.84	5.16
467.77	6.88
499.02	11.96
582.01	5.16
627.73	29.51
672.10	8.07
702.97	2.17
722.48	20.52
786.88	10.27
918.65	12.92
976.75	1.78
1040.81	18.67
1106.49	36.49
1134.91	1.58
1146.02	5.87
1171.40	35.35
1232.30	36.06
1271.90	50.34
1325.84	62.79
1368.33	121.43
1398.53	9.28
1408.42	77.61
1432.24	6.89
1453.41	168.58
1484.04	3.49
1487.33	21.61
1503.13	7.57
1504.92	43.13
1585.90	82.82
1710.62	198.48
3081.65	38.37
3097.79	28.59
3174.07	14.45
3196.23	12.05
3219.56	12.81
3235.58	0.02
3240.88	0.27
3247.37	2.98

Table 24: Vibrational spectrum of the 3-methylthymine ground state at RI-CC2/cc-pVDZ level(unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
86.95	1.37
100.96	0.17
123.16	4.39
149.10	0.37
208.72	4.41
265.51	1.69
290.19	0.60
342.51	8.07
394.83	21.57
395.67	11.93
466.49	11.42
497.30	5.55
567.48	77.95
607.90	2.39
666.38	1.40
725.40	15.42
740.88	0.22
796.56	3.76
879.21	16.29
932.86	2.11
982.68	8.84
1056.76	0.81
1059.31	9.09
1137.82	49.47
1150.34	0.33
1223.58	27.11
1269.31	43.94
1284.69	4.21
1368.62	17.46
1405.90	23.05
1412.54	5.45
1435.00	65.46
1464.38	6.60
1482.36	10.15
1488.42	8.12
1498.67	44.83
1508.01	92.32
1673.00	145.63
1713.48	249.31
1766.30	460.75
3078.41	26.60
3104.78	22.54
3168.95	8.32
3181.83	12.07
3198.01	10.46
3234.54	5.71
3244.79	0.27
3642.59	109.33

Table 25: Vibrational spectrum of the 3-methylthymine S_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
64.57	0.05
84.80	0.13
92.00	3.17
111.08	0.87
186.08	3.34
228.85	2.05
239.89	1.66
309.61	12.13
317.50	4.24
361.01	4.58
391.64	78.94
460.98	2.83
474.43	2.98
555.62	40.86
563.90	9.21
588.46	31.45
651.65	2.60
692.47	19.60
742.54	14.16
855.34	4.60
943.82	3.53
1048.06	2.96
1065.40	5.03
1071.39	5.12
1119.10	13.59
1138.42	9.44
1219.12	23.12
1260.13	5.40
1301.04	10.03
1353.00	76.58
1406.01	0.61
1410.05	9.95
1425.19	25.37
1455.77	21.93
1474.54	5.90
1485.18	17.87
1491.97	4.24
1504.72	9.57
1670.00	108.10
1748.27	431.10
3058.93	47.99
3080.68	38.51
3146.54	19.33
3154.53	16.55
3174.57	12.37
3222.65	9.29
3225.71	0.34
3617.64	60.55

Table 26: Vibrational spectrum of the 3-methylthymine T_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
67.84	1.07
79.06	0.21
112.13	5.17
147.84	0.64
175.05	0.47
197.67	2.01
277.92	4.11
311.11	7.79
345.77	7.62
382.88	20.87
448.84	15.19
477.96	4.97
559.82	56.25
588.29	29.23
641.99	10.58
664.32	10.08
700.19	6.74
724.07	26.26
791.11	14.39
904.67	3.13
959.68	0.46
979.41	1.58
1046.42	45.54
1101.44	74.95
1146.11	5.68
1212.29	4.37
1256.68	23.06
1269.03	23.57
1354.45	141.05
1377.74	23.02
1403.98	55.89
1420.74	0.95
1430.28	22.08
1455.25	64.09
1466.97	16.10
1479.99	27.41
1497.01	101.95
1503.76	10.95
1577.97	91.12
1738.99	270.24
3039.56	16.75
3097.12	29.98
3107.56	10.80
3195.25	11.66
3197.94	1.81
3213.96	14.91
3240.94	0.45
3595.07	71.16

Table 27: Vibrational spectrum of the 1-methylthymine ground state at RI-CC2/cc-pVDZ level(unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
55.92	0.00
95.85	0.00
126.68	0.09
144.75	0.65
194.73	4.45
259.65	3.24
291.55	0.55
327.37	1.75
378.95	17.76
391.92	3.73
433.09	19.09
509.76	2.50
634.24	1.02
681.22	50.00
697.89	6.62
733.31	36.65
744.06	9.85
767.48	3.27
862.22	3.30
880.54	15.74
1013.98	0.72
1056.06	1.29
1081.52	31.36
1147.10	0.09
1156.35	15.76
1204.66	38.33
1249.30	7.85
1346.82	31.42
1373.72	3.14
1391.50	84.81
1414.77	26.81
1448.45	2.37
1464.63	4.56
1467.82	104.66
1468.99	8.66
1489.73	14.48
1515.52	48.34
1681.90	0.22
1722.90	357.17
1767.30	613.61
3077.09	27.63
3096.08	36.24
3166.04	8.56
3181.18	11.39
3192.46	8.56
3216.54	1.48
3224.19	10.39
3589.63	64.12

Table 28: Vibrational spectrum of the 1-methylthymine S_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
15.86	1.90
85.93	0.12
100.95	0.24
105.42	0.42
188.80	2.43
230.99	2.50
240.35	6.27
294.49	1.99
304.54	2.78
359.04	2.66
373.15	41.28
375.05	109.19
426.98	10.24
484.18	1.04
566.51	0.58
586.38	3.83
685.59	10.88
703.26	7.97
718.79	4.47
839.49	1.26
974.83	1.50
1043.30	11.42
1050.92	0.15
1081.49	3.89
1143.56	2.96
1181.52	1.39
1214.58	50.84
1223.51	55.10
1269.02	4.50
1360.70	3.32
1404.01	0.67
1409.17	6.11
1428.03	14.40
1458.71	39.34
1473.94	6.26
1490.40	8.35
1492.30	7.16
1507.87	4.05
1686.65	89.79
1742.68	477.43
3059.91	44.90
3080.25	45.91
3147.67	19.30
3155.48	15.97
3168.04	20.83
3210.93	8.82
3229.77	0.02
3625.66	148.12

Table 29: Vibrational spectrum of the 1-methylthymine T_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
76.07	0.59
98.45	0.27
111.66	0.03
149.94	1.61
159.80	1.83
243.90	5.10
267.38	4.42
315.93	4.47
345.18	0.81
386.64	17.76
416.46	20.86
468.55	6.80
594.26	13.80
613.35	2.06
657.09	45.65
686.79	7.47
716.97	87.61
726.40	3.81
769.16	7.24
821.82	1.46
971.79	4.14
981.69	0.85
1067.14	19.33
1136.02	46.79
1139.13	10.32
1185.70	25.73
1240.40	31.79
1308.93	143.12
1351.17	7.16
1379.50	86.34
1380.78	12.87
1408.19	41.92
1436.68	71.23
1445.06	1.07
1464.97	8.44
1485.94	24.14
1492.86	15.12
1505.37	53.27
1600.17	90.07
1738.88	294.05
3041.84	15.04
3081.46	37.99
3110.81	11.06
3171.83	15.38
3195.40	2.49
3208.51	10.84
3232.31	0.14
3589.44	70.34

Table 30: Vibrational spectrum of the 1,3-dimethylthymine ground state at RI-CC2/cc-pVDZ level(unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
73.79	0.22
92.24	0.27
105.77	1.98
130.44	6.01
145.54	2.27
157.44	0.03
243.96	0.01
262.35	2.36
294.94	0.09
308.72	0.90
360.51	9.89
396.92	22.93
414.02	0.15
449.28	16.52
494.90	4.02
576.47	1.92
660.83	1.98
728.72	17.27
734.97	2.10
765.72	2.83
875.08	14.86
917.26	4.85
976.61	1.82
1047.30	2.41
1055.34	1.04
1068.43	33.60
1101.42	21.82
1146.72	0.20
1150.70	0.32
1198.79	22.93
1280.02	8.36
1302.51	10.17
1355.08	23.01
1388.78	69.47
1412.89	3.57
1415.95	64.93
1448.16	3.41
1463.89	4.73
1467.91	8.94
1472.17	135.90
1488.42	12.51
1492.11	7.59
1499.15	11.62
1517.54	65.09
1668.64	130.50
1709.93	340.24
1735.99	370.96
3076.43	30.01
3095.30	38.64
3101.76	25.98
3166.56	8.72
3179.98	12.25
3192.44	8.40
3196.75	11.70
3215.02	2.29
3223.59	10.39

