# Electronic Supplementary Information

for

# Enhanced reactivity of pyrimidine peroxyl radical towards C - H bond in duplex DNA – A theoretical study

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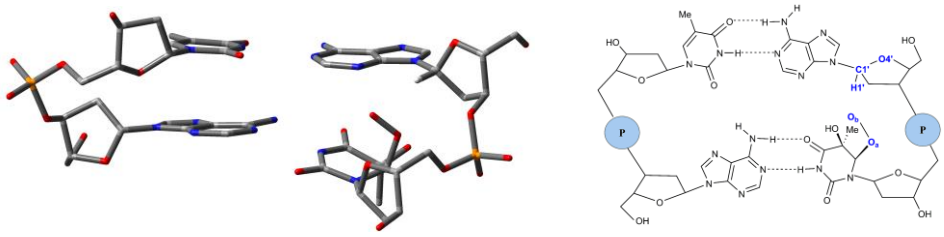
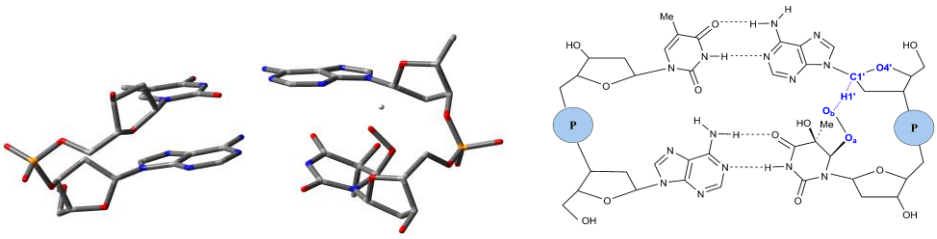


ds - 5' A T* 3' - Reactant

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | X | Y | Z | | | | | |
| O | -8.962847 | -3.535350 | 1.409181 | C | 6.681768 | 1.203281 | -2.561714 |
| C | -8.809335 | -2.707301 | 2.545363 | H | 6.122589 | 0.669612 | -1.371452 |
| H | -9.744321 | -2.180328 | 2.788825 | C | 5.765977 | 1.471961 | -0.718143 |
| H | -8.490094 | -3.279133 | 3.426049 | H | 8.498522 | 0.526211 | -1.202249 |
| C | -7.736273 | -1.685183 | 2.226854 | C | 9.370064 | -0.132120 | -1.233337 |
| H | -7.718536 | -0.908482 | 3.002754 | H | 7.232458 | -0.166365 | -0.725500 |
| O | -6.482299 | -2.354997 | 2.169465 | H | 7.217001 | -1.182834 | -1.124316 |
| C | -5.795448 | -1.895661 | 1.012826 | O | 7.137015 | -0.193790 | 0.359793 |
| N | -5.267481 | -0.963690 | 1.233952 | N | 8.803219 | 1.669699 | -0.370314 |
| C | 3.690039 | -0.966498 | 1.591968 | C | 4.954296 | -0.112274 | -1.700046 |
| H | 4.584046 | -1.866056 | 1.050507 | H | 4.935396 | -1.269324 | -2.451575 |
| C | 5.627351 | -1.604149 | 1.193602 | N | 5.855410 | -1.667796 | -2.860833 |
| C | 4.203341 | -2.966292 | 0.369386 | C | 3.740842 | -1.766783 | -2.618044 |
| H | 5.146157 | -3.929728 | -0.279507 | C | 2.920260 | -0.877489 | -1.955353 |
| H | 5.033933 | -4.931636 | 0.144896 | N | 1.523461 | -0.864184 | -1.751226 |
| H | 4.915082 | -4.000479 | -1.346456 | H | 0.738358 | -1.856780 | -2.182365 |
| C | 6.183590 | -3.608595 | -0.154546 | H | 1.183837 | -2.709195 | -2.487725 |
| O | 2.768715 | -3.206087 | 0.210193 | N | -0.245598 | -1.858255 | -1.929495 |
| N | 2.297547 | -4.140753 | -0.436203 | C | 0.999951 | 0.189915 | -1.095994 |
| H | 1.942375 | -2.308730 | 0.851273 | H | 1.823850 | 1.143793 | -0.619529 |
| C | 0.901428 | -2.437001 | 0.723472 | N | 1.322159 | 1.959126 | -0.103863 |
| O | 2.313469 | -1.173829 | 1.523870 | C | 3.146017 | 1.202862 | -0.694751 |
| C | 1.512362 | -0.407966 | 2.032510 | P | 3.643078 | 0.166140 | -1.390364 |
| H | -7.952026 | -1.024173 | 0.847662 | O | 9.407307 | 1.372502 | 1.088523 |
| C | -8.975799 | -1.147774 | 0.485307 | O | 9.909287 | 2.828538 | 1.520947 |
| H | -6.903376 | -1.697211 | -0.014337 | O | 10.36672 | 0.266058 | 1.146362 |
| H | -7.290905 | -2.671380 | -0.325840 | C | 8.141833 | 1.189621 | 2.043208 |
| O | -6.604980 | -1.111811 | -0.880726 | H | 7.142279 | 2.218357 | 2.087952 |
| P | -7.654918 | 0.393970 | 0.979844 | H | 7.474790 | 2.999687 | 2.779397 |
| O | -8.026550 | 1.338367 | -0.247275 | C | 7.008592 | 2.658636 | 1.093985 |
| O | -9.479805 | 1.866961 | 0.202915 | H | 5.840941 | 1.641337 | 2.578646 |
| O | -7.978506 | 0.791016 | -1.610712 | O | 5.160886 | 2.488621 | 2.769470 |
| C | -7.049364 | 2.585103 | -0.093867 | C | 5.268714 | 0.766670 | 1.619338 |
| H | -6.653471 | 3.148012 | 1.161950 | H | 4.130635 | 0.230443 | 2.282850 |
| H | -7.533315 | 3.584139 | 1.649212 | C | 3.299017 | 0.936312 | 2.212404 |
| C | -6.220101 | 2.364291 | 1.791061 | H | 5.891056 | 0.790131 | 3.855505 |
| H | -5.609534 | 4.221113 | 0.895979 | C | 6.746356 | 0.107462 | 3.786891 |
| O | -5.538206 | 4.840764 | 1.798004 | H | 4.570742 | 0.015123 | 3.750483 |
| C | -4.329940 | 3.654903 | 0.651206 | H | 4.686670 | -1.047122 | 3.974467 |
| H | -3.956402 | 3.752925 | -0.720766 | O | 3.840616 | 0.438498 | 4.443508 |
| N | -3.070168 | 4.386441 | -0.784432 | N | 5.943723 | 1.570052 | 5.026949 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -3.515572 | 2.458304 | -1.230460 | C | -4.773728 | -2.836259 | 0.627493 |
| C | -4.458908 | 1.392403 | -1.329006 | H | -4.903586 | -4.086130 | 0.061030 |
| C | -3.925395 | 0.247196 | -2.192862 | N | -5.878013 | -4.538817 | -0.066017 |
| H | -3.877771 | 0.688549 | -3.661313 | C | -3.764398 | -4.638631 | -0.264812 |
| H | -3.272888 | 1.587592 | -3.799863 | C | -2.821032 | -3.702765 | 0.113311 |
| H | -3.457765 | -0.124252 | -4.257952 | N | -1.411959 | -3.660477 | 0.022932 |
| C | -4.900788 | 0.878157 | -3.996235 | H | -0.674306 | -4.620117 | -0.557227 |
| O | -2.518192 | -0.130182 | -1.761907 | H | -1.131997 | -5.464302 | -0.859404 |
| N | -2.136835 | -1.282151 | -1.922992 | N | 0.342727 | -4.563804 | -0.518300 |
| H | -1.738736 | 0.870099 | -1.296011 | C | -0.788255 | -2.582629 | 0.529956 |
| C | -0.727031 | 0.647855 | -1.119778 | H | -1.504111 | -1.573568 | 1.055725 |
| O | -2.160452 | 2.164898 | -0.996920 | N | -0.911489 | -0.742054 | 1.434648 |
| C | -1.363269 | 2.989924 | -0.613645 | C | -2.819315 | -1.491859 | 1.156366 |
| H | -5.882717 | 5.120913 | -0.322191 | H | -3.424006 | -2.583022 | 0.675282 |
| C | -6.949850 | 5.236847 | -0.524601 | O | -5.410213 | 1.730966 | -1.744703 |
| H | -5.151056 | 4.380860 | -1.448564 | O | -4.871822 | 0.893205 | -0.018733 |
| H | -5.810377 | 3.630710 | -1.885222 | O | -3.929349 | 0.960145 | 0.884062 |
| O | -4.831866 | 5.073561 | -2.228588 | H | -4.749682 | -0.873029 | -2.046492 |
| O | -5.373118 | 6.421861 | -0.115605 | H | -4.158384 | -1.644334 | -2.081091 |
| C | 8.139370 | -1.175624 | -3.378491 | H | 8.309627 | -1.748655 | -4.133175 |
| H | 8.511565 | 0.149523 | -3.715463 | H | -4.454429 | 6.343700 | 0.171921 |
| H | 9.598472 | 0.229514 | -3.863556 | H | -9.561951 | -4.255851 | 1.626886 |
| C | 8.004847 | 0.490615 | -4.627154 | H | 6.865990 | 1.708582 | 5.264809 |
| H | 8.096459 | 1.066807 | -2.578628 | H | -9.996494 | 2.128661 | -0.570619 |
| O | 8.547682 | 2.053885 | -2.732772 | H | 10.79346 | 3.028697 | 1.187989 |

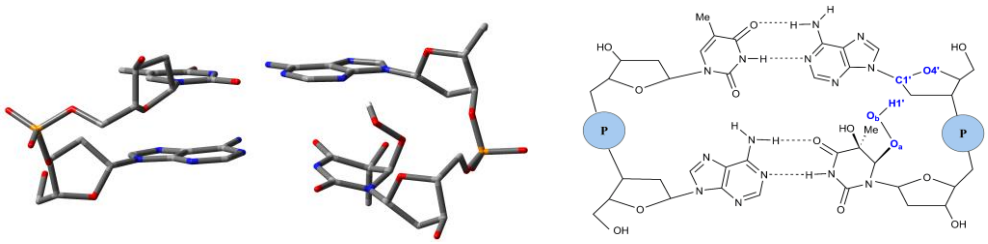


ds - 5' A T* 3' - TS

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | X | Y | Z | | | | | |
| O | -8.201353 | -3.631548 | 1.650677 | O | 6.463904 | 1.311061 | -2.591642 |
| C | -8.154659 | -2.728154 | 2.737385 | C | 5.980842 | 0.745677 | -1.382558 |
| H | -9.162600 | -2.407243 | 3.039954 | H | 5.630681 | 1.528340 | -0.702429 |
| H | -7.651708 | -3.167054 | 3.608156 | C | 8.365209 | 0.679463 | -1.329322 |
| C | -7.363412 | -1.508541 | 2.303816 | H | 9.255620 | 0.051620 | -1.412311 |
| H | -7.412923 | -0.740133 | 3.081814 | C | 7.147373 | -0.062268 | -0.804636 |
| O | -5.999993 | -1.890491 | 2.117013 | H | 7.144652 | -1.072091 | -1.220556 |
| C | -5.634316 | -1.748471 | 0.787743 | H | 7.107805 | -0.110342 | 0.283363 |
| H | -4.993850 | -0.648580 | 0.681045 | O | 8.671511 | 1.819364 | -0.493459 |
| N | 3.767719 | -1.040177 | 1.667914 | N | 4.823371 | -0.068340 | -1.666653 |
| C | 4.661444 | -1.891674 | 1.053401 | C | 4.803043 | -1.203441 | -2.450337 |
| H | 5.701603 | -1.599854 | 1.153282 | H | 5.713925 | -1.560172 | -2.915069 |
| C | 4.282180 | -2.981669 | 0.355131 | N | 3.617593 | -1.734328 | -2.573799 |
| C | 5.222344 | -3.892529 | -0.369426 | C | 2.804015 | -0.891798 | -1.844268 |
| H | 5.167309 | -4.909351 | 0.030312 | C | 1.416789 | -0.918335 | -1.585117 |
| H | 4.938834 | -3.941694 | -1.424640 | N | 0.635993 | -1.912073 | -2.022320 |
| H | 6.253261 | -3.537877 | -0.288374 | H | 1.081234 | -2.737523 | -2.393198 |
| C | 2.849506 | -3.260999 | 0.254210 | H | -0.345983 | -1.930922 | -1.762731 |
| O | 2.375886 | -4.183181 | -0.408115 | N | 0.892758 | 0.099164 | -0.876347 |
| N | 2.029537 | -2.418852 | 0.973449 | C | 1.710177 | 1.061588 | -0.407836 |
| H | 0.988389 | -2.581541 | 0.899917 | H | 1.209993 | 1.850698 | 0.147989 |
| C | 2.397591 | -1.294286 | 1.664582 | N | 3.026740 | 1.160246 | -0.537891 |
| O | 1.600261 | -0.575223 | 2.242755 | C | 3.521218 | 0.158058 | -1.283403 |
| C | -7.821974 | -0.926886 | 0.960594 | P | 9.355601 | 1.520630 | 0.929380 |
| H | -8.884672 | -1.102324 | 0.767200 | O | 9.830386 | 2.986070 | 1.360857 |
| C | -6.894869 | -1.598305 | -0.044177 | O | 10.352486 | 0.446361 | 0.923787 |
| H | -7.306303 | -2.581459 | -0.290270 | O | 8.145660 | 1.280402 | 1.941257 |
| H | -6.738702 | -1.010336 | -0.948639 | C | 7.112676 | 2.270521 | 2.050889 |
| O | -7.567234 | 0.486185 | 1.033741 | H | 7.449122 | 3.054488 | 2.737466 |
| P | -8.090459 | 1.463827 | -0.115855 | H | 6.914465 | 2.719065 | 1.071485 |
| O | -9.647945 | 1.600087 | 0.276661 | C | 5.859614 | 1.636623 | 2.593847 |
| O | -7.918970 | 1.092580 | -1.531747 | H | 5.153555 | 2.453466 | 2.820026 |
| O | -7.436205 | 2.845109 | 0.294912 | O | 5.284716 | 0.745134 | 1.652896 |
| C | -6.527857 | 3.096677 | 1.382693 | C | 4.200147 | 0.158530 | 2.360463 |
| H | -7.128072 | 3.487518 | 2.209568 | H | 3.342192 | 0.835440 | 2.344408 |
| H | -6.024335 | 2.175068 | 1.683232 | C | 6.001526 | 0.780108 | 3.860640 |
| C | -5.474922 | 4.127398 | 0.970761 | H | 6.887337 | 0.142526 | 3.754944 |
| H | -5.256085 | 4.743718 | 1.850808 | C | 4.719190 | -0.062041 | 3.800416 |
| O | -4.254710 | 3.519174 | 0.565584 | H | 4.902286 | -1.120561 | 3.994855 |
| C | -4.057761 | 3.640906 | -0.843683 | H | 4.000901 | 0.307301 | 4.535254 |
| H | -3.229478 | 4.333796 | -1.012897 | O | 6.058644 | 1.553866 | 5.036384 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | -3.604907 | 2.369414 | -1.389654 | N | -4.670654 | -2.727923 | 0.403033 |
| C | -4.595037 | 1.337895 | -1.610761 | C | -4.802611 | -3.852948 | -0.390888 |
| C | -3.969354 | 0.118719 | -2.297510 | H | -5.770038 | -4.170882 | -0.753887 |
| C | -3.713596 | 0.452001 | -3.775231 | N | -3.671537 | -4.460348 | -0.625350 |
| H | -3.096828 | 1.347344 | -3.885720 | C | -2.734608 | -3.703950 | 0.051135 |
| H | -3.208377 | -0.392162 | -4.250359 | C | -1.323804 | -3.728499 | 0.080040 |
| H | -4.676715 | 0.609253 | -4.266175 | N | -0.582049 | -4.638301 | -0.569384 |
| C | -2.630563 | -0.260282 | -1.690544 | H | -1.045090 | -5.389825 | -1.052550 |
| O | -2.261936 | -1.427910 | -1.749470 | H | 0.434962 | -4.597150 | -0.508023 |
| N | -1.865052 | 0.749042 | -1.230068 | N | -0.703020 | -2.751152 | 0.761947 |
| H | -0.880273 | 0.531210 | -0.957659 | C | -1.416681 | -1.778632 | 1.357466 |
| C | -2.287236 | 2.062660 | -1.031577 | H | -0.820285 | -1.026062 | 1.869573 |
| O | -1.509845 | 2.888500 | -0.607571 | N | -2.732413 | -1.643299 | 1.374899 |
| C | -5.863658 | 5.033282 | -0.208628 | C | -3.328888 | -2.626717 | 0.694874 |
| H | -6.935275 | 5.232379 | -0.256635 | H | -5.391854 | 1.711501 | -2.259743 |
| C | -5.366313 | 4.204703 | -1.398089 | O | -5.308290 | 1.048004 | -0.427715 |
| H | -6.100639 | 3.425718 | -1.611972 | O | -4.466189 | 0.486694 | 0.513408 |
| H | -5.210326 | 4.821715 | -2.284172 | O | -4.837844 | -0.973975 | -2.180262 |
| O | -5.218487 | 6.287172 | -0.121516 | H | -4.263552 | -1.759464 | -2.186203 |
| O | 7.955011 | -1.000391 | -3.516340 | H | 8.125498 | -1.558310 | -4.282140 |
| C | 8.275371 | 0.340305 | -3.844083 | H | -4.290148 | 6.134753 | 0.096630 |
| H | 9.353329 | 0.454701 | -4.028336 | H | -8.529232 | -4.480273 | 1.963693 |
| H | 7.727297 | 0.680017 | -4.731629 | H | 6.980663 | 1.746299 | 5.234803 |
| C | 7.879603 | 1.225728 | -2.676197 | H | -10.178531 | 1.689483 | -0.525543 |
| H | 8.289353 | 2.230065 | -2.834901 | H | 10.689763 | 3.220489 | 0.988017 |

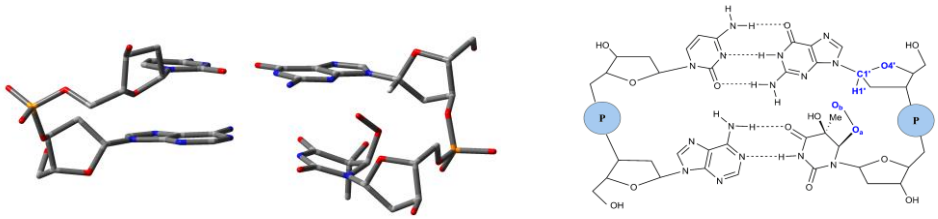


ds - 5' A T* 3' - Product

## Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| O | -8.496189 | -3.514840 | 2.072404 | C | 6.119623 | 0.684863 | -1.376351 |
| C | -8.256520 | -2.521062 | 3.048412 | H | 5.758606 | 1.496320 | -0.736701 |
| H | -9.191889 | -2.047735 | 3.382739 | C | 8.489592 | 0.538198 | -1.160920 |
| H | -7.738034 | -2.928328 | 3.925818 | H | 9.362249 | -0.119024 | -1.168463 |
| C | -7.372892 | -1.461877 | 2.420941 | C | 7.214438 | -0.150455 | -0.704821 |
| H | -7.274218 | -0.606499 | 3.096103 | H | 7.203737 | -1.168318 | -1.100565 |
| O | -6.075370 | -2.021451 | 2.198173 | H | 7.099422 | -0.171795 | 0.378743 |
| C | -5.822795 | -2.045848 | 0.854646 | O | 8.775730 | 1.687694 | -0.331121 |
| N | 3.650391 | -0.946761 | 1.566119 | N | 4.951921 | -0.092749 | -1.715062 |
| C | 4.556828 | -1.837270 | 1.030960 | C | 4.936612 | -1.251232 | -2.464143 |
| H | 5.595946 | -1.563648 | 1.179832 | H | 5.859030 | -1.650699 | -2.867076 |
| C | 4.193049 | -2.943701 | 0.349976 | N | 3.742346 | -1.748018 | -2.636233 |
| C | 5.151771 | -3.897791 | -0.289317 | C | 2.918641 | -0.856935 | -1.979195 |
| H | 5.045899 | -4.900495 | 0.134937 | C | 1.520699 | -0.839314 | -1.782719 |
| H | 4.932420 | -3.971142 | -1.358389 | N | 0.732489 | -1.831036 | -2.208375 |
| H | 6.184452 | -3.565854 | -0.153874 | H | 1.168525 | -2.667569 | -2.564204 |
| C | 2.763039 | -3.198896 | 0.181368 | H | -0.264259 | -1.804483 | -2.007097 |
| O | 2.303313 | -4.137627 | -0.467633 | N | 0.995971 | 0.216183 | -1.132072 |
| N | 1.925061 | -2.311290 | 0.820752 | C | 1.817156 | 1.170857 | -0.655785 |
| H | 0.890695 | -2.456822 | 0.700282 | H | 1.313082 | 1.989954 | -0.148326 |
| C | 2.278195 | -1.172765 | 1.497133 | N | 3.140701 | 1.227775 | -0.723662 |
| O | 1.464297 | -0.422206 | 2.008516 | C | 3.639266 | 0.187874 | -1.412662 |
| C | -7.882400 | -0.991620 | 1.047325 | P | 9.353985 | 1.400590 | 1.140249 |
| H | -8.963339 | -1.124934 | 0.941381 | O | 9.853441 | 2.858413 | 1.569267 |
| C | -7.065974 | -1.826085 | 0.060056 | O | 10.307402 | 0.290500 | 1.222546 |
| H | -7.608188 | -2.764013 | -0.124954 | O | 8.072900 | 1.230768 | 2.076246 |
| H | -6.873263 | -1.312332 | -0.882930 | C | 7.074397 | 2.261327 | 2.091494 |
| O | -7.563490 | 0.409086 | 0.959317 | H | 7.393634 | 3.049549 | 2.781425 |
| P | -7.991743 | 1.252218 | -0.319979 | H | 6.960442 | 2.691631 | 1.090883 |
| O | -9.518600 | 1.612562 | 0.054689 | C | 5.763728 | 1.688562 | 2.561564 |
| O | -7.847099 | 0.667941 | -1.663497 | H | 5.073502 | 2.535027 | 2.715479 |
| O | -7.161336 | 2.591999 | -0.164579 | O | 5.223693 | 0.789297 | 1.606643 |
| C | -6.692742 | 3.140601 | 1.077160 | C | 4.072418 | 0.261344 | 2.251119 |
| H | -7.553928 | 3.549416 | 1.617920 | H | 3.241322 | 0.964646 | 2.152262 |
| H | -6.201894 | 2.355932 | 1.657195 | C | 5.785767 | 0.865686 | 3.858154 |
| C | -5.689435 | 4.247191 | 0.780225 | H | 6.652588 | 0.194902 | 3.832186 |
| H | -5.664796 | 4.903201 | 1.658580 | C | 4.479774 | 0.068395 | 3.730570 |
| O | -4.373376 | 3.755058 | 0.582222 | H | 4.608937 | -0.989747 | 3.966681 |
| C | -4.017801 | 3.740740 | -0.798389 | H | 3.726192 | 0.485390 | 4.401772 |
| H | -3.138010 | 4.375488 | -0.917031 | O | 5.790141 | 1.673055 | 5.012554 |
| N | -3.576945 | 2.421210 | -1.227051 | N | -4.801134 | -2.930552 | 0.465549 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -4.521733 | 1.324868 | -1.200618 | C | -4.893583 | -4.131641 | -0.219781 |
| C | -3.995526 | 0.162104 | -2.054790 | H | -5.859823 | -4.559759 | -0.450344 |
| C | -4.076627 | 0.545544 | -3.538464 | N | -3.737763 | -4.651446 | -0.532057 |
| H | -3.532661 | 1.469190 | -3.749798 | C | -2.819732 | -3.754323 | -0.022832 |
| H | -3.660154 | -0.263481 | -4.143762 | C | -1.408311 | -3.697717 | -0.060778 |
| H | -5.131575 | 0.673403 | -3.795279 | N | -0.642667 | -4.616005 | -0.660019 |
| C | -2.548334 | -0.157247 | -1.730788 | H | -1.081321 | -5.428715 | -1.060789 |
| O | -2.131059 | -1.298060 | -1.915667 | H | 0.374087 | -4.535372 | -0.614347 |
| N | -1.776379 | 0.869146 | -1.322556 | N | -0.811859 | -2.643043 | 0.527661 |
| H | -0.759149 | 0.679540 | -1.177728 | C | -1.547633 | -1.664194 | 1.063504 |
| C | -2.219152 | 2.166222 | -1.031742 | H | -0.981388 | -0.832697 | 1.480990 |
| O | -1.411343 | 3.008007 | -0.705736 | N | -2.871667 | -1.607267 | 1.130904 |
| C | -5.979246 | 5.083997 | -0.476486 | C | -3.455672 | -2.680631 | 0.585004 |
| H | -7.046802 | 5.175118 | -0.688328 | H | -5.468791 | 1.637265 | -1.648673 |
| C | -5.224735 | 4.306653 | -1.560894 | O | -4.915639 | 0.958738 | 0.102429 |
| H | -5.859792 | 3.520489 | -1.969749 | O | -3.783910 | 0.930109 | 0.959841 |
| H | -4.915182 | 4.969796 | -2.370238 | O | -4.764955 | -0.983310 | -1.805553 |
| O | -5.484665 | 6.399792 | -0.324995 | H | -4.174680 | -1.733472 | -1.988331 |
| O | 8.157265 | -1.177570 | -3.339705 | H | 8.361420 | -1.759503 | -4.078970 |
| C | 8.556740 | 0.141333 | -3.668573 | H | -4.571927 | 6.336193 | -0.014907 |
| H | 9.648895 | 0.208147 | -3.776970 | H | -8.951117 | -4.256128 | 2.483983 |
| H | 8.088376 | 0.484089 | -4.599659 | H | 6.701960 | 1.826308 | 5.279726 |
| C | 8.115590 | 1.067195 | -2.549469 | H | -10.036224 | 1.745773 | -0.750127 |
| H | 8.569413 | 2.053299 | -2.702220 | H | 10.734076 | 3.063034 | 1.230034 |
| O | 6.700867 | 1.200594 | -2.563820 | H | -3.638403 | -0.041764 | 1.098656 |

