Supplementary Material for Organic & Biomolecular Chemistry

Coordinates for uracil, 5-hydroxy-uracil and 5-formyl–uracil base-paired with standard DNA bases, determined at the BSSE-free MP2 theory level.

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TITLE      AFoU 1-methyl-adenine:1-methyl-5-hydroxy-uracil base pair
REMARK     6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK     Delta E = -13.5 kcal/mol
MODEL        1
ATOM      1 C1'  FOU     1      -4.383   2.827   0.000
ATOM      2 H1'1 FOU     1      -3.620   3.602  -0.004
ATOM      3 N1   FOU     1      -3.697   1.535  -0.000
ATOM      4 C6   FOU     1      -4.413   0.382   0.000
ATOM      5 H6   FOU     1      -5.496   0.482   0.000
ATOM      6 C5   FOU     1      -3.847  -0.857   0.000
ATOM      7 C7   FOU     1      -4.710  -2.057   0.001
ATOM      8 C4   FOU     1      -2.393  -0.969   0.000
ATOM      9 O4   FOU     1      -1.768  -2.026   0.001
ATOM     10 N3   FOU     1      -1.736   0.258   0.000
ATOM     11 H3   FOU     1      -0.696   0.230   0.000
ATOM     12 C2   FOU     1      -2.285   1.523  -0.000
ATOM     13 O2   FOU     1      -1.626   2.544   0.000
ATOM     14 H7   FOU     1      -4.163  -3.016   0.001
ATOM     15 O8   FOU     1      -5.929  -2.012   0.001
ATOM     16 H1'2 FOU     1      -5.007   2.918  -0.892
ATOM     17 H1'3 FOU     1      -4.999   2.922   0.897
TER
ATOM     18 C1'  ADE     2       6.170   1.332  -0.000
ATOM     19 H1'1 ADE     2       5.614   2.270  -0.001
ATOM     20 N9   ADE     2       5.190   0.257  -0.001
ATOM     21 C8   ADE     2       5.408  -1.097  -0.001
ATOM     22 H8   ADE     2       6.412  -1.503  -0.001
ATOM     23 N7   ADE     2       4.297  -1.825  -0.001
ATOM     24 C5   ADE     2       3.302  -0.875  -0.000
ATOM     25 C6   ADE     2       1.892  -0.982   0.000
ATOM     26 N6   ADE     2       1.263  -2.171  -0.000
ATOM     27 H61  ADE     2       0.249  -2.215   0.001
ATOM     28 H62  ADE     2       1.817  -3.010  -0.000
ATOM     29 N1   ADE     2       1.175   0.157   0.000
ATOM     30 C2   ADE     2       1.824   1.347   0.000
ATOM     31 H2   ADE     2       1.173   2.218   0.001
ATOM     32 N3   ADE     2       3.137   1.578  -0.000
ATOM     33 C4   ADE     2       3.824   0.423  -0.000
ATOM     34 H1'2 ADE     2       6.795   1.277  -0.894
ATOM     35 H1'3 ADE     2       6.794   1.277   0.894
ENDMDL
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TITLE     A:5HOdU   A:1-methyl-5-hydroxy-uracil base pair
REMARK     6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK     Delta E = -13.3 kcal/mol
REMARK     H-Bonds N1-H3=1.87 and H61-O4=2.04
MODEL        2
ATOM      1 C1'  HOU A   1      -4.803  -2.466  -0.000
ATOM      2 H1'1 HOU A   1      -4.099  -3.296  -0.000
ATOM      3 N1   HOU A   1      -4.026  -1.232   0.000
ATOM      4 C6   HOU A   1      -4.700  -0.019   0.001
ATOM      5 H6   HOU A   1      -5.783  -0.069   0.002
ATOM      6 C5   HOU A   1      -4.033   1.160   0.001
ATOM      7 O5   HOU A   1      -4.640   2.370   0.002
ATOM      8 HO5  HOU A   1      -3.899   2.996   0.002
ATOM      9 C4   HOU A   1      -2.576   1.157   0.000
ATOM     10 O4   HOU A   1      -1.939   2.218   0.000
ATOM     11 N3   HOU A   1      -1.998  -0.085  -0.001
ATOM     12 H3   HOU A   1      -0.959  -0.125  -0.001