Table 31: Vibrational spectrum of the 1,3-dimethylthymine S_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
74.45	0.59
87.28	0.66
92.58	0.25
99.16	0.89
110.20	1.35
125.82	6.05
225.00	2.26
235.91	1.96
262.48	0.84
307.71	4.62
313.53	2.56
327.65	4.75
394.11	11.20
416.40	61.53
443.35	11.37
475.33	3.56
565.68	6.06
578.56	3.49
606.85	6.20
686.98	8.37
702.32	5.19
859.36	1.68
947.55	1.03
1021.76	11.56
1047.90	2.10
1070.01	3.79
1079.30	5.31
1098.01	4.86
1137.34	15.24
1145.40	0.38
1203.48	11.93
1256.80	51.54
1305.94	1.10
1347.86	69.98
1373.05	19.91
1406.25	1.73
1413.11	23.27
1422.22	12.43
1460.11	53.90
1473.59	5.26
1477.85	12.46
1491.26	5.42
1493.77	8.53
1505.61	7.85
1507.12	1.45
1673.20	84.06
1717.61	408.28
3057.75	50.25
3077.72	70.14
3079.94	19.37
3144.73	19.83
3153.43	16.80
3165.66	21.14
3173.98	13.18
3202.78	11.00
3224.88	0.61

Table 32: Vibrational spectrum of the 1,3-dimethylthymine T_1 state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies)

wavenumber [1/cm]	intensity [km/mol]
65.66	1.03
76.77	0.11
84.25	0.42
100.35	0.31
124.01	7.93
156.36	0.18
187.74	0.70
247.63	1.96
276.42	4.52
312.92	2.59
329.49	4.72
374.24	6.84
392.01	25.86
431.30	15.88
471.23	5.88
562.61	3.76
625.43	2.67
642.72	25.22
694.54	6.42
719.36	16.13
766.22	5.92
878.72	1.68
947.99	3.10
981.10	1.45
1020.84	3.53
1051.88	58.10
1100.33	32.55
1134.25	3.83
1145.82	5.62
1180.39	26.71
1261.43	10.77
1304.11	17.75
1315.30	166.57
1374.16	82.25
1380.93	15.21
1403.69	70.48
1415.17	4.38
1445.42	1.69
1447.50	100.44
1466.66	9.77
1479.47	27.13
1483.14	3.23
1489.04	34.08
1503.08	5.47
1508.71	62.76
1580.40	97.57
1710.55	222.64
3039.08	18.11
3080.33	40.36
3096.06	32.37
3107.68	11.73
3173.32	14.67
3190.88	2.33
3193.71	12.69
3200.57	14.02
3234.93	0.01

Table 33: Geometry of the ground state of uracil in atomic units obtained at RI-CC2/cc-pVDZ level

1.80276131503938	-3.82523577877818	-0.00001843121476	c
-0.76911959552013	-3.60787322393067	-0.00007500514995	c
-1.94412134408134	-1.10454937651617	0.00002508530838	c
-0.14550597259914	0.88615452904312	0.00017510886307	n
2.48204977900901	0.75797537834155	0.00023770292495	c
3.36151866289513	-1.73799691500085	0.00013053376173	n
-4.22669268030672	-0.64209232037238	-0.00000930583133	o
3.89552706152535	2.59733451753509	0.00037114273740	o
5.27279481407985	-1.92595057138397	0.00017209542869	h
-0.87594766368821	2.67228606501715	0.00025076303206	h
2.76550865539636	-5.65443235453763	-0.00008760001027	h
-1.98531788402312	-5.27108030126895	-0.00019329108878	h

Table 34: Geometry of the S_1 state of uracil in atomic units obtained at RI-CC2/cc-pVDZ level

0.33897033221462	1.36132036952789	-0.71354640950436	c
-2.16830967216996	0.27921600085562	-0.55259778778755	c
-2.33291781271658	-2.23250800809978	-0.12483561008593	c
-0.22143039872179	-3.74915347578373	0.21200756656727	n
2.27161351679411	-2.80420926445030	0.25197377565216	c
2.38079163497256	-0.23449154572517	-0.16599513219088	n
-3.85075421208677	1.43897566732052	-0.82824054100883	h
-4.53991708654283	-3.78289851094835	0.06201268861541	o
4.11105733844260	-4.18360201279782	0.62476047658149	o
-0.41352184865411	-5.63002979361522	0.56716080078631	h
4.17622188098919	0.45468528231244	-0.20606788408108	h
0.71559577364017	3.38976059942737	-0.69108040928701	h

Table 35: Geometry of the T_1 state of uracil in atomic units obtained at RI-CC2/cc-pVDZ level

1.91164001968400	-3.84894454808797	0.76085934370093	c
-0.80480063599536	-3.55410211096836	-0.05576329127888	c
-1.92939839894834	-1.06654822108889	0.07178595469496	c
-0.14940202847252	0.86449654246044	0.64216133438314	n
2.43153503217761	0.71567056781175	0.08782439180786	c
3.30666121126855	-1.77911271016009	-0.13529134932617	n
-4.20035084227332	-0.56795061284651	-0.24597887642145	o
3.82104193628791	2.55612524845929	-0.17004733482631	o
5.21906293952542	-1.89260554848371	-0.35009209010192	h
-0.85510646934687	2.65950378661802	0.63044996769175	h
2.84401224282969	-5.68197431665829	0.56296480531994	h
-1.87734509750552	-5.06855912797309	-0.96463511177476	h

Table 36: Geometry of the ground state of 1-methyluracil in atomic units obtained at RI-CC2/cc-pVDZ level

3.19927492493216	-1.61294411458012	0.00002496572308	n
1.78994513815827	-3.80490875530421	0.00000425774160	c
-0.79562455592143	-3.82574497399391	-0.00005200096061	c
-2.19814316354062	-1.45135065988189	-0.00008777859003	c
-0.57447546404974	0.68307490368417	-0.00007282818888	n
2.05084777304719	0.78296736363196	-0.00000626022137	c
-1.84216337645154	-5.60143284488652	-0.00006587108237	h
-4.51337583495722	-1.18600662462670	-0.00012714570564	o
-1.45042543968538	2.40315870417777	-0.00009288771281	h
3.29104096638268	2.75002496504491	0.00002452016135	o
5.96445752662432	-1.63530129680317	0.00009268440858	c
2.89459639181716	-5.55345191094566	0.00003828359882	h
6.59797914498682	-3.61316638311048	0.00008717986953	h
6.69023167873668	-0.65768880411026	-1.68559838758938	h
6.69017693650958	-0.65777544186486	1.68595990868878	h

Table 37: Geometry of the S_1 state of 1-methyluracil in atomic units obtained at RI-CC2/cc-pVDZ level

2.47284219790390	-1.21883476261733	0.35097373278242	c
1.01471465551930	-3.38649220409950	0.53677103998948	n
-1.63486694404622	-3.40483785631362	0.57155080828315	c
-2.96583384584748	-1.01430645907590	0.74559106965191	c
-1.56362896608391	1.10351097005636	0.54104936098563	c
1.03302848194054	1.02335132300095	0.22110284039145	n
2.33846925714895	-5.81022268346566	0.57477312468215	c
-2.34970005387219	3.68917577919150	0.58742271762857	o
2.06308892529937	2.64930787963247	0.23651621729449	h
4.80586872183922	-1.14431584641531	0.27256638258338	o
-5.01612029820632	-0.94840912581698	0.95565215848534	h
-2.50903283175285	-5.20965661974894	1.07059000464394	h
1.91080736843675	-6.82204050660228	2.34595047606720	h
1.72708949018737	-6.96826125760383	-1.04554565629915	h
4.37369743813411	-5.43050654877564	0.45132462265113	h

Table 38: Geometry of the T_1 state of 1-methyluracil in atomic units obtained at RI-CC2/cc-pVDZ level