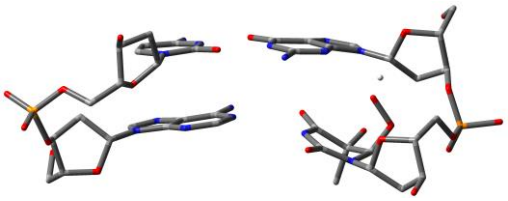


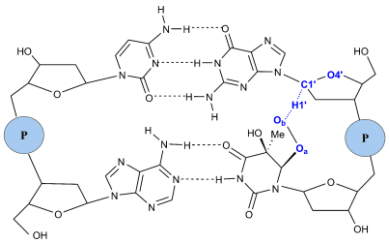
ds - 5' G T* 3' - Reactant

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| O | -9.009631 | -3.534033 | 1.633326 | C | 7.323324 | -0.472426 | -0.762034 |
| C | -8.727479 | -2.621076 | 2.676025 | H | 7.259967 | -1.532402 | -1.015782 |
| H | -9.622088 | -2.044824 | 2.956588 | H | 7.262765 | -0.344685 | 0.318435 |
| H | -8.343371 | -3.128202 | 3.570560 | O | 8.987411 | 1.312840 | -0.665088 |
| C | -7.659219 | -1.665277 | 2.182473 | N | 5.024738 | -0.464276 | -1.698144 |
| H | -7.580607 | -0.811534 | 2.869195 | C | 4.948542 | -1.684743 | -2.337172 |
| O | -6.421650 | -2.358709 | 2.110496 | H | 5.845422 | -2.150928 | -2.725658 |
| C | -5.808845 | -2.003567 | 0.871677 | N | 3.732284 | -2.148766 | -2.437652 |
| H | -5.333343 | -1.022961 | 0.958736 | C | 2.957427 | -1.168145 | -1.850809 |
| N | 3.900885 | -0.752431 | 1.754271 | C | 1.562628 | -1.067047 | -1.648718 |
| C | 4.765822 | -1.710539 | 1.327581 | N | 0.724191 | -2.043226 | -1.996600 |
| H | 5.817404 | -1.476585 | 1.446254 | H | 1.094639 | -2.903122 | -2.367322 |
| C | 4.317728 | -2.862873 | 0.779240 | H | -0.276175 | -1.923064 | -1.863728 |
| C | 2.890403 | -3.014332 | 0.661299 | N | 1.092159 | 0.057512 | -1.071214 |
| N | 2.050679 | -2.110615 | 1.160506 | C | 1.964841 | 1.001915 | -0.678110 |
| H | 0.179118 | -2.253958 | 0.807258 | H | 1.510464 | 1.874875 | -0.213841 |
| C | 2.507058 | -0.966798 | 1.723444 | N | 3.288632 | 1.001918 | -0.778615 |
| O | 1.776246 | -0.100284 | 2.204388 | C | 3.730461 | -0.110039 | -1.390660 |
| C | -7.952859 | -1.140348 | 0.757809 | P | 9.620827 | 1.150971 | 0.803691 |
| H | -9.004946 | -1.243005 | 0.479403 | O | 10.260126 | 2.599408 | 1.030622 |
| C | -6.984738 | -1.943740 | -0.095396 | O | 10.483671 | -0.020918 | 0.976749 |
| H | -7.406135 | -2.944248 | -0.233140 | O | 8.383674 | 1.202675 | 1.810183 |
| H | -6.750670 | -1.474210 | -1.048794 | C | 7.471156 | 2.307847 | 1.744682 |
| O | -7.589551 | 0.271664 | 0.742254 | H | 7.878703 | 3.138002 | 2.330116 |
| P | -7.918903 | 1.145194 | -0.542097 | H | 7.347461 | 2.633434 | 0.706622 |
| O | -9.458250 | 1.535108 | -0.275235 | C | 6.141633 | 1.898196 | 2.318347 |
| O | -7.665287 | 0.600746 | -1.885452 | H | 5.513514 | 2.804009 | 2.365236 |
| O | -7.076017 | 2.478130 | -0.316470 | O | 5.522310 | 0.913871 | 1.507939 |
| C | -6.782638 | 3.095269 | 0.941223 | C | 4.359454 | 0.540416 | 2.235649 |
| H | -7.708460 | 3.510013 | 1.355974 | H | 3.548875 | 1.240533 | 2.020835 |
| H | -6.360331 | 2.352387 | 1.623774 | C | 6.143128 | 1.260324 | 3.713951 |
| C | -5.772623 | 4.211991 | 0.707532 | H | 6.948798 | 0.516851 | 3.757925 |
| H | -5.803476 | 4.863236 | 1.589367 | C | 4.769382 | 0.576355 | 3.727325 |
| O | -4.443077 | 3.723155 | 0.582324 | H | 4.798319 | -0.427452 | 4.155116 |
| C | -3.970175 | 3.778878 | -0.761724 | H | 4.069448 | 1.180113 | 4.309191 |
| H | -3.091260 | 4.425079 | -0.784385 | O | 6.254887 | 2.209268 | 4.748275 |
| N | -3.482343 | 2.475229 | -1.204261 | N | -4.746138 | -2.913452 | 0.549225 |
| C | -4.404450 | 1.389019 | -1.202412 | C | -4.770307 | -4.193773 | 0.019325 |
| C | -3.903953 | 0.209270 | -2.032991 | H | -5.705461 | -4.706155 | -0.160524 |
| C | -3.988091 | 0.572837 | -3.521177 | N | -3.583615 | -4.677930 | -0.213513 |
| H | -3.427310 | 1.482124 | -3.752000 | C | -2.715181 | -3.678111 | 0.187037 |

| | | | |
|---|---|---|---|
| H | -3.588913 | -0.256902 | -4.108981 |
| H | -5.042916 | 0.711319 | -3.773967 |
| C | -2.460017 | -0.109900 | -1.692762 |
| O | -2.048048 | -1.249200 | -1.867432 |
| N | -1.686021 | 0.921891 | -1.282360 |
| H | -0.690757 | 0.697190 | -1.080787 |
| C | -2.123030 | 2.211418 | -0.971431 |
| O | -1.334715 | 3.049213 | -0.597414 |
| C | -5.997774 | 5.059673 | -0.556813 |
| H | -7.049098 | 5.102313 | -0.849887 |
| C | -5.128393 | 4.344640 | -1.597315 |
| H | -5.697954 | 3.555498 | -2.090787 |
| H | -4.775018 | 5.046572 | -2.354329 |
| O | -5.587538 | 6.395741 | -0.347158 |
| O | 8.109128 | -1.817846 | -3.315476 |
| C | 8.538526 | -0.557562 | -3.801548 |
| H | 9.626054 | -0.546284 | -3.958788 |
| H | 8.042269 | -0.299211 | -4.744586 |
| C | 8.179181 | 0.497541 | -2.771554 |
| H | 8.658257 | 1.444518 | -3.047201 |
| O | 6.770982 | 0.681714 | -2.742020 |
| C | 6.223281 | 0.312636 | -1.485425 |
| H | 5.905741 | 1.198487 | -0.926483 |
| C | 8.600529 | 0.100719 | -1.351956 |
| H | 9.439178 | -0.599442 | -1.331876 |
| C | -1.281764 | -3.585838 | 0.177356 |
| N | -0.843230 | -2.371517 | 0.725035 |
| C | -1.646081 | -1.345382 | 1.146561 |
| N | -2.961685 | -1.409188 | 1.131675 |
| C | -3.420016 | -2.583119 | 0.666237 |
| H | -5.373958 | 1.691936 | -1.595108 |
| O | -4.745241 | 0.975841 | 0.162503 |
| O | -3.771639 | 1.143828 | 1.012343 |
| O | -4.688281 | -0.915087 | -1.760736 |
| H | -4.091758 | -1.681973 | -1.811388 |
| H | 8.292268 | -2.487053 | -3.982814 |
| H | -4.687673 | 6.381236 | 0.003189 |
| H | -9.549082 | -4.249701 | 1.982716 |
| H | 7.185775 | 2.323766 | 4.964486 |
| H | -9.916525 | 1.684548 | -1.112781 |
| H | 11.143182 | 2.678542 | 0.647838 |
| O | -0.453739 | -4.400252 | -0.237700 |
| N | -1.034368 | -0.217856 | 1.553961 |
| H | -1.641494 | 0.486044 | 1.943404 |
| H | -0.034603 | -0.189750 | 1.757787 |
| N | 2.367833 | -4.076210 | 0.048854 |
| H | 1.346115 | -4.184058 | -0.034981 |
| H | 2.974093 | -4.742617 | -0.398828 |
| H | 5.001280 | -3.619212 | 0.418300 |



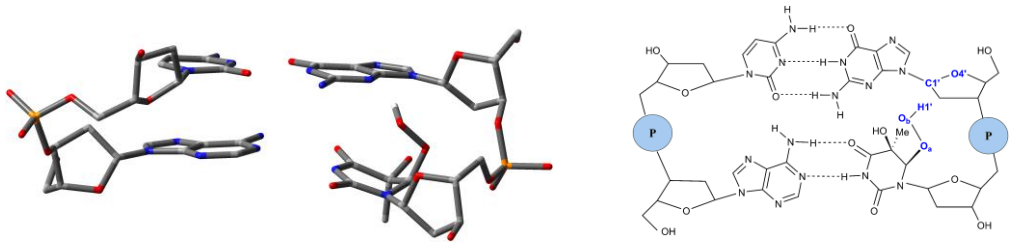


ds - 5' G T* 3' - TS

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z | | | | |
|---|---|---|---|---|---|---|---|
| O | -8.126594 | -3.808093 | 1.335628 | C | 7.240397 | -0.345440 | -0.913869 |
| C | -8.253722 | -2.904729 | 2.415463 | H | 7.183283 | -1.393822 | -1.213850 |
| H | -9.308294 | -2.663064 | 2.616131 | H | 7.260460 | -0.270253 | 0.173045 |
| H | -7.807671 | -3.305904 | 3.333890 | O | 8.876741 | 1.467936 | -0.842309 |
| C | -7.515931 | -1.626110 | 2.062317 | N | 4.883786 | -0.369896 | -1.688108 |
| H | -7.699937 | -0.872487 | 2.834467 | C | 4.807904 | -1.553139 | -2.393842 |
| O | -6.116557 | -1.900015 | 2.010722 | H | 5.693362 | -1.964537 | -2.861937 |
| C | -5.641078 | -1.780820 | 0.710851 | N | 3.603632 | -2.054223 | -2.450159 |
| H | -5.044813 | -0.662640 | 0.630041 | C | 2.835072 | -1.138635 | -1.759535 |
| N | 4.040169 | -0.826153 | 1.828390 | C | 1.452080 | -1.096554 | -1.475651 |
| C | 4.893508 | -1.737600 | 1.291302 | N | 0.623448 | -2.071463 | -1.851546 |
| H | 5.945065 | -1.481351 | 1.346263 | H | 0.997028 | -2.892049 | -2.299365 |
| C | 4.433027 | -2.870985 | 0.714084 | H | -0.369144 | -2.002706 | -1.647194 |
| C | 3.005177 | -3.052889 | 0.688240 | N | 0.980106 | -0.031453 | -0.797584 |
| N | 2.182574 | -2.195312 | 1.288283 | C | 1.843772 | 0.917246 | -0.396805 |
| H | 0.296686 | -2.335874 | 1.066101 | H | 1.391181 | 1.742375 | 0.149374 |
| C | 2.652809 | -1.072204 | 1.878838 | N | 3.158927 | 0.972949 | -0.576643 |
| O | 1.938944 | -0.249544 | 2.454318 | C | 3.599697 | -0.082194 | -1.281836 |
| C | -7.875401 | -1.063144 | 0.682690 | P | 9.627419 | 1.234668 | 0.559932 |
| H | -8.908568 | -1.277401 | 0.392345 | O | 10.261209 | 2.680096 | 0.820352 |
| C | -6.831050 | -1.691669 | -0.229750 | O | 10.516965 | 0.070453 | 0.596737 |
| H | -7.168169 | -2.692111 | -0.513794 | O | 8.473854 | 1.207350 | 1.661990 |
| H | -6.619044 | -1.095000 | -1.117009 | C | 7.546017 | 2.299703 | 1.731407 |
| O | -7.681839 | 0.359048 | 0.784668 | H | 7.988512 | 3.101987 | 2.331009 |
| P | -8.144576 | 1.346880 | -0.380474 | H | 7.337560 | 2.681643 | 0.726135 |
| O | -9.727884 | 1.451216 | -0.095508 | C | 6.270095 | 1.834034 | 2.379933 |
| O | -7.871258 | 1.010161 | -1.788891 | H | 5.637861 | 2.724547 | 2.535477 |
| O | -7.549540 | 2.733029 | 0.108425 | O | 5.600798 | 0.893542 | 1.556931 |
| C | -6.705686 | 2.954009 | 1.253378 | C | 4.500697 | 0.453521 | 2.343108 |
| H | -7.359034 | 3.289701 | 2.064138 | H | 3.660761 | 1.140192 | 2.218556 |
| H | -6.194742 | 2.031328 | 1.536796 | C | 6.385174 | 1.104075 | 3.723666 |
| C | -5.657399 | 4.029548 | 0.955813 | H | 7.185394 | 0.357452 | 3.645655 |
| H | -5.525679 | 4.621257 | 1.869409 | C | 5.010976 | 0.426391 | 3.803780 |
| O | -4.385252 | 3.478594 | 0.628840 | H | 5.057356 | -0.591964 | 4.193118 |
| C | -4.095721 | 3.630622 | -0.761547 | H | 4.358608 | 1.014900 | 4.452479 |
| H | -3.270412 | 4.340630 | -0.858394 | O | 6.589758 | 1.976539 | 4.808634 |
| N | -3.585382 | 2.378891 | -1.306272 | N | -4.612697 | -2.727257 | 0.435895 |
| C | -4.547291 | 1.347270 | -1.634061 | C | -4.652598 | -3.941740 | -0.243552 |
| C | -3.861864 | 0.145011 | -2.294204 | H | -5.586580 | -4.347197 | -0.606704 |
| C | -3.496057 | 0.511914 | -3.741199 | N | -3.483702 | -4.499837 | -0.353880 |
| H | -2.878189 | 1.412284 | -3.785390 | C | -2.615662 | -3.634631 | 0.286461 |

| | | | |
|---|---|---|---|
| H | -2.952733 | -0.320406 | -4.194452 |
| H | -4.420623 | 0.675363 | -4.299738 |
| C | -2.568945 | -0.237858 | -1.599879 |
| O | -2.189846 | -1.400892 | -1.652917 |
| N | -1.844298 | 0.769196 | -1.067831 |
| H | -0.886176 | 0.547438 | -0.742996 |
| C | -2.300064 | 2.069874 | -0.849443 |
| O | -1.569864 | 2.883236 | -0.327769 |
| C | -5.977776 | 4.964398 | -0.220008 |
| H | -7.046600 | 5.145135 | -0.343017 |
| C | -5.374839 | 4.183642 | -1.392480 |
| H | -6.073336 | 3.396062 | -1.680770 |
| H | -5.170671 | 4.829606 | -2.247559 |
| O | -5.364570 | 6.225652 | -0.046499 |
| O | 7.890116 | -1.531338 | -3.585935 |
| C | 8.225617 | -0.230400 | -4.038079 |
| H | 9.294109 | -0.164107 | -4.288446 |
| H | 7.637347 | 0.053921 | -4.919097 |
| C | 7.919058 | 0.754715 | -2.924559 |
| H | 8.352390 | 1.728947 | -3.179336 |
| O | 6.513137 | 0.897478 | -2.779630 |
| C | 6.067422 | 0.439291 | -1.512364 |
| H | 5.760945 | 1.280733 | -0.883273 |
| C | 8.456692 | 0.289279 | -1.567163 |
| H | 9.305360 | -0.393435 | -1.652131 |
| C | -1.183430 | -3.604236 | 0.358941 |
| N | -0.728112 | -2.433483 | 0.982357 |
| C | -1.515557 | -1.412270 | 1.447113 |
| N | -2.832411 | -1.436462 | 1.397653 |
| C | -3.297966 | -2.534185 | 0.784076 |
| H | -5.288600 | 1.730343 | -2.340061 |
| O | -5.351305 | 1.033076 | -0.518211 |
| O | -4.568076 | 0.512576 | 0.492955 |
| O | -4.727775 | -0.952871 | -2.267868 |
| H | -4.156573 | -1.737418 | -2.196534 |
| H | 8.026812 | -2.155145 | -4.306410 |
| H | -4.453703 | 6.079425 | 0.238928 |
| H | -8.350225 | -4.692733 | 1.640132 |
| H | 7.536503 | 2.086153 | 4.944172 |
| H | -10.202380 | 1.524778 | -0.933543 |
| H | 11.095874 | 2.809836 | 0.352276 |
| O | -0.369420 | -4.422943 | -0.075026 |
| N | -0.889834 | -0.334946 | 1.947404 |
| H | -1.484742 | 0.403147 | 2.286887 |
| H | 0.116886 | -0.307295 | 2.111093 |
| N | 2.463047 | -4.097919 | 0.064524 |
| H | 1.439275 | -4.213869 | 0.035856 |
| H | 3.047801 | -4.720147 | -0.467517 |
| H | 5.105943 | -3.590861 | 0.268632 |

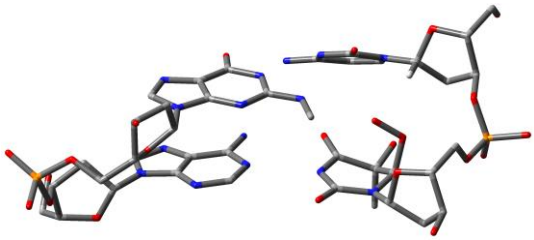


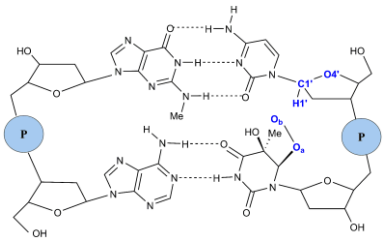
ds - 5' G T* 3' - Product

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| O | -8.482992 | -3.597470 | 1.849215 | H | 7.233989 | -1.553451 | -0.927262 |
| C | -8.366125 | -2.577316 | 2.820319 | H | 7.227213 | -0.288374 | 0.335670 |
| H | -9.345393 | -2.140229 | 3.067916 | O | 8.949407 | 1.315346 | -0.735309 |
| H | -7.905033 | -2.946840 | 3.744996 | N | 5.008103 | -0.522838 | -1.688862 |
| C | -7.476721 | -1.490591 | 2.248564 | C | 4.929397 | -1.774075 | -2.264351 |
| H | -7.464469 | -0.626158 | 2.919405 | H | 5.824596 | -2.256991 | -2.636417 |
| O | -6.147251 | -1.999715 | 2.131494 | N | 3.713605 | -2.246051 | -2.328049 |
| C | -5.803440 | -2.067513 | 0.806648 | C | 2.942157 | -1.240630 | -1.779693 |
| N | 3.877709 | -0.674649 | 1.778855 | C | 1.549794 | -1.134066 | -1.563795 |
| C | 4.758029 | -1.638211 | 1.398826 | N | 0.708945 | -2.126157 | -1.858049 |
| H | 5.805593 | -1.380879 | 1.501332 | H | 1.071837 | -2.984844 | -2.238922 |
| C | 4.328059 | -2.823577 | 0.910351 | H | -0.292978 | -1.986205 | -1.751709 |
| C | 2.904066 | -3.004345 | 0.803391 | N | 1.082701 | 0.010192 | -1.023584 |
| N | 2.049629 | -2.094842 | 1.267367 | C | 1.956095 | 0.977847 | -0.695474 |
| H | 0.187298 | -2.299696 | 0.958472 | H | 1.504654 | 1.870608 | -0.266127 |
| C | 2.489478 | -0.914154 | 1.764298 | N | 3.278019 | 0.981243 | -0.821094 |
| O | 1.744564 | -0.034810 | 2.199675 | C | 3.716720 | -0.157867 | -1.382541 |
| C | -7.895972 | -1.053927 | 0.835507 | P | 9.567565 | 1.256301 | 0.747752 |
| H | -8.964581 | -1.206307 | 0.655468 | O | 10.188352 | 2.723703 | 0.887002 |
| C | -6.995621 | -1.890114 | -0.074172 | O | 10.440584 | 0.107537 | 1.004824 |
| H | -7.502439 | -2.843279 | -0.277517 | O | 8.319160 | 1.357737 | 1.736580 |
| H | -6.750303 | -1.388172 | -1.010315 | C | 7.391651 | 2.442683 | 1.591170 |
| O | -7.596844 | 0.353630 | 0.747518 | H | 7.784356 | 3.318734 | 2.117948 |
| P | -7.944706 | 1.172264 | -0.570699 | H | 7.268368 | 2.691720 | 0.531703 |
| O | -9.517050 | 1.454508 | -0.344691 | C | 6.064836 | 2.050930 | 2.184855 |
| O | -7.653913 | 0.598185 | -1.895347 | H | 5.416570 | 2.942687 | 2.156552 |
| O | -7.208603 | 2.559432 | -0.349598 | O | 5.477893 | 0.994775 | 1.443971 |
| C | -6.754823 | 3.085136 | 0.906255 | C | 4.316324 | 0.651250 | 2.185973 |
| H | -7.622793 | 3.491165 | 1.437644 | H | 3.498089 | 1.326265 | 1.925935 |
| H | -6.279377 | 2.292036 | 1.487027 | C | 6.062988 | 1.522652 | 3.626471 |
| C | -5.742627 | 4.195591 | 0.649130 | H | 6.896533 | 0.819737 | 3.745592 |
| H | -5.751823 | 4.846764 | 1.531402 | C | 4.717106 | 0.783513 | 3.673134 |
| O | -4.414357 | 3.716469 | 0.496318 | H | 4.788941 | -0.194843 | 4.151978 |
| C | -4.008074 | 3.713876 | -0.869810 | H | 3.988711 | 1.384588 | 4.221102 |
| H | -3.131788 | 4.359183 | -0.951965 | O | 6.114402 | 2.554908 | 4.582769 |
| N | -3.535609 | 2.399537 | -1.288720 | N | -4.738529 | -2.939179 | 0.522904 |
| C | -4.483883 | 1.304825 | -1.325635 | C | -4.742083 | -4.208792 | -0.053332 |
| C | -3.898308 | 0.114702 | -2.103019 | H | -5.673818 | -4.695959 | -0.306244 |
| C | -3.865815 | 0.456361 | -3.599241 | N | -3.549730 | -4.697895 | -0.227723 |
| H | -3.312355 | 1.378322 | -3.793654 | C | -2.697424 | -3.724567 | 0.260780 |
| H | -3.400741 | -0.366552 | -4.147452 | C | -1.263644 | -3.639779 | 0.307394 |

| | | | |
|---|---|---|---|
| H | -4.898780 | 0.568830 | -3.938717 |
| C | -2.481895 | -0.195843 | -1.665533 |
| O | -2.057823 | -1.342875 | -1.770861 |
| N | -1.733133 | 0.847404 | -1.252067 |
| H | -0.741789 | 0.650145 | -1.028939 |
| C | -2.198563 | 2.142849 | -0.987770 |
| O | -1.417524 | 2.979054 | -0.588260 |
| C | -5.989308 | 5.039783 | -0.611269 |
| H | -7.048364 | 5.127770 | -0.862627 |
| C | -5.192168 | 4.272642 | -1.672272 |
| H | -5.808942 | 3.484484 | -2.104446 |
| H | -4.860187 | 4.941282 | -2.468029 |
| O | -5.505860 | 6.356577 | -0.432864 |
| O | 8.117060 | -1.998331 | -3.169677 |
| C | 8.547042 | -0.774853 | -3.741667 |
| H | 9.636040 | -0.771377 | -3.892589 |
| H | 8.056278 | -0.586514 | -4.704620 |
| C | 8.178690 | 0.351210 | -2.792702 |
| H | 8.661541 | 1.275486 | -3.130589 |
| O | 6.769632 | 0.538755 | -2.790762 |
| C | 6.209295 | 0.260447 | -1.517576 |
| H | 5.891639 | 1.183489 | -1.022543 |
| C | 8.582096 | 0.056259 | -1.343905 |
| H | 9.424359 | -0.634702 | -1.262169 |
| C | 7.298520 | -0.480556 | -0.734431 |
| N | -0.835799 | -2.426811 | 0.873701 |
| C | -1.640598 | -1.391753 | 1.252657 |
| N | -2.962210 | -1.469725 | 1.214265 |
| C | -3.417393 | -2.634691 | 0.718379 |
| H | -5.389459 | 1.606346 | -1.858702 |
| O | -4.986680 | 0.974331 | -0.053275 |
| O | -3.935773 | 0.940854 | 0.897775 |
| O | -4.686607 | -1.019866 | -1.878208 |
| H | -4.083893 | -1.779571 | -1.944788 |
| H | 8.305342 | -2.713314 | -3.786349 |
| H | -4.606136 | 6.294665 | -0.086540 |
| H | -8.887081 | -4.370895 | 2.254162 |
| H | 7.034032 | 2.718736 | 4.814477 |
| H | -9.964705 | 1.535319 | -1.196802 |
| H | 11.075932 | 2.787023 | 0.511355 |
| O | -0.428161 | -4.456251 | -0.079204 |
| N | -1.050952 | -0.262411 | 1.662589 |
| H | -1.648853 | 0.510229 | 1.913477 |
| H | -0.038069 | -0.179726 | 1.776928 |
| N | 2.400674 | -4.102338 | 0.240755 |
| H | 1.383541 | -4.221309 | 0.142853 |
| H | 3.018066 | -4.765127 | -0.197230 |
| H | 5.022751 | -3.585287 | 0.583866 |
| H | -3.789040 | -0.039724 | 1.036050 |



