

The Supporting Information gives the geometries for all thymine and thymine water tautomers and transition states discussed in the article.

Geometry of T1 tautomer in xyz

```
C 0.159744 0.734796 0.000000
C -1.221710 0.230746 0.000000
N -1.321697 -1.172608 0.000000
C -0.302812 -2.118790 0.000000
N 0.959382 -1.534749 0.000000
C 1.178902 -0.170615 0.000000
O -2.225226 0.935171 0.000000
O -0.486451 -3.325227 0.000000
C 0.358620 2.223113 0.000000
H -2.266877 -1.554151 0.000000
H 1.735410 -2.188497 0.000000
H 2.229564 0.134881 0.000000
H -0.117502 2.676199 -0.884993
H -0.117502 2.676199 0.884993
H 1.429363 2.481205 0.000000
```

Geometry of T2 tautomer in xyz

C 0.151927 0.720896 0.000000
C -1.225527 0.233810 0.000000
C -0.197837 -1.984308 0.000000
C 1.180687 -0.192301 0.000000
C 0.349971 2.209430 0.000000
N -1.292618 -1.178893 0.000000
N 1.038531 -1.569014 0.000000
O -2.248901 0.911183 0.000000
O -0.495840 -3.297456 0.000000
H -2.222478 -1.597165 0.000000
H 0.371733 -3.738454 0.000000
H 2.218973 0.160140 0.000000
H -0.127820 2.662216 -0.884686
H -0.127820 2.662216 0.884686
H 1.420668 2.466312 0.000000

Geometry of T3 tautomer in xyz

C -0.004875 -0.004509 0.000000
C 0.014391 1.358811 0.000000
C 1.318810 2.066615 0.000000
C 2.359044 -0.019140 0.000000
C -1.228451 2.199624 0.000000
N 2.488282 1.271319 0.000000
N 1.186225 -0.713338 0.000000
O 1.381682 3.292999 0.000000
O 3.436781 -0.831203 0.000000
H 1.209952 -1.727144 0.000000
H -0.920332 -0.602270 0.000000
H -1.238507 2.859472 -0.882886
H -1.238507 2.859472 0.882886
H -2.139601 1.579953 0.000000
H 4.189845 -0.213895 0.000000

Geometry of T4 tautomer in xyz

C 0.142116 0.718607 0.000000
C -1.143127 0.130633 0.000000
C -0.261315 -1.947507 0.000000
C 1.186913 -0.205265 0.000000
C 0.327949 2.210459 0.000000
N -1.365879 -1.182486 0.000000
N 1.013750 -1.546735 0.000000
O -2.217885 0.947551 0.000000
O -0.495364 -3.275532 0.000000
H -2.983149 0.344830 0.000000
H 0.392665 -3.671347 0.000000
H 2.227041 0.145051 0.000000
H -0.143162 2.665009 -0.887148
H -0.143162 2.665009 0.887148
H 1.398539 2.468524 0.000000

Geometry of T5 tautomer in xyz

C 0.158539 0.733347 0.000000
C -1.143841 0.116401 0.000000
C -0.355598 -2.081293 0.000000
C 1.192186 -0.168445 0.000000
C 0.330726 2.226385 0.000000
N -1.406819 -1.166892 0.000000
N 0.939317 -1.509029 0.000000
O -2.185447 0.973759 0.000000
O -0.485442 -3.295076 0.000000
H -2.969354 0.393124 0.000000
H 1.702561 -2.181015 0.000000
H 2.243946 0.134485 0.000000
H -0.143251 2.677691 -0.887070
H -0.143251 2.677691 0.887070
H 1.399220 2.494731 0.000000

Geometry of T6 tautomer in xyz

C 0.065460 -0.014990 0.000000
C 0.031537 1.411658 0.000000
C 1.282533 2.002025 0.000000
C -1.243254 2.216090 0.000000
C 2.385608 -0.202834 0.000000
N 2.388501 1.223887 0.000000
N 1.125652 -0.800100 0.000000
O 1.547617 3.326335 0.000000
O 3.451153 -0.796220 0.000000
H 3.305932 1.668366 0.000000
H -0.904700 -0.536442 0.000000
H -1.335884 2.858287 -0.895186
H -1.335884 2.858287 0.895186
H -2.112365 1.540030 0.000000
H 0.696680 3.791701 0.000000

Geometry of T12 transition state in xyz

C 0.000000 0.000000 0.000000
C 0.000000 1.375656 0.000000
C 1.271039 2.109002 0.000000
C 2.353015 -0.074444 0.000000
C -1.252979 2.206155 0.000000
N 2.428431 1.273793 0.000000
N 1.173527 -0.715124 0.000000
O 1.398580 3.327232 0.000000
O 3.288625 -0.949895 0.000000
H 3.336355 1.736714 0.000000
H 2.116222 -1.627364 0.000000
H -0.929752 -0.577750 0.000000
H -1.283174 2.862895 0.885185
H -1.283174 2.862895 -0.885185
H -2.149492 1.566699 0.000000