3.18157937103570	-1.56546529340471	-0.19908503173766	n
1.86108769455372	-3.51999772934431	-1.41790837067647	c
-0.76419869649515	-3.73351884410390	-0.35948272913945	c
-2.14452357794707	-1.43099959305454	0.11864455759113	c
-0.61257534096132	0.76051054615996	-0.16697665278039	n
2.00000175395557	0.78937301014925	0.24010419890510	c
-1.59042379869529	-5.52567244436657	0.25461851104780	h
-4.41103073072179	-1.26223950584482	0.70653053736305	o
-1.47733853300773	2.41804600240129	0.31348324620631	h
3.16887922497788	2.69172741685061	0.88947741691412	o
5.93152051002599	-1.68861624840196	0.02220804682170	c
2.97584469454787	-5.23712989886609	-1.71340101944579	h
6.45611531560184	-3.32605043424284	1.19458050540891	h
6.78483017450763	-1.89063712563655	-1.86953495447500	h
6.58906488429483	0.07147470583668	0.89977094324186	h

Table 39: Geometry of the ground state of 3-methyluracil in atomic units obtained at RI-CC2/cc-pVDZ level

2.79714164681303	-1.01045026890339	-0.00001791287129	n
1.25389811567673	-3.10246603675422	-0.00016362255182	c
-1.31316486967807	-2.86480407908371	-0.00019078434808	c
-2.46708517483147	-0.35814027765836	-0.00004321799133	c
-0.70637677397164	1.68439222856346	0.00011010194934	n
1.93172230778643	1.48817325204744	0.00012419304869	c
-4.75997781109014	0.08483868394174	-0.00004457760902	o
3.40669124058504	3.28784921728753	0.00024450508516	o
4.70991562415775	-1.18565781259049	-0.00000271805855	h
-1.80814868627959	4.22833202252713	0.00027392507107	c
2.21805379681193	-4.93065827999989	-0.00025498588686	h
-2.55202819089705	-4.51140317880031	-0.00030746949353	h
-0.24216752498826	5.58527638286228	0.00023659189750	h
-3.00170726765816	4.47177526002970	-1.68451421451066	h
-3.00150048836956	4.47165857068938	1.68524425825438	h

Table 40: Geometry of the S_1 state of 3-methyluracil in atomic units obtained at RI-CC2/cc-pVDZ level

2.79138538550787	-1.00126223373660	-0.00546091480648	n
1.31851909173905	-3.19358690560213	-0.19016565115791	c
-1.39057205504203	-2.84124138944154	-0.03995018936935	c
-2.25943674890140	-0.43899347441420	-0.00905220466464	c
-0.72254069131865	1.69010288475517	-0.02080268754906	n
1.95094690981076	1.46013393063429	-0.00297684870678	c
-4.84924166816676	0.36268602110326	0.04531837702526	o
3.36006519094605	3.32488766050975	0.01784991779591	o
4.71074444075797	-1.13048533087093	-0.05950886105723	h
-1.83134024939790	4.22521958412281	0.00101014415586	c
2.26709584373131	-4.97895644865622	0.23324658801925	h
-2.68628389356617	-4.44614134099931	-0.03391910470826	h
-0.24077256896263	5.55844591597488	-0.00295003475465	h
-3.01382116786823	4.51256121809166	-1.68828726474870	h
-2.98979477651223	4.49882248322404	1.70964727142755	h

Table 41: Geometry of the T_1 state of 3-methyluracil in atomic units obtained at RI-CC2/cc-pVDZ level

2.71861610000044	-1.08596160297985	0.30224905701576	n
1.35722643246798	-3.03251202058339	-0.87153392097581	c
-1.36374806596261	-2.81511148066425	-0.06150908122873	c
-2.48008058133044	-0.32704113202667	0.06626659604168	c
-0.72479109306228	1.70273515596575	-0.17078448166096	n
1.85840518654597	1.42577898884371	0.35057184104708	c
-4.77591715712352	0.10511291570904	0.33710668625788	o
3.30560783556969	3.18916083447132	0.80863503575888	o
4.63087739504241	-1.20985161521849	0.51736423640308	h
-1.78782258403116	4.26100948014373	-0.09533836044030	c
2.28988725584137	-4.87643849392636	-0.86047103144193	h
-2.46778964157149	-4.40908405382381	0.65222459141879	h
-0.22121226262804	5.59991182561404	-0.32316126556842	h
-3.16725440752885	4.46425187322566	-1.63282577445189	h
-2.75894842630412	4.59841946280791	1.71529468009731	h

Table 42: Geometry of the ground state of thymine in atomic units obtained at RI-CC2/cc-pVDZ level

1.80467847639010	-3.82768331030142	0.00017256838633	c
-0.77248595387687	-3.63715673109377	0.00009956818093	c
-1.91223731068656	-1.10615996119000	-0.00001345376157	c
-0.13325138697833	0.88607774948266	0.00006043219334	n
2.49742541157605	0.75781269840660	0.00016968217022	c
3.36633735052051	-1.73267815721277	0.00017162516731	n
-2.52517525947582	-5.86967207941727	-0.00011090060169	c
-4.20520534526542	-0.66663501949474	-0.00012031812041	o
3.90557677004676	2.60333217734376	0.00025724699882	o
5.27719578200499	-1.92437168113128	0.00028652361625	h
-0.86707905183507	2.67044871394354	0.00004753420255	h
2.77662425317857	-5.65380172744093	0.00023370848073	h
-1.46082419896370	-7.65950025416043	0.00159308281278	h
-3.76783570463527	-5.82206043476818	1.67202990970417	h
-3.76544811641981	-5.82382518070266	-1.67383435239424	h

Table 43: Geometry of the S_1 state of thymine in atomic units obtained at RI-CC2/cc-pVDZ level

0.33048389411507	1.35823498295451	-0.60788074196863	c
-1.99829401997630	0.32372925580859	-0.73053867035561	c
-2.48302784291670	-2.22090104994847	-0.30328930827534	n
-0.56469944559451	-4.01329444491755	0.12845925347989	c
1.80361011676503	-2.92739345546888	0.25505578583550	n
2.36962494693841	-0.35082951276319	0.05984930677219	c
-4.35311019801620	1.56382175445597	-1.28736868505487	o
-1.01129248596558	-6.28737552721796	0.37417760966081	o
0.79802652207934	4.13455280311244	-1.02645337985241	c
-4.25598685339039	-2.93035960172474	-0.53587411844264	h
3.19949428914101	-4.19350611884565	0.64125351240329	h
4.36538369425570	0.14415601534491	-0.14668333048302	h
-0.92800727853156	5.06124499599545	-1.74270164759363	h
1.35496104465238	5.09792261866155	0.73886474406704	h
2.31196958965884	4.43913007824831	-2.42887452606781	h

Table 44: Geometry of the T_1 state of thymine in atomic units obtained at RI-CC2/cc-pVDZ level

1.72319817829857	-3.81070065882309	0.33444147963110	c
-1.04751040804398	-3.60247394114372	-0.34387701763916	c
-2.19372203297843	-1.12462397459517	-0.25649553148946	c
-0.44358463517930	0.86183706947456	0.22000472614834	n
2.12172647585424	0.76064964484094	-0.39957879520916	c
3.04844219130333	-1.71564588458133	-0.59264027858918	n
-2.49860724661829	-5.83617994946672	-1.23682436566550	c
-4.48300554916687	-0.66040096580886	-0.54530654106213	o
3.46297465935337	2.62564101983094	-0.73621890723532	o
4.95713320713838	-1.79013302125016	-0.84852909721381	h
-1.19525297885639	2.63763729646820	0.15597975326328	h
2.67700977239451	-5.62691621708028	0.06752265026983	h
-1.65236227217059	-6.61387478786286	-2.98658531096922	h
-2.43744005778862	-7.36809460725325	0.18520405639556	h
-4.47548506978080	-5.30760971594959	-1.60218691104771	h

Table 45: Geometry of the ground state of 1,3-dimethyluracil in atomic units obtained at RI-CC2/cc-pVDZ level

3.19487805647921	-1.63418343850067	-0.00000045797039	n
1.80761237791159	-3.83314070846399	-0.00005056092074	c
-0.77514484268780	-3.83912033153101	-0.00005432409450	c
-2.18689302853849	-1.47637497315650	-0.00007207416626	c
-0.60604136361164	0.71676014179638	-0.00003234890558	n
2.03099431564135	0.75178190575228	-0.00005437760932	c
-1.83634731574708	-5.60616582432924	-0.00009455239072	h
-4.51627433945057	-1.29417339675079	-0.00005854152488	o
-1.81535970560174	3.21118575053244	-0.00002312043575	c
3.28754496569621	2.71614246275426	-0.00008784442589	o
5.96001730513952	-1.63045771771152	-0.00003635427253	c
2.91505281614476	-5.58014992074299	-0.00003471686971	h
6.61078640894986	-3.60301813763702	0.00055082927020	h
6.67678034843274	-0.64574511272398	-1.68552567258794	h
6.67675553721488	-0.64473356285251	1.68488789946477	h
-3.86202526192372	2.88043971071654	-0.00004371655041	h
-1.23605125174251	4.27861358688822	1.68778529482087	h
-1.23603947092308	4.27863727623410	-1.68780849509750	h