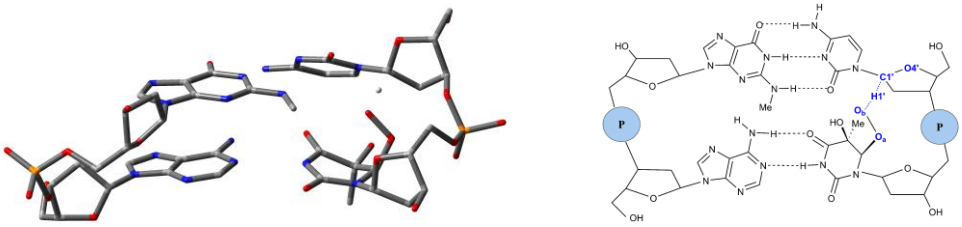


ds - 5' $C_a$ T* 3' - Reactant

## Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z | | | | |
|---|---|---|---|---|---|---|---|
| O | -9.155654 | -2.929097 | 1.876554 | H | 7.119233 | -0.277180 | 0.550735 |
| C | -8.805902 | -1.992838 | 2.877083 | O | 8.974008 | 0.970026 | -0.778558 |
| H | -9.640566 | -1.311126 | 3.098380 | N | 5.063030 | -1.042746 | -1.519552 |
| H | -8.499139 | -2.485233 | 3.808485 | C | 4.997329 | -2.399968 | -1.763386 |
| C | -7.634121 | -1.184764 | 2.360366 | H | 5.906722 | -2.969449 | -1.905674 |
| H | -7.471612 | -0.304996 | 2.997674 | N | 3.779794 | -2.862965 | -1.829384 |
| O | -6.479091 | -2.015017 | 2.354091 | C | 2.995818 | -1.750612 | -1.623252 |
| C | -5.770184 | -1.685206 | 1.167017 | C | 1.598314 | -1.590385 | -1.547806 |
| H | -5.281469 | -0.718237 | 1.301647 | N | 0.754844 | -2.630964 | -1.667109 |
| N | -4.700893 | -2.627588 | 0.910043 | H | 1.153806 | -3.545965 | -1.514593 |
| C | -4.825730 | -3.670157 | 0.044766 | H | -0.227700 | -2.493079 | -1.450675 |
| H | -5.815706 | -3.841548 | -0.359558 | N | 1.123427 | -0.344800 | -1.372672 |
| C | -3.767915 | -4.438452 | -0.305472 | C | 1.986258 | 0.683111 | -1.235250 |
| C | -2.496236 | -4.092682 | 0.274994 | H | 1.513870 | 1.653799 | -1.100026 |
| N | -2.382836 | -3.108081 | 1.151282 | N | 3.307917 | 0.643240 | -1.238803 |
| C | -3.447213 | -2.348821 | 1.517914 | C | 3.762958 | -0.605496 | -1.439518 |
| O | -3.364487 | -1.429902 | 2.321742 | P | 9.507412 | 1.307534 | 0.698055 |
| C | -7.843303 | -0.714564 | 0.898104 | O | 10.132907 | 2.765252 | 0.478029 |
| H | -8.884199 | -0.802202 | 0.577715 | O | 10.359377 | 0.277843 | 1.299989 |
| C | -6.878402 | -1.596511 | 0.126648 | O | 8.206704 | 1.661466 | 1.550839 |
| H | -7.364552 | -2.569649 | 0.009451 | C | 7.315441 | 2.684254 | 1.082316 |
| H | -6.577486 | -1.187745 | -0.836544 | H | 7.705851 | 3.658226 | 1.394780 |
| O | -7.425691 | 0.674244 | 0.809975 | H | 7.252516 | 2.658997 | -0.010981 |
| P | -7.734030 | 1.458304 | -0.540317 | C | 5.949526 | 2.475719 | 1.681507 |
| O | -9.155057 | 2.129106 | -0.194357 | H | 5.356862 | 3.381670 | 1.467466 |
| O | -7.709075 | 0.730597 | -1.818433 | O | 5.321449 | 1.333245 | 1.126808 |
| O | -6.674912 | 2.644306 | -0.534036 | C | 4.133714 | 1.155287 | 1.889972 |
| C | -6.169732 | 3.289486 | 0.639948 | H | 3.317449 | 1.741492 | 1.452177 |
| H | -6.970774 | 3.882893 | 1.095360 | C | 5.885175 | 2.215875 | 3.190896 |
| H | -5.809716 | 2.534990 | 1.345633 | H | 6.640318 | 1.461997 | 3.444986 |
| C | -5.019159 | 4.186419 | 0.214921 | C | 4.473637 | 1.635825 | 3.323052 |
| H | -4.813701 | 4.882743 | 1.036888 | H | 4.407583 | 0.817570 | 4.041934 |
| O | -3.843295 | 3.424517 | -0.031094 | H | 3.792486 | 2.431184 | 3.636964 |
| C | -3.521435 | 3.384368 | -1.423223 | O | 6.038721 | 3.386573 | 3.959045 |
| H | -2.596472 | 3.942477 | -1.577917 | N | 3.724619 | -0.220442 | 1.788419 |
| N | -3.195236 | 2.020246 | -1.815995 | C | 4.497443 | -1.365344 | 1.711944 |
| C | -4.220630 | 1.025414 | -1.775846 | H | 5.575722 | -1.313244 | 1.759037 |
| C | -3.764081 | -0.287584 | -2.419351 | N | 3.790839 | -2.452238 | 1.579080 |
| C | -3.633175 | -0.106595 | -3.936105 | C | 2.482625 | -2.014751 | 1.587991 |
| H | -2.958660 | 0.712360 | -4.193900 | C | 1.243045 | -2.716005 | 1.414459 |
| H | -3.253878 | -1.034681 | -4.369818 | N | 0.154248 | -1.843465 | 1.503442 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -4.626137 | 0.091021 | -4.346992 | C | 0.215900 | -0.478079 | 1.642836 |
| C | -2.403338 | -0.677618 | -1.857123 | N | 1.349235 | 0.187137 | 1.764412 |
| O | -2.149980 | -1.858064 | -1.655638 | C | 2.420959 | -0.631214 | 1.715957 |
| N | -1.511859 | 0.327268 | -1.717865 | H | -5.146809 | 1.366936 | -2.243717 |
| H | -0.498547 | 0.076673 | -1.492909 | O | -4.659356 | 0.755606 | -0.407494 |
| C | -1.842967 | 1.669210 | -1.626774 | O | -3.644805 | 0.538825 | 0.376007 |
| O | -0.981941 | 2.500266 | -1.429724 | O | -4.682594 | -1.298382 | -2.122593 |
| C | -5.263644 | 4.978869 | -1.081986 | H | -4.147908 | -2.090329 | -1.934434 |
| H | -6.322408 | 5.195791 | -1.240734 | H | 8.432737 | -3.720728 | -2.681994 |
| C | -4.694430 | 4.041834 | -2.153672 | H | -3.679214 | 6.079489 | -0.817130 |
| H | -5.453176 | 3.318363 | -2.452304 | H | -9.795244 | -3.549448 | 2.239308 |
| H | -4.364362 | 4.602336 | -3.029449 | H | 6.972829 | 3.496763 | 4.163695 |
| O | -4.604124 | 6.226917 | -1.052423 | H | -9.663453 | 2.280323 | -1.002065 |
| O | 8.227171 | -2.863817 | -2.294504 | H | 11.032969 | 2.729766 | 0.129578 |
| C | 8.725116 | -1.841720 | -3.138739 | H | -3.875771 | -5.260675 | -0.999671 |
| H | 9.821731 | -1.885618 | -3.208115 | N | -1.380826 | -4.750612 | -0.057527 |
| H | 8.304351 | -1.913067 | -4.149680 | H | -0.503087 | -4.524741 | 0.432799 |
| C | 8.323309 | -0.500369 | -2.551743 | H | -1.425305 | -5.547350 | -0.669755 |
| H | 8.860117 | 0.295264 | -3.081341 | O | 1.058092 | -3.913065 | 1.179934 |
| O | 6.926293 | -0.297905 | -2.710300 | H | -0.776670 | -2.293959 | 1.424756 |
| C | 6.261372 | -0.240841 | -1.455795 | N | -0.965233 | 0.175241 | 1.611040 |
| H | 5.924499 | 0.778930 | -1.244332 | H | -1.803624 | -0.350198 | 1.859872 |
| C | 8.610274 | -0.403815 | -1.050537 | C | -1.000612 | 1.617151 | 1.762590 |
| H | 9.424086 | -1.055639 | -0.723860 | H | -2.008489 | 1.963373 | 1.525015 |
| C | 7.270796 | -0.748621 | -0.420897 | H | -0.728863 | 1.932851 | 2.776961 |
| H | 7.193567 | -1.833645 | -0.323704 | H | -0.300882 | 2.072088 | 1.059137 |

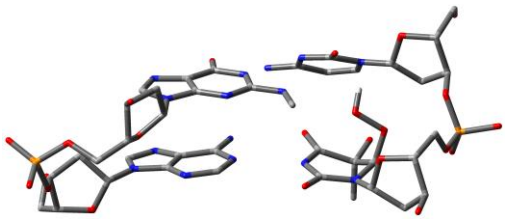


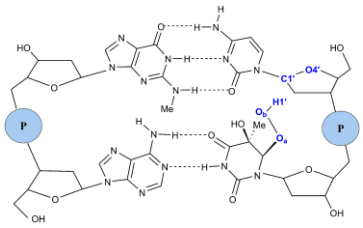
ds - 5' $C_a$ T* 3' - TS

## Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z | | | | |
|---|---|---|---|---|---|---|---|
| O | -8.389197 | -3.254563 | 1.884131 | H | 7.106025 | -0.238079 | 0.500412 |
| C | -8.298145 | -2.226253 | 2.850295 | O | 8.931566 | 1.015754 | -0.869253 |
| H | -9.282666 | -1.783915 | 3.062842 | N | 5.013100 | -0.998433 | -1.530605 |
| H | -7.867239 | -2.589696 | 3.791514 | C | 4.939120 | -2.354990 | -1.775252 |
| C | -7.389061 | -1.142479 | 2.303592 | H | 5.844148 | -2.925865 | -1.938418 |
| H | -7.415460 | -0.271849 | 2.966770 | N | 3.719568 | -2.815693 | -1.814843 |
| O | -6.053293 | -1.641991 | 2.248259 | C | 2.942209 | -1.701930 | -1.589579 |
| C | -5.587620 | -1.642498 | 0.943976 | C | 1.547747 | -1.539274 | -1.475709 |
| H | -4.922265 | -0.587297 | 0.748042 | N | 0.698821 | -2.581029 | -1.575213 |
| N | -4.588254 | -2.660650 | 0.758616 | H | 1.102709 | -3.492410 | -1.410882 |
| C | -4.711304 | -3.707049 | -0.105027 | H | -0.267639 | -2.434866 | -1.298357 |
| H | -5.679617 | -3.832786 | -0.575353 | N | 1.077875 | -0.294871 | -1.285365 |
| C | -3.668582 | -4.530178 | -0.364072 | C | 1.945809 | 0.730915 | -1.171181 |
| C | -2.424391 | -4.243953 | 0.309285 | H | 1.479802 | 1.703351 | -1.025134 |
| N | -2.325705 | -3.267164 | 1.196255 | N | 3.267562 | 0.689948 | -1.207405 |
| C | -3.352749 | -2.419296 | 1.424276 | C | 3.715829 | -0.558581 | -1.420604 |
| O | -3.274449 | -1.440618 | 2.156031 | P | 9.490253 | 1.364108 | 0.595083 |
| C | -7.732000 | -0.718670 | 0.870892 | O | 10.100484 | 2.825112 | 0.356696 |
| H | -8.790532 | -0.855679 | 0.630230 | O | 10.362198 | 0.344585 | 1.185287 |
| C | -6.795596 | -1.573195 | 0.024599 | O | 8.203682 | 1.710795 | 1.471468 |
| H | -7.257222 | -2.559536 | -0.082682 | C | 7.288876 | 2.718103 | 1.015144 |
| H | -6.574982 | -1.135827 | -0.948316 | H | 7.673543 | 3.699844 | 1.310074 |
| O | -7.384882 | 0.672508 | 0.779289 | H | 7.201217 | 2.682326 | -0.076120 |
| P | -7.790870 | 1.535207 | -0.501913 | C | 5.940206 | 2.495886 | 1.648260 |
| O | -9.357307 | 1.795828 | -0.235383 | H | 5.327335 | 3.388796 | 1.437192 |
| O | -7.558480 | 0.990265 | -1.852870 | O | 5.319408 | 1.336480 | 1.121938 |
| O | -7.096027 | 2.922035 | -0.192762 | C | 4.152445 | 1.150944 | 1.914445 |
| C | -6.131435 | 3.214610 | 0.837265 | H | 3.321852 | 1.732649 | 1.497701 |
| H | -6.680916 | 3.713882 | 1.639786 | C | 5.916697 | 2.254727 | 3.162421 |
| H | -5.672779 | 2.295474 | 1.208147 | H | 6.699654 | 1.527969 | 3.409429 |
| C | -5.038968 | 4.144202 | 0.300317 | C | 4.527054 | 1.633624 | 3.337771 |
| H | -4.783886 | 4.852275 | 1.097099 | H | 4.512584 | 0.808190 | 4.050717 |
| O | -3.843623 | 3.447438 | -0.040302 | H | 3.833144 | 2.403958 | 3.682310 |
| C | -3.677656 | 3.369686 | -1.460362 | O | 6.052942 | 3.440632 | 3.910404 |
| H | -2.823853 | 3.992004 | -1.736763 | N | 3.749250 | -0.226997 | 1.822253 |
| N | -3.294102 | 2.018037 | -1.833260 | C | 4.528785 | -1.366949 | 1.732053 |
| C | -4.326297 | 1.003469 | -1.867949 | H | 5.607325 | -1.307598 | 1.763650 |
| C | -3.753723 | -0.334160 | -2.345970 | N | 3.827670 | -2.457967 | 1.606874 |
| C | -3.445686 | -0.248102 | -3.848879 | C | 2.516471 | -2.029495 | 1.634724 |
| H | -2.784315 | 0.588156 | -4.084735 | C | 1.280918 | -2.737958 | 1.465699 |
| H | -2.971526 | -1.178892 | -4.170130 | N | 0.187588 | -1.870294 | 1.557269 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -4.389023 | -0.130858 | -4.387106 | C | 0.241725 | -0.501117 | 1.689166 |
| C | -2.454953 | -0.654274 | -1.631602 | N | 1.372898 | 0.167313 | 1.819639 |
| O | -2.184485 | -1.819406 | -1.359100 | C | 2.447395 | -0.645806 | 1.765828 |
| N | -1.606388 | 0.379236 | -1.465915 | H | -5.123781 | 1.298010 | -2.556556 |
| H | -0.595494 | 0.159877 | -1.244921 | O | -5.029772 | 0.937789 | -0.644906 |
| C | -1.958496 | 1.720518 | -1.542223 | O | -4.235188 | 0.441556 | 0.371528 |
| O | -1.117691 | 2.580071 | -1.375387 | O | -4.668810 | -1.363111 | -2.096986 |
| C | -5.405734 | 4.913639 | -0.978268 | H | -4.115317 | -2.143688 | -1.917485 |
| H | -6.466466 | 5.161064 | -1.035865 | H | 8.363695 | -3.684527 | -2.747780 |
| C | -4.972961 | 3.917159 | -2.059294 | H | -3.771299 | 5.958935 | -0.845040 |
| H | -5.743347 | 3.150923 | -2.164320 | H | -8.840021 | -4.010080 | 2.273773 |
| H | -4.808336 | 4.409032 | -3.018924 | H | 6.987212 | 3.578900 | 4.096374 |
| O | -4.696644 | 6.132069 | -1.060436 | H | -9.835744 | 1.785640 | -1.074457 |
| O | 8.163226 | -2.826918 | -2.359289 | H | 11.000403 | 2.794202 | 0.008104 |
| C | 8.646756 | -1.806598 | -3.213989 | H | -3.766314 | -5.356872 | -1.054676 |
| H | 9.742076 | -1.850580 | -3.301648 | N | -1.320324 | -4.952221 | 0.061992 |
| H | 8.209287 | -1.880435 | -4.217648 | H | -0.449938 | -4.691157 | 0.547332 |
| C | 8.255156 | -0.463536 | -2.624020 | H | -1.332074 | -5.716388 | -0.591465 |
| H | 8.782293 | 0.330230 | -3.166043 | O | 1.100619 | -3.935562 | 1.229500 |
| O | 6.855529 | -0.261645 | -2.757565 | H | -0.731473 | -2.332227 | 1.472210 |
| C | 6.214483 | -0.200125 | -1.490770 | N | -0.936299 | 0.145514 | 1.634755 |
| H | 5.884661 | 0.821141 | -1.275365 | H | -1.786990 | -0.388883 | 1.805418 |
| C | 8.569130 | -0.360936 | -1.128530 | C | -1.003572 | 1.589654 | 1.728441 |
| H | 9.391676 | -1.007849 | -0.814250 | H | -2.018600 | 1.899652 | 1.469866 |
| C | 7.242170 | -0.707915 | -0.474225 | H | -0.751577 | 1.949070 | 2.733062 |
| H | 7.167830 | -1.793179 | -0.377260 | H | -0.310070 | 2.038888 | 1.014759 |



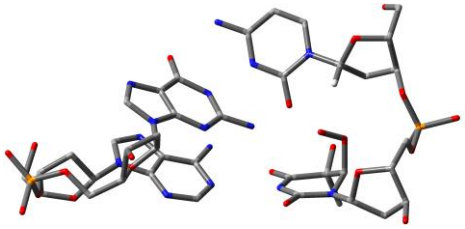


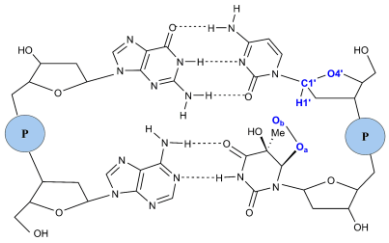
ds - 5'$C_a$ T* 3' - Product

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) | | | | | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | | | |
| O | -8.672505 | -3.180140 | 2.075373 | H | 7.148492 | -0.287931 | 0.504298 |
| C | -8.443695 | -2.132907 | 2.996052 | O | 8.991741 | 1.033800 | -0.775692 |
| H | -9.368978 | -1.581904 | 3.221135 | N | 5.072434 | -0.913794 | -1.583194 |
| H | -8.019345 | -2.502800 | 3.937922 | C | 4.990350 | -2.255370 | -1.898543 |
| C | -7.450562 | -1.174692 | 2.371026 | H | 5.892305 | -2.824238 | -2.084119 |
| H | -7.359913 | -0.276059 | 2.988949 | N | 3.767872 | -2.703304 | -1.973113 |
| O | -6.172064 | -1.813721 | 2.303949 | C | 2.997014 | -1.595993 | -1.698308 |
| C | -5.793041 | -1.914298 | 0.997581 | C | 1.601989 | -1.428073 | -1.594586 |
| H | -4.027041 | -0.116732 | 1.098906 | N | 0.749042 | -2.457753 | -1.751301 |
| N | -4.715655 | -2.786788 | 0.750206 | H | 1.144441 | -3.380723 | -1.642602 |
| C | -4.793528 | -3.772401 | -0.193296 | H | -0.225069 | -2.316258 | -1.498833 |
| H | -5.771497 | -3.929515 | -0.633277 | N | 1.137436 | -0.191109 | -1.349126 |
| C | -3.705365 | -4.490126 | -0.559258 | C | 2.012050 | 0.819048 | -1.171356 |
| C | -2.467782 | -4.189951 | 0.109555 | H | 1.551933 | 1.786910 | -0.981582 |
| N | -2.398785 | -3.250564 | 1.047682 | N | 3.334703 | 0.770310 | -1.192004 |
| C | -3.459084 | -2.479617 | 1.344673 | C | 3.777005 | -0.468853 | -1.464673 |
| O | -3.398344 | -1.503929 | 2.097679 | P | 9.531207 | 1.303154 | 0.712442 |
| C | -7.811366 | -0.787701 | 0.927641 | O | 10.145449 | 2.774012 | 0.559569 |
| H | -8.884352 | -0.874652 | 0.732422 | O | 10.393779 | 0.252017 | 1.259506 |
| C | -6.961280 | -1.739910 | 0.085629 | O | 8.234073 | 1.606120 | 1.589385 |
| H | -7.534450 | -2.671194 | -0.036017 | C | 7.323170 | 2.632568 | 1.170055 |
| H | -6.685724 | -1.330298 | -0.886784 | H | 7.700410 | 3.599484 | 1.518449 |
| O | -7.400680 | 0.582215 | 0.758903 | H | 7.251696 | 2.650714 | 0.077172 |
| P | -7.759665 | 1.335909 | -0.599070 | C | 5.966280 | 2.375613 | 1.771096 |
| O | -9.283794 | 1.769276 | -0.303952 | H | 5.350348 | 3.272641 | 1.588390 |
| O | -7.597063 | 0.632510 | -1.881867 | O | 5.361930 | 1.236504 | 1.184566 |
| O | -6.894260 | 2.660179 | -0.525595 | C | 4.181322 | 1.018788 | 1.946545 |
| C | -6.361321 | 3.256518 | 0.666210 | H | 3.363919 | 1.633064 | 1.550642 |
| H | -7.173809 | 3.783707 | 1.178078 | C | 5.919469 | 2.070403 | 3.273774 |
| H | -5.942282 | 2.479472 | 1.309190 | H | 6.710727 | 1.348063 | 3.506110 |
| C | -5.264049 | 4.238715 | 0.278628 | C | 4.538122 | 1.417942 | 3.399711 |
| H | -5.155927 | 4.947796 | 1.108354 | H | 4.535085 | 0.548404 | 4.058353 |
| O | -4.007769 | 3.605010 | 0.087876 | H | 3.828284 | 2.152094 | 3.787397 |
| C | -3.674222 | 3.506342 | -1.299695 | O | 6.021802 | 3.227362 | 4.071401 |
| H | -2.767803 | 4.090871 | -1.464983 | N | 3.764808 | -0.347422 | 1.771963 |
| N | -3.302214 | 2.144836 | -1.649521 | C | 4.529936 | -1.491765 | 1.626636 |
| C | -4.318872 | 1.108620 | -1.591175 | H | 5.609151 | -1.447771 | 1.662459 |
| C | -3.795836 | -0.181373 | -2.236087 | N | 3.815044 | -2.565975 | 1.445933 |
| C | -3.669444 | 0.007612 | -3.753460 | C | 2.509627 | -2.122043 | 1.491660 |
| H | -3.040458 | 0.863193 | -4.007659 | C | 1.265764 | -2.804827 | 1.290334 |
| H | -3.240312 | -0.895583 | -4.194490 | N | 0.182566 | -1.930367 | 1.421941 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -4.671810 | 0.155203 | -4.162936 | C | 0.255774 | -0.572192 | 1.631205 |
| C | -2.424354 | -0.523423 | -1.683015 | N | 1.394201 | 0.075024 | 1.791154 |
| O | -2.118768 | -1.697564 | -1.495803 | C | 2.458751 | -0.746191 | 1.691741 |
| N | -1.571264 | 0.511469 | -1.542838 | H | -5.215252 | 1.420622 | -2.134801 |
| H | -0.560194 | 0.291653 | -1.352893 | O | -4.813046 | 0.904867 | -0.294024 |
| C | -1.947678 | 1.847744 | -1.461235 | O | -3.686817 | 0.596316 | 0.519047 |
| O | -1.102007 | 2.699333 | -1.272251 | O | -4.666879 | -1.239112 | -1.948400 |
| C | -5.513082 | 5.011468 | -1.027023 | H | -4.089194 | -2.016562 | -1.855752 |
| H | -6.574611 | 5.179970 | -1.220768 | H | 8.422063 | -3.559038 | -2.909871 |
| C | -4.861022 | 4.097084 | -2.069608 | H | -3.988833 | 6.170768 | -0.703068 |
| H | -5.568930 | 3.332814 | -2.390233 | H | -9.199153 | -3.863003 | 2.502154 |
| H | -4.533357 | 4.668931 | -2.939126 | H | 6.949544 | 3.371962 | 4.283128 |
| O | -4.906242 | 6.286743 | -0.981998 | H | -9.776199 | 1.850147 | -1.131243 |
| O | 8.224905 | -2.721781 | -2.477764 | H | 11.044003 | 2.761797 | 0.206430 |
| C | 8.726303 | -1.660990 | -3.270268 | H | -3.772924 | -5.259648 | -1.316471 |
| H | 9.822540 | -1.706766 | -3.344767 | N | -1.342136 | -4.837421 | -0.189889 |
| H | 8.302851 | -1.678551 | -4.282542 | H | -0.468472 | -4.594398 | 0.305589 |
| C | 8.332629 | -0.349085 | -2.615245 | H | -1.343123 | -5.566255 | -0.883215 |
| H | 8.868197 | 0.470137 | -3.109101 | O | 1.071762 | -3.989858 | 1.003256 |
| O | 6.934972 | -0.137223 | -2.754219 | H | -0.746432 | -2.366148 | 1.317612 |
| C | 6.281389 | -0.131896 | -1.492336 | N | -0.914892 | 0.091385 | 1.633474 |
| H | 5.960921 | 0.880843 | -1.228536 | H | -1.764496 | -0.445028 | 1.791116 |
| C | 8.629570 | -0.326344 | -1.112477 | C | -0.947474 | 1.527948 | 1.834950 |
| H | 9.446807 | -0.991281 | -0.822739 | H | -1.964325 | 1.873506 | 1.644692 |
| C | 7.293775 | -0.702410 | -0.493747 | H | -0.636947 | 1.804223 | 2.849273 |
| H | 7.212653 | -1.791050 | -0.460412 | H | -0.275185 | 2.011389 | 1.123028 |



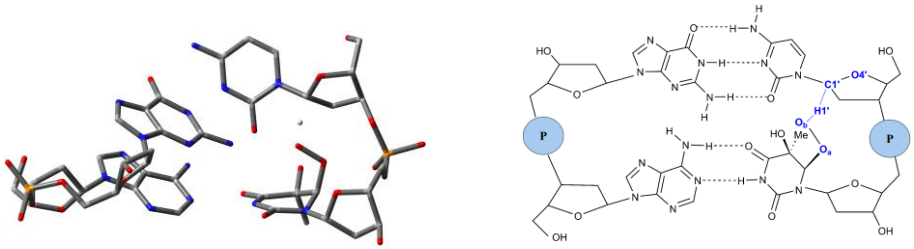


ds - 5' C T* 3' - Reactant

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z | | | | |
|---|---|---|---|---|---|---|---|
| O | 7.653275 | -4.125926 | -1.662002 | H | -6.645429 | -1.808540 | 0.154294 |
| C | 7.837469 | -3.179385 | -2.697963 | H | -6.778252 | -0.227864 | -0.655021 |
| H | 8.895598 | -2.902587 | -2.810717 | O | -8.758182 | 0.743291 | 0.680623 |
| H | 7.474013 | -3.564104 | -3.660004 | N | -4.641541 | -0.773115 | 1.428443 |
| C | 7.037566 | -1.937321 | -2.352838 | C | -4.395842 | -2.116156 | 1.646528 |
| H | 7.208336 | -1.179554 | -3.126008 | H | -5.199943 | -2.836529 | 1.583011 |
| O | 5.653297 | -2.261534 | -2.315817 | N | -3.154776 | -2.381670 | 1.947217 |
| C | 5.112614 | -2.011064 | -1.027801 | C | -2.544449 | -1.144964 | 1.943625 |
| H | 4.548057 | -1.077638 | -1.031520 | C | -1.218435 | -0.758634 | 2.211499 |
| N | 4.128984 | -3.068015 | -0.752689 | N | -0.259646 | -1.659844 | 2.469499 |
| C | 4.249448 | -4.303964 | -1.310213 | H | -0.536617 | -2.627365 | 2.530252 |
| H | 5.213731 | -4.512452 | -1.761736 | H | 0.645269 | -1.366261 | 2.828565 |
| C | 3.210319 | -5.172511 | -1.295703 | N | -0.926761 | 0.556418 | 2.161110 |
| C | 1.963596 | -4.681800 | -0.773965 | C | -1.895573 | 1.426391 | 1.819867 |
| N | 1.890429 | -3.514550 | -0.134335 | H | -1.573332 | 2.463464 | 1.761037 |
| C | 2.973198 | -2.716950 | -0.041157 | N | -3.168493 | 1.179137 | 1.545471 |
| O | 2.981770 | -1.665983 | 0.619951 | C | -3.441665 | -0.130481 | 1.635270 |
| C | 7.363352 | -1.343830 | -0.977086 | P | -9.350737 | 1.047128 | -0.779177 |
| H | 8.393056 | -1.537836 | -0.661453 | O | -10.136669 | 2.417046 | -0.510416 |
| C | 6.304788 | -1.955014 | -0.075876 | O | -10.078511 | -0.066652 | -1.394088 |
| H | 6.609778 | -2.969534 | 0.192783 | O | -8.130207 | 1.579889 | -1.657150 |
| H | 6.125364 | -1.355171 | 0.818417 | C | -7.374215 | 2.717214 | -1.216602 |
| O | 7.147123 | 0.082944 | -1.100770 | H | -7.876225 | 3.625948 | -1.563793 |
| P | 7.706341 | 1.052368 | 0.031863 | H | -7.318377 | 2.735401 | -0.122774 |
| O | 9.202639 | 1.312888 | -0.502135 | C | -5.983237 | 2.642412 | -1.796148 |
| O | 7.639135 | 0.628452 | 1.437225 | H | -5.500172 | 3.621271 | -1.638401 |
| O | 6.901460 | 2.400401 | -0.223037 | O | -5.256172 | 1.611082 | -1.157577 |
| C | 6.389632 | 2.821734 | -1.494638 | C | -4.090558 | 1.350889 | -1.938853 |
| H | 7.222369 | 3.174265 | -2.113714 | H | -3.225455 | 1.861188 | -1.503356 |
| H | 5.886738 | 1.981040 | -1.980119 | C | -5.875293 | 2.291099 | -3.284008 |
| C | 5.389475 | 3.940631 | -1.260528 | H | -6.548732 | 1.450438 | -3.493718 |
| H | 5.192462 | 4.409461 | -2.232866 | C | -4.414665 | 1.850639 | -3.366141 |
| O | 4.167147 | 3.426258 | -0.753223 | H | -4.230627 | 1.080135 | -4.115690 |
| C | 3.944201 | 3.813535 | 0.600450 | H | -3.809087 | 2.726871 | -3.613005 |
| H | 3.076640 | 4.476067 | 0.630734 | O | -6.125675 | 3.383477 | -4.135761 |
| N | 3.561902 | 2.665208 | 1.409662 | N | -3.795187 | -0.054647 | -1.840751 |
| C | 4.467524 | 1.572582 | 1.505283 | C | -4.637022 | -1.130983 | -2.062319 |
| C | 4.150019 | 0.609010 | 2.662914 | H | -5.643793 | -0.985944 | -2.431235 |
| C | 4.669623 | 1.221596 | 3.961682 | N | -4.088389 | -2.278588 | -1.784454 |
| H | 4.272249 | 2.228508 | 4.114919 | C | -2.810318 | -1.957730 | -1.370333 |
| H | 4.375436 | 0.578341 | 4.792297 | C | -1.715108 | -2.781675 | -0.942200 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 5.760891 | 1.257204 | 3.902415 | N | -0.593324 | -1.996744 | -0.634900 |
| C | 2.646626 | 0.371888 | 2.792047 | C | -0.505625 | -0.630513 | -0.724745 |
| O | 2.228938 | -0.581278 | 3.422114 | N | -1.507864 | 0.134845 | -1.106472 |
| N | 1.814983 | 1.273161 | 2.190973 | C | -2.608933 | -0.582771 | -1.402309 |
| H | 0.779840 | 1.078631 | 2.231254 | H | 5.495745 | 1.912489 | 1.617573 |
| C | 2.186291 | 2.390733 | 1.462280 | O | 4.544782 | 0.818275 | 0.240678 |
| O | 1.344914 | 3.107684 | 0.961555 | O | 3.418767 | 0.787651 | -0.409490 |
| C | 5.827194 | 5.024198 | -0.258184 | O | 4.795390 | -0.614623 | 2.482868 |
| H | 6.913792 | 5.125548 | -0.206215 | H | 4.230260 | -1.160415 | 1.903009 |
| C | 5.222625 | 4.524901 | 1.057318 | H | -7.541983 | -3.874388 | 2.504019 |
| H | 5.911367 | 3.838816 | 1.552629 | H | 4.375393 | 6.220822 | -0.756317 |
| H | 5.008361 | 5.356470 | 1.730285 | H | 8.175370 | -4.911019 | -1.857126 |
| O | 5.330203 | 6.293163 | -0.630635 | H | -7.070870 | 3.418674 | -4.316226 |
| O | -7.513767 | -2.996416 | 2.110446 | H | 9.792227 | 1.525722 | 0.233444 |
| C | -8.148926 | -2.077560 | 2.979733 | H | -10.931765 | 2.290418 | 0.023103 |
| H | -9.227657 | -2.281325 | 3.050209 | H | 3.292768 | -6.155317 | -1.739550 |
| H | -7.717260 | -2.110139 | 3.988149 | N | 0.836599 | -5.383289 | -0.912528 |
| C | -7.947975 | -0.676920 | 2.427299 | H | -0.069094 | -4.933733 | -0.716594 |
| H | -8.598684 | 0.015630 | 2.974456 | H | 0.839903 | -6.216220 | -1.477413 |
| O | -6.600104 | -0.267682 | 2.595507 | O | -1.654423 | -4.005073 | -0.836912 |
| C | -5.933950 | -0.133315 | 1.343994 | H | 0.225158 | -2.513540 | -0.289252 |
| H | -5.723842 | 0.921050 | 1.142346 | N | 0.691142 | -0.080901 | -0.441078 |
| C | -8.238784 | -0.587517 | 0.927819 | H | 1.403557 | -0.602158 | 0.063453 |
| H | -8.969103 | -1.321777 | 0.580071 | H | 0.702764 | 0.926822 | -0.361604 |
| C | -6.865268 | -0.748771 | 0.297097 | | | | |