ATOM     13 C2   HOU A   1      -2.642  -1.322  -0.001
ATOM     14 O2   HOU A   1      -2.024  -2.373  -0.002
ATOM     15 H1'2 HOU A   1      -5.430  -2.516   0.894
ATOM     16 H1'3 HOU A   1      -5.430  -2.516  -0.894
TER
ATOM     17 C1'  ADE B   2       5.838  -1.556   0.002
ATOM     18 H1'1 ADE B   2       5.235  -2.465   0.003
ATOM     19 N9   ADE B   2       4.914  -0.433   0.001
ATOM     20 C8   ADE B   2       5.201   0.909   0.001
ATOM     21 H8   ADE B   2       6.224   1.264   0.002
ATOM     22 N7   ADE B   2       4.128   1.693  -0.000
ATOM     23 C5   ADE B   2       3.086   0.794  -0.001
ATOM     24 C6   ADE B   2       1.683   0.972  -0.002
ATOM     25 N6   ADE B   2       1.113   2.190  -0.003
ATOM     26 H61  ADE B   2       0.104   2.286  -0.002
ATOM     27 H62  ADE B   2       1.709   3.001  -0.001
ATOM     28 N1   ADE B   2       0.910  -0.130  -0.002
ATOM     29 C2   ADE B   2       1.497  -1.352  -0.001
ATOM     30 H2   ADE B   2       0.803  -2.188  -0.001
ATOM     31 N3   ADE B   2       2.797  -1.648   0.000
ATOM     32 C4   ADE B   2       3.541  -0.529   0.000
ATOM     33 H1'2 ADE B   2       6.465  -1.532   0.896
ATOM     34 H1'3 ADE B   2       6.464  -1.534  -0.892
ENDMDL
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TITLE      A:T WC  1-methyl-adenine:1-methyl-thymine base pair
REMARK     6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK     Delta E = -12.9 kcal/mol
REMARK     H-Bonds (A->T): H61-O4=2.01A; N1-H3=1.90A
MODEL        3
ATOM      1 C1'  THY     1      -4.781  -2.515   0.001
ATOM      2 H1'1 THY     1      -4.067  -3.336  -0.010
ATOM      3 N1   THY     1      -4.016  -1.272  -0.001
ATOM      4 C6   THY     1      -4.678  -0.065  -0.002
ATOM      5 H6   THY     1      -5.762  -0.140  -0.002
ATOM      6 C5   THY     1      -4.049   1.138  -0.002
ATOM      7 C7   THY     1      -4.768   2.453  -0.003
ATOM      8 H71  THY     1      -4.488   3.040  -0.882
ATOM      9 H72  THY     1      -4.489   3.041   0.876
ATOM     10 H73  THY     1      -5.852   2.308  -0.003
ATOM     11 C4   THY     1      -2.590   1.147  -0.001
ATOM     12 O4   THY     1      -1.911   2.174  -0.001
ATOM     13 N3   THY     1      -2.001  -0.110   0.000
ATOM     14 H3   THY     1      -0.964  -0.140   0.001
ATOM     15 C2   THY     1      -2.622  -1.346   0.001
ATOM     16 O2   THY     1      -2.007  -2.399   0.002
ATOM     17 H1'2 THY     1      -5.397  -2.578   0.902
ATOM     18 H1'3 THY     1      -5.416  -2.569  -0.886
TER
ATOM     19 C1'  ADE     2       5.880  -1.509  -0.003
ATOM     20 H1'1 ADE     2       5.288  -2.425  -0.004
ATOM     21 N9   ADE     2       4.943  -0.397  -0.002
ATOM     22 C8   ADE     2       5.213   0.947  -0.001
ATOM     23 H8   ADE     2       6.231   1.315  -0.002
ATOM     24 N7   ADE     2       4.130   1.718   0.001
ATOM     25 C5   ADE     2       3.100   0.806   0.001
ATOM     26 C6   ADE     2       1.694   0.966   0.002
ATOM     27 N6   ADE     2       1.106   2.175   0.005
ATOM     28 H61  ADE     2       0.094   2.253   0.003
ATOM     29 H62  ADE     2       1.690   2.995   0.002
ATOM     30 N1   ADE     2       0.935  -0.146   0.002
ATOM     31 C2   ADE     2       1.538  -1.359   0.001
ATOM     32 H2   ADE     2       0.855  -2.205   0.000
ATOM     33 N3   ADE     2       2.842  -1.639  -0.001
ATOM     34 C4   ADE     2       3.571  -0.512  -0.000