Table 46: Geometry of the S_1 state of 1,3-dimethyluracil in atomic units obtained at RI-CC2/cc-pVDZ level

3.19657706133500	-0.27959186500231	-0.21380079612269	n
1.72503189379741	-2.47449058566074	-0.03479926925016	c
-0.99952962854711	-2.18726370270642	-0.03607628293705	c
-1.92424136225011	0.12884075893475	-0.56713702772406	c
-0.40673597728440	2.21907393893384	-1.02546243112466	n
2.25347387632616	2.10827612821651	-0.71401584530144	c
-2.24681711280759	-3.79874769134090	0.28525300446282	h
-4.53249601474360	0.84454336962315	-0.74488416007837	o
-1.52659429023360	4.72309154079865	-1.39369739208208	c
3.54841529884353	4.05033623097569	-0.92287981199247	o
5.93733753319334	-0.53896943096926	0.02102154420208	c
2.67052993280888	-4.10885915483510	0.80993409187034	h
6.41719000967623	-1.26363642408884	1.91558679024887	h
6.63746619367226	-1.86926690183019	-1.42125945729460	h
6.78778681513269	1.33156354544335	-0.25809036238614	h
-3.33695894186822	4.49279694254495	-2.39279726366681	h
-1.84924147019142	5.68616080816421	0.42736968612467	h
-0.20696117930998	5.84991486214330	-2.52979747908413	h

Table 47: Geometry of the T_1 state of 1,3-dimethyluracil in atomic units obtained at RI-CC2/cc-pVDZ level

3.16598306624989	-1.62123370548290	-0.19089244236726	n
1.89380635623001	-3.64761615989383	-1.33680049227005	c
-0.75881622851074	-3.76019035894362	-0.34563961701311	c
-2.14936722023074	-1.43137795770768	-0.08439540460184	c
-0.62921373246135	0.77536164333595	-0.40894076587898	n
1.98314897278520	0.76826855968050	0.02121295167338	c
-1.62626065131307	-5.49642960542688	0.36556214485372	h
-4.45534590970225	-1.27788067840425	0.35472445930235	o
-1.87035528369115	3.24485288798938	-0.21901703767695	c
3.17847922641252	2.70430606318817	0.52373859413624	o
5.90772551301192	-1.72380152259630	0.12872969408048	c
3.00670421829344	-5.38882342654781	-1.44647895218452	h
6.39215740128130	-3.34581779339239	1.33868081188091	h
6.83270687835152	-1.94611016103819	-1.72722418542289	h
6.52856405975947	0.05033988587982	1.00334983681971	h
-3.84311390137086	2.98840686231833	-0.80297446532233	h
-1.81551710264107	3.96956411524181	1.73346070217385	h
-0.89243993477409	4.59077974660956	-1.45987686497576	h

Table 48: Geometry of the ground state of 1-methylthymine in atomic units obtained at RI-CC2/cc-pVDZ level

1.80009646109859	-3.79367496258727	-0.00000434755469	c
-0.96041289307839	-3.59768898832893	-0.00005085454695	c
-1.84519808002703	-1.07904910119822	-0.00000705555262	n
-0.46866939786484	1.16223559255944	-0.00003682334017	c
2.15161902225160	0.78039103005411	-0.00012369119249	n
3.19794815147379	-1.61519555813003	-0.00004697737567	c
-2.44984354509549	-5.39788932379239	-0.00002568233492	o
-1.42394490874515	3.28430991839479	0.00001820187420	o
2.94024720500453	-6.39380591975310	0.00018433635829	c
-3.76207866626817	-0.85505767310422	0.00005491374233	h
5.26752080186618	-1.66009065613468	0.00002223952075	h
5.02093369740000	-6.30308861163562	0.00239606878034	h
2.31102894411247	-7.46739294770402	1.67203858880720	h
2.31465350984262	-7.46640880575342	-1.67382602380108	h
3.71025681322392	3.06436102013922	-0.00000310057013	c
5.70600006193744	2.48992557996942	-0.00004039320419	h
3.30313386186607	4.21291831669698	-1.68565847026297	h
3.30301459264579	4.21297360901402	1.68579586372074	h

Table 49: Geometry of the S_1 state of 1-methylthymine in atomic units obtained at RI-CC2/cc-pVDZ level

1.75694348405518	-3.86302668834292	-0.10573923199763	c
-0.73318493981853	-3.49338152339869	-0.48611186610730	c
-1.80638579187829	-1.11184914764683	-0.68900126258495	n
-0.42808093876766	1.15590289900441	-0.52336738847694	c
2.14499332084592	0.78109709460693	-0.17155511377464	n
3.27099335468673	-1.58712983068312	0.18258473793598	c
-2.69412843607505	-5.35416167892345	-0.77249737470039	o
-1.48894361611972	3.23089154857949	-0.69471834589261	o
2.92913383090123	-6.44563721456626	0.11526006620164	c
-3.70654438907027	-0.90576046072651	-0.90889395822077	h
5.33688497172864	-1.62167454789001	0.05226105451245	h
4.51806091122568	-6.66862085369079	-1.21900997067085	h
3.65693194403028	-6.79518581368055	2.03934017051093	h
1.52243419396860	-7.92431877156596	-0.31624120526742	h
3.72606046963373	3.03030573773633	0.09646420405260	c
5.39382036290413	2.84794459003546	-1.13773603599701	h
2.59946748581980	4.68023269172386	-0.45903429751845	h
4.35460735525122	3.23955622544125	2.07277163327346	h

Table 50: Geometry of the T_1 state of 1-methylthymine in atomic units obtained at RI-CC2/cc-pVDZ level

1.70317472271263	-3.79443751663497	0.33352932017741	c
-0.93215173175741	-3.59854658290513	-0.33201141109121	c
-1.88248906706653	-1.08790200370039	-0.15367510351754	n
-0.40859850386869	1.07880881477306	-0.48303806986134	c
2.16780549675742	0.72476665528667	0.11625849267273	n
2.97821031637011	-1.46648122311994	1.36419262742017	c
-2.33355532575316	-5.36979046732614	-0.99970890804119	o
-1.27627527971744	3.11561483785489	-1.19838161622194	o
3.13454881191105	-6.17693864033697	-0.08287906722256	c
-3.69767892927891	-0.87250689008700	-0.77282408738826	h
5.02053332522328	-1.53457650968469	1.70170520015803	h
4.69804236805812	-5.87502288424652	-1.44127443157291	h
4.01317371307205	-6.82380931164785	1.70116079112503	h
1.86701685907941	-7.65794481078225	-0.80532548845107	h
3.83751574194105	2.91965749490436	-0.02022528344893	c
5.49823782787563	2.45676846829236	-1.18760505895278	h
2.77483069726809	4.48675013229941	-0.86605020329665	h
4.46583718900752	3.44646906017225	1.89640818740489	h

Table 51: Geometry of the ground state of 3-methylthymine in atomic units obtained at RI-CC2/cc-pVDZ level

3.14946711210703	-0.41275705147510	0.00053346949426	n
1.60314300851682	-2.51179212560755	0.00140958415783	c
-0.96937282252128	-2.30195248280986	0.00124921144154	c
-2.08734982180744	0.23320972239033	0.00035973314173	c
-0.34570721222286	2.27588782260790	0.00033500638825	n
2.29592248286051	2.08087040978639	0.00013928635212	c
-2.74327282387610	-4.51772348699393	0.00029327420880	c
-4.38966802564336	0.65759343857975	-0.00008416465033	o
3.76557009287884	3.88670422653790	-0.00025869941060	o
5.06175887416944	-0.59390556574169	0.00051315309004	h
-1.45413460732821	4.81670161185104	-0.00007098016509	c
2.57594747970426	-4.33734539341452	0.00211230088294	h
-1.69475477624520	-6.31730809393687	0.00626186646524	h
-3.98973436906758	-4.45604708262536	1.66897110383713	h
-3.97990329689299	-4.46206414379222	-1.67583302886671	h
0.10941609499852	6.17670907488858	-0.00012890643601	h
-2.64848693673059	5.05674041756014	-1.68486820851823	h
-2.64865926039994	5.05709305453598	1.68453341251554	h