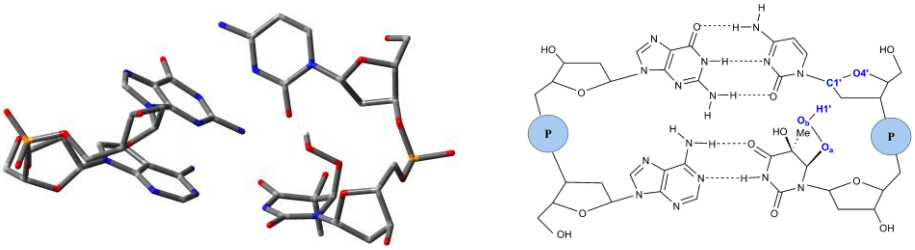


ds - 5' C T* 3' - TS

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) | | | | | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | | | |
| O | 7.161630 | -4.006456 | -2.077432 | H | -6.621693 | -1.735378 | 0.185702 |
| C | 7.141738 | -2.985671 | -3.059442 | H | -6.743004 | -0.153550 | -0.621764 |
| H | 8.157131 | -2.730760 | -3.392945 | O | -8.698893 | 0.842838 | 0.726820 |
| H | 6.548085 | -3.279054 | -3.935141 | N | -4.593519 | -0.725060 | 1.440710 |
| C | 6.519094 | -1.751677 | -2.438035 | C | -4.360459 | -2.069278 | 1.664464 |
| H | 6.600274 | -0.915091 | -3.138190 | H | -5.173175 | -2.781025 | 1.614629 |
| O | 5.133218 | -1.982900 | -2.182013 | N | -3.118438 | -2.346891 | 1.951443 |
| C | 4.848092 | -2.016914 | -0.825841 | C | -2.493737 | -1.117328 | 1.933055 |
| H | 4.191147 | -0.909665 | -0.512093 | C | -1.160363 | -0.741737 | 2.181435 |
| N | 3.917732 | -3.112641 | -0.596146 | N | -0.199453 | -1.647133 | 2.422128 |
| C | 4.022257 | -4.248428 | -1.359752 | H | -0.479623 | -2.612857 | 2.499218 |
| H | 4.979625 | -4.386196 | -1.849894 | H | 0.706051 | -1.358548 | 2.786864 |
| C | 2.996401 | -5.119298 | -1.466319 | N | -0.857517 | 0.569658 | 2.114055 |
| C | 1.751043 | -4.731857 | -0.855277 | C | -1.820210 | 1.446965 | 1.777464 |
| N | 1.684381 | -3.690804 | -0.031457 | H | -1.487797 | 2.479767 | 1.703516 |
| C | 2.758803 | -2.902543 | 0.185201 | N | -3.099112 | 1.210457 | 1.521413 |
| O | 2.747310 | -1.979000 | 1.002351 | C | -3.383927 | -0.095170 | 1.627648 |
| C | 7.134475 | -1.364619 | -1.089336 | P | -9.286654 | 1.152641 | -0.732906 |
| H | 8.156063 | -1.739701 | -0.972583 | O | -10.068085 | 2.525900 | -0.469106 |
| C | 6.170666 | -1.964768 | -0.064539 | O | -10.024162 | 0.047060 | -1.351365 |
| H | 6.487691 | -2.988487 | 0.161375 | O | -8.056330 | 1.676646 | -1.603424 |
| H | 6.119657 | -1.379144 | 0.857589 | C | -7.295378 | 2.808107 | -1.155986 |
| O | 7.147819 | 0.068814 | -1.092132 | H | -7.798724 | 3.721615 | -1.488475 |
| P | 7.785641 | 0.935491 | 0.081927 | H | -7.231165 | 2.813082 | -0.062463 |
| O | 9.307597 | 1.051890 | -0.434776 | C | -5.908816 | 2.738195 | -1.746933 |
| O | 7.673907 | 0.474907 | 1.473056 | H | -5.421564 | 3.712764 | -1.577137 |
| O | 7.129357 | 2.366098 | -0.152534 | O | -5.181777 | 1.694128 | -1.129216 |
| C | 6.618475 | 2.814262 | -1.418848 | C | -4.029914 | 1.425166 | -1.927195 |
| H | 7.461401 | 3.165859 | -2.024477 | H | -3.147523 | 1.900926 | -1.487459 |
| H | 6.107605 | 1.988454 | -1.917868 | C | -5.812658 | 2.410071 | -3.240714 |
| C | 5.621301 | 3.940751 | -1.206868 | H | -6.491507 | 1.575928 | -3.459562 |
| H | 5.499649 | 4.436437 | -2.178539 | C | -4.354532 | 1.964817 | -3.338852 |
| O | 4.351884 | 3.451379 | -0.804100 | H | -4.175360 | 1.214485 | -4.109673 |
| C | 4.079190 | 3.749809 | 0.563499 | H | -3.746070 | 2.845333 | -3.562664 |
| H | 3.208754 | 4.408537 | 0.593296 | O | -6.062099 | 3.516616 | -4.073749 |
| N | 3.672322 | 2.566749 | 1.302769 | N | -3.775535 | 0.008281 | -1.863633 |
| C | 4.609337 | 1.475658 | 1.439013 | C | -4.667771 | -1.027494 | -2.075933 |
| C | 4.223095 | 0.515938 | 2.588426 | H | -5.669268 | -0.835163 | -2.437924 |
| C | 4.767715 | 1.103172 | 3.891569 | N | -4.173048 | -2.199256 | -1.797170 |
| H | 4.441029 | 2.138663 | 4.027609 | C | -2.881119 | -1.936307 | -1.387838 |
| H | 4.418215 | 0.493821 | 4.726224 | C | -1.831654 | -2.809700 | -0.947098 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 5.859207 | 1.062863 | 3.843769 | N | -0.677198 | -2.077526 | -0.632717 |
| C | 2.713743 | 0.343811 | 2.738998 | C | -0.518032 | -0.719211 | -0.739472 |
| O | 2.269568 | -0.541477 | 3.448222 | N | -1.475482 | 0.090122 | -1.138675 |
| N | 1.904185 | 1.207055 | 2.063887 | C | -2.613304 | -0.573081 | -1.428398 |
| H | 0.866854 | 1.052573 | 2.131992 | H | 5.597084 | 1.872728 | 1.674181 |
| C | 2.304653 | 2.298433 | 1.309803 | O | 4.875317 | 0.859663 | 0.189177 |
| O | 1.474526 | 2.995650 | 0.758979 | O | 3.756661 | 0.223165 | -0.315084 |
| C | 6.004700 | 4.991687 | -0.152731 | O | 4.802372 | -0.743605 | 2.409950 |
| H | 7.086505 | 5.096352 | -0.041174 | H | 4.126133 | -1.326435 | 2.015125 |
| C | 5.333311 | 4.447410 | 1.109863 | H | -7.515264 | -3.780372 | 2.561467 |
| H | 6.000726 | 3.750027 | 1.617737 | H | 4.573169 | 6.187185 | -0.699699 |
| H | 5.080559 | 5.255630 | 1.797929 | H | 7.620194 | -4.776816 | -2.429126 |
| O | 5.516872 | 6.269111 | -0.511122 | H | -7.008552 | 3.562200 | -4.245182 |
| O | -7.482521 | -2.905101 | 2.162305 | H | 9.904267 | 1.185818 | 0.313401 |
| C | -8.100802 | -1.975245 | 3.032018 | H | -10.926741 | 2.385663 | -0.050095 |
| H | -9.181118 | -2.166710 | 3.112004 | H | 3.083184 | -6.020802 | -2.057960 |
| H | -7.661538 | -2.007866 | 4.037070 | N | 0.626601 | -5.402623 | -1.103975 |
| C | -7.888276 | -0.579652 | 2.471492 | H | -0.279249 | -4.992122 | -0.829567 |
| H | -8.524917 | 0.123396 | 3.021637 | H | 0.627504 | -6.130491 | -1.799226 |
| O | -6.533675 | -0.186984 | 2.625077 | O | -1.832067 | -4.034562 | -0.838435 |
| C | -5.877831 | -0.067751 | 1.367132 | H | 0.101615 | -2.628940 | -0.251633 |
| H | -5.654157 | 0.982680 | 1.159705 | N | 0.713942 | -0.229765 | -0.458642 |
| C | -8.192342 | -0.492856 | 0.974353 | H | 1.311945 | -0.737143 | 0.189399 |
| H | -8.934542 | -1.219964 | 0.636719 | H | 0.751360 | 0.779887 | -0.387088 |
| C | -6.827202 | -0.673168 | 0.331077 | | | | |

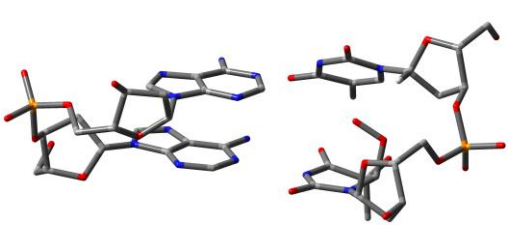


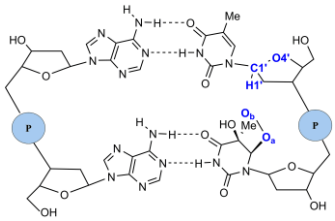
ds - 5' C T* 3' - Product

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) | | | | | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | | | |
| O | -7.290171 | 4.205879 | -1.466456 | H | 6.641480 | 0.238083 | -0.700670 |
| C | -7.712194 | 3.332770 | -2.493748 | O | 8.649294 | -1.100580 | 0.206972 |
| H | -8.792103 | 3.130589 | -2.447680 | N | 4.719338 | 0.416571 | 1.627067 |
| H | -7.479301 | 3.739137 | -3.487766 | C | 4.586013 | 1.687744 | 2.153232 |
| C | -6.959866 | 2.026847 | -2.320271 | H | 5.437517 | 2.353403 | 2.192448 |
| H | -7.216053 | 1.337267 | -3.128545 | N | 3.387998 | 1.950011 | 2.598568 |
| O | -5.554668 | 2.294463 | -2.391692 | C | 2.691903 | 0.781941 | 2.369747 |
| C | -5.010441 | 2.261253 | -1.139996 | C | 1.359681 | 0.423526 | 2.644573 |
| N | -4.008441 | 3.248079 | -0.969400 | N | 0.507470 | 1.290896 | 3.207280 |
| C | -3.884939 | 4.295860 | -1.837633 | H | 0.842702 | 2.222186 | 3.395267 |
| H | -4.691108 | 4.398311 | -2.551349 | H | -0.471296 | 1.050100 | 3.331039 |
| C | -2.814056 | 5.122578 | -1.787951 | N | 0.959253 | -0.819794 | 2.314652 |
| C | -1.798724 | 4.822905 | -0.821812 | C | 1.837755 | -1.644469 | 1.713251 |
| N | -1.956001 | 3.845714 | 0.073306 | H | 1.432677 | -2.618155 | 1.445593 |
| C | -3.045850 | 3.057249 | 0.048441 | N | 3.109686 | -1.419734 | 1.411074 |
| O | -3.240078 | 2.141064 | 0.863062 | C | 3.489996 | -0.186679 | 1.776352 |
| C | -7.162424 | 1.356503 | -0.959791 | P | 9.067792 | -1.114237 | -1.341909 |
| H | -8.158282 | 1.541251 | -0.546041 | O | 9.784414 | -2.541881 | -1.456568 |
| C | -6.035272 | 1.917407 | -0.095152 | O | 9.804173 | 0.069243 | -1.795021 |
| H | -6.373373 | 2.826931 | 0.414953 | O | 7.726797 | -1.391018 | -2.161526 |
| H | -5.703812 | 1.190846 | 0.651445 | C | 6.945639 | -2.562123 | -1.884263 |
| O | -6.974932 | -0.051905 | -1.190641 | H | 7.349110 | -3.397789 | -2.465105 |
| P | -7.587744 | -1.092273 | -0.149903 | H | 6.998851 | -2.810653 | -0.818664 |
| O | -9.066999 | -1.284876 | -0.764941 | C | 5.511112 | -2.306979 | -2.276193 |
| O | -7.594802 | -0.752897 | 1.279972 | H | 4.981327 | -3.273833 | -2.256113 |
| O | -6.804264 | -2.434297 | -0.474535 | O | 4.925572 | -1.390135 | -1.371225 |
| C | -6.110968 | -2.697949 | -1.705909 | C | 3.713997 | -0.909993 | -1.950174 |
| H | -6.855436 | -2.924471 | -2.477632 | H | 2.855297 | -1.421842 | -1.504192 |
| H | -5.521954 | -1.821574 | -1.983706 | C | 5.272531 | -1.660045 | -3.644183 |
| C | -5.180535 | -3.886132 | -1.515502 | H | 5.966829 | -0.817258 | -3.756020 |
| H | -4.951905 | -4.274258 | -2.515802 | C | 3.838252 | -1.164776 | -3.469909 |
| O | -3.952340 | -3.520281 | -0.905768 | H | 3.605765 | -0.271937 | -4.051282 |
| C | -3.897183 | -3.937801 | 0.457914 | H | 3.163406 | -1.967395 | -3.780434 |
| H | -3.064966 | -4.636731 | 0.557386 | O | 5.371503 | -2.563392 | -4.718269 |
| N | -3.555928 | -2.829613 | 1.336381 | N | 3.568079 | 0.477076 | -1.583596 |
| C | -4.479098 | -1.714115 | 1.435972 | C | 4.487517 | 1.502249 | -1.715937 |
| C | -4.144584 | -0.822792 | 2.645479 | H | 5.443523 | 1.335836 | -2.194485 |
| C | -4.564505 | -1.536512 | 3.935298 | N | 4.074727 | 2.631967 | -1.216923 |
| H | -4.119753 | -2.532014 | 4.011181 | C | 2.812475 | 2.352655 | -0.733034 |
| H | -4.261108 | -0.934092 | 4.794052 | C | 1.815388 | 3.202511 | -0.144885 |
| H | -5.654384 | -1.618852 | 3.930375 | N | 0.660775 | 2.464531 | 0.166038 |

| | | | |
|---|---|---|---|
| C | -2.652432 | -0.550013 | 2.715302 |
| O | -2.253622 | 0.518244 | 3.161464 |
| N | -1.821260 | -1.547647 | 2.328075 |
| H | -0.790654 | -1.367402 | 2.391696 |
| C | -2.193559 | -2.659552 | 1.569921 |
| O | -1.340663 | -3.437113 | 1.194776 |
| C | -5.727688 | -5.025549 | -0.641199 |
| H | -6.814912 | -5.115308 | -0.697381 |
| C | -5.238348 | -4.623966 | 0.753299 |
| H | -5.953215 | -3.946425 | 1.219754 |
| H | -5.111509 | -5.500601 | 1.390481 |
| O | -5.201003 | -6.271230 | -1.052209 |
| O | 7.790870 | 2.299778 | 2.510040 |
| C | 8.433119 | 1.183119 | 3.096892 |
| H | 9.525597 | 1.311339 | 3.099166 |
| H | 8.095453 | 1.018246 | 4.127894 |
| C | 8.084363 | -0.051678 | 2.284028 |
| H | 8.722979 | -0.882038 | 2.607899 |
| O | 6.726442 | -0.408907 | 2.490556 |
| C | 5.959460 | -0.249687 | 1.302207 |
| H | 5.671630 | -1.227945 | 0.907337 |
| C | 8.246603 | 0.169530 | 0.777894 |
| H | 8.996736 | 0.923366 | 0.527222 |
| C | 6.842014 | 0.532984 | 0.327795 |
| H | 6.684922 | 1.607812 | 0.436497 |
| C | 0.438553 | 1.141370 | -0.121104 |
| N | 1.332580 | 0.362311 | -0.687730 |
| C | 2.477619 | 1.021910 | -0.959735 |
| H | -5.495446 | -2.087782 | 1.571570 |
| O | -4.590471 | -0.986219 | 0.237451 |
| O | -3.327254 | -0.404175 | -0.049798 |
| O | -4.828753 | 0.390928 | 2.533972 |
| H | -4.171247 | 1.106323 | 2.581852 |
| H | 7.930491 | 3.072709 | 3.066440 |
| H | -4.240797 | -6.182617 | -1.109908 |
| H | -7.768588 | 5.037804 | -1.540235 |
| H | 6.289968 | -2.596344 | -5.005837 |
| H | -9.686421 | -1.541697 | -0.069400 |
| H | 10.680707 | -2.535378 | -1.097672 |
| H | -2.712887 | 5.946637 | -2.481202 |
| N | -0.660280 | 5.523875 | -0.795899 |
| H | 0.147687 | 5.205275 | -0.248987 |
| H | -0.476434 | 6.186933 | -1.530841 |
| O | 1.833205 | 4.412707 | 0.065402 |
| H | -0.139544 | 3.003465 | 0.506190 |
| N | -0.790930 | 0.673681 | 0.173608 |
| H | -1.388774 | 1.164294 | 0.831271 |
| H | -0.940120 | -0.317763 | 0.055392 |
| H | -3.475383 | 0.536380 | 0.206785 |



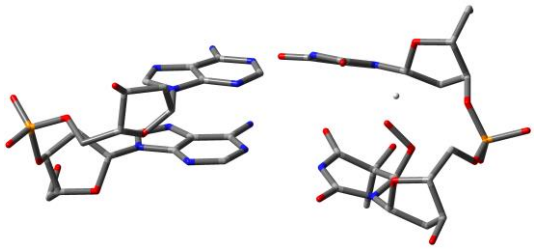


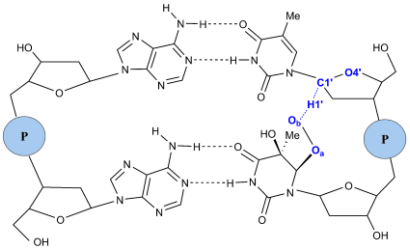
ds - 5' T T* 3' - Reactant

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| O | -8.866483 | -2.572421 | 2.674339 | O | 6.959612 | -0.842311 | -2.366745 |
| C | -8.505831 | -1.485730 | 3.504521 | C | 6.228937 | -0.779391 | -1.149157 |
| H | -9.350110 | -0.795274 | 3.650331 | H | 5.894328 | 0.251388 | -0.972087 |
| H | -8.153249 | -1.821505 | 4.487793 | C | 8.546926 | -0.918523 | -0.623626 |
| C | -7.373058 | -0.743172 | 2.825972 | H | 9.354656 | -1.534899 | -0.221957 |
| H | -7.222417 | 0.233688 | 3.305604 | C | 7.184317 | -1.285205 | -0.063563 |
| O | -6.193620 | -1.531476 | 2.918941 | H | 7.135699 | -2.370916 | 0.013640 |
| C | -5.527022 | -1.371757 | 1.671955 | H | 6.992912 | -0.872010 | 0.925838 |
| H | -5.087691 | -0.371095 | 1.634553 | O | 8.868539 | 0.475627 | -0.402839 |
| N | -4.421375 | -2.290770 | 1.521554 | N | 5.024792 | -1.568416 | -1.258524 |
| C | -4.482699 | -3.410327 | 0.717571 | C | 4.896653 | -2.937531 | -1.161162 |
| H | -5.474980 | -3.674368 | 0.370106 | H | 5.769891 | -3.568482 | -1.070526 |
| C | -3.406318 | -4.140452 | 0.361109 | N | 3.662287 | -3.357883 | -1.233617 |
| C | -3.454792 | -5.327182 | -0.549854 | C | 2.932115 | -2.199867 | -1.401739 |
| H | -2.881690 | -5.120857 | -1.459267 | C | 1.544427 | -1.974250 | -1.506930 |
| H | -2.998558 | -6.199551 | -0.074685 | N | 0.655522 | -2.972215 | -1.490031 |
| H | -4.483028 | -5.572244 | -0.826125 | H | 0.976895 | -3.890975 | -1.228118 |
| C | -2.093861 | -3.696914 | 0.830765 | H | -0.336604 | -2.776797 | -1.396486 |
| O | -1.034984 | -4.247667 | 0.529255 | N | 1.134268 | -0.697194 | -1.636574 |
| N | -2.107792 | -2.597797 | 1.656652 | C | 2.042806 | 0.296389 | -1.638639 |
| H | -1.183047 | -2.147523 | 1.831292 | H | 1.618108 | 1.293651 | -1.735112 |
| C | -3.198308 | -1.853757 | 2.052428 | N | 3.360013 | 0.201082 | -1.530750 |
| O | -3.106983 | -0.887735 | 2.777009 | C | 3.750805 | -1.078056 | -1.419565 |
| C | -7.635980 | -0.525016 | 1.313608 | P | 8.966232 | 0.996744 | 1.111945 |
| H | -8.682357 | -0.683930 | 1.042931 | O | 9.980893 | 2.229021 | 0.974429 |
| C | -6.666995 | -1.498263 | 0.669692 | O | 9.279561 | -0.041967 | 2.097306 |
| H | -7.118504 | -2.492264 | 0.744250 | O | 7.596531 | 1.771379 | 1.381750 |
| H | -6.412873 | -1.255577 | -0.361327 | C | 7.305385 | 2.975338 | 0.647982 |
| O | -7.253095 | 0.839257 | 0.986526 | H | 8.013932 | 3.752513 | 0.950594 |
| P | -7.606662 | 1.389786 | -0.462613 | H | 7.411320 | 2.785060 | -0.425610 |
| O | -9.010418 | 2.125497 | -0.183000 | C | 5.898493 | 3.423176 | 0.956123 |
| O | -7.631086 | 0.462469 | -1.604338 | H | 5.787627 | 4.445240 | 0.560429 |
| O | -6.540235 | 2.548365 | -0.691190 | O | 4.971982 | 2.547079 | 0.333513 |
| C | -5.975791 | 3.360181 | 0.343926 | C | 3.771928 | 2.494668 | 1.087214 |
| H | -6.747803 | 4.032814 | 0.735029 | H | 2.915042 | 2.772686 | 0.467156 |
| H | -5.592742 | 2.719336 | 1.143340 | C | 5.489347 | 3.447729 | 2.433496 |
| C | -4.834408 | 4.154023 | -0.267024 | H | 5.840707 | 2.529142 | 2.922273 |
| H | -4.556513 | 4.942903 | 0.442899 | C | 3.972314 | 3.425550 | 2.288242 |
| O | -3.703257 | 3.320502 | -0.481046 | H | 3.436320 | 3.077289 | 3.171441 |
| C | -3.459193 | 3.109321 | -1.870327 | H | 3.636774 | 4.438604 | 2.044073 |
| H | -2.533869 | 3.620538 | -2.142812 | O | 5.932083 | 4.599971 | 3.107214 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | -3.184195 | 1.699496 | -2.114750 | N | 3.552867 | 1.106813 | 1.467624 |
| C | -4.213428 | 0.743010 | -1.851925 | C | 4.501001 | 0.120441 | 1.589113 |
| C | -3.857778 | -0.643514 | -2.399191 | H | 5.551034 | 0.380718 | 1.582785 |
| C | -3.928666 | -0.630056 | -3.930490 | N | 4.002331 | -1.084000 | 1.697666 |
| H | -3.286825 | 0.140316 | -4.363576 | C | 2.637293 | -0.878119 | 1.646317 |
| H | -3.621052 | -1.608581 | -4.305891 | C | 1.530879 | -1.753137 | 1.612814 |
| H | -4.966378 | -0.452824 | -4.223576 | N | 1.638602 | -3.094791 | 1.614665 |
| C | -2.439957 | -1.009762 | -1.980546 | H | 2.547963 | -3.488558 | 1.421255 |
| O | -2.176146 | -2.176863 | -1.720540 | H | 0.808299 | -3.620297 | 1.346242 |
| N | -1.526178 | -0.015780 | -2.018945 | N | 0.306334 | -1.202092 | 1.569200 |
| H | -0.506386 | -0.259199 | -1.842607 | C | 0.167758 | 0.130888 | 1.474927 |
| C | -1.826379 | 1.341056 | -2.023964 | H | -0.860061 | 0.487460 | 1.447888 |
| O | -0.934660 | 2.159782 | -1.995384 | N | 1.127331 | 1.042696 | 1.409713 |
| C | -5.139739 | 4.784090 | -1.638615 | C | 2.337015 | 0.475935 | 1.505623 |
| H | -6.200291 | 5.015490 | -1.762444 | H | -5.179896 | 1.060701 | -2.247958 |
| C | -4.658190 | 3.703118 | -2.612860 | O | -4.500213 | 0.628752 | -0.422518 |
| H | -5.446797 | 2.967734 | -2.774775 | O | -3.414557 | 0.428073 | 0.262470 |
| H | -4.368273 | 4.137849 | -3.570577 | O | -4.742292 | -1.591004 | -1.876461 |
| O | -4.445358 | 6.002788 | -1.806267 | H | -4.198195 | -2.362046 | -1.635591 |
| O | 8.142042 | -3.439149 | -1.826126 | H | 8.268844 | -4.301998 | -2.233501 |
| C | 8.731989 | -2.451716 | -2.651942 | H | -3.513956 | 5.853632 | -1.599520 |
| H | 9.828679 | -2.536412 | -2.648030 | H | -9.457079 | -3.155508 | 3.160408 |
| H | 8.377369 | -2.530067 | -3.687066 | H | 6.781861 | 4.408937 | 3.517555 |
| C | 8.340230 | -1.079335 | -2.132189 | H | -9.537303 | 2.167347 | -0.991968 |
| H | 8.924155 | -0.321840 | -2.668084 | H | 10.902717 | 1.941520 | 0.941475 |