ATOM     35 H1'2 ADE     2       6.507  -1.480   0.891
ATOM     36 H1'3 ADE     2       6.507  -1.478  -0.897
ENDMDL
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TITLE      A:U  1-methyl-adenine:1-methyl-5-hydroxy-uracil base pair
REMARK     6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK     Delta E = -12.9 kcal/mol
REMARK     H-Bonds (A->U): H61-O4=2.01A; N1-H3=1.90A
MODEL        4
ATOM      1  C1' URA     1      -0.943  -1.944  -0.192  1.00  0.00
ATOM      2  N1  URA     1      -0.306  -0.637  -0.062  1.00  0.00
ATOM      3  C2  URA     1       1.066  -0.588   0.220  1.00  0.00
ATOM      4  O2  URA     1       1.749  -1.585   0.363  1.00  0.00
ATOM      5  N3  URA     1       1.567   0.696   0.323  1.00  0.00
ATOM      6 3H   URA     1       2.583   0.754   0.532  1.00  0.00
ATOM      7  C4  URA     1       0.891   1.906   0.181  1.00  0.00
ATOM      8  O4  URA     1       1.474   2.980   0.300  1.00  0.00
ATOM      9  C5  URA     1      -0.525   1.751  -0.110  1.00  0.00
ATOM     10 5H   URA     1      -1.135   2.635  -0.237  1.00  0.00
ATOM     11  C6  URA     1      -1.049   0.505  -0.217  1.00  0.00
ATOM     12 6H   URA     1      -2.102   0.341  -0.433  1.00  0.00
ATOM     13 1H1' URA     1      -0.175  -2.698  -0.031  1.00  0.00
ATOM     14 2H1' URA     1      -1.730  -2.057   0.558  1.00  0.00
ATOM     15 3H1' URA     1      -1.366  -2.060  -1.194  1.00  0.00
TER
ATOM      1  C1' ADE     2       9.366  -0.062   1.939  1.00  0.00
ATOM      2  N9  ADE     2       8.364   0.971   1.730  1.00  0.00
ATOM      3  C4  ADE     2       7.035   0.748   1.455  1.00  0.00
ATOM      4  N3  ADE     2       6.411  -0.435   1.327  1.00  0.00
ATOM      5  C2  ADE     2       5.116  -0.260   1.058  1.00  0.00
ATOM      6 2H   ADE     2       4.516  -1.158   0.935  1.00  0.00
ATOM      7  N1  ADE     2       4.433   0.902   0.915  1.00  0.00
ATOM      8  C6  ADE     2       5.087   2.070   1.048  1.00  0.00
ATOM      9  N6  ADE     2       4.421   3.229   0.907  1.00  0.00
ATOM     10 1H6  ADE     2       3.426   3.227   0.703  1.00  0.00
ATOM     11 2H6  ADE     2       4.927   4.093   1.012  1.00  0.00
ATOM     12  C5  ADE     2       6.472   2.023   1.336  1.00  0.00
ATOM     13  N7  ADE     2       7.407   3.014   1.527  1.00  0.00
ATOM     14  C8  ADE     2       8.524   2.333   1.761  1.00  0.00
ATOM     15 8H   ADE     2       9.489   2.782   1.960  1.00  0.00
ATOM     16 1H1' ADE     2       8.860  -1.023   1.836  1.00  0.00
ATOM     17 2H1' ADE     2       9.795   0.019   2.941  1.00  0.00
ATOM     18 3H1' ADE     2      10.158   0.015   1.190  1.00  0.00
TER
ENDMDL
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TITLE     C:FoU(1)   1-methyl-cytosine:1-methyl-5-formyl-uracil
REMARK    6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK    Delta E = -13.1 kcal/mol
REMARK    H-bonds   H41-O4=1.98A; N3-H3=1.97A
MODEL        5
ATOM      1 C1'  FOU     1       3.490   2.885  -0.538
ATOM      2 H1'1 FOU     1       3.072   3.610   0.163
ATOM      3 N1   FOU     1       2.923   1.563  -0.279
ATOM      4 C6   FOU     1       3.696   0.491   0.008
ATOM      5 H6   FOU     1       4.769   0.653   0.055
ATOM      6 C5   FOU     1       3.188  -0.756   0.230
ATOM      7 C7   FOU     1       4.104  -1.873   0.528