Geometry of T13 transition state in xyz

C 0.002970 1.403892 0.000000
C 1.375954 1.988915 0.000000
C 2.475636 1.182525 0.000000
C 1.116026 -0.741255 0.000000
C 1.467777 3.488268 0.000000
N 0.000929 0.001916 0.000000
N 2.357940 -0.209584 0.000000
O -1.011074 2.090329 0.000000
O 0.784363 -1.981295 0.000000
H 3.167311 -0.820523 0.000000
H 3.498509 1.567698 0.000000
H 0.953232 3.899406 0.883672
H 0.953232 3.899406 -0.883672
H 2.514850 3.830076 0.000000
H -0.346445 -1.293277 0.000000

Geometry of T15 transition state in xyz

C 0.000000 0.000000 0.000000
C 0.000000 1.374526 0.000000
C 1.322259 1.936044 0.000000
C 2.471738 -0.201145 0.000000
C -1.225432 2.242682 0.000000
N 1.155794 -0.734130 0.000000
N 2.445437 1.181586 0.000000
O 1.702225 3.162761 0.000000
O 3.450877 -0.924840 0.000000
H 2.830037 2.440301 0.000000
H 1.114579 -1.750044 0.000000
H -0.929529 -0.578707 0.000000
H -1.239815 2.896480 0.887572
H -1.239815 2.896480 -0.887572
H -2.141630 1.631339 0.000000

Geometry of 1-TW₁ water cluster in xyz

C -0.018464 0.061634 0.074157
C -0.022952 -0.002330 1.437465
C 1.267335 -0.047173 2.136869
C 2.400966 0.052293 -0.104597
C -1.269771 -0.027834 2.273811
N 1.142283 0.083829 -0.669950
N 2.384289 -0.015207 1.277552
O 1.411927 -0.106268 3.352939
O 3.443873 0.082580 -0.762024
H 3.298914 -0.037558 1.726946
H 1.142504 0.132031 -1.698662
H -0.944136 0.099055 -0.508168
H -1.303184 -0.941273 2.890149
H -1.285645 0.826842 2.969954
H -2.171810 0.009798 1.643041
O 2.163298 0.212284 -3.267585
H 2.898452 0.269355 -2.625093
H 2.315296 -0.652057 -3.673712

Geometry of 2-TW₁ water cluster in xyz

C -0.097408 0.048850 -0.072470
C -0.098755 0.004400 1.291210
C 1.195636 -0.069418 1.975812
C 2.342648 -0.039115 -0.247357
C -1.342312 0.023643 2.132483
N 2.313329 -0.088412 1.140962
N 1.068236 0.028518 -0.807995
O 1.313481 -0.115943 3.207134
O 3.363507 -0.051257 -0.915021
H 3.224435 -0.147014 1.624301
H 1.046974 0.063813 -1.822083
H -1.022099 0.102715 -0.655166
H -1.398496 -0.881008 2.759815
H -1.332676 0.886975 2.817865
H -2.245386 0.078098 1.504291
O 4.130189 -0.229700 3.304183
H 3.208395 -0.272777 3.625403
H 4.400086 0.657633 3.577304

Geometry of 1-TW₂ water cluster in xyz

C -0.074490 -0.038932 0.160823
C -0.068673 -0.045193 1.525918
C 1.220675 0.083900 2.213076
C 2.320392 0.198608 -0.046212
C -1.301645 -0.177335 2.372588
N 2.319559 0.196274 1.337737
N 1.068882 0.082659 -0.601822
O 1.381634 0.096444 3.428801
O 3.367356 0.298630 -0.695705
H 3.236075 0.283562 1.775038
H 0.995074 0.090727 -1.640261
H -0.999912 -0.132813 -0.415964
H -1.230272 -1.063899 3.024045
H -1.410859 0.696806 3.035476
H -2.204380 -0.266121 1.747996
O 0.882238 0.045676 -3.368779
H 1.837559 -0.122967 -3.553723
H 0.747107 0.914580 -3.771056
H 3.615364 0.080701 -2.473676
O 3.570542 -0.168986 -3.421464
H 3.962581 -1.052320 -3.422637

Geometry of 1-TW₂ water cluster in xyz

C -0.028425 0.087095 0.044865
C 0.109289 0.003707 1.401435
C 1.464775 -0.082226 1.946731
C 2.359642 0.023097 -0.376994
C -1.041423 -0.006224 2.365963
N 2.489798 -0.068021 0.996446
N 1.048233 0.093433 -0.811261
O 1.716443 -0.164772 3.156017
O 3.324901 0.043176 -1.143669
H 3.448496 -0.128906 1.377391
H 0.945054 0.155594 -1.834494
H -1.008938 0.153512 -0.436637
H -1.031120 -0.927650 2.971048
H -0.964042 0.838491 3.070090
H -2.003991 0.060550 1.834934
O 4.524688 -0.253519 2.941678
H 4.819876 0.625278 3.216358
H 3.643669 -0.315431 3.360287
O 1.799276 0.231479 -3.495936
H 1.888673 -0.631794 -3.922520
H 2.596014 0.263130 -2.928827