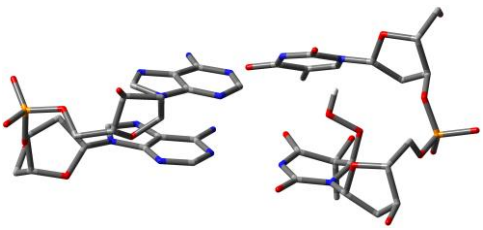


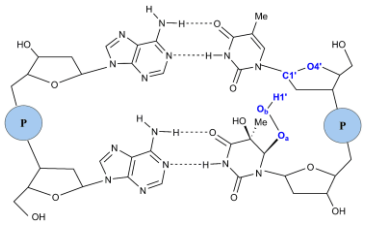

ds - 5' T T* 3' - TS

## Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| O | -7.707571 | -3.151922 | 2.831538 | O | 6.545443 | 0.125489 | -2.667641 |
| C | -7.501721 | -2.011343 | 3.640938 | C | 6.084560 | -0.244392 | -1.374788 |
| H | -8.455118 | -1.581194 | 3.981763 | H | 5.805952 | 0.659125 | -0.817906 |
| H | -6.887140 | -2.241200 | 4.520262 | C | 8.460914 | -0.450921 | -1.425879 |
| C | -6.770816 | -0.974839 | 2.810227 | H | 9.311913 | -1.135524 | -1.412619 |
| H | -6.747068 | -0.019782 | 3.345316 | C | 7.238876 | -1.008356 | -0.716162 |
| O | -5.433869 | -1.420990 | 2.592523 | H | 7.181908 | -2.072581 | -0.937644 |
| C | -5.171044 | -1.519179 | 1.233687 | H | 7.280130 | -0.893798 | 0.366074 |
| H | -4.676465 | -0.428910 | 0.849249 | O | 8.876658 | 0.820286 | -0.873437 |
| N | -4.114650 | -2.460178 | 0.988020 | N | 4.872638 | -1.024549 | -1.482456 |
| C | -4.261018 | -3.613931 | 0.244025 | C | 4.736897 | -2.378453 | -1.703027 |
| H | -5.274111 | -3.835783 | -0.073619 | H | 5.600385 | -3.003248 | -1.879123 |
| C | -3.228520 | -4.417753 | -0.082480 | N | 3.497609 | -2.790550 | -1.713368 |
| C | -3.358848 | -5.661396 | -0.905133 | C | 2.768706 | -1.638757 | -1.505667 |
| H | -2.740358 | -5.588610 | -1.804130 | C | 1.381755 | -1.416371 | -1.379819 |
| H | -3.002877 | -6.531744 | -0.346699 | N | 0.494826 | -2.412778 | -1.462368 |
| H | -4.396045 | -5.832300 | -1.201716 | H | 0.824506 | -3.364202 | -1.495598 |
| C | -1.886961 | -4.045833 | 0.382272 | H | -0.485782 | -2.230277 | -1.275867 |
| O | -0.867411 | -4.668701 | 0.091009 | N | 0.964201 | -0.151981 | -1.171775 |
| N | -1.829961 | -2.937021 | 1.192225 | C | 1.882601 | 0.824605 | -1.050854 |
| H | -0.877173 | -2.565587 | 1.451544 | H | 1.469703 | 1.815757 | -0.875693 |
| C | -2.847384 | -2.052586 | 1.441536 | N | 3.204202 | 0.729393 | -1.113442 |
| O | -2.684556 | -0.994710 | 2.012412 | C | 3.592971 | -0.531950 | -1.356855 |
| C | -7.383527 | -0.774305 | 1.416345 | P | 9.283670 | 0.867676 | 0.677505 |
| H | -8.442864 | -1.044779 | 1.380905 | O | 10.252855 | 2.142035 | 0.729714 |
| C | -6.508064 | -1.650329 | 0.523791 | O | 9.795159 | -0.393296 | 1.223143 |
| H | -6.886237 | -2.674724 | 0.604775 | O | 7.990304 | 1.434517 | 1.423815 |
| H | -6.482514 | -1.320542 | -0.515009 | C | 7.528290 | 2.759507 | 1.107292 |
| O | -7.228492 | 0.621293 | 1.112192 | H | 8.247487 | 3.487225 | 1.495922 |
| P | -7.914006 | 1.266318 | -0.177573 | H | 7.449713 | 2.872267 | 0.020390 |
| O | -9.435675 | 1.434652 | 0.327167 | C | 6.181136 | 2.983385 | 1.745226 |
| O | -7.847653 | 0.567955 | -1.473817 | H | 5.947954 | 4.056498 | 1.652828 |
| O | -7.312661 | 2.732012 | -0.179990 | O | 5.207772 | 2.198618 | 1.077649 |
| C | -6.342576 | 3.279194 | 0.732370 | C | 4.122017 | 1.936831 | 1.953258 |
| H | -6.902302 | 3.825422 | 1.497346 | H | 3.197741 | 2.373645 | 1.563983 |
| H | -5.755491 | 2.480622 | 1.191052 | C | 6.039545 | 2.599214 | 3.221254 |
| C | -5.396245 | 4.234944 | 0.002876 | H | 6.501117 | 1.616082 | 3.383382 |
| H | -5.150179 | 5.045125 | 0.699492 | C | 4.521576 | 2.502530 | 3.324310 |
| O | -4.170550 | 3.613526 | -0.367272 | H | 4.162591 | 1.879940 | 4.143948 |
| C | -4.102575 | 3.394591 | -1.776256 | H | 4.124192 | 3.514506 | 3.448971 |
| H | -3.325446 | 4.046096 | -2.183652 | O | 6.554485 | 3.570234 | 4.098283 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | -3.639769 | 2.038977 | -2.045189 | N | 3.902810 | 0.499920 | 1.958702 |
| C | -4.597963 | 0.962690 | -1.923142 | C | 4.825895 | -0.491585 | 1.728846 |
| C | -3.973551 | -0.360570 | -2.365649 | H | 5.878947 | -0.248450 | 1.681733 |
| C | -3.758153 | -0.347696 | -3.886338 | N | 4.299942 | -1.679226 | 1.574551 |
| H | -3.155476 | 0.504626 | -4.206380 | C | 2.943999 | -1.457096 | 1.713401 |
| H | -3.257614 | -1.272674 | -4.183309 | C | 1.811631 | -2.281847 | 1.542641 |
| H | -4.735646 | -0.307001 | -4.372495 | N | 1.890546 | -3.577271 | 1.187260 |
| C | -2.621436 | -0.557388 | -1.711874 | H | 2.772040 | -3.903067 | 0.818217 |
| O | -2.273130 | -1.693482 | -1.408865 | H | 1.035606 | -4.042757 | 0.890734 |
| N | -1.834326 | 0.533525 | -1.624263 | N | 0.604506 | -1.724555 | 1.733473 |
| H | -0.839047 | 0.396208 | -1.346769 | C | 0.498788 | -0.410273 | 2.005815 |
| C | -2.284067 | 1.853278 | -1.745246 | H | -0.520211 | -0.052004 | 2.129579 |
| O | -1.504215 | 2.769397 | -1.623860 | N | 1.481452 | 0.471186 | 2.116495 |
| C | -5.932922 | 4.828757 | -1.308601 | C | 2.676210 | -0.111117 | 1.953818 |
| H | -7.015277 | 4.966177 | -1.302687 | H | -5.469467 | 1.149985 | -2.555663 |
| C | -5.481637 | 3.771123 | -2.321577 | O | -5.177896 | 0.933104 | -0.636516 |
| H | -6.187146 | 2.939042 | -2.288578 | O | -4.224433 | 0.659342 | 0.324976 |
| H | -5.431835 | 4.175223 | -3.333595 | O | -4.809380 | -1.420994 | -1.999293 |
| O | -5.360694 | 6.094701 | -1.565223 | H | -4.208387 | -2.165447 | -1.819343 |
| O | 7.668081 | -2.501969 | -3.198112 | H | 7.635011 | -3.194964 | -3.865096 |
| C | 8.123327 | -1.305877 | -3.803135 | H | -4.411083 | 6.034085 | -1.400235 |
| H | 9.189840 | -1.375087 | -4.064247 | H | -8.033911 | -3.871329 | 3.380617 |
| H | 7.554117 | -1.072837 | -4.711406 | H | 7.480047 | 3.368739 | 4.270365 |
| C | 7.926473 | -0.157151 | -2.829095 | H | -10.039348 | 1.291823 | -0.413179 |
| H | 8.420634 | 0.733476 | -3.234488 | H | 11.173534 | 1.899685 | 0.566984 |



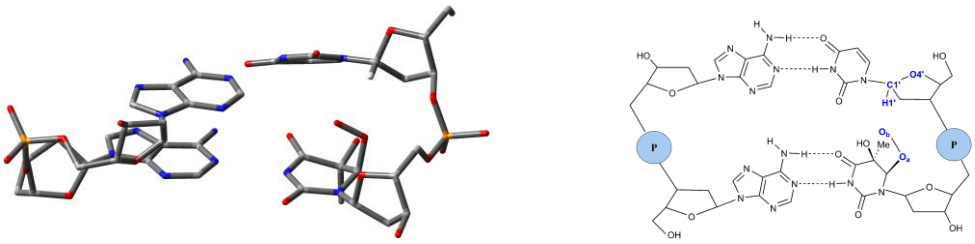


ds - 5' T T* 3' - Product

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z | | | | |
|---|---|---|---|---|---|---|---|
| O | -8.306087 | -2.688171 | 3.078049 | C | 6.214561 | -0.607287 | -1.204312 |
| C | -7.972694 | -1.514162 | 3.790201 | H | 5.869839 | 0.391818 | -0.906817 |
| H | -8.862611 | -0.902258 | 4.000524 | C | 8.550275 | -0.790493 | -0.763912 |
| H | -7.471885 | -1.740034 | 4.740240 | H | 9.367376 | -1.445858 | -0.453826 |
| C | -7.020075 | -0.706795 | 2.932804 | C | 7.203592 | -1.211640 | -0.201822 |
| H | -6.872305 | 0.285503 | 3.370722 | H | 7.157752 | -2.299549 | -0.221988 |
| O | -5.760393 | -1.381806 | 2.885282 | H | 7.041124 | -0.891491 | 0.826520 |
| C | -5.450133 | -1.638701 | 1.578691 | O | 8.886067 | 0.572808 | -0.411535 |
| N | -4.348490 | -2.493762 | 1.377459 | N | 5.017815 | -1.399472 | -1.366361 |
| C | -4.437544 | -3.615092 | 0.567607 | C | 4.893572 | -2.772561 | -1.367756 |
| H | -5.446636 | -3.877368 | 0.267708 | H | 5.767368 | -3.407437 | -1.326560 |
| C | -3.367517 | -4.328613 | 0.161679 | N | 3.659984 | -3.190389 | -1.462821 |
| C | -3.439249 | -5.509079 | -0.755224 | C | 2.924725 | -2.026101 | -1.543399 |
| H | -2.893083 | -5.294974 | -1.678975 | C | 1.534849 | -1.794624 | -1.607027 |
| H | -2.963865 | -6.380956 | -0.298097 | N | 0.643503 | -2.790557 | -1.635433 |
| H | -4.473545 | -5.756082 | -1.003629 | H | 0.966711 | -3.729294 | -1.463700 |
| C | -2.042130 | -3.891176 | 0.600825 | H | -0.345941 | -2.589855 | -1.513547 |
| O | -0.992486 | -4.436918 | 0.269440 | N | 1.120338 | -0.513346 | -1.641376 |
| N | -2.031418 | -2.798393 | 1.441841 | C | 2.027620 | 0.478201 | -1.589760 |
| H | -1.098403 | -2.321604 | 1.571391 | H | 1.602760 | 1.479937 | -1.617029 |
| C | -3.098508 | -2.032318 | 1.809858 | N | 3.347112 | 0.379471 | -1.501349 |
| O | -2.978979 | -1.004231 | 2.459765 | C | 3.740427 | -0.903136 | -1.484524 |
| C | -7.492895 | -0.570694 | 1.474787 | P | 8.990782 | 0.948841 | 1.143669 |
| H | -8.574753 | -0.700768 | 1.378913 | O | 9.997832 | 2.194466 | 1.122736 |
| C | -6.683668 | -1.636636 | 0.738240 | O | 9.321353 | -0.170099 | 2.031604 |
| H | -7.237320 | -2.584887 | 0.812258 | O | 7.610758 | 1.678084 | 1.483883 |
| H | -6.494622 | -1.386707 | -0.306271 | C | 7.297409 | 2.926176 | 0.838742 |
| O | -7.126291 | 0.756016 | 1.043060 | H | 7.998185 | 3.690444 | 1.188855 |
| P | -7.644930 | 1.270724 | -0.372518 | H | 7.395497 | 2.812903 | -0.246442 |
| O | -9.091614 | 1.854790 | 0.031818 | C | 5.887378 | 3.329496 | 1.189539 |
| O | -7.684743 | 0.336739 | -1.508178 | H | 5.752779 | 4.371968 | 0.859677 |
| O | -6.724345 | 2.528231 | -0.668162 | O | 4.971223 | 2.474058 | 0.525525 |
| C | -6.129151 | 3.364870 | 0.333266 | C | 3.773797 | 2.368787 | 1.277730 |
| H | -6.915882 | 3.982172 | 0.782095 | H | 2.914542 | 2.686752 | 0.680570 |
| H | -5.652120 | 2.740403 | 1.092066 | C | 5.495153 | 3.254036 | 2.669073 |
| C | -5.080314 | 4.248489 | -0.325484 | H | 5.867579 | 2.312758 | 3.094676 |
| H | -4.894695 | 5.089934 | 0.353470 | C | 3.977275 | 3.216404 | 2.538963 |
| O | -3.850607 | 3.567938 | -0.519481 | H | 3.458094 | 2.798775 | 3.401787 |
| C | -3.645509 | 3.230040 | -1.892491 | H | 3.622953 | 4.238297 | 2.371017 |
| H | -2.753813 | 3.758286 | -2.234597 | O | 5.925360 | 4.368734 | 3.410917 |
| N | -3.319584 | 1.821493 | -2.044704 | N | 3.556638 | 0.957374 | 1.561529 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -4.319190 | 0.834077 | -1.675948 | C | 4.507213 | -0.032298 | 1.630077 |
| C | -3.917642 | -0.544836 | -2.218455 | H | 5.556676 | 0.229876 | 1.652465 |
| C | -4.045708 | -0.559075 | -3.747311 | N | 4.011711 | -1.242987 | 1.650157 |
| H | -3.465052 | 0.239484 | -4.214208 | C | 2.647347 | -1.037641 | 1.590868 |
| H | -3.700994 | -1.523619 | -4.128039 | C | 1.547183 | -1.913189 | 1.477596 |
| H | -5.102426 | -0.440314 | -4.000033 | N | 1.667839 | -3.251391 | 1.402451 |
| C | -2.477099 | -0.852563 | -1.854141 | H | 2.587043 | -3.623540 | 1.213297 |
| O | -2.156920 | -2.010431 | -1.598840 | H | 0.853515 | -3.775686 | 1.088744 |
| N | -1.604719 | 0.172428 | -1.939021 | N | 0.320974 | -1.365327 | 1.435376 |
| H | -0.583617 | -0.033793 | -1.799864 | C | 0.176234 | -0.027908 | 1.421815 |
| C | -1.955224 | 1.522590 | -1.982473 | H | -0.851833 | 0.325868 | 1.376555 |
| O | -1.083645 | 2.365247 | -2.015961 | N | 1.132458 | 0.887358 | 1.448436 |
| C | -5.456128 | 4.787563 | -1.715849 | C | 2.343581 | 0.321256 | 1.535208 |
| H | -6.532729 | 4.928947 | -1.836346 | H | -5.288759 | 1.098058 | -2.105904 |
| C | -4.895451 | 3.705448 | -2.644026 | O | -4.590363 | 0.821865 | -0.300707 |
| H | -5.627410 | 2.908019 | -2.773655 | O | -3.344775 | 0.528325 | 0.331541 |
| H | -4.644850 | 4.121005 | -3.621304 | O | -4.735340 | -1.529888 | -1.653895 |
| O | -4.859059 | 6.048435 | -1.944232 | H | -4.154341 | -2.299304 | -1.521166 |
| O | 8.078911 | -3.171463 | -2.201128 | H | 8.172299 | -3.987345 | -2.702992 |
| C | 8.654055 | -2.110717 | -2.941875 | H | -3.917594 | 5.972417 | -1.742156 |
| H | 9.749235 | -2.205644 | -2.983244 | H | -8.780551 | -3.286192 | 3.663586 |
| H | 8.265355 | -2.079463 | -3.967253 | H | 6.794827 | 4.177311 | 3.776050 |
| C | 8.296664 | -0.794804 | -2.273410 | H | -9.691470 | 1.819609 | -0.724808 |
| H | 8.873629 | 0.007358 | -2.747922 | H | 10.918856 | 1.913301 | 1.196274 |
| O | 6.914094 | -0.517933 | -2.437845 | H | -3.629915 | 0.211689 | 1.210867 |

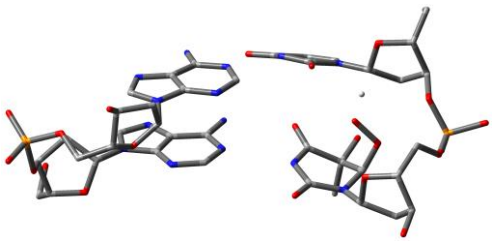


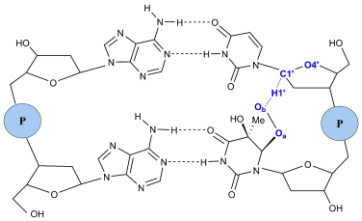
ds - 5' U T* 3' - Reactant

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z | | | | |
|---|---|---|---|---|---|---|---|
| O | -8.753365 | -2.890697 | 2.647270 | C | 8.505123 | -0.788786 | -0.840111 |
| C | -8.376867 | -1.832920 | 3.507280 | H | 9.334336 | -1.441512 | -0.558265 |
| H | -9.225341 | -1.164104 | 3.715454 | C | 7.174791 | -1.230923 | -0.255991 |
| H | -7.979920 | -2.202836 | 4.460874 | H | 7.136874 | -2.318639 | -0.293066 |
| C | -7.284635 | -1.043700 | 2.815199 | H | 7.033474 | -0.929597 | 0.781030 |
| H | -7.124355 | -0.087658 | 3.331988 | O | 8.835240 | 0.571472 | -0.471293 |
| O | -6.092354 | -1.819462 | 2.821375 | N | 4.965731 | -1.417751 | -1.377748 |
| C | -5.482870 | -1.600471 | 1.554428 | C | 4.853840 | -2.791499 | -1.398593 |
| H | -5.047638 | -0.598453 | 1.541895 | H | 5.733327 | -3.419337 | -1.381381 |
| N | -4.378913 | -2.506411 | 1.324537 | N | 3.622425 | -3.219341 | -1.479305 |
| C | -4.482157 | -3.648798 | 0.567311 | C | 2.876109 | -2.060968 | -1.529048 |
| H | -5.489845 | -3.919168 | 0.276335 | C | 1.483642 | -1.843705 | -1.576748 |
| C | -3.417148 | -4.387514 | 0.195448 | N | 0.604665 | -2.849189 | -1.618039 |
| C | -2.079546 | -3.956599 | 0.584468 | H | 0.938900 | -3.787194 | -1.463001 |
| O | -1.030993 | -4.504289 | 0.251459 | H | -0.386676 | -2.669707 | -1.490527 |
| N | -2.062298 | -2.844593 | 1.397865 | N | 1.056894 | -0.565102 | -1.586564 |
| H | -1.125685 | -2.411306 | 1.584207 | C | 1.955535 | 0.435215 | -1.523167 |
| C | -3.128449 | -2.083038 | 1.811344 | H | 1.520658 | 1.432897 | -1.528272 |
| O | -3.005049 | -1.110244 | 2.523297 | N | 3.275652 | 0.347320 | -1.450918 |
| C | -7.616736 | -0.762590 | 1.326955 | C | 3.682270 | -0.931844 | -1.463856 |
| H | -8.671250 | -0.929643 | 1.095893 | P | 8.979125 | 0.917727 | 1.088666 |
| C | -6.664046 | -1.691042 | 0.597213 | O | 9.971882 | 2.174575 | 1.062692 |
| H | -7.103677 | -2.692332 | 0.638620 | O | 9.340604 | -0.218381 | 1.941456 |
| H | -6.456992 | -1.392135 | -0.428969 | O | 7.605451 | 1.629783 | 1.485175 |
| O | -7.274148 | 0.622010 | 1.043274 | C | 7.266278 | 2.893136 | 0.884980 |
| P | -7.710728 | 1.221232 | -0.364738 | H | 7.967039 | 3.653550 | 1.243062 |
| O | -9.125508 | 1.891098 | 0.008597 | H | 7.341633 | 2.813902 | -0.204983 |
| O | -7.754688 | 0.339770 | -1.541572 | C | 5.860940 | 3.271872 | 1.279095 |
| O | -6.700283 | 2.429047 | -0.593195 | H | 5.709521 | 4.322744 | 0.984660 |
| C | -6.127654 | 3.227003 | 0.448174 | O | 4.936555 | 2.428716 | 0.610228 |
| H | -6.910330 | 3.854112 | 0.890426 | C | 3.757736 | 2.290282 | 1.386546 |
| H | -5.689952 | 2.575090 | 1.209799 | H | 2.882530 | 2.619214 | 0.819178 |
| C | -5.041167 | 4.089731 | -0.171157 | C | 5.503426 | 3.148752 | 2.764507 |
| H | -4.786849 | 4.874550 | 0.551815 | H | 5.893446 | 2.199166 | 3.154164 |
| O | -3.872369 | 3.323997 | -0.431320 | C | 3.983199 | 3.101138 | 2.667884 |
| C | -3.658870 | 3.142984 | -1.830060 | H | 3.487325 | 2.652585 | 3.528844 |
| H | -2.762131 | 3.694691 | -2.117904 | H | 3.616643 | 4.124425 | 2.539493 |
| N | -3.335440 | 1.748429 | -2.104384 | O | 5.941467 | 4.245700 | 3.527724 |
| C | -4.328240 | 0.752428 | -1.848148 | N | 3.558569 | 0.869454 | 1.631866 |
| C | -3.921945 | -0.611561 | -2.413436 | C | 4.517128 | -0.114183 | 1.641742 |
| C | -3.968664 | -0.578296 | -3.945197 | H | 5.564335 | 0.156871 | 1.643171 |

| | | | |
|---|---|---|---|
| H | -3.343188 | 0.216078 | -4.357790 |
| H | -3.626595 | -1.542300 | -4.328242 |
| H | -5.005997 | -0.427813 | -4.253991 |
| C | -2.500867 | -0.930917 | -1.972763 |
| O | -2.210275 | -2.087693 | -1.697688 |
| N | -1.617531 | 0.089895 | -2.007766 |
| H | -0.596763 | -0.125090 | -1.812525 |
| C | -1.964943 | 1.436748 | -2.010143 |
| O | -1.103607 | 2.286317 | -1.973210 |
| C | -5.407668 | 4.735678 | -1.519744 |
| H | -6.480145 | 4.920733 | -1.614930 |
| C | -4.900865 | 3.699867 | -2.529934 |
| H | -5.662111 | 2.936164 | -2.690613 |
| H | -4.654277 | 4.169250 | -3.483397 |
| O | -4.773595 | 5.988633 | -1.673298 |
| O | 8.015895 | -3.148251 | -2.308208 |
| C | 8.570992 | -2.071927 | -3.041395 |
| H | 9.665768 | -2.159215 | -3.104960 |
| H | 8.162955 | -2.025706 | -4.058731 |
| C | 8.218847 | -0.770030 | -2.343487 |
| H | 8.779217 | 0.044266 | -2.817156 |
| O | 6.830942 | -0.500621 | -2.472899 |
| C | 6.159326 | -0.617691 | -1.226356 |
| H | 5.812707 | 0.373022 | -0.904543 |
| N | 4.031160 | -1.328698 | 1.639214 |
| C | 2.663886 | -1.132973 | 1.627962 |
| C | 1.564988 | -2.011445 | 1.518827 |
| N | 1.685816 | -3.344861 | 1.380130 |
| H | 2.594303 | -3.704507 | 1.124926 |
| H | 0.856744 | -3.857176 | 1.084507 |
| N | 0.336482 | -1.469870 | 1.548346 |
| C | 0.182047 | -0.135704 | 1.594091 |
| H | -0.850886 | 0.206196 | 1.619946 |
| N | 1.133179 | 0.786576 | 1.607950 |
| C | 2.349093 | 0.225350 | 1.626273 |
| H | -5.308232 | 1.037632 | -2.236548 |
| O | -4.601403 | 0.611575 | -0.419124 |
| O | -3.503788 | 0.481247 | 0.265596 |
| O | -4.777430 | -1.599212 | -1.918758 |
| H | -4.207462 | -2.355425 | -1.688775 |
| H | 8.113103 | -3.956878 | -2.821011 |
| H | -3.832432 | 5.878726 | -1.487128 |
| H | -9.323258 | -3.497874 | 3.128548 |
| H | 6.814729 | 4.046083 | 3.879935 |
| H | -9.691090 | 1.945115 | -0.773090 |
| H | 10.898347 | 1.905720 | 1.017482 |
| H | -3.524125 | -5.279685 | -0.404624 |