ATOM      8 H7   FOU     1       3.605  -2.844   0.691
ATOM      9 O8   FOU     1       5.317  -1.756   0.595
ATOM     10 C4   FOU     1       1.747  -0.960   0.158
ATOM     11 O4   FOU     1       1.186  -2.043   0.304
ATOM     12 N3   FOU     1       1.022   0.202  -0.098
ATOM     13 H3   FOU     1      -0.010   0.111  -0.082
ATOM     14 C2   FOU     1       1.515   1.465  -0.369
ATOM     15 O2   FOU     1       0.840   2.428  -0.661
ATOM     16 H1'2 FOU     1       3.248   3.203  -1.553
ATOM     17 H1'3 FOU     1       4.571   2.821  -0.412
TER
ATOM     18 C1'  CYT     2      -4.995   1.584   0.649
ATOM     19 H1'1 CYT     2      -4.873   1.777   1.717
ATOM     20 N1   CYT     2      -4.141   0.474   0.243
ATOM     21 C2   CYT     2      -2.740   0.660   0.424
ATOM     22 O2   CYT     2      -2.347   1.705   0.914
ATOM     23 N3   CYT     2      -1.918  -0.371   0.024
ATOM     24 C4   CYT     2      -2.426  -1.502  -0.436
ATOM     25 N4   CYT     2      -1.554  -2.474  -0.815
ATOM     26 C5   CYT     2      -3.835  -1.714  -0.601
ATOM     27 H5   CYT     2      -4.238  -2.638  -0.995
ATOM     28 C6   CYT     2      -4.651  -0.681  -0.247
ATOM     29 H6   CYT     2      -5.732  -0.732  -0.337
ATOM     30 H41  CYT     2      -1.920  -3.407  -0.917
ATOM     31 H42  CYT     2      -0.608  -2.395  -0.447
ATOM     32 H1'2 CYT     2      -6.031   1.325   0.429
ATOM     33 H1'3 CYT     2      -4.708   2.486   0.106
ENDMDL
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Supplementary Material for Organic & Biomolecular Chemistry


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TITLE   C:FoU(2) 1-methyl-cytosine:1-methyl-5-formyl-uracil
REMARK  6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK    Delta E = - 13.1 kcal/mol
REMARK    H-Bonds H41-O4=1.98A; N3-H3=1.97A
MODEL        6
ATOM      1 C1'  FOU     1      -3.488   2.885  -0.539
ATOM      2 H1'1 FOU     1      -3.071   3.610   0.162
ATOM      3 N1   FOU     1      -2.921   1.564  -0.280
ATOM      4 C6   FOU     1      -3.695   0.492   0.007
ATOM      5 H6   FOU     1      -4.769   0.655   0.053
ATOM      6 C5   FOU     1      -3.189  -0.755   0.230
ATOM      7 C7   FOU     1      -4.105  -1.872   0.528
ATOM      8 H7   FOU     1      -3.607  -2.843   0.691
ATOM      9 O8   FOU     1      -5.319  -1.754   0.593
ATOM     10 C4   FOU     1      -1.747  -0.960   0.158
ATOM     11 O4   FOU     1      -1.187  -2.044   0.305
ATOM     12 N3   FOU     1      -1.021   0.201  -0.096
ATOM     13 H3   FOU     1       0.010   0.110  -0.078
ATOM     14 C2   FOU     1      -1.513   1.464  -0.368
ATOM     15 O2   FOU     1      -0.837   2.427  -0.660
ATOM     16 H1'2 FOU     1      -4.569   2.822  -0.415
ATOM     17 H1'3 FOU     1      -3.244   3.204  -1.554
TER
ATOM     18 C1'  CYT     2       4.994   1.585   0.648
ATOM     19 H1'1 CYT     2       4.707   2.487   0.105
ATOM     20 N1   CYT     2       4.140   0.475   0.242
ATOM     21 C2   CYT     2       2.739   0.659   0.424
ATOM     22 O2   CYT     2       2.346   1.704   0.915
ATOM     23 N3   CYT     2       1.917  -0.372   0.025
ATOM     24 C4   CYT     2       2.426  -1.503  -0.436
ATOM     25 N4   CYT     2       1.554  -2.475  -0.814
ATOM     26 C5   CYT     2       3.835  -1.714  -0.601
ATOM     27 H5   CYT     2       4.239  -2.637  -0.995
ATOM     28 C6   CYT     2       4.650  -0.680  -0.248