Table 52: Geometry of the S_1 state of 3-methylthymine in atomic units obtained at RI-CC2/cc-pVDZ level

3.17079742195367	-0.27302193348822	-0.29815330267392	n
1.74662817815072	-2.48460530986634	-0.03526655230835	c
-0.98016051026892	-2.20386882247723	0.00599917046298	c
-1.87538663038570	0.13188751060959	-0.50769335427706	c
-0.38950081301224	2.25095708014972	-0.98149722940953	n
2.27558476042378	2.12119102903554	-0.79535190476729	c
-2.69868969685729	-4.42928013397127	0.44729660080411	c
-4.50372918285828	0.84871195417280	-0.65242451371758	o
-1.54810589999866	4.74020735023111	-1.31582177379016	c
3.63878654000801	4.00054135942653	-1.07619056144190	o
5.09289704380023	-0.35507881329861	-0.24421194626128	h
2.72213546111375	-4.11722038502498	0.77791587479589	h
-2.21276949474299	-5.41786473456112	2.21945762878087	h
-4.68193741700863	-3.79906348000587	0.59348479279861	h
-2.58069960675278	-5.81405320128446	-1.10968259967018	h
-3.18347103385977	4.56629023400847	-2.59010540400668	h
-2.17008932842736	5.53735639847158	0.50779981858715	h
-0.10310332436763	5.97392205201868	-2.14973163559362	h

Table 53: Geometry of the T_1 state of 3-methylthymine in atomic units obtained at RI-CC2/cc-pVDZ level

3.07612027953311	-0.46956712664860	-0.10158209562820	n
1.69078853921876	-2.40112213160309	1.05654794704982	c
-1.04960707350744	-2.19868307341915	0.27724040565678	c
-2.12466713721060	0.29570597572547	0.00970021622783	c
-0.36844955749579	2.33340138921892	0.22321690173647	n
2.22278670708296	2.03998756795290	-0.22998732646877	c
-2.56328446708613	-4.49026163097253	-0.31841180300075	c
-4.41073262364906	0.74500757026330	-0.35982897891141	o
3.68346218195969	3.78976485574302	-0.70110359598302	o
4.99286903090337	-0.59928596413905	-0.26450758462516	h
-1.41074323720271	4.89165899253447	0.02469872355864	c
2.59907285143407	-4.26083052004204	1.01265779979170	h
-1.69551991620561	-5.56046311672936	-1.89463409229413	h
-2.60683414511113	-5.78457145826451	1.32442751534212	h
-4.50585712658759	-3.95520030063839	-0.82819705361124	h
0.10862386266246	6.23145724198106	0.46600631307883	h
-2.13363176327004	5.26042096304816	-1.89438367225566	h
-2.98206711724819	5.07452360020470	1.36834155010402	h

Table 54: Geometry of the ground state of 1,3-dimethythymine in atomic units obtained at RI-CC2/cc-pVDZ level

3.22022206759642	-1.61810362002763	-0.00036295455137	c
1.81064727119988	-3.78582386899000	-0.00048404588510	c
-0.94679032023300	-3.59783569447014	-0.00062241852478	c
-1.89724306989047	-1.08086387292953	-0.00037438737916	n
-0.45891780010703	1.13343895425780	-0.00023298438301	c
2.16054066682242	0.76455570691268	-0.00032429416619	n
2.94147168502109	-6.39101399589123	0.00004586806911	c
-2.38242656770763	-5.44897201431080	-0.00065979676045	o
-1.39985228212658	3.26888875090063	-0.00000171837400	o
3.70477503887431	3.05787140425583	-0.00005976413685	c
-4.64332219668209	-0.70096525529496	-0.00001531400698	c
5.28976399329761	-1.66098549764283	-0.00013287715343	h
5.02276566837948	-6.30560134205046	0.00215572096999	h
2.30760150318596	-7.46168378088604	1.67187640694232	h
2.31112281874473	-7.46178875510787	-1.67308907979160	h
5.70343888482066	2.49198838852881	-0.00016360892074	h
3.29070762561144	4.20463655321774	-1.68523495035336	h
3.29077150203346	4.20427717117211	1.68538338703080	h
-5.50784205485698	-2.58544729299901	0.00003041658681	h
-5.20703008134354	0.37524313585782	1.68741160714135	h
-5.20751307875564	0.37534246677784	-1.68727949189804	h

Table 55: Geometry of the S_1 state of 1,3-dimethythymine in atomic units obtained at RI-CC2/cc-pVDZ level

3.34423783187624	-1.57387095394669	-0.21715014902200	c
1.81084748725883	-3.84318437414594	-0.02189692910309	c
-0.71196323270138	-3.48344812619288	-0.02761937419443	c
-1.87022946091366	-1.12661190343336	-0.12360101241250	n
-0.44524730237160	1.12983408144647	0.02112965593496	c
2.14984982404813	0.77826811879935	-0.03025078689677	n
2.99788039927517	-6.42846624317660	0.03320579781754	c
-2.62049701060881	-5.42820549236140	0.07706692092673	o
-1.51623457814315	3.21182391030306	0.15001386979725	o
3.73786763083025	3.03888516512866	0.01433484559948	c
-4.61909295760209	-0.89387343193003	0.08374731684139	c
5.36726203269419	-1.58043475172154	0.22831302463228	h
4.37542085490132	-6.59437391738315	1.59219022670765	h
1.54029438865189	-7.89454146302391	0.31276914762834	h
3.99781149094855	-6.85200204814555	-1.74920687780790	h
4.96882521375446	3.00215167821869	1.69625438804492	h
4.91963957320500	3.09492177700918	-1.70040717175835	h
2.49393935692247	4.69689997842814	0.08140530644834	h
-5.49192926328418	-2.53683239600133	-0.84828353574838	h
-5.22858010614451	-0.81432230715085	2.07645746901502	h
-5.18112855721669	0.86314246902952	-0.86502378066685	h

Table 56: Geometry of the T_1 state of 1,3-dimethythymine in atomic units obtained at RI-CC2/cc-pVDZ level

3.08020666545311	-1.48329741794633	-1.27091819037057	c
1.65080608387439	-3.79349648666961	-0.43159514805397	c
-1.04752643959361	-3.57802473381045	-0.10833420846736	c
-1.98500138771968	-1.05175193163846	-0.30519870268449	n
-0.48071008873980	1.06520793790759	0.19459718708529	c
2.15094604587869	0.67605937161420	-0.05528142202139	n
2.98573593359227	-6.19674936521245	0.15585288377319	c
-2.50965154158843	-5.38542141292416	0.29253818337726	o
-1.37640949502193	3.13405763585407	0.78786245662715	o
3.79291380557765	2.87081495165712	0.28881786438992	c
-4.71610618190924	-0.65962730159544	-0.05987439844398	c
5.14888430875660	-1.58331734783496	-1.34033922315504	h
4.35146916999977	-5.92300054202723	1.71842462844205	h
1.61478665374569	-7.66810942493160	0.68616671394871	h
4.09377364912200	-6.84539070670200	-1.49577712158644	h
5.50653123725664	2.27613547681779	1.30784332991358	h
4.33160637758893	3.66663660817401	-1.56264253785227	h
2.75470260369881	4.29992905347564	1.37406537711483	h
-5.64730906619838	-2.40228879953969	-0.68781180273935	h
-5.24997142993222	-0.26299488729608	1.91478006616045	h
-5.27547768682413	0.95411918657795	-1.23971179184900	h

Table 57: Geometry of the ground state of uracil+6H_2O in atomic units obtained at B3-LYP/TZVP level