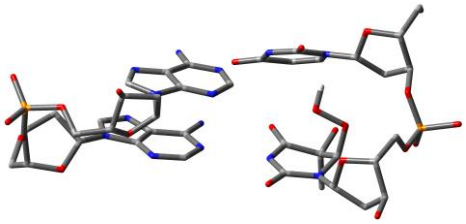


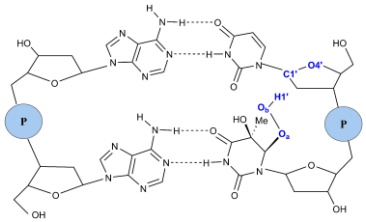
ds - 5' U T* 3' - TS

## Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z | | | | |
|---|---|---|---|---|---|---|---|
| O | -7.719559 | -3.419987 | 2.624226 | C | 8.415654 | -0.454270 | -1.398696 |
| C | -7.556206 | -2.313445 | 3.488769 | H | 9.27382 | -1.129615 | -1.376509 |
| H | -8.525507 | -1.921720 | 3.830861 | C | 7.193586 | -1.022527 | -0.697725 |
| H | -6.952477 | -2.569865 | 4.368251 | H | 7.14851 | -2.087568 | -0.917795 |
| C | -6.835192 | -1.220974 | 2.723405 | H | 7.22518 | -0.906112 | 0.384563 |
| H | -6.837637 | -0.296154 | 3.309167 | O | 8.813098 | 0.823030 | -0.846671 |
| O | -5.485565 | -1.627611 | 2.502151 | N | 4.83407 | -1.062587 | -1.484097 |
| C | -5.210131 | -1.676028 | 1.144011 | C | 4.712823 | -2.417936 | -1.702651 |
| H | -4.718269 | -0.568010 | 0.798071 | H | 5.583613 | -3.035287 | -1.868769 |
| N | -4.141134 | -2.598215 | 0.877344 | N | 3.477304 | -2.841350 | -1.723280 |
| C | -4.272501 | -3.747065 | 0.132651 | C | 2.736017 | -1.695780 | -1.524600 |
| H | -5.280429 | -3.976364 | -0.193197 | C | 1.345821 | -1.485052 | -1.413735 |
| C | -3.223387 | -4.532874 | -0.179657 | N | 0.467148 | -2.487148 | -1.505761 |
| C | -1.886210 | -4.168926 | 0.282698 | H | 0.8008 | -3.436885 | -1.547446 |
| O | -0.855564 | -4.774290 | 0.001906 | H | -0.518976 | -2.310514 | -1.344198 |
| N | -1.848990 | -3.056874 | 1.097083 | N | 0.916868 | -0.223887 | -1.208212 |
| H | -0.903567 | -2.678080 | 1.373337 | C | 1.825263 | 0.760840 | -1.078510 |
| C | -2.876740 | -2.188287 | 1.350526 | H | 1.401256 | 1.747940 | -0.906490 |
| O | -2.733923 | -1.139299 | 1.941382 | N | 3.147922 | 0.676763 | -1.130303 |
| C | -7.428278 | -0.957894 | 1.332160 | C | 3.54913 | -0.581510 | -1.369892 |
| H | -8.487070 | -1.225487 | 1.267547 | P | 9.202532 | 0.880961 | 0.708364 |
| C | -6.537321 | -1.789405 | 0.413364 | O | 10.156143 | 2.166833 | 0.766089 |
| H | -6.909065 | -2.818681 | 0.443688 | O | 9.722734 | -0.371802 | 1.264463 |
| H | -6.501446 | -1.414270 | -0.609418 | O | 7.894688 | 1.435251 | 1.438856 |
| O | -7.266485 | 0.449456 | 1.095577 | C | 7.421041 | 2.754457 | 1.115174 |
| P | -7.948893 | 1.161509 | -0.161013 | H | 8.130753 | 3.490616 | 1.505308 |
| O | -9.471939 | 1.304322 | 0.346238 | H | 7.347526 | 2.862620 | 0.027445 |
| O | -7.879748 | 0.529350 | -1.490856 | C | 6.067959 | 2.966641 | 1.744879 |
| O | -7.350324 | 2.625723 | -0.078288 | H | 5.825006 | 4.037282 | 1.649220 |
| C | -6.342218 | 3.106720 | 0.831795 | O | 5.10608 | 2.171654 | 1.072669 |
| H | -6.871495 | 3.615715 | 1.642206 | C | 4.020394 | 1.894625 | 1.943711 |
| H | -5.753274 | 2.276066 | 1.226978 | H | 3.091444 | 2.316225 | 1.548972 |
| C | -5.402496 | 4.090031 | 0.128708 | C | 5.921764 | 2.583725 | 3.220857 |
| H | -5.145350 | 4.871822 | 0.853037 | H | 6.393442 | 1.606196 | 3.387844 |
| O | -4.182495 | 3.481145 | -0.280335 | C | 4.40445 | 2.469617 | 3.314982 |
| C | -4.133163 | 3.317379 | -1.697853 | H | 4.047662 | 1.845901 | 4.134715 |
| H | -3.363545 | 3.986414 | -2.090674 | H | 3.994506 | 3.477373 | 3.433160 |
| N | -3.671671 | 1.973853 | -2.023684 | O | 6.419821 | 3.562404 | 4.099061 |
| C | -4.630706 | 0.894816 | -1.939863 | N | 3.823325 | 0.454244 | 1.950914 |
| C | -4.005202 | -0.414128 | -2.422564 | C | 4.763082 | -0.522413 | 1.725029 |
| C | -3.786004 | -0.352657 | -3.941560 | H | 5.812709 | -0.262965 | 1.687357 |

| | | | |
|---|---|---|---|
| H | -3.182013 | 0.508737 | -4.233482 |
| H | -3.285425 | -1.268307 | -4.266141 |
| H | -4.762270 | -0.295989 | -4.428602 |
| C | -2.654796 | -0.632117 | -1.771409 |
| O | -2.309653 | -1.777258 | -1.499436 |
| N | -1.867025 | 0.454422 | -1.649899 |
| H | -0.870010 | 0.307883 | -1.376980 |
| C | -2.315114 | 1.777051 | -1.733195 |
| O | -1.533885 | 2.688482 | -1.586991 |
| C | -5.952054 | 4.734929 | -1.152683 |
| H | -7.033042 | 4.879983 | -1.128101 |
| C | -5.520600 | 3.711243 | -2.208049 |
| H | -6.225535 | 2.877886 | -2.188758 |
| H | -5.488178 | 4.147689 | -3.207287 |
| O | -5.372334 | 6.004740 | -1.370533 |
| O | 7.653231 | -2.517473 | -3.172544 |
| C | 8.103469 | -1.318939 | -3.776430 |
| H | 9.172504 | -1.380104 | -4.029057 |
| H | 7.539596 | -1.092497 | -4.689707 |
| C | 7.889765 | -0.169399 | -2.806890 |
| H | 8.379479 | 0.724149 | -3.211220 |
| O | 6.505336 | 0.102688 | -2.656207 |
| C | 6.037410 | -0.270605 | -1.366870 |
| H | 5.745061 | 0.630624 | -0.813270 |
| N | 4.256536 | -1.717328 | 1.562310 |
| C | 2.896082 | -1.516476 | 1.690577 |
| C | 1.77727 | -2.356552 | 1.503898 |
| N | 1.877813 | -3.647568 | 1.137668 |
| H | 2.763268 | -3.951936 | 0.759012 |
| H | 1.031033 | -4.121381 | 0.830721 |
| N | 0.560521 | -1.818263 | 1.689509 |
| C | 0.433567 | -0.507348 | 1.969034 |
| H | -0.591301 | -0.164722 | 2.087907 |
| N | 1.401951 | 0.388197 | 2.090705 |
| C | 2.606336 | -0.175562 | 1.934288 |
| H | -5.500182 | 1.103170 | -2.568721 |
| O | -5.216117 | 0.826438 | -0.656399 |
| O | -4.26534 | 0.525899 | 0.300360 |
| O | -4.840835 | -1.487044 | -2.093471 |
| H | -4.237374 | -2.235069 | -1.937952 |
| H | 7.628232 | -3.211285 | -3.839014 |
| H | -4.422517 | 5.932844 | -1.211369 |
| H | -8.045803 | -4.168713 | 3.132803 |
| H | 7.347113 | 3.373319 | 4.275924 |
| H | -10.07343 | 1.198705 | -0.402094 |
| H | 11.08118 | 1.934763 | 0.613594 |
| H | -3.339812 | -5.427862 | -0.773855 |



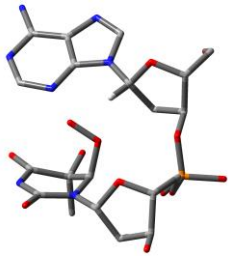


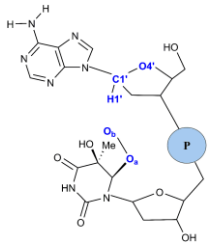
ds - 5' U T* 3' - Product

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) | | | | | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | | | |
| O | -8.297406 | -2.950562 | 2.989246 | H | 9.332904 | -1.413944 | -0.444688 |
| C | -7.976333 | -1.793335 | 3.733777 | C | 7.164130 | -1.202001 | -0.216539 |
| H | -8.873060 | -1.199879 | 3.966265 | H | 7.127197 | -2.289494 | -0.261125 |
| H | -7.467308 | -2.040098 | 4.674143 | H | 6.985328 | -0.906568 | 0.816338 |
| C | -7.039086 | -0.948909 | 2.895152 | O | 8.835379 | 0.599344 | -0.361040 |
| H | -6.898356 | 0.031185 | 3.361553 | N | 4.996525 | -1.381580 | -1.416688 |
| O | -5.772050 | -1.608149 | 2.818816 | C | 4.885638 | -2.755125 | -1.457027 |
| C | -5.472905 | -1.832524 | 1.504750 | H | 5.764928 | -3.382705 | -1.422326 |
| N | -4.369189 | -2.678669 | 1.275141 | N | 3.657124 | -3.181645 | -1.577472 |
| C | -4.458334 | -3.789775 | 0.460496 | C | 2.911588 | -2.022476 | -1.634947 |
| H | -5.467900 | -4.062209 | 0.174761 | C | 1.519656 | -1.803042 | -1.702272 |
| C | -3.379082 | -4.481216 | 0.042186 | N | 0.639312 | -2.807213 | -1.762986 |
| C | -2.048074 | -4.044836 | 0.444305 | H | 0.973615 | -3.747712 | -1.625248 |
| O | -0.992996 | -4.559081 | 0.088702 | H | -0.352203 | -2.621075 | -1.635188 |
| N | -2.043036 | -2.960505 | 1.304084 | N | 1.092614 | -0.525097 | -1.703475 |
| H | -1.116179 | -2.467610 | 1.427944 | C | 1.990200 | 0.472691 | -1.615988 |
| C | -3.112209 | -2.216072 | 1.701666 | H | 1.556426 | 1.471108 | -1.617499 |
| O | -2.999379 | -1.202382 | 2.373407 | N | 3.309760 | 0.384622 | -1.519004 |
| C | -7.522427 | -0.774313 | 1.444747 | C | 3.715611 | -0.894259 | -1.535457 |
| H | -8.604139 | -0.908243 | 1.352151 | P | 8.916587 | 0.938600 | 1.204050 |
| C | -6.711797 | -1.814208 | 0.672776 | O | 9.910603 | 2.194836 | 1.224930 |
| H | -7.260125 | -2.767014 | 0.723813 | O | 9.248420 | -0.196891 | 2.069891 |
| H | -6.529972 | -1.533503 | -0.365338 | O | 7.524224 | 1.644376 | 1.544119 |
| O | -7.166017 | 0.565821 | 1.049280 | C | 7.203569 | 2.903897 | 0.925358 |
| P | -7.695879 | 1.117892 | -0.348270 | H | 7.894412 | 3.666485 | 1.298050 |
| O | -9.149108 | 1.668734 | 0.078099 | H | 7.310462 | 2.816381 | -0.161407 |
| O | -7.726499 | 0.218233 | -1.511833 | C | 5.786732 | 3.284840 | 1.274930 |
| O | -6.793239 | 2.395441 | -0.606552 | H | 5.644187 | 4.334509 | 0.972147 |
| C | -6.203083 | 3.209436 | 0.416717 | O | 4.884713 | 2.438504 | 0.580477 |
| H | -6.996188 | 3.798555 | 0.891219 | C | 3.682683 | 2.299309 | 1.319970 |
| H | -5.709042 | 2.569048 | 1.150900 | H | 2.824553 | 2.624187 | 0.724865 |
| C | -5.174125 | 4.131699 | -0.220763 | C | 5.383732 | 3.165184 | 2.748628 |
| H | -5.001474 | 4.955502 | 0.482720 | H | 5.763347 | 2.217017 | 3.151800 |
| O | -3.931341 | 3.483572 | -0.441220 | C | 3.867233 | 3.113911 | 2.605671 |
| C | -3.730409 | 3.183531 | -1.823671 | H | 3.346779 | 2.666447 | 3.452596 |
| H | -2.849289 | 3.733972 | -2.157448 | H | 3.502162 | 4.135865 | 2.463349 |
| N | -3.383438 | 1.784340 | -2.013755 | O | 5.794787 | 4.264000 | 3.523956 |
| C | -4.364905 | 0.773140 | -1.660581 | N | 3.479534 | 0.878141 | 1.562447 |
| C | -3.944576 | -0.587964 | -2.231771 | C | 4.442281 | -0.100389 | 1.616745 |
| C | -4.085607 | -0.577497 | -3.759314 | H | 5.487761 | 0.175012 | 1.660345 |
| H | -3.522356 | 0.239053 | -4.216313 | N | 3.963434 | -1.317660 | 1.596059 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -3.727429 | -1.528938 | -4.160138 | C | 2.597280 | -1.129041 | 1.523139 |
| H | -5.146258 | -0.472287 | -4.001338 | C | 1.510542 | -2.015380 | 1.370331 |
| C | -2.496391 | -0.877194 | -1.884186 | N | 1.649661 | -3.349193 | 1.258337 |
| O | -2.156716 | -2.033084 | -1.649326 | H | 2.575246 | -3.703866 | 1.066628 |
| N | -1.640520 | 0.162501 | -1.959602 | H | 0.845746 | -3.875773 | 0.922215 |
| H | -0.616456 | -0.035700 | -1.836358 | N | 0.277724 | -1.482398 | 1.327208 |
| C | -2.013174 | 1.506953 | -1.971477 | C | 0.115196 | -0.147063 | 1.348917 |
| O | -1.156548 | 2.364969 | -1.995371 | H | -0.916512 | 0.195209 | 1.298572 |
| C | -5.566430 | 4.704469 | -1.592924 | N | 1.058568 | 0.779309 | 1.413103 |
| H | -6.645768 | 4.831580 | -1.704412 | C | 2.275767 | 0.226969 | 1.500793 |
| C | -4.992689 | 3.658685 | -2.554503 | H | -5.340920 | 1.031360 | -2.079616 |
| H | -5.712036 | 2.853069 | -2.702129 | O | -4.627755 | 0.727467 | -0.284229 |
| H | -4.755329 | 4.105880 | -3.521072 | O | -3.373134 | 0.448367 | 0.336523 |
| O | -4.990898 | 5.980948 | -1.786750 | O | -4.738342 | -1.598477 | -1.676749 |
| O | 8.082405 | -3.106771 | -2.250393 | H | -4.144342 | -2.363800 | -1.580865 |
| C | 8.658780 | -2.024106 | -2.957608 | H | 8.191407 | -3.910178 | -2.768966 |
| H | 9.755191 | -2.109279 | -2.985858 | H | -4.048009 | 5.914998 | -1.587648 |
| H | 8.284065 | -1.971403 | -3.987296 | H | -8.764867 | -3.569652 | 3.558168 |
| C | 8.281741 | -0.727543 | -2.262777 | H | 6.664279 | 4.072988 | 3.890172 |
| H | 8.858832 | 0.090032 | -2.710159 | H | -9.751830 | 1.647514 | -0.676830 |
| O | 6.899528 | -0.456534 | -2.439047 | H | 10.832119 | 1.921354 | 1.318765 |
| C | 6.183446 | -0.582914 | -1.218199 | H | -3.648199 | 0.061528 | 1.190541 |
| H | 5.824399 | 0.405106 | -0.901980 | H | -3.470896 | -5.343204 | -0.603027 |
| C | 8.514982 | -0.757580 | -0.750342 | | | | |

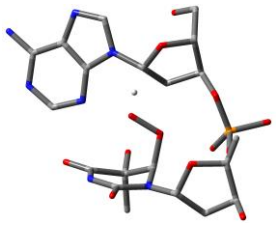


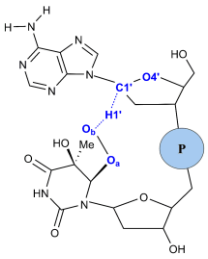


ss - 5' A T* 3' - Reactant

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| O | 3.022095 | 4.395092 | -0.011582 |
| C | 2.111143 | 4.523628 | -1.087565 |
| H | 1.488085 | 5.423545 | -0.979193 |
| H | 2.631105 | 4.571460 | -2.053005 |
| C | 1.212700 | 3.300362 | -1.096053 |
| H | 0.415428 | 3.451733 | -1.833101 |
| O | 1.965279 | 2.153120 | -1.456975 |
| C | 1.991736 | 1.202085 | -0.405425 |
| H | 1.354812 | 0.345791 | -0.642625 |
| C | 0.593062 | 2.994410 | 0.272581 |
| H | 0.490312 | 3.887752 | 0.896187 |
| C | 1.515418 | 1.934971 | 0.850207 |
| H | 2.364640 | 2.430475 | 1.326536 |
| H | 1.016118 | 1.263546 | 1.551925 |
| O | -0.720604 | 2.444816 | 0.010512 |
| P | -1.752261 | 2.305818 | 1.210471 |
| O | -2.088962 | 3.845859 | 1.528764 |
| O | -1.387981 | 1.512929 | 2.393639 |
| O | -3.018699 | 1.694072 | 0.472400 |
| C | -3.421449 | 1.965357 | -0.877095 |
| H | -3.962585 | 2.917373 | -0.899891 |
| H | -2.540175 | 2.013470 | -1.521688 |
| C | -4.318786 | 0.823442 | -1.319834 |
| H | -4.822187 | 1.124934 | -2.246727 |
| O | -3.533485 | -0.334652 | -1.577175 |
| C | -3.851083 | -1.393228 | -0.682327 |
| H | -4.402678 | -2.174979 | -1.211188 |
| N | -2.622385 | -2.029845 | -0.233524 |
| C | -1.546128 | -1.194271 | 0.200716 |
| C | -0.558199 | -1.911701 | 1.135133 |
| C | -1.228326 | -2.082188 | 2.503812 |
| H | -2.186606 | -2.603638 | 2.430218 |
| H | -0.554947 | -2.645242 | 3.152733 |
| H | -1.378261 | -1.083627 | 2.923989 |
| C | -0.221935 | -3.294499 | 0.584835 |
| O | 0.840311 | -3.838867 | 0.774515 |
| N | -1.262219 | -3.935123 | -0.059858 |
| H | -1.093424 | -4.883003 | -0.373050 |
| C | -2.443100 | -3.372418 | -0.532764 |
| O | -3.262207 | -4.049966 | -1.114721 |
| C | -5.376474 | 0.401392 | -0.279636 |
| H | -5.628941 | 1.220481 | 0.397679 |
| C | -4.683094 | -0.759103 | 0.436530 |
| H | -4.033471 | -0.385313 | 1.231807 |
| H | -5.405007 | -1.458780 | 0.861062 |
| O | -6.587212 | 0.017629 | -0.896547 |
| N | 3.346691 | 0.695913 | -0.306529 |
| C | 4.509973 | 1.427730 | -0.421179 |
| H | 4.458976 | 2.501591 | -0.541226 |
| N | 5.594228 | 0.700436 | -0.374639 |
| C | 5.120345 | -0.586510 | -0.218440 |
| C | 5.761263 | -1.835232 | -0.112039 |
| N | 7.103490 | -1.947276 | -0.140087 |
| H | 7.666848 | -1.134391 | -0.324169 |
| H | 7.511275 | -2.866890 | -0.130832 |
| N | 5.018146 | -2.941408 | 0.031905 |
| C | 3.687788 | -2.814986 | 0.086315 |
| H | 3.120265 | -3.729076 | 0.231193 |
| N | 2.963262 | -1.699133 | -0.006470 |
| C | 3.730366 | -0.612750 | -0.172080 |
| H | -1.943006 | -0.317599 | 0.710768 |
| O | -0.833950 | -0.616282 | -0.932419 |
| O | -0.113051 | -1.518475 | -1.537602 |
| O | 0.586630 | -1.143105 | 1.294555 |
| H | 1.350558 | -1.526085 | 0.792741 |
| H | -6.411615 | -0.725553 | -1.486951 |
| H | 3.640135 | 5.133029 | -0.032281 |
| H | -2.306853 | 3.960460 | 2.463369 |

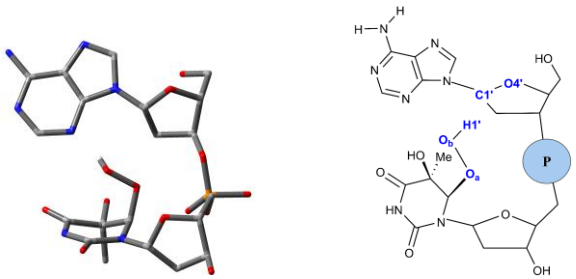





ss - 5' A T* 3 ' - TS

# Coordinates of optimized geometries

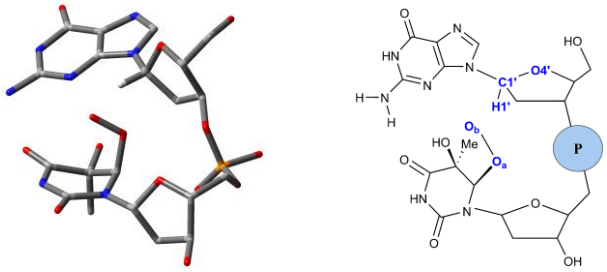
| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| O | 3.129733 | 3.783496 | 0.006351 |
| C | 2.177581 | 4.307610 | -0.894864 |
| H | 1.784355 | 5.277767 | -0.557188 |
| H | 2.596342 | 4.436392 | -1.902229 |
| C | 1.033416 | 3.315343 | -0.980162 |
| H | 0.244559 | 3.712727 | -1.624153 |
| O | 1.498906 | 2.094088 | -1.562802 |
| C | 1.744085 | 1.146491 | -0.586999 |
| H | 1.002131 | 0.119272 | -0.851945 |
| C | 0.462922 | 2.911769 | 0.379701 |
| H | 0.529225 | 3.716303 | 1.118899 |
| C | 1.275979 | 1.676490 | 0.768215 |
| H | 2.146115 | 1.975425 | 1.356835 |
| H | 0.684529 | 0.946505 | 1.327541 |
| O | -0.916139 | 2.597173 | 0.127422 |
| P | -1.913343 | 2.241700 | 1.315986 |
| O | -2.516586 | 3.698076 | 1.647237 |
| O | -1.407472 | 1.520078 | 2.490121 |
| O | -3.067794 | 1.450512 | 0.561803 |
| C | -3.494403 | 1.762396 | -0.772320 |
| H | -4.058253 | 2.702035 | -0.751108 |
| H | -2.618071 | 1.856059 | -1.418409 |
| C | -4.365379 | 0.626778 | -1.277672 |
| H | -4.894185 | 0.991163 | -2.167384 |
| O | -3.577147 | -0.490722 | -1.655238 |
| C | -3.720186 | -1.573282 | -0.738004 |
| H | -4.186157 | -2.406306 | -1.268398 |
| N | -2.425800 | -2.082191 | -0.321318 |
| C | -1.518936 | -1.227513 | 0.418379 |
| C | -0.481665 | -2.050222 | 1.203240 |
| C | -1.199867 | -2.768204 | 2.355938 |
| H | -2.033473 | -3.384292 | 2.009835 |
| H | -0.473425 | -3.393381 | 2.878689 |
| H | -1.567376 | -2.006430 | 3.048399 |
| C | 0.145135 | -3.120655 | 0.318332 |
| O | 1.252445 | -3.570725 | 0.507369 |
| N | -0.684979 | -3.623825 | -0.660539 |
| H | -0.326709 | -4.386001 | -1.221790 |
| C | -1.947314 | -3.171984 | -1.035714 |
| O | -2.572180 | -3.756100 | -1.895012 |
| C | -5.390191 | 0.080321 | -0.268122 |
| H | -5.716012 | 0.839218 | 0.447054 |
| C | -4.618594 | -1.063052 | 0.396390 |
| H | -4.038180 | -0.687376 | 1.239599 |
| H | -5.298697 | -1.838001 | 0.753790 |
| O | -6.557406 | -0.370370 | -0.925400 |
| N | 3.104771 | 0.703622 | -0.685489 |
| C | 4.114770 | 1.241839 | -1.464437 |
| H | 3.918666 | 2.102539 | -2.085110 |
| N | 5.249722 | 0.609389 | -1.361645 |
| C | 4.981912 | -0.414781 | -0.473563 |
| C | 5.762722 | -1.466243 | 0.040866 |
| N | 7.068536 | -1.601493 | -0.265642 |
| H | 7.466310 | -1.025711 | -0.989017 |
| H | 7.539084 | -2.441502 | 0.028687 |
| N | 5.194502 | -2.354113 | 0.870088 |
| C | 3.904926 | -2.203054 | 1.182387 |
| H | 3.471919 | -2.958841 | 1.830573 |
| N | 3.070930 | -1.242396 | 0.782882 |
| C | 3.659153 | -0.378896 | -0.047681 |
| H | -2.088646 | -0.641503 | 1.139875 |
| O | -0.956322 | -0.215709 | -0.407317 |
| O | 0.112289 | -0.714636 | -1.135716 |
| O | 0.480905 | -1.209879 | 1.743934 |
| H | 1.364235 | -1.349534 | 1.323411 |
| H | -6.293870 | -0.998220 | -1.610227 |
| H | 3.936974 | 4.306371 | -0.034664 |
| H | -2.817266 | 3.737723 | 2.564791 |




ss - 5' A T* 3' - Product

# Coordinates of optimized geometries

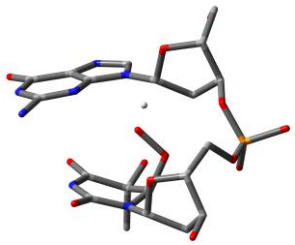
| Atom | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| O | 3.449591 | 3.789946 | 0.714990 |
| C | 2.601420 | 4.530056 | -0.137530 |
| H | 2.155290 | 5.395566 | 0.374418 |
| H | 3.135330 | 4.890570 | -1.027245 |
| C | 1.492991 | 3.600350 | -0.593333 |
| H | 0.802866 | 4.135757 | -1.250872 |
| O | 2.070014 | 2.520593 | -1.332833 |
| C | 2.110304 | 1.396606 | -0.555834 |
| H | 0.877103 | -1.219725 | -0.443965 |
| C | 0.731617 | 2.932470 | 0.554915 |
| H | 0.677406 | 3.568151 | 1.443869 |
| C | 1.477971 | 1.621863 | 0.790445 |
| H | 2.256932 | 1.768652 | 1.546787 |
| H | 0.805218 | 0.822247 | 1.114684 |
| O | -0.592718 | 2.677517 | 0.049814 |
| P | -1.759597 | 2.390768 | 1.091163 |
| O | -2.276854 | 3.885505 | 1.397498 |
| O | -1.463233 | 1.615739 | 2.304860 |
| O | -2.869968 | 1.714154 | 0.182913 |
| C | -2.975372 | 1.867679 | -1.241498 |
| H | -3.359127 | 2.871136 | -1.457873 |
| H | -1.991055 | 1.725234 | -1.692900 |
| C | -3.931926 | 0.809416 | -1.762668 |
| H | -4.241292 | 1.113520 | -2.770220 |
| O | -3.299460 | -0.457012 | -1.858927 |
| C | -3.752714 | -1.351267 | -0.847240 |
| H | -4.267928 | -2.181611 | -1.333151 |
| N | -2.633357 | -1.968514 | -0.153105 |
| C | -1.676759 | -1.123808 | 0.545313 |
| C | -0.885010 | -1.931764 | 1.588505 |
| C | -1.783909 | -2.236042 | 2.791896 |
| H | -2.708865 | -2.735685 | 2.491808 |
| H | -1.242026 | -2.868588 | 3.498526 |
| H | -2.018489 | -1.284476 | 3.275842 |
| C | -0.397841 | -3.246236 | 0.999333 |
| O | 0.654595 | -3.744017 | 1.351580 |
| N | -1.257411 | -3.860707 | 0.136064 |
| H | -0.986500 | -4.762390 | -0.236161 |
| C | -2.337992 | -3.266797 | -0.527279 |
| O | -2.977178 | -3.921983 | -1.321526 |
| C | -5.178660 | 0.571466 | -0.893012 |
| H | -5.489092 | 1.469095 | -0.352966 |
| C | -4.711493 | -0.548504 | 0.042147 |
| H | -4.203906 | -0.131397 | 0.913076 |
| H | -5.554629 | -1.155291 | 0.376372 |
| O | -6.282323 | 0.181791 | -1.684957 |
| N | 3.338842 | 0.721889 | -0.676057 |
| C | 4.546802 | 1.247691 | -1.105919 |
| H | 4.605771 | 2.286013 | -1.395890 |
| N | 5.523986 | 0.383773 | -1.108459 |
| C | 4.938568 | -0.778505 | -0.651674 |
| C | 5.442125 | -2.075415 | -0.440931 |
| N | 6.737782 | -2.375896 | -0.649544 |
| H | 7.345137 | -1.689228 | -1.064635 |
| H | 7.026628 | -3.336943 | -0.574098 |
| N | 4.609474 | -3.033539 | -0.011787 |
| C | 3.326755 | -2.721023 | 0.199372 |
| H | 2.687554 | -3.531797 | 0.534142 |
| N | 2.727220 | -1.534976 | 0.048956 |
| C | 3.585719 | -0.598147 | -0.382314 |
| H | -2.220301 | -0.340134 | 1.072684 |
| O | -0.835976 | -0.396579 | -0.312432 |
| O | 0.036656 | -1.324135 | -0.950481 |
| O | 0.224718 | -1.184020 | 1.997781 |
| H | 1.000431 | -1.767288 | 1.948756 |
| H | -6.004249 | -0.550115 | -2.250513 |
| H | 4.204960 | 4.331549 | 0.965320 |
| H | -2.663445 | 3.930929 | 2.281886 |