ATOM     29 H6   CYT     2       5.731  -0.731  -0.338
ATOM     30 H42  CYT     2       1.920  -3.408  -0.917
ATOM     31 H41  CYT     2       0.608  -2.396  -0.446
ATOM     32 H1'2 CYT     2       6.030   1.325   0.429
ATOM     33 H1'3 CYT     2       4.871   1.778   1.716
ENDMDL
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TITLE      C(1):5-HOdU  1-methyl-cytosine:1-methyl-5-hydroxy-uracil BP
REMARK     6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK     Delta E = -12.2 kcal/mol
REMARK     H-Bonds (C->U): H41-O4=1.99A; N3-H3=1.99A
MODEL        7
ATOM      1 C1'  HOU     1      -3.981  -2.488  -0.540
ATOM      2 H1'1 HOU     1      -3.487  -3.326  -0.047
ATOM      3 N1   HOU     1      -3.284  -1.252  -0.200
ATOM      4 C6   HOU     1      -3.994  -0.101   0.098
ATOM      5 H6   HOU     1      -5.074  -0.189   0.140
ATOM      6 C5   HOU     1      -3.357   1.072   0.331
ATOM      7 O5   HOU     1      -3.997   2.230   0.629
ATOM      8 HO5  HOU     1      -3.271   2.863   0.741
ATOM      9 C4   HOU     1      -1.904   1.128   0.265
ATOM     10 O4   HOU     1      -1.307   2.196   0.459
ATOM     11 N3   HOU     1      -1.284  -0.062  -0.016
ATOM     12 H3   HOU     1      -0.250  -0.060  -0.014
ATOM     13 C2   HOU     1      -1.902  -1.278  -0.321
ATOM     14 O2   HOU     1      -1.288  -2.272  -0.661
ATOM     15 H1'2 HOU     1      -3.965  -2.662  -1.619
ATOM     16 H1'3 HOU     1      -5.012  -2.408  -0.193
TER
ATOM     17 C1'  CYT     2       4.663  -1.838   0.516
ATOM     18 H1'1 CYT     2       4.583  -2.034   1.587
ATOM     19 N1   CYT     2       3.866  -0.668   0.164
ATOM     20 C2   CYT     2       2.466  -0.762   0.415
ATOM     21 O2   CYT     2       2.031  -1.784   0.918
ATOM     22 N3   CYT     2       1.696   0.324   0.064
ATOM     23 C4   CYT     2       2.255   1.425  -0.411
ATOM     24 N4   CYT     2       1.432   2.456  -0.740
ATOM     25 C5   CYT     2       3.665   1.546  -0.643
ATOM     26 H5   CYT     2       4.109   2.445  -1.049
ATOM     27 C6   CYT     2       4.427   0.457  -0.341
ATOM     28 H6   CYT     2       5.503   0.438  -0.484
ATOM     29 H42  CYT     2       1.854   3.364  -0.850
ATOM     30 H41  CYT     2       0.501   2.436  -0.328
ATOM     31 H1'2 CYT     2       5.702  -1.645   0.244
ATOM     32 H1'3 CYT     2       4.288  -2.712  -0.018
ENDMDL
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TITLE      C(2):5-HOdU  1-methyl-cytosine:1-methyl-5-hydroxy-uracil BP
REMARK     6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK     Delta E = -12.2 kcal/mol
REMARK     H-Bonds (C->U): H41-O4=1.99A; N3-H3=1.99A
MODEL        8
ATOM      1 C1'  HOU     1       3.984  -2.486  -0.539
ATOM      2 H1'1 HOU     1       3.479  -3.327  -0.062
ATOM      3 N1   HOU     1       3.285  -1.252  -0.198
ATOM      4 C6   HOU     1       3.994  -0.101   0.101
ATOM      5 H6   HOU     1       5.073  -0.188   0.145
ATOM      6 C5   HOU     1       3.356   1.073   0.333
ATOM      7 O7   HOU     1       3.995   2.230   0.631
ATOM      8 H7   HOU     1       3.269   2.863   0.743
ATOM      9 C4   HOU     1       1.903   1.128   0.265
ATOM     10 O4   HOU     1       1.306   2.195   0.458
ATOM     11 H1'2 HOU     1       5.009  -2.413  -0.175
ATOM     12 H1'3 HOU     1       3.985  -2.650  -1.620