0.20775884851906	0.07356579155689	-0.18583725755595	c
2.75542656646271	0.10921949251565	-0.19811629007736	c
4.03859892217919	2.51096456750382	0.00629832362615	c
2.47420371902501	4.61753899695527	0.15520149844033	n
-0.11053574465878	4.57728725441861	0.22576607900870	c
-1.19899088309171	2.23234253650130	0.02031314468237	n
6.36186758772745	2.77053202076443	0.05824039529974	o
-1.38753555221199	6.52412865946944	0.46335435492745	o
-6.63055983955597	6.95545586622821	0.80914828039623	o
9.00724360991960	6.99577752979754	2.05290005228129	o
4.72764593062309	9.24819415812061	0.14150201239204	o
8.51358529778579	-2.15556066874047	-0.64607132120292	o
-0.87538501512077	-1.65503881545369	-0.32183443716260	h
3.88169731440990	-1.58581930395065	-0.35063123190850	h
-3.14625791358345	2.11419872139255	0.01974447169321	h
3.34198635143741	6.41335240655113	0.17657017055059	h
8.31411874756676	5.42477734454378	1.37462718886730	h
10.73896919940333	7.06974102153183	1.50503217469076	h
-4.78861984406421	7.04296999717046	0.66436416403294	h
-7.29613759519175	8.36520472949074	-0.12609321276769	h
3.69267987909263	10.41679414157753	1.11742788545413	h
6.37118575633656	9.04764912702211	0.95511483657746	h
8.13755958991254	-0.37460833792154	-0.37862988217304	h
9.70320907796294	-2.20237014313860	-2.02008454003956	h
-6.50546066361992	1.89185213680599	0.08268688030569	o
-7.02129164240121	3.66258065824330	0.31717875458856	h
-7.63277931910630	1.16945339093923	-1.14637121845757	h
0.40472472700385	11.29178694357122	2.32454676673698	o
-0.08505558793455	11.42865246078496	4.07056677275929	h
-0.36490414885324	9.73742231222933	1.70199668381254	h

Table 58: Geometry of the ground state of 1-methyluracil+6H_2O in atomic units obtained at B3-LYP/TZVP level

-0.13705077365498	-4.46526820248801	-1.97764871973731	c
-1.53514374077158	-2.74050498921006	-0.72679637497714	c
-0.29504036018351	-0.93641550883741	0.90115733093591	c
2.30979072704645	-1.18486327893064	1.03750186475539	n
3.74777551572894	-2.89345747733471	-0.26218631044655	c
2.44103401805596	-4.58749405244288	-1.78589389627164	n
-1.38676989239756	0.72811225798093	2.11936408403053	o
6.07172406092344	-2.94731547305762	-0.12926131374754	o
3.91464129262494	-6.45039841266624	-3.22723162348765	c
4.84811318968798	2.03128248591896	4.03156988585176	o
0.96441838226472	5.34405083402967	4.31130784034817	o
8.96397011915433	-7.58444833527424	0.09225067595407	o
-5.44221724373955	3.92340282814047	1.11962899815226	o
-2.49175008253470	8.29114488651116	1.47413528447037	o
-3.56346923311232	-2.66965447885093	-0.91828835902092	h
3.31219612059476	0.09305525068295	2.22427372370098	h
-0.98444707282478	-5.85282132263140	-3.21689113554248	h
2.60513352465221	-7.57175684317764	-4.34606815050119	h
5.23692887565364	-5.48695971546975	-4.47694007252918	h
4.98130663570882	-7.67327007437414	-1.96170692409485	h
10.08178286744034	-7.75958128551867	1.51585748166401	h
8.30125818352243	-5.87764602189238	0.18864698738966	h
6.57182336741404	2.31851365509659	3.46102973446611	h
3.93593170412064	3.63674371219051	4.18018900144553	h
-0.01284654143582	3.84043057226858	3.93687667986748	h
0.10737261809811	6.68566026156295	3.38250974137547	h
-6.72760252462060	3.74526380143916	2.39496064139433	h
-4.19199545506852	2.60845545355365	1.47363361378550	h
-3.70007394970101	6.91016533878569	1.22486684252013	h
-2.32693216618152	9.11873916576614	-0.13561226109581	h
9.39636890893124	0.98688007365715	1.59625637733187	o
10.29864364969004	1.71596514656351	0.19682053239570	h
8.43886980127959	-0.42692717565059	0.90937033623703	h

Table 59: Geometry of the ground state of 3-methyluracil+6H_2O in atomic units obtained at B3-LYP/TZVP level

3.31737502599818	-2.97301667966542	1.70472941814529	c
0.84103925007676	-3.42932963963523	2.29437281036969	n
-1.09559815725935	-2.01709935976916	1.34804983138934	c
-0.68497793014013	-0.05140518321719	-0.21681232242397	c
1.86694401003919	0.60890645048335	-0.90523885070932	c
3.78264726459327	-0.91247870947746	0.15553666487175	n
2.40939997894637	2.37655056117788	-2.32372751961804	o
6.44726152339651	-0.38097473471977	-0.43095819545051	c
5.04120916532578	-4.32531896485262	2.50128006511140	o
6.75818034520726	4.88189128462177	-4.48600526315331	o
-2.26401332702036	4.54728968456235	-4.08044625795563	o
4.38323766993921	-9.10057088831958	5.31500689059719	o
-0.32711362672314	-7.33775437642017	5.56816193852855	o
9.98371522879333	-4.69696031358476	4.46477348638454	o
0.45109793381607	-4.89199289366533	3.54873973385240	h
-2.20119763076544	1.06731358090840	-1.00189405526455	h
-2.96468863848893	-2.60052373410256	1.93586766503370	h
6.56795866639185	1.41288912783034	-1.41076687613714	h
7.52635298370910	-0.29862297533339	1.31732668035003	h
7.21750892211933	-1.86992898636115	-1.62870206610260	h
-2.36741634091562	4.61227799999399	-5.89470339717469	h
-0.52486978677291	4.08908652186659	-3.70355232131826	h
4.82233705304750	-7.77466337525243	4.12618422434292	h
5.64680629644812	-8.93072875174180	6.65615436728338	h
11.06958745893924	-5.37004794050526	3.16951267684176	h
8.36586312036673	-4.37365553567294	3.64341370762852	h
6.70183079038571	6.63387095171079	-4.00137341698454	h
5.15242277559096	4.18155393266305	-3.94693458984485	h
1.30596256509135	-8.24949356308166	5.73531225740997	h
-0.98677590661986	-7.14188600611683	7.25107289363387	h
8.34655685469292	-7.71363859571859	8.48347004102239	o
9.63932883752764	-8.67320190630909	9.32654964138259	h
9.20653783343126	-6.62053866053222	7.26210367035799	h

Table 60: Geometry of the ground state of thymine+6H_2O in atomic units obtained at B3-LYP/TZVP level

-0.01100761848085	0.03118286725459	-0.00997088909594	n
2.57875544097952	0.03770633955610	-0.00899851473635	c
3.96745557049116	2.18098747204169	-0.01335197066473	c
2.59622820128255	4.56294073365719	-0.02478899290225	c
-0.01879516108975	4.39657489158725	-0.08414573546729	n
-1.39892252959417	2.21222961058877	-0.02017343434104	c
3.62470704296005	6.66049172086266	0.01592446062030	o
-3.74086439085501	2.21128100853809	0.03001734678422	o
-2.65327560534475	8.80640072725248	-0.54309931488339	o
1.33500851874032	11.20328511865171	1.78788701666162	o
-6.85422764875447	6.38698002872555	1.50523763982058	o
-6.92610542147003	-1.95163824625216	0.37172955257205	o
-2.57633147627910	-4.62874432443094	0.12237689066391	o
8.61243122575779	8.82581220552308	0.03045730613765	o
3.43567326735110	-1.81936099469630	0.01267819041805	h
6.79904135875267	2.21640785946487	0.01761054209331	c
-0.95859397884207	-1.67504914337654	0.00550470370375	h
-1.04227632244809	6.10208921717744	-0.23197886359168	h
2.34732328691296	9.76413458583503	1.23798674244444	h
2.39313755440965	12.66942002018615	1.59910460126961	h
-5.99724889924823	-0.35932379466824	0.20393993211774	h
-8.37069690503042	-1.83238710429059	-0.72557053131239	h
-4.26765718113707	8.60466230273994	0.31961233521538	h
-1.67594631666172	10.12421672474679	0.29815973854320	h
6.98428490627409	7.97692948754943	0.03003272357724	h
8.74841891138506	9.58464484213980	-1.61619024863917	h
-4.35093198823132	-4.07641202345145	0.20947321128351	h
-2.50680011691415	-5.97679307545862	-1.09528337514503	h
-7.32078774899183	6.14943615513953	3.24666878303059	h
-5.93994797643887	4.86443405656278	1.01394973568473	h
7.55505142416379	0.29890653412917	0.00301739640611	h
7.55117208451496	3.22810020357646	-1.61653984491027	h
7.51910469992414	3.18769559767972	1.69041094079048	h

Table 61: Geometry of the ground state of 1,3dimethyluracil+6H_2O in atomic units obtained at B3-LYP/TZVP level