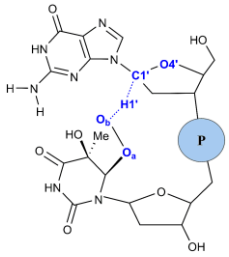



ss - 5' G T* 3' - Reactant

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| O | 0.843605 | 4.894452 | -1.691276 |
| C | 0.081148 | 3.885201 | -2.310245 |
| H | -0.965807 | 4.203447 | -2.289182 |
| H | 0.374479 | 3.737860 | -3.358359 |
| C | 0.221785 | 2.575089 | -1.557577 |
| H | -0.326433 | 1.760717 | -2.052548 |
| O | 1.608438 | 2.277991 | -1.485458 |
| C | 1.771954 | 1.348824 | -0.426746 |
| H | 1.541222 | 0.337769 | -0.767355 |
| H | 6.593798 | -2.198052 | 0.334533 |
| C | -0.234879 | 2.652084 | -0.090960 |
| H | -0.240435 | 3.691025 | 0.248410 |
| C | 0.795791 | 1.808616 | 0.671479 |
| H | 1.328406 | 2.419734 | 1.404670 |
| H | 0.359496 | 0.953004 | 1.190839 |
| O | -1.591678 | 2.165595 | -0.041760 |
| P | -2.361231 | 2.012708 | 1.338561 |
| O | -2.089439 | 3.395684 | 2.095862 |
| O | -2.028682 | 0.842003 | 2.180467 |
| O | -3.883252 | 2.119335 | 0.900877 |
| C | -4.399222 | 1.883632 | -0.414841 |
| H | -5.343084 | 2.430691 | -0.457026 |
| H | -3.707589 | 2.278794 | -1.162841 |
| C | -4.651688 | 0.411708 | -0.658459 |
| H | -5.296176 | 0.317564 | -1.546198 |
| O | -3.407662 | -0.237289 | -0.895181 |
| C | -3.541163 | -1.564585 | -0.410138 |
| H | -4.114788 | -2.180267 | -1.113639 |
| N | -2.226337 | -2.168025 | -0.329716 |
| C | -1.151282 | -1.369947 | 0.162858 |
| C | -0.011130 | -2.212013 | 0.749677 |
| C | -0.500445 | -2.839213 | 2.062555 |
| H | -1.392693 | -3.452732 | 1.918939 |
| H | 0.302864 | -3.450176 | 2.478413 |
| H | -0.725303 | -2.027580 | 2.759491 |
| C | 0.342440 | -3.338465 | -0.212504 |
| O | 1.468286 | -3.770726 | -0.347989 |
| N | -0.736022 | -3.914602 | -0.838653 |
| H | -0.556090 | -4.717207 | -1.429767 |
| C | -2.016922 | -3.370187 | -0.982580 |
| O | -2.869761 | -3.966140 | -1.600528 |
| C | -5.341376 | -0.340369 | 0.519866 |
| H | -5.567798 | 0.342408 | 1.340533 |
| C | -4.281564 | -1.376449 | 0.912666 |
| H | -3.594384 | -0.951774 | 1.652311 |
| H | -4.730052 | -2.292762 | 1.301260 |
| O | -6.577193 | -0.902940 | 0.137846 |
| N | 3.156994 | 1.342666 | -0.038388 |
| C | 3.950368 | 2.436767 | 0.255774 |
| N | 5.185275 | 2.118657 | 0.513727 |
| C | 5.218744 | 0.747918 | 0.389659 |
| C | 6.316034 | -0.173914 | 0.539105 |
| N | 5.854891 | -1.507257 | 0.296735 |
| C | 4.580475 | -1.895750 | -0.008572 |
| N | 3.588255 | -1.044344 | -0.144175 |
| C | 3.972347 | 0.248094 | 0.046776 |
| H | -1.509586 | -0.661162 | 0.911958 |
| O | -0.630989 | -0.490990 | -0.883219 |
| O | -0.061588 | -1.167705 | -1.839145 |
| O | 1.077356 | -1.395525 | 1.029474 |
| H | 1.845892 | -1.542943 | 0.433517 |
| H | -6.417008 | -1.605103 | -0.504524 |
| H | 1.753704 | 4.570551 | -1.680946 |
| H | -1.854189 | 3.240004 | 3.019960 |
| O | 7.480738 | 0.008995 | 0.809883 |
| N | 4.362893 | -3.218347 | -0.210839 |
| H | 3.388600 | -3.493702 | -0.284159 |
| H | 4.994546 | -3.884065 | 0.203443 |
| H | 3.541310 | 3.437916 | 0.243426 |

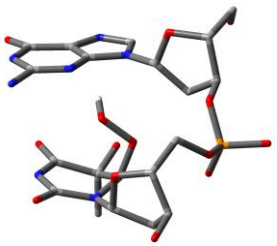


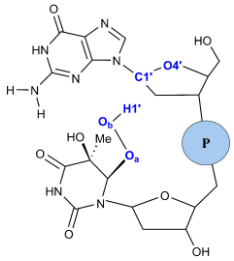



ss - 5' G T* 3' - TS

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| O | 1.845759 | 4.856730 | -0.123738 |
| C | 1.062670 | 4.841494 | -1.301155 |
| H | 0.362030 | 5.689033 | -1.330724 |
| H | 1.687386 | 4.872294 | -2.202194 |
| C | 0.271218 | 3.546416 | -1.328031 |
| H | -0.413911 | 3.550848 | -2.181209 |
| O | 1.182766 | 2.457259 | -1.478186 |
| C | 1.256246 | 1.713866 | -0.310379 |
| H | 0.620471 | 0.624852 | -0.525447 |
| H | 5.072255 | -2.843713 | -1.064591 |
| C | -0.495379 | 3.264610 | -0.031506 |
| H | -0.828316 | 4.179948 | 0.467877 |
| C | 0.491042 | 2.441014 | 0.784053 |
| H | 1.154389 | 3.117883 | 1.327792 |
| H | 0.007099 | 1.756835 | 1.481559 |
| O | -1.637169 | 2.475375 | -0.408864 |
| P | -2.769766 | 2.136896 | 0.665127 |
| O | -3.605009 | 3.514208 | 0.684198 |
| O | -2.392585 | 1.706753 | 2.022962 |
| O | -3.678061 | 1.106738 | -0.123556 |
| C | -3.467649 | 0.601255 | -1.452829 |
| H | -4.081737 | 1.207423 | -2.125201 |
| H | -2.413390 | 0.679601 | -1.727826 |
| C | -3.893740 | -0.864058 | -1.533073 |
| H | -4.309646 | -1.034149 | -2.533214 |
| O | -2.789852 | -1.749031 | -1.373961 |
| C | -2.850494 | -2.430620 | -0.122332 |
| H | -3.079971 | -3.481835 | -0.317477 |
| N | -1.530280 | -2.443853 | 0.497947 |
| C | -1.080600 | -1.241361 | 1.168773 |
| C | 0.256678 | -1.475445 | 1.890051 |
| C | -0.004182 | -2.267055 | 3.179252 |
| H | -0.523211 | -3.207059 | 2.974138 |
| H | 0.950326 | -2.482342 | 3.665015 |
| H | -0.611458 | -1.653127 | 3.848159 |
| C | 1.246590 | -2.277941 | 1.061897 |
| O | 2.441055 | -2.168600 | 1.262452 |
| N | 0.709915 | -3.169842 | 0.183087 |
| H | 1.355168 | -3.691670 | -0.404709 |
| C | -0.633296 | -3.259337 | -0.191675 |
| O | -0.966891 | -4.057917 | -1.037415 |
| C | -4.908475 | -1.316446 | -0.470884 |
| H | -5.586138 | -0.518194 | -0.164230 |
| C | -3.977557 | -1.761777 | 0.663114 |
| H | -3.641554 | -0.875770 | 1.204377 |
| H | -4.473932 | -2.450580 | 1.347973 |
| O | -5.713270 | -2.372745 | -0.951581 |
| N | 2.592499 | 1.300862 | -0.022640 |
| C | 3.538966 | 1.918161 | 0.783487 |
| H | 3.336519 | 2.872334 | 1.248427 |
| N | 4.647904 | 1.243074 | 0.873047 |
| C | 4.443178 | 0.129978 | 0.087819 |
| C | 5.279620 | -1.025620 | -0.134005 |
| N | 4.592913 | -1.956748 | -0.974363 |
| C | 3.332712 | -1.811508 | -1.475923 |
| N | 2.597124 | -0.752194 | -1.306610 |
| C | 3.184934 | 0.153577 | -0.485406 |
| H | -1.810641 | -0.933602 | 1.922077 |
| O | -1.100983 | -0.135898 | 0.290569 |
| O | -0.188030 | -0.321284 | -0.729177 |
| O | 0.838515 | -0.233251 | 2.174314 |
| H | 1.797589 | -0.391936 | 2.206623 |
| H | -5.139613 | -3.023349 | -1.375837 |
| H | 2.502942 | 5.556493 | -0.192714 |
| H | -3.937091 | 3.684982 | 1.575119 |
| O | 6.387165 | -1.294123 | 0.272490 |
| N | 2.798193 | -2.898837 | -2.146349 |
| H | 1.950190 | -2.639357 | -2.637388 |
| H | 3.440675 | -3.425439 | -2.723647 |

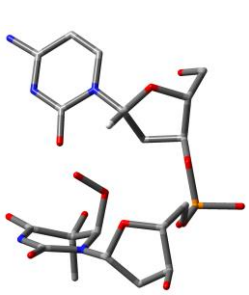


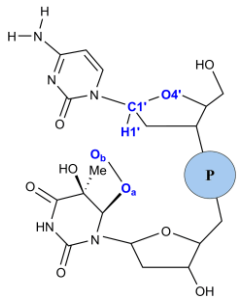



ss - 5' G T* 3' - Product

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| O | 2.254718 | 4.901722 | 0.277708 | C | -5.021090 | -0.613102 | -0.354327 |
| C | 1.533364 | 5.034476 | -0.931655 | H | -5.519632 | 0.326148 | -0.115511 |
| H | 0.845090 | 5.892028 | -0.899854 | C | -4.110084 | -1.108761 | 0.774612 |
| H | 2.205147 | 5.156571 | -1.790704 | H | -3.551230 | -0.266109 | 1.187343 |
| C | 0.727616 | 3.766221 | -1.139862 | H | -4.678074 | -1.593550 | 1.569851 |
| H | 0.094775 | 3.868333 | -2.026156 | O | -6.033656 | -1.545772 | -0.671278 |
| O | 1.630861 | 2.678545 | -1.347495 | N | 2.867552 | 1.234794 | -0.002846 |
| C | 1.630277 | 1.863855 | -0.248805 | C | 3.963189 | 1.714790 | 0.703931 |
| H | 0.659942 | -0.585297 | -1.048680 | H | 3.940907 | 2.706453 | 1.135333 |
| H | 4.601525 | -3.249280 | -1.160789 | N | 4.949072 | 0.867032 | 0.756323 |
| C | -0.119112 | 3.371771 | 0.076877 | C | 4.502485 | -0.228161 | 0.046236 |
| H | -0.450411 | 4.242972 | 0.650718 | C | 5.137562 | -1.493209 | -0.237813 |
| C | 0.790386 | 2.426477 | 0.854441 | N | 4.261613 | -2.304053 | -1.034895 |
| H | 1.397605 | 3.004559 | 1.561548 | C | 2.994013 | -1.991655 | -1.419011 |
| H | 0.241097 | 1.654124 | 1.392105 | N | 2.436611 | -0.834623 | -1.170851 |
| O | -1.270468 | 2.680889 | -0.445462 | C | 3.222958 | -0.013589 | -0.429750 |
| P | -2.466418 | 2.325168 | 0.546359 | H | -1.685097 | -0.597858 | 1.735723 |
| O | -3.122419 | 3.761607 | 0.844829 | O | -0.901765 | -0.226477 | -0.008428 |
| O | -2.152637 | 1.609331 | 1.800135 | O | -0.286603 | -0.870382 | -1.117222 |
| O | -3.519420 | 1.657083 | -0.421430 | O | 1.049746 | -0.526966 | 1.803072 |
| C | -3.255237 | 0.844088 | -1.584975 | H | 1.950373 | -0.892745 | 1.819339 |
| H | -3.618902 | 1.430135 | -2.432072 | H | -5.616693 | -2.321670 | -1.067056 |
| H | -2.186084 | 0.653879 | -1.695260 | H | 2.874312 | 5.634362 | 0.352432 |
| C | -4.012915 | -0.491333 | -1.507416 | H | -3.364638 | 3.823807 | 1.777858 |
| H | -4.527038 | -0.647558 | -2.462043 | O | 6.219757 | -1.928221 | 0.078795 |
| O | -3.144640 | -1.604332 | -1.320842 | N | 2.266908 | -2.962596 | -2.057783 |
| C | -3.217844 | -2.092896 | 0.019779 | H | 1.395864 | -2.621395 | -2.443840 |
| H | -3.674250 | -3.085453 | -0.011326 | H | 2.769603 | -3.601086 | -2.656485 |
| N | -1.879453 | -2.315421 | 0.552720 | | | | |
| C | -1.107521 | -1.174556 | 1.009519 | | | | |
| C | 0.186699 | -1.628094 | 1.710699 | | | | |
| C | -0.157838 | -2.174867 | 3.102939 | | | | |
| H | -0.891120 | -2.983439 | 3.045274 | | | | |
| H | 0.751348 | -2.547121 | 3.581226 | | | | |
| H | -0.564937 | -1.357959 | 3.703307 | | | | |
| C | 0.906115 | -2.734344 | 0.958746 | | | | |
| O | 2.112359 | -2.869995 | 1.047561 | | | | |
| N | 0.100198 | -3.595899 | 0.278169 | | | | |
| H | 0.541961 | -4.363418 | -0.212990 | | | | |
| C | -1.260481 | -3.422292 | -0.012747 | | | | |
| O | -1.830576 | -4.255845 | -0.679822 | | | | |

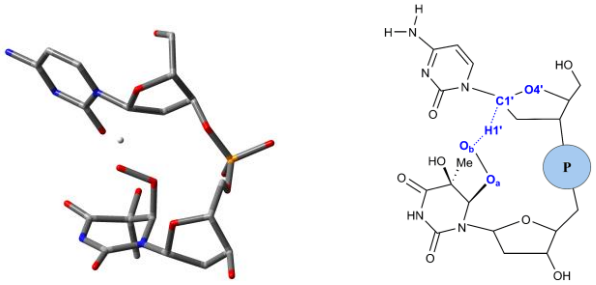





ss - 5' C T* 3' - Reactant

# Coordinates of optimized geometries

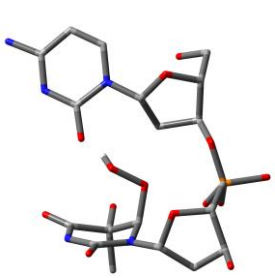
| Atom | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| O | -2.623310 | -3.702183 | -1.592980 |
| C | -1.566902 | -3.113584 | -2.330768 |
| H | -0.702360 | -3.789381 | -2.406185 |
| H | -1.887871 | -2.837558 | -3.342883 |
| C | -1.142280 | -1.861745 | -1.592022 |
| H | -0.264504 | -1.409812 | -2.074288 |
| O | -2.232770 | -0.966469 | -1.603592 |
| C | -2.297241 | -0.224354 | -0.404313 |
| H | -1.867453 | 0.766329 | -0.524292 |
| N | -3.711270 | -0.019377 | -0.101317 |
| C | -4.570366 | -1.061491 | -0.242606 |
| H | -4.125330 | -1.985131 | -0.605815 |
| C | -5.888847 | -0.915845 | 0.028015 |
| C | -6.302666 | 0.392712 | 0.448293 |
| N | -5.483413 | 1.411697 | 0.578075 |
| C | -4.151666 | 1.264235 | 0.322165 |
| O | -3.340153 | 2.171835 | 0.437914 |
| C | -0.797386 | -2.128827 | -0.114035 |
| H | -1.110828 | -3.131548 | 0.185450 |
| C | -1.553049 | -1.048822 | 0.666875 |
| H | -2.275180 | -1.512617 | 1.343850 |
| H | -0.896130 | -0.406525 | 1.256981 |
| O | 0.642811 | -2.088460 | -0.013714 |
| P | 1.402088 | -2.235178 | 1.369163 |
| O | 0.726246 | -3.524226 | 2.043059 |
| O | 1.420511 | -1.075100 | 2.284075 |
| O | 2.840475 | -2.737863 | 0.917118 |
| C | 3.369664 | -2.720223 | -0.413487 |
| H | 4.099554 | -3.532085 | -0.449037 |
| H | 2.572310 | -2.905762 | -1.136974 |
| C | 4.055794 | -1.404613 | -0.715029 |
| H | 4.665113 | -1.538819 | -1.622428 |
| O | 3.068099 | -0.406656 | -0.937544 |
| C | 3.593155 | 0.822849 | -0.450421 |
| H | 4.295889 | 1.257574 | -1.171003 |
| N | 2.517305 | 1.777706 | -0.316885 |
| C | 1.296399 | 1.326027 | 0.257225 |
| C | 0.484372 | 2.469318 | 0.871814 |
| C | 1.231745 | 3.011022 | 2.097846 |
| H | 2.230715 | 3.375682 | 1.848745 |
| H | 0.643373 | 3.823358 | 2.529104 |
| H | 1.309076 | 2.204650 | 2.832122 |
| C | 0.353180 | 3.586178 | -0.155186 |
| O | -0.646212 | 4.249831 | -0.279501 |
| N | 1.519306 | 3.838462 | -0.860384 |
| H | 1.503772 | 4.616139 | -1.508643 |
| C | 2.584437 | 2.958840 | -1.048415 |
| O | 3.519188 | 3.254653 | -1.759567 |
| C | 4.987583 | -0.882362 | 0.418528 |
| H | 5.055136 | -1.603068 | 1.235304 |
| C | 4.287334 | 0.410621 | 0.846585 |
| H | 3.531086 | 0.197872 | 1.610532 |
| H | 4.993939 | 1.152909 | 1.222385 |
| O | 6.311347 | -0.688637 | -0.032017 |
| H | 1.472164 | 0.556482 | 1.010600 |
| O | 0.474682 | 0.619335 | -0.733044 |
| O | 0.288682 | 1.324419 | -1.809542 |
| O | -0.751150 | 1.972676 | 1.265458 |
| H | -1.501542 | 2.455122 | 0.863319 |
| H | 6.316088 | 0.016597 | -0.690669 |
| H | -2.956489 | -4.462782 | -2.078679 |
| H | 0.566862 | -3.366480 | 2.982907 |
| H | -6.585777 | -1.735707 | -0.079515 |
| N | -7.606137 | 0.608480 | 0.751526 |
| H | -7.878717 | 1.561258 | 0.934785 |
| H | -8.311887 | -0.062653 | 0.504414 |

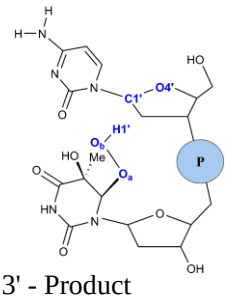



ss - 5' C T* 3' - TS

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| O | 3.827453 | 3.034518 | -0.138119 |
| C | 2.939986 | 3.603130 | -1.076104 |
| H | 2.699501 | 4.649260 | -0.835006 |
| H | 3.350897 | 3.571878 | -2.095216 |
| C | 1.657831 | 2.792275 | -1.056090 |
| H | 0.939832 | 3.226017 | -1.756893 |
| O | 1.914934 | 1.450440 | -1.479121 |
| C | 2.065936 | 0.608910 | -0.388428 |
| H | 1.172875 | -0.309768 | -0.573520 |
| N | 3.373420 | -0.016020 | -0.420323 |
| C | 4.216099 | 0.177727 | -1.470958 |
| H | 3.850319 | 0.837613 | -2.245367 |
| C | 5.425630 | -0.427789 | -1.518161 |
| C | 5.759855 | -1.273687 | -0.408883 |
| N | 4.958684 | -1.475397 | 0.611818 |
| C | 3.736996 | -0.880953 | 0.656812 |
| O | 2.939984 | -1.028675 | 1.568691 |
| C | 1.027383 | 2.640259 | 0.327000 |
| H | 1.194111 | 3.511557 | 0.968396 |
| C | 1.656474 | 1.360408 | 0.879466 |
| H | 2.545625 | 1.600472 | 1.464705 |
| H | 0.965040 | 0.785929 | 1.499828 |
| O | -0.379029 | 2.500836 | 0.062827 |
| P | -1.466057 | 2.362009 | 1.214900 |
| O | -1.857163 | 3.909940 | 1.441478 |
| O | -1.137380 | 1.644202 | 2.452288 |
| O | -2.698990 | 1.714199 | 0.442109 |
| C | -2.978094 | 1.965989 | -0.942210 |
| H | -3.383896 | 2.979868 | -1.038312 |
| H | -2.055734 | 1.867387 | -1.519800 |
| C | -3.986945 | 0.946750 | -1.443293 |
| H | -4.398242 | 1.336606 | -2.382703 |
| O | -3.376647 | -0.304878 | -1.719328 |
| C | -3.710694 | -1.282841 | -0.733963 |
| H | -4.259604 | -2.084037 | -1.232463 |
| N | -2.518761 | -1.926370 | -0.209326 |
| C | -1.567812 | -1.152555 | 0.560147 |
| C | -0.650642 | -2.065696 | 1.384237 |
| C | -1.475944 | -2.799980 | 2.451421 |
| H | -2.295828 | -3.379502 | 2.021844 |
| H | -0.809611 | -3.464475 | 3.005711 |
| H | -1.875386 | -2.055348 | 3.144322 |
| C | -0.024917 | -3.106607 | 0.469673 |
| O | 1.106970 | -3.510154 | 0.599970 |
| N | -0.903572 | -3.628336 | -0.460076 |
| H | -0.566365 | -4.382059 | -1.045076 |
| C | -2.113471 | -3.075569 | -0.879897 |
| O | -2.761545 | -3.620452 | -1.747715 |
| C | -5.141700 | 0.622481 | -0.481217 |
| H | -5.402353 | 1.467170 | 0.160531 |
| C | -4.583656 | -0.566177 | 0.305210 |
| H | -4.001828 | -0.210072 | 1.155610 |
| H | -5.388076 | -1.207686 | 0.668476 |
| O | -6.314148 | 0.287804 | -1.196561 |
| H | -2.096109 | -0.493284 | 1.250934 |
| O | -0.857663 | -0.226585 | -0.252011 |
| O | 0.125465 | -0.870755 | -0.981821 |
| O | 0.313350 | -1.284133 | 1.999702 |
| H | 1.210370 | -1.614185 | 1.800745 |
| H | -6.085376 | -0.398710 | -1.836160 |
| H | 4.676680 | 3.484829 | -0.185530 |
| H | -2.174453 | 4.044014 | 2.344244 |
| H | 6.100904 | -0.270179 | -2.348141 |
| N | 6.968334 | -1.884285 | -0.378082 |
| H | 7.113215 | -2.562581 | 0.353711 |
| H | 7.538980 | -1.934891 | -1.204150 |

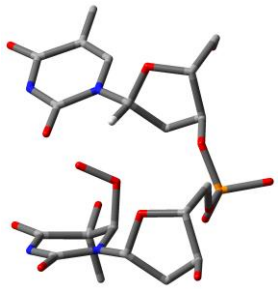


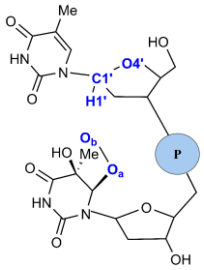



ss - 5' C T* 3' - Product

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| O | -4.170239 | -2.921675 | 0.673798 |
| C | -3.440042 | -3.804715 | -0.152716 |
| H | -3.146144 | -4.720958 | 0.379650 |
| H | -4.015554 | -4.092494 | -1.043452 |
| C | -2.189797 | -3.072289 | -0.602421 |
| H | -1.604753 | -3.704060 | -1.275282 |
| O | -2.580068 | -1.895725 | -1.320786 |
| C | -2.446469 | -0.798321 | -0.519102 |
| H | -0.784259 | 1.355325 | -0.488815 |
| N | -3.555232 | 0.077847 | -0.608169 |
| C | -4.725180 | -0.297415 | -1.194480 |
| H | -4.746254 | -1.308641 | -1.577443 |
| C | -5.772260 | 0.561655 | -1.269302 |
| C | -5.584403 | 1.849359 | -0.677253 |
| N | -4.453609 | 2.226252 | -0.109101 |
| C | -3.397551 | 1.388920 | -0.076527 |
| O | -2.295272 | 1.684193 | 0.388662 |
| C | -1.321087 | -2.561745 | 0.549106 |
| H | -1.375850 | -3.210045 | 1.429023 |
| C | -1.831378 | -1.146666 | 0.810037 |
| H | -2.607289 | -1.166944 | 1.583856 |
| H | -1.028458 | -0.476193 | 1.129081 |
| O | 0.024472 | -2.533668 | 0.041410 |
| P | 1.226844 | -2.474934 | 1.085042 |
| O | 1.512503 | -4.048689 | 1.297603 |
| O | 1.045726 | -1.738095 | 2.342569 |
| O | 2.428762 | -1.930177 | 0.205712 |
| C | 2.517957 | -2.086124 | -1.219305 |
| H | 2.718787 | -3.140064 | -1.443464 |
| H | 1.578366 | -1.765425 | -1.674699 |
| C | 3.648564 | -1.209317 | -1.728076 |
| H | 3.922073 | -1.572597 | -2.726420 |
| O | 3.245125 | 0.144413 | -1.849460 |
| C | 3.802868 | 0.954475 | -0.815647 |
| H | 4.450770 | 1.695500 | -1.287166 |
| N | 2.779016 | 1.737012 | -0.146501 |
| C | 1.725418 | 1.064042 | 0.596033 |
| C | 1.034451 | 2.033274 | 1.577421 |
| C | 1.991845 | 2.353553 | 2.731001 |
| H | 2.947511 | 2.743908 | 2.372781 |
| H | 1.521258 | 3.085410 | 3.390806 |
| H | 2.159072 | 1.431318 | 3.293668 |
| C | 0.675273 | 3.336837 | 0.878380 |
| O | -0.318692 | 3.969362 | 1.153827 |
| N | 1.618556 | 3.786370 | -0.016845 |
| H | 1.440832 | 4.675739 | -0.465916 |
| C | 2.621529 | 3.031410 | -0.622803 |
| O | 3.330660 | 3.540984 | -1.465062 |
| C | 4.901240 | -1.175898 | -0.836133 |
| H | 5.050621 | -2.110009 | -0.289650 |
| C | 4.610284 | 0.011025 | 0.086653 |
| H | 4.038197 | -0.312094 | 0.956400 |
| H | 5.537622 | 0.475692 | 0.426103 |
| O | 6.066547 | -0.977949 | -1.611658 |
| H | 2.161398 | 0.252941 | 1.182278 |
| O | 0.811101 | 0.380241 | -0.226259 |
| O | 0.076811 | 1.348907 | -0.968285 |
| O | -0.116311 | 1.437463 | 2.093472 |
| H | -0.888541 | 1.962646 | 1.819021 |
| H | 5.927504 | -0.195951 | -2.161233 |
| H | -4.969950 | -3.360594 | 0.980414 |
| H | 1.901148 | -4.201969 | 2.168882 |
| H | -6.704069 | 0.270876 | -1.735116 |
| N | -6.598812 | 2.742381 | -0.666935 |
| H | -6.394637 | 3.667319 | -0.322534 |
| H | -7.438066 | 2.587300 | -1.197068 |