0.17848931754453	-3.40158859983297	1.68800448752252	c
-1.64131596298701	-1.71802795698958	0.56142165727877	c
-0.62468574541251	0.30562757081940	-0.81897450735801	n
1.91945734560409	0.90317178832349	-0.88645061317851	c
3.54887948803791	-0.78949552593377	0.27165446842966	n
2.65937797592769	-2.88968517552567	1.50026081935222	c
-3.94508073912187	-1.96946719810034	0.76164286242022	o
-2.38745472647133	1.94390569633612	-2.22095742157526	c
2.72682050650705	2.82182716674335	-1.91290294862128	o
6.26226942881613	-0.22789863136363	0.16236375914580	c
-0.50869091908837	-5.06209725348995	2.65065232803669	h
-8.39144894022867	-2.16556877664229	-2.22547619114407	o
7.00105933515903	6.02255414121792	-2.46616995105556	o
-5.02179387351447	-7.27049881281418	0.39918679809951	o
0.52685919025057	7.00779634031569	-5.28681056933811	o
5.54245914134818	8.03048657980176	-7.20420419723974	o
-4.37499573235832	-5.08360426025836	-4.81344854268691	o
4.08934985467439	-4.09834807338692	2.31858332710626	h
7.27688889016328	-1.78464025982836	1.03805817094383	h
6.86989317221313	-0.02375366325129	-1.79254851291066	h
6.68557664166552	1.51806953273564	1.16864959843081	h
-3.90196939854341	0.76378802909446	-2.94230819289825	h
-3.16020560073961	3.40078738870011	-0.98530946840167	h
-1.39681775050866	2.82978869508840	-3.78006843193929	h
-4.36662846263778	-6.24173075510544	-3.39406574154698	h
-5.91852388277037	-4.13219067493347	-4.56498536306417	h
-6.76899311242895	-7.77464314847687	0.48549226225057	h
-5.01239720023606	-5.48350021862656	0.82843408009159	h
5.56532753398407	4.91230143490389	-2.15938156249546	h
6.80568110219452	7.41273502333984	-1.30683851661482	h
1.97210120399603	7.53014577286327	-6.29501870720182	h
1.24247561724518	5.84285093935866	-4.08080392303295	h
-9.53693057256830	-0.76099906382045	-2.37403033210482	h
-7.07595509682456	-1.64940492378533	-1.05438349767858	h
6.37011919411720	7.31167627771102	-8.65384744418247	h
6.37438851940230	7.31395351925287	-5.72102835127612	h

Table 62: Geometry of the ground state of 1-methylthymine+6H_2O in atomic units obtained at B3-LYP/TZVP level

-1.44625145301301	-0.62074483935181	-0.03778731782524	n
-0.07338752142000	1.56941625292619	0.02315120868794	c
2.52482965316527	1.27970133340476	0.07634187598565	n
3.59816433353045	-1.08576413424905	0.06085828545232	c
2.25396907599734	-3.25655583245909	0.02470569160883	c
-0.48421438271682	-3.05218953596134	0.02497160468317	c
-1.06048083691332	3.68054752762267	0.02696109498873	o
4.08943258880553	3.57297270512440	0.14372273255123	c
3.44305651233888	-5.82749985603096	0.01520486252309	c
-1.93320104523483	-4.88253229776341	0.08427418303227	o
-6.50870563443338	-0.15305050460989	-0.44541805122299	o
-7.14198578707571	-4.52721505495767	2.12327136656684	o
-6.26126987761248	4.99446999062398	0.81861273760195	o
-3.16712552027675	-10.03822968396557	-0.54186663589811	o
0.88558100933269	8.66985947284277	1.37065149994670	o
-3.44132788001463	-0.42132300327349	-0.16832307222115	h
5.64302538333086	-1.09727176228965	0.08924479491851	h
5.49741475047387	-5.69307999128709	0.10877451946501	h
2.78557945690987	-6.95340658672232	1.61529818437402	h
2.94290546828938	-6.87084982702046	-1.69631438694076	h
6.06396454648176	3.00517713905372	0.15315284896804	h
3.71692835551723	4.74014312175989	-1.50974633448731	h
3.67885827463470	4.68756561098421	1.82334614119852	h
-5.38113028409535	-4.80433650064784	1.69674466992908	h
-7.94172931712397	-6.15670156219601	1.78950612548910	h
-7.28894327421277	-1.56291636636749	0.47703331532199	h
-7.07312324593050	1.44910365827217	0.25952897210998	h
-4.47588791180891	4.68640253748512	0.48652488961268	h
-6.83048384484169	6.08591580289772	-0.52106291393525	h
-2.50362981084732	-8.32415239669131	-0.38797549329982	h
-2.91908307672929	-10.51213035863850	-2.28004190603862	h
-0.34636209383675	9.62455698993157	2.30721744841796	h
0.04205853726307	7.11162111749101	0.90080112934498	h
-8.20043274523463	-9.65265727293228	1.06177138566157	o
-6.47860628689332	-10.01826884390634	0.48896243817188	h
-8.50494566829859	-10.76753546769608	2.46588765565475	h

Table 63: Geometry of the ground state of 3-methylthymine+6H_2O in atomic units obtained at B3-LYP/TZVP level

3.64422902673796	-0.58915796046853	0.28349100881177	c
2.96463883110200	-2.40863492631315	1.98724377925835	n
0.52460128201728	-3.16750508491528	2.35787108723969	c
-1.43802349301295	-2.13323371362658	1.09854409529688	c
-0.88152814993953	-0.13191440965491	-0.68868811567437	c
1.66311575778261	0.51700421803761	-1.02837763679494	n
-4.13234457748212	-2.93616653072640	1.44441138304283	c
-2.53411595445175	0.99297246018260	-1.89382711089316	o
2.22658348099607	2.43021463803532	-2.97125335347930	c
5.87209499407408	0.00964299533255	-0.04835362228038	o
10.24909737720142	-2.18629268873618	2.13895735531876	o
9.44224249246397	3.67084657875004	-2.00367365062396	o
-3.88588622504048	3.87659400745773	-6.22895220665086	o
6.76298834085126	-4.64766737997755	4.92492703380163	o
-5.37517063570895	-1.75768477423624	-5.75242435206366	o
-0.60345170705598	-0.06607005519701	-8.32679573422793	o
4.38551139462440	-3.20869060915189	3.06463483186750	h
0.28784895639901	-4.66267078719062	3.73225097591228	h
1.67877252673398	1.69939263255281	-4.81976457766377	h
1.16257674709739	4.14208503297546	-2.55923770484835	h
4.23021393320589	2.84145128725707	-2.91964534924538	h
-1.89078311369595	-1.24475777695086	-7.76688358139531	h
-1.49045130720743	1.53443779360781	-8.28258852685925	h
-6.20746111295765	-0.39818223287211	-6.63884709257042	h
-4.72344100689191	-0.93968727251599	-4.24622709029708	h
-4.18127798392981	5.66442321017768	-6.08096250658705	h
-3.31191122980779	3.29722086708990	-4.58059222884021	h
-5.31489000893390	-1.34027250794163	2.00604199059011	h
-4.91803688921652	-3.68150492078916	-0.31410441835020	h
-4.27768749903452	-4.39895764055905	2.88951185359576	h
9.72390312468294	3.15716509101273	-3.72560229425317	h
8.13804203824122	2.54450802552789	-1.38406540295683	h
11.62692377109716	-1.01713675641093	2.33329589977661	h
8.94113179745638	-1.29633664953514	1.19473061976196	h
8.33277858443138	-3.94421773505794	4.21977084996564	h
6.93592341898159	-4.59952473538910	6.73447120178750	h

Table 64: Geometry of the ground state of 1,3dimethylthymine+6H_2O in atomic units obtained at B3-LYP/TZVP level

3.03530875278916	-2.39879091206728	2.06287009398612	c
0.60929188646876	-3.13604234632587	2.31396318645218	c
-1.27301594184477	-1.89520046725856	0.75786156742643	c
-0.39622372084718	-0.08105458228314	-0.94706136316907	n
2.10183542963071	0.70023851435267	-1.13099448278665	c
3.79742014924442	-0.53923413370751	0.42275097904936	n
-3.55188499193935	-2.37700421509539	0.88244316857125	o
-2.26629560453031	1.04524536808912	-2.67795265831364	c
2.79454846730262	2.37428895783591	-2.57721970859911	o
6.46265522911241	0.21355082896030	0.25286124725520	c
-8.46626933106025	-2.22270257436469	-1.30410394636005	o
6.84786943207557	6.14472724634545	-2.95245816435014	o
5.04925477528836	8.60761560112675	-7.34119778281254	o
-4.96756898030737	-7.38200517153488	-0.85229991373907	o
1.77515826416818	8.18974948435423	-3.06995055555841	o
-5.27091129321603	-4.04063724303246	-5.40793457806604	o
-0.22758200147863	-5.16751878273422	4.10284015943465	c
4.53481614122252	-3.24297436731624	3.16691846355625	h
7.54138577973149	-0.93000584912758	1.57516618890231	h
7.16992064355321	-0.09944290935856	-1.65518439158086	h
6.68776937682563	2.20434447463749	0.72276055797479	h
-3.25024377288897	-0.46762078493248	-3.67303994519737	h
-3.61057372725354	2.17972007265683	-1.60635125029607	h
-1.26255391725852	2.23240105705794	-4.01055259170263	h
-4.86144952224512	-5.49435601532461	-4.36864008188484	h
-6.76268061116765	-3.36432297046149	-4.58732656380863	h
-6.75822438671467	-7.67899979973192	-0.70040957747568	h
-4.68739326644961	-5.80073671772475	0.03556485088509	h
5.88902111938084	4.58672690580294	-3.05987806735307	h
5.58260513006481	7.30878451607835	-2.29778725358013	h
2.33180649864633	8.62144623063036	-4.77005828337086	h
1.40740699865627	6.40350827050022	-3.15081984793882	h
-9.66697206256088	-0.93915572937437	-0.83980668084738	h
-6.90648371987246	-1.83127763248807	-0.41587932138283	h
5.33246332049825	7.97368438976008	-9.02025084563180	h
6.19919092914230	7.69573747457423	-6.22363529837477	h
-1.63408049352387	-4.44628574821918	5.43041072371758	h
-1.10368377811526	-6.73482771327852	3.08363179541174	h
1.37084107815854	-5.90127437921210	5.17619343105264	h

Table 65: Geometry of the ground state of uracil+6H_2O in atomic units obtained at RI-CC2/cc-pVDZ level

0.23692480981438	0.05576598148804	-0.07498313408757	c
2.82264907336489	0.12050370870882	-0.03261556142092	c
4.07378861650596	2.55671445687344	0.11662256501894	c
2.46941611589819	4.65520053103928	0.12379944840583	n
-0.13253270134293	4.58921362171002	0.13121545931984	c
-1.20344278143533	2.21529053912459	0.00944468886697	n
6.42715292757197	2.85187439339721	0.23967063739002	o
-1.45154726592058	6.55873016249886	0.24372358241806	o
-6.65608725195599	6.73469749238877	1.07819323832713	o
8.81010841601509	7.22931441293897	2.21050490660456	o
4.65705321615838	9.19729525954321	-0.19413682021329	o
8.33440140189478	-2.20504490986321	-0.34709990718092	o
-0.83712509325709	-1.70875264947070	-0.16114905534333	h
3.98927320801713	-1.57973582940308	-0.07450721842173	h
-3.17740640110477	2.07913333536771	-0.04060972370896	h
3.33166059880634	6.49144048575337	0.02703202342620	h
8.12014632176078	5.60024992389316	1.66217465808295	h
10.21098346581279	7.45197793438629	1.05463199294309	h
-4.81494628483581	6.84902279296351	0.88601598750950	h
-7.26036784842638	7.87627882608585	-0.21656505249308	h
3.54356512399200	10.24766529331347	0.85218012783704	h
6.18495589828943	8.92366850848644	0.82652669126646	h
8.04555156775454	-0.43330007522215	0.07641348031509	h
8.42901071451564	-2.10973800536472	-2.17047959626843	h
-6.38146017608209	1.77521076491644	-0.07812149893912	o
-6.84510248506503	3.51097640845396	0.44162850337373	h
-7.06028033318493	1.67412384643212	-1.77440881609085	h
0.54985246295512	11.05183835217842	2.41380969325795	o
0.54775465276973	10.47247288940412	4.14886879748809	h
-0.30902375610839	9.66129437179458	1.54958249595566	h

Table 66: Geometry of the S_1 state of uracil+6H_2O in atomic units obtained at RI-CC2/cc-pVDZ level

0.13753994197352	-0.03378175112134	0.02079904816826	c
2.84145639841666	0.09728018089448	-0.22452401673673	c
3.85402225029866	2.43568827208900	-0.41460487882597	c
2.45158774708917	4.66239224106747	-0.33272181653378	n
-0.14606518479180	4.58147321890922	0.03157761220368	c
-1.20382244572652	2.24061361226901	0.18555774141812	n
6.48689362638243	3.10438322818994	-0.70387552350906	o
-1.41304344899608	6.60297433169741	0.19265470459190	o
-6.53569159000147	7.04533533231374	1.13147683782802	o
8.49029051027716	6.68785175975168	2.99592879279212	o
5.02829146985114	9.06815285963085	-0.28306418536396	o
8.52448234479389	-1.12697297883361	-1.35031502472631	o
-0.94127669312485	-1.76894025587674	0.28649065746396	h
4.03869625082451	-1.57739418293837	-0.30264104211645	h
-3.16212691340916	2.16817168952160	0.38977338871043	h
3.37318347573987	6.43880148158998	-0.44407518638621	h
7.98104278986957	5.12147624188406	2.17386390604722	h
10.02750767580052	7.10624109751613	2.09373339374818	h
-4.69044379705560	7.00611171281471	0.91738500533929	h
-7.07402561044779	7.93152015080401	-0.37574361068381	h
3.73034839266194	10.14496074611448	0.50819271750723	h
6.16457094680377	8.64777782331636	1.11417002013655	h
9.57648047940572	-0.22185557297952	-0.15807669952048	h
8.50108283624989	0.02768380035678	-2.77222040887144	h
-6.46714311345280	1.94166129437781	0.66100967954946	o
-6.83771829383460	3.74621723368920	0.96783756867508	h
-7.18457858495776	1.67360514769181	-1.00082309358541	h
0.77308702459023	11.08547811561825	1.84100440509342	o
0.70655144399943	10.73111491946350	3.63480987820094	h
-0.15211520846849	9.63872086067443	1.13768700476890	h

Table 67: Geometry of the T_1 state of uracil+6H_2O in atomic units obtained at RI-CC2/cc-pVDZ level

0.08773872419271	0.29109553531883	-1.51176348237959	c
2.80447415889115	0.28092610994330	-0.66067336322638	c
4.04760787265428	2.68590397441205	-0.36599074226878	c
2.48594946455019	4.81090908204393	-0.55254966028251	n
-0.09820866664332	4.67040585232282	-0.13888670885711	c
-1.19734746042445	2.31687132857104	-0.38953629826773	n
6.38826848850807	2.91305679319921	0.04523533170141	o
-1.37368487346487	6.58279165100326	0.43697517127482	o
-6.61108892000997	6.88016487928839	1.31857710423743	o
8.74182996541381	7.28969937448729	2.15903248891270	o
4.70584040774010	9.39880607466151	-0.38960871757121	o
8.03442717541909	-2.29792075824363	0.54592556715542	o
-0.97361969990782	-1.48221357779816	-1.52508934724430	h
3.83308377772126	-1.41608354651984	-0.07535969356056	h
-3.16004559863216	2.21112929221348	-0.15243151513557	h
3.33867084234793	6.63659717646667	-0.47157499945464	h
8.07506665881304	5.67616393301062	1.55217704102700	h
10.22815602708458	7.50665702053519	1.11429117411020	h
-4.76907251521734	6.94446722706024	1.14503597309066	h
-7.16838675192954	7.99865358683354	-0.01700442812130	h
3.58897920774260	10.34964696196752	0.74500384938032	h
6.20597370145785	9.03720162196049	0.64164377379846	h
7.86118173349222	-0.46409158978043	0.57434927962548	h
8.45984771263475	-2.58420904035877	-1.20920315741128	h
-6.38535435985333	1.88970359093203	0.18164344427118	o
-6.83012544482953	3.62588431557353	0.70420384099943	h
-7.23995672869273	1.72391089453474	-1.42766597779129	h
0.77405928851166	11.00931771799872	2.64922375676063	o
1.02767543745781	10.36379629206014	4.34224464835416	h
-0.14190401720634	9.62230839586122	1.84372114315563	h