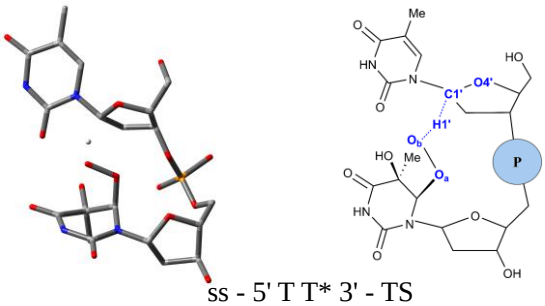





ss - 5' T T* 3' - Reactant

# Coordinates of optimized geometries

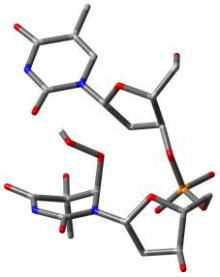
| Atom | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| O | -3.831452 | -3.525103 | 0.128856 |
| C | -3.026640 | -3.819504 | -0.999899 |
| H | -2.570142 | -4.815716 | -0.912639 |
| H | -3.606720 | -3.777924 | -1.930413 |
| C | -1.925717 | -2.779367 | -1.075346 |
| H | -1.198998 | -3.082468 | -1.838599 |
| O | -2.482396 | -1.522072 | -1.428204 |
| C | -2.189841 | -0.540463 | -0.444878 |
| H | -1.375739 | 0.108939 | -0.774795 |
| N | -3.371620 | 0.306821 | -0.308538 |
| C | -4.613671 | -0.290540 | -0.172079 |
| H | -4.577060 | -1.375846 | -0.128310 |
| C | -5.766465 | 0.400537 | -0.115111 |
| C | -7.118584 | -0.224889 | 0.031785 |
| H | -7.618376 | 0.149355 | 0.929484 |
| H | -7.755687 | 0.036701 | -0.817519 |
| H | -7.040739 | -1.312167 | 0.096175 |
| C | -5.711348 | 1.859616 | -0.216684 |
| O | -6.671206 | 2.602149 | -0.188198 |
| N | -4.414481 | 2.371109 | -0.353187 |
| H | -4.324315 | 3.378885 | -0.405528 |
| C | -3.229321 | 1.677131 | -0.397010 |
| O | -2.150722 | 2.245615 | -0.497719 |
| C | -1.200606 | -2.574976 | 0.262908 |
| H | -1.284356 | -3.446833 | 0.918802 |
| C | -1.837314 | -1.315318 | 0.825244 |
| H | -2.752381 | -1.593619 | 1.355771 |
| H | -1.172250 | -0.753973 | 1.485025 |
| O | 0.191903 | -2.350697 | -0.056733 |
| P | 1.255249 | -2.381762 | 1.123740 |
| O | 1.366102 | -3.961241 | 1.409331 |
| O | 1.028104 | -1.571582 | 2.329517 |
| O | 2.590030 | -1.952955 | 0.380416 |
| C | 2.937513 | -2.271643 | -0.973314 |
| H | 3.219551 | -3.328889 | -1.029467 |
| H | 2.084451 | -2.069222 | -1.625938 |
| C | 4.106157 | -1.382314 | -1.359452 |
| H | 4.529224 | -1.769505 | -2.294440 |
| O | 3.665347 | -0.049257 | -1.577867 |
| C | 4.154221 | 0.840574 | -0.577808 |
| H | 4.871114 | 1.526468 | -1.033570 |
| N | 3.077595 | 1.693950 | -0.097596 |
| C | 1.885259 | 1.078560 | 0.399662 |
| C | 1.001061 | 2.021411 | 1.236957 |
| C | 1.633538 | 2.168286 | 2.623010 |
| H | 2.673024 | 2.501320 | 2.561086 |
| H | 1.050894 | 2.887849 | 3.200837 |
| H | 1.585435 | 1.192274 | 3.113859 |
| C | 0.905740 | 3.401876 | 0.592671 |
| O | -0.050694 | 4.123011 | 0.733654 |
| N | 2.038514 | 3.807226 | -0.087242 |
| H | 2.025564 | 4.741189 | -0.478081 |
| C | 3.096860 | 3.020274 | -0.522486 |
| O | 3.995084 | 3.504501 | -1.175531 |
| C | 5.217382 | -1.285664 | -0.296283 |
| H | 5.262247 | -2.178727 | 0.331427 |
| C | 4.812023 | -0.037247 | 0.492297 |
| H | 4.105041 | -0.297582 | 1.282399 |
| H | 5.682240 | 0.447294 | 0.937928 |
| O | 6.490943 | -1.162033 | -0.893522 |
| H | 2.134638 | 0.208760 | 1.004410 |
| O | 1.095404 | 0.494985 | -0.678351 |
| O | 0.595260 | 1.427124 | -1.440995 |
| O | -0.270514 | 1.474352 | 1.390654 |
| H | -0.880064 | 1.896094 | 0.751564 |
| H | 6.474412 | -0.411452 | -1.500704 |
| H | -4.556241 | -4.157385 | 0.171933 |
| H | 1.605411 | -4.123544 | 2.331581 |

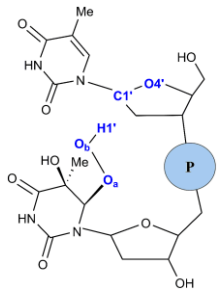



ss - 5' T T* 3' - TS

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| O | -2.793831 | -3.616228 | -1.031129 | N | 2.636161 | 1.685966 | -0.610895 |
| C | -1.702845 | -3.319942 | -1.884370 | C | 1.514435 | 1.124916 | 0.105483 |
| H | -0.951836 | -4.122594 | -1.878407 | C | 0.909331 | 2.171156 | 1.051608 |
| H | -2.031930 | -3.152061 | -2.917537 | C | 1.923083 | 2.501209 | 2.154053 |
| C | -1.063728 | -2.055120 | -1.352527 | H | 2.875579 | 2.858376 | 1.755842 |
| H | -0.173455 | -1.784226 | -1.930458 | H | 1.486291 | 3.266650 | 2.798253 |
| O | -2.030022 | -1.014582 | -1.464910 | H | 2.083775 | 1.595791 | 2.746720 |
| C | -2.110266 | -0.260323 | -0.319646 | C | 0.604293 | 3.441406 | 0.262882 |
| H | -1.388435 | 0.804353 | -0.566842 | O | -0.308884 | 4.180540 | 0.539983 |
| N | -3.479915 | 0.164581 | -0.140026 | N | 1.502696 | 3.721161 | -0.752181 |
| C | -4.516911 | -0.691890 | -0.493293 | H | 1.384361 | 4.596596 | -1.245950 |
| H | -4.181473 | -1.649500 | -0.879900 | C | 2.563175 | 2.932447 | -1.197540 |
| C | -5.815319 | -0.367870 | -0.361466 | O | 3.361727 | 3.359170 | -2.005654 |
| C | -6.949196 | -1.273174 | -0.730257 | C | 5.346714 | -0.758069 | -0.134185 |
| H | -7.581792 | -1.469927 | 0.139694 | H | 5.638193 | -1.370769 | 0.722127 |
| H | -7.585050 | -0.800006 | -1.483570 | C | 4.669320 | 0.542226 | 0.283547 |
| H | -6.579162 | -2.222165 | -1.122988 | H | 4.052870 | 0.375147 | 1.172603 |
| C | -6.159269 | 0.948461 | 0.181177 | H | 5.388211 | 1.339256 | 0.483173 |
| O | -7.286450 | 1.366942 | 0.343426 | O | 6.527250 | -0.558844 | -0.883060 |
| N | -5.049886 | 1.729444 | 0.529313 | H | 1.880020 | 0.279991 | 0.691629 |
| H | -5.242574 | 2.643713 | 0.921042 | O | 0.578239 | 0.545600 | -0.806125 |
| C | -3.716949 | 1.413372 | 0.413188 | O | -0.459742 | 1.417903 | -1.098001 |
| O | -2.833029 | 2.172794 | 0.766130 | O | -0.240749 | 1.680948 | 1.663423 |
| C | -0.678641 | -2.154929 | 0.136208 | H | -1.025469 | 2.146932 | 1.318918 |
| H | -0.934358 | -3.138148 | 0.542045 | H | 6.339470 | 0.050713 | -1.607334 |
| C | -1.464432 | -1.038055 | 0.828675 | H | -3.213404 | -4.430397 | -1.327055 |
| H | -2.262181 | -1.465547 | 1.444975 | H | 1.381306 | -4.009330 | 2.735753 |
| H | -0.831060 | -0.406663 | 1.457207 | | | | |
| O | 0.745712 | -2.003355 | 0.199542 | | | | |
| P | 1.558405 | -2.223834 | 1.547437 | | | | |
| O | 1.355326 | -3.801303 | 1.792219 | | | | |
| O | 1.254600 | -1.377528 | 2.707540 | | | | |
| O | 3.045529 | -2.024443 | 1.017482 | | | | |
| C | 3.506258 | -2.548681 | -0.237620 | | | | |
| H | 4.179703 | -3.385551 | -0.029720 | | | | |
| H | 2.661584 | -2.893726 | -0.838345 | | | | |
| C | 4.240783 | -1.444951 | -0.971540 | | | | |
| H | 4.701047 | -1.879319 | -1.869878 | | | | |
| O | 3.306024 | -0.437661 | -1.342432 | | | | |
| C | 3.767970 | 0.839081 | -0.916269 | | | | |
| H | 4.309874 | 1.344609 | -1.723120 | | | | |

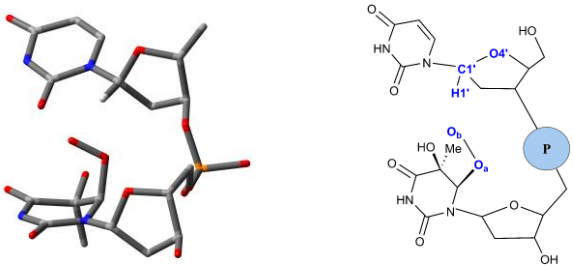





ss - 5' T T* 3' - Product

# Coordinates of optimized geometries

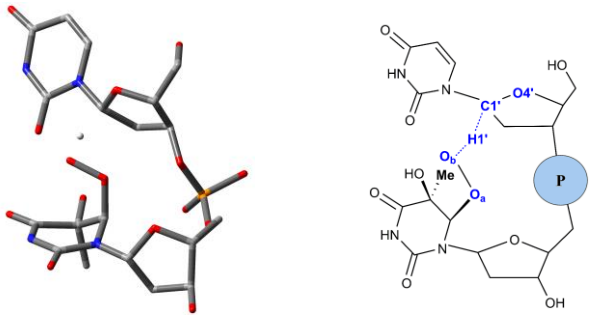
| Atom | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| O | -2.661218 | -3.657543 | -1.156790 |
| C | -1.624114 | -3.290118 | -2.051382 |
| H | -0.864090 | -4.080305 | -2.133699 |
| H | -2.014700 | -3.068629 | -3.052108 |
| C | -0.980445 | -2.043442 | -1.481160 |
| H | -0.105501 | -1.731288 | -2.060144 |
| O | -1.961113 | -1.010618 | -1.525904 |
| C | -2.116103 | -0.430845 | -0.307289 |
| H | -1.082063 | 1.747226 | -1.038659 |
| N | -3.440922 | 0.048570 | -0.112401 |
| C | -4.487819 | -0.867033 | -0.055491 |
| H | -4.167695 | -1.898705 | -0.183747 |
| C | -5.772410 | -0.511789 | 0.117965 |
| C | -6.917243 | -1.473387 | 0.190112 |
| H | -7.444488 | -1.366165 | 1.141911 |
| H | -7.643674 | -1.264297 | -0.599832 |
| H | -6.569722 | -2.503442 | 0.090551 |
| C | -6.087749 | 0.915481 | 0.230641 |
| O | -7.197486 | 1.375396 | 0.397778 |
| N | -4.975599 | 1.761910 | 0.110036 |
| H | -5.161938 | 2.757454 | 0.135135 |
| C | -3.663990 | 1.413062 | -0.098454 |
| O | -2.784786 | 2.249548 | -0.253556 |
| C | -0.574821 | -2.227005 | -0.004557 |
| H | -0.791776 | -3.241945 | 0.336088 |
| C | -1.396226 | -1.189339 | 0.771195 |
| H | -2.109707 | -1.688630 | 1.439331 |
| H | -0.769421 | -0.524131 | 1.373400 |
| O | 0.849095 | -2.043295 | 0.059251 |
| P | 1.672912 | -2.237399 | 1.403599 |
| O | 1.094495 | -3.619351 | 1.985264 |
| O | 1.645726 | -1.148534 | 2.397619 |
| O | 3.126269 | -2.574248 | 0.865428 |
| C | 3.530116 | -2.707235 | -0.504797 |
| H | 4.269116 | -3.511707 | -0.524751 |
| H | 2.674143 | -2.972195 | -1.128638 |
| C | 4.156445 | -1.414088 | -0.981848 |
| H | 4.666296 | -1.605112 | -1.937881 |
| O | 3.129721 | -0.446165 | -1.156666 |
| C | 3.635384 | 0.807085 | -0.718762 |
| H | 4.248421 | 1.275091 | -1.498843 |
| N | 2.536704 | 1.711607 | -0.468381 |
| C | 1.329663 | 1.186043 | 0.135821 |
| C | 0.690603 | 2.242689 | 1.047849 |
| C | 1.567221 | 2.442625 | 2.289220 |
| H | 2.578119 | 2.765862 | 2.027489 |
| H | 1.103776 | 3.194961 | 2.930971 |
| H | 1.617726 | 1.491056 | 2.826218 |
| C | 0.572903 | 3.566460 | 0.302026 |
| O | -0.369607 | 4.310861 | 0.457999 |
| N | 1.657485 | 3.882781 | -0.482558 |
| H | 1.660223 | 4.786626 | -0.937567 |
| C | 2.663823 | 3.010521 | -0.905502 |
| O | 3.593244 | 3.420458 | -1.571002 |
| C | 5.192268 | -0.816268 | 0.014098 |
| H | 5.411205 | -1.517744 | 0.821576 |
| C | 4.469251 | 0.435570 | 0.508647 |
| H | 3.794493 | 0.186915 | 1.336773 |
| H | 5.162326 | 1.219664 | 0.820657 |
| O | 6.430449 | -0.544495 | -0.607290 |
| H | 1.598456 | 0.326875 | 0.750220 |
| O | 0.433565 | 0.648526 | -0.806303 |
| O | -0.208036 | 1.725118 | -1.485316 |
| O | -0.580348 | 1.809284 | 1.437785 |
| H | -1.225024 | 2.488944 | 1.174068 |
| H | 6.318406 | 0.193438 | -1.218948 |
| H | -3.124610 | -4.422652 | -1.511565 |
| H | 0.994042 | -3.563715 | 2.944768 |




ss - 5' U T* 3' - Reactant

# Coordinates of optimized geometries

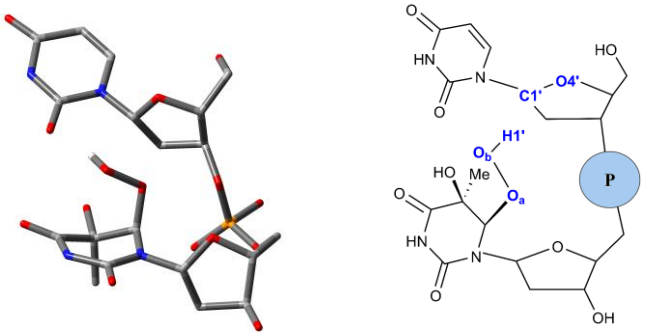
| Atom | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| O | -3.992809 | -3.566421 | 0.150064 |
| C | -3.185755 | -3.869890 | -0.974680 |
| H | -2.721528 | -4.861191 | -0.874547 |
| H | -3.766230 | -3.844987 | -1.905519 |
| C | -2.093660 | -2.821643 | -1.062986 |
| H | -1.367575 | -3.123959 | -1.827018 |
| O | -2.663688 | -1.572012 | -1.423613 |
| C | -2.377066 | -0.580362 | -0.449557 |
| H | -1.573198 | 0.076723 | -0.789294 |
| N | -3.569580 | 0.254062 | -0.313342 |
| C | -4.802844 | -0.351222 | -0.178227 |
| H | -4.758301 | -1.435691 | -0.134967 |
| C | -5.952724 | 0.342512 | -0.119633 |
| C | -5.930653 | 1.796683 | -0.214563 |
| O | -6.887289 | 2.539766 | -0.183598 |
| N | -4.630466 | 2.314873 | -0.351000 |
| H | -4.546050 | 3.323435 | -0.399006 |
| C | -3.441455 | 1.630729 | -0.395670 |
| O | -2.366086 | 2.203731 | -0.492194 |
| C | -1.364932 | -2.599498 | 0.270447 |
| H | -1.439136 | -3.466265 | 0.934200 |
| C | -2.010176 | -1.340755 | 0.825160 |
| H | -2.919745 | -1.623045 | 1.363048 |
| H | -1.346975 | -0.768018 | 1.477041 |
| O | 0.024200 | -2.366396 | -0.056393 |
| P | 1.090881 | -2.378663 | 1.121897 |
| O | 1.224751 | -3.955562 | 1.411172 |
| O | 0.853327 | -1.568521 | 2.325701 |
| O | 2.417859 | -1.932723 | 0.375169 |
| C | 2.766674 | -2.248971 | -0.978806 |
| H | 3.060263 | -3.303073 | -1.034671 |
| H | 1.910273 | -2.056405 | -1.630107 |
| C | 3.924474 | -1.346845 | -1.367335 |
| H | 4.348706 | -1.728159 | -2.304216 |
| O | 3.468132 | -0.018452 | -1.582219 |
| C | 3.950339 | 0.874969 | -0.582086 |
| H | 4.658926 | 1.568711 | -1.038872 |
| N | 2.866306 | 1.716626 | -0.097955 |
| C | 1.683285 | 1.089048 | 0.406280 |
| C | 0.791724 | 2.024661 | 1.244023 |
| C | 1.427633 | 2.183111 | 2.627177 |
| H | 2.462528 | 2.529138 | 2.560288 |
| H | 0.838163 | 2.896601 | 3.205579 |
| H | 1.394032 | 1.207913 | 3.120845 |
| C | 0.677725 | 3.401645 | 0.595352 |
| O | -0.288021 | 4.110503 | 0.735447 |
| N | 1.803950 | 3.818833 | -0.087820 |
| H | 1.778883 | 4.751361 | -0.481569 |
| C | 2.869334 | 3.042488 | -0.525265 |
| O | 3.759640 | 3.535328 | -1.182557 |
| C | 5.038175 | -1.239162 | -0.307724 |
| H | 5.095951 | -2.132945 | 0.317989 |
| C | 4.620868 | 0.002909 | 0.484700 |
| H | 3.919424 | -0.267350 | 1.276322 |
| H | 5.486851 | 0.496447 | 0.928688 |
| O | 6.307883 | -1.098921 | -0.909374 |
| H | 1.944368 | 0.223676 | 1.012624 |
| O | 0.895229 | 0.493215 | -0.666612 |
| O | 0.382725 | 1.417028 | -1.431097 |
| O | -0.473262 | 1.464127 | 1.404330 |
| H | -1.088730 | 1.877323 | 0.766130 |
| H | 6.279549 | -0.348498 | -1.516326 |
| H | -4.712664 | -4.203688 | 0.202386 |
| H | 1.471222 | -4.112555 | 2.332457 |
| H | -6.910226 | -0.146266 | -0.012566 |




ss - 5' U T* 3' - TS

# Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| O | -2.842715 | -3.753056 | -1.070806 |
| C | -1.756544 | -3.441647 | -1.925195 |
| H | -0.987085 | -4.226305 | -1.907476 |
| H | -2.086901 | -3.293607 | -2.960932 |
| C | -1.150162 | -2.155991 | -1.404441 |
| H | -0.265568 | -1.869314 | -1.982934 |
| O | -2.141385 | -1.140054 | -1.531380 |
| C | -2.273898 | -0.399996 | -0.381517 |
| H | -1.596313 | 0.699664 | -0.605909 |
| N | -3.664913 | -0.035448 | -0.223621 |
| C | -4.658402 | -0.922918 | -0.605373 |
| H | -4.282015 | -1.864916 | -0.990925 |
| C | -5.965919 | -0.635355 | -0.492536 |
| C | -6.389453 | 0.650932 | 0.048205 |
| O | -7.528793 | 1.035126 | 0.193178 |
| N | -5.309304 | 1.467881 | 0.426519 |
| H | -5.542252 | 2.370414 | 0.823700 |
| C | -3.965228 | 1.200995 | 0.338287 |
| O | -3.115617 | 1.984313 | 0.719168 |
| C | -0.770060 | -2.234281 | 0.086483 |
| H | -0.978516 | -3.228486 | 0.492285 |
| C | -1.616058 | -1.158289 | 0.772256 |
| H | -2.404886 | -1.626336 | 1.370343 |
| H | -1.021526 | -0.505690 | 1.417080 |
| O | 0.644183 | -2.010300 | 0.161325 |
| P | 1.455830 | -2.222805 | 1.511917 |
| O | 1.322546 | -3.812827 | 1.720087 |
| O | 1.102526 | -1.416438 | 2.686405 |
| O | 2.936539 | -1.944899 | 1.000812 |
| C | 3.434614 | -2.426472 | -0.257346 |
| H | 4.138288 | -3.239711 | -0.055722 |
| H | 2.612083 | -2.793070 | -0.875946 |
| C | 4.134207 | -1.280823 | -0.960478 |
| H | 4.628173 | -1.680760 | -1.856808 |
| O | 3.164967 | -0.307678 | -1.333304 |
| C | 3.559018 | 0.979008 | -0.871041 |
| H | 4.091628 | 1.526334 | -1.656478 |
| N | 2.383693 | 1.765898 | -0.571059 |
| C | 1.277595 | 1.140818 | 0.115842 |
| C | 0.615258 | 2.141274 | 1.074067 |
| C | 1.599672 | 2.494264 | 2.195538 |
| H | 2.539657 | 2.901934 | 1.816670 |
| H | 1.120828 | 3.226495 | 2.848357 |
| H | 1.794407 | 1.585713 | 2.772976 |
| C | 0.264211 | 3.411382 | 0.304013 |
| O | -0.683136 | 4.105121 | 0.584453 |
| N | 1.158266 | 3.747308 | -0.697832 |
| H | 1.005850 | 4.625136 | -1.177850 |
| C | 2.259871 | 3.016118 | -1.141116 |
| O | 3.047559 | 3.490978 | -1.932698 |
| C | 5.194482 | -0.561680 | -0.091994 |
| H | 5.499887 | -1.177523 | 0.757210 |
| C | 4.450965 | 0.697788 | 0.339583 |
| H | 3.826833 | 0.483328 | 1.212960 |
| H | 5.128362 | 1.522502 | 0.569323 |
| O | 6.376219 | -0.293749 | -0.816912 |
| H | 1.672281 | 0.300105 | 0.688517 |
| O | 0.380415 | 0.540754 | -0.821901 |
| O | -0.693773 | 1.370745 | -1.104319 |
| O | -0.520181 | 1.590687 | 1.661663 |
| H | -1.318980 | 2.028854 | 1.313828 |
| H | 6.172257 | 0.321488 | -1.531858 |
| H | -3.238324 | -4.584364 | -1.351938 |
| H | 1.350575 | -4.041012 | 2.658924 |
| H | -6.730260 | -1.338794 | -0.789792 |




ss - 5' U T* 3' - Product

## Coordinates of optimized geometries

| Atom | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| O | -2.676466 | -3.829827 | -1.107015 |
| C | -1.654107 | -3.435760 | -2.007924 |
| H | -0.865427 | -4.198193 | -2.080293 |
| H | -2.053772 | -3.242514 | -3.010827 |
| C | -1.059027 | -2.158065 | -1.453387 |
| H | -0.199182 | -1.816194 | -2.038164 |
| O | -2.081631 | -1.166711 | -1.507892 |
| C | -2.278176 | -0.600211 | -0.289616 |
| H | -1.352041 | 1.628287 | -1.005804 |
| N | -3.628180 | -0.188184 | -0.106969 |
| C | -4.630265 | -1.146960 | -0.076267 |
| H | -4.262885 | -2.161305 | -0.210121 |
| C | -5.927205 | -0.837525 | 0.083473 |
| C | -6.326975 | 0.560164 | 0.211472 |
| O | -7.452052 | 0.977712 | 0.370849 |
| N | -5.244442 | 1.455982 | 0.114966 |
| H | -5.474129 | 2.442344 | 0.148233 |
| C | -3.917654 | 1.168562 | -0.078671 |
| O | -3.072299 | 2.041648 | -0.211558 |
| C | -0.644849 | -2.309890 | 0.024412 |
| H | -0.799102 | -3.334837 | 0.369301 |
| C | -1.528667 | -1.320316 | 0.794483 |
| H | -2.219300 | -1.859372 | 1.455728 |
| H | -0.942516 | -0.624139 | 1.402855 |
| O | 0.764160 | -2.036543 | 0.092032 |
| P | 1.591916 | -2.192078 | 1.439274 |
| O | 1.148299 | -3.648860 | 1.954266 |
| O | 1.451063 | -1.147950 | 2.469204 |
| O | 3.078015 | -2.338894 | 0.903378 |
| C | 3.479616 | -2.546862 | -0.458302 |
| H | 4.255715 | -3.315978 | -0.439633 |
| H | 2.633013 | -2.885309 | -1.058929 |
| C | 4.038051 | -1.251728 | -1.009323 |
| H | 4.529040 | -1.460988 | -1.970920 |
| O | 2.964815 | -0.335671 | -1.192827 |
| C | 3.402246 | 0.947797 | -0.768967 |
| H | 3.962207 | 1.452724 | -1.565291 |
| N | 2.256910 | 1.784676 | -0.487929 |
| C | 1.095534 | 1.186488 | 0.136552 |
| C | 0.409363 | 2.197746 | 1.067239 |
| C | 1.287013 | 2.433344 | 2.301404 |
| H | 2.277604 | 2.809492 | 2.032213 |
| H | 0.792936 | 3.157153 | 2.953049 |
| H | 1.389432 | 1.481841 | 2.831004 |
| C | 0.208803 | 3.521138 | 0.338800 |
| O | -0.771136 | 4.210012 | 0.518243 |
| N | 1.262444 | 3.906324 | -0.455976 |
| H | 1.211011 | 4.815788 | -0.896745 |
| C | 2.307809 | 3.095152 | -0.905084 |
| O | 3.204598 | 3.564306 | -1.576261 |
| C | 5.071568 | -0.572131 | -0.067265 |
| H | 5.369794 | -1.243343 | 0.740800 |
| C | 4.289218 | 0.637894 | 0.437524 |
| H | 3.653631 | 0.355592 | 1.285372 |
| H | 4.939946 | 1.466717 | 0.723852 |
| O | 6.262057 | -0.229341 | -0.744208 |
| H | 1.427323 | 0.342186 | 0.740706 |
| O | 0.215371 | 0.601630 | -0.791516 |
| O | -0.483450 | 1.647002 | -1.462500 |
| O | -0.831725 | 1.690873 | 1.465116 |
| H | -1.515641 | 2.337168 | 1.217098 |
| H | 6.074343 | 0.488634 | -1.360943 |
| H | -3.105784 | -4.621382 | -1.446543 |
| H | 1.076910 | -3.660355 | 2.917923 |
| H | -6.699707 | -1.592549 | 0.110492 |

**Fig. S1** The optimized geometries and Coordinates of optimized geometries for the studied duplex and single-stranded 5' X T* 3'.