ATOM     13 N3   HOU     1       1.284  -0.062  -0.018
ATOM     14 H3   HOU     1       0.250  -0.060  -0.018
ATOM     15 C2   HOU     1       1.903  -1.278  -0.322
ATOM     16 O2   HOU     1       1.290  -2.271  -0.665
TER
ATOM     17 C1'  CYT     2      -4.662  -1.839   0.519
ATOM     18 H1'1 CYT     2      -4.287  -2.713  -0.015
ATOM     19 N1   CYT     2      -3.866  -0.669   0.165
ATOM     20 C2   CYT     2      -2.466  -0.763   0.414
ATOM     21 O2   CYT     2      -2.029  -1.785   0.916
ATOM     22 N3   CYT     2      -1.696   0.324   0.062
ATOM     23 C4   CYT     2      -2.256   1.424  -0.412
ATOM     24 N4   CYT     2      -1.434   2.456  -0.743
ATOM     25 C5   CYT     2      -3.667   1.545  -0.641
ATOM     26 H5   CYT     2      -4.112   2.445  -1.046
ATOM     27 C6   CYT     2      -4.428   0.456  -0.338
ATOM     28 H6   CYT     2      -5.505   0.437  -0.479
ATOM     29 H42  CYT     2      -1.856   3.364  -0.851
ATOM     30 H41  CYT     2      -0.503   2.435  -0.332
ATOM     31 H1'2 CYT     2      -5.701  -1.647   0.248
ATOM     32 H1'3 CYT     2      -4.581  -2.035   1.590
ENDMDL
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```
TITLE      C(1):U  1-methyl-cytosine:1-methyl-uracil base pair
REMARK     6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK     Delta E = -12.0 kcal/mol
REMARK     H-Bonds (C->U): H41-O4=1.95A; N3-H3=2.01A
MODEL        9
ATOM      1 C1'  URA     1      -4.423  -1.957  -0.488
ATOM      2 H1'  URA     1      -4.107  -2.804   0.124
ATOM      3 N1   URA     1      -3.632  -0.778  -0.153
ATOM      4 C6   URA     1      -4.211   0.399   0.238
ATOM      5 H6   URA     1      -5.294   0.383   0.306
ATOM      6 C5   URA     1      -3.488   1.511   0.521
ATOM      7 H5   URA     1      -3.964   2.433   0.822
ATOM      8 C4   URA     1      -2.040   1.475   0.408
ATOM      9 O4   URA     1      -1.298   2.434   0.608
ATOM     10 N3   URA     1      -1.532   0.230   0.043
ATOM     11 H3   URA     1      -0.503   0.142   0.019
ATOM     12 C2   URA     1      -2.242  -0.911  -0.292
ATOM     13 O2   URA     1      -1.739  -1.949  -0.674
ATOM     14 H1'2 URA     1      -4.285  -2.222  -1.538
ATOM     15 H1'3 URA     1      -5.472  -1.731  -0.296
TER
ATOM     16 C1'  CYT     2       4.285  -2.103   0.379
ATOM     17 H1'1 CYT     2       4.188  -2.359   1.436
ATOM     18 N1   CYT     2       3.585  -0.853   0.103
ATOM     19 C2   CYT     2       2.182  -0.849   0.353
ATOM     20 O2   CYT     2       1.666  -1.863   0.791
ATOM     21 N3   CYT     2       1.502   0.316   0.076
ATOM     22 C4   CYT     2       2.149   1.395  -0.334
ATOM     23 N4   CYT     2       1.414   2.507  -0.594
ATOM     24 C5   CYT     2       3.566   1.415  -0.564
ATOM     25 H5   CYT     2       4.081   2.299  -0.916
ATOM     26 C6   CYT     2       4.236   0.252  -0.333
ATOM     27 H6   CYT     2       5.308   0.154  -0.482
ATOM     28 H42  CYT     2       1.908   3.383  -0.651
ATOM     29 H41  CYT     2       0.482   2.536  -0.183
ATOM     30 H1'2 CYT     2       5.336  -1.978   0.116
ATOM     31 H1'3 CYT     2       3.842  -2.909  -0.208
ENDMDL
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```
TITLE      C(2):U  1-methyl-cytosine:1-methyl-uracil base pair
REMARK     6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK     Delta E = -12.0 kcal/mol
REMARK     H-Bonds (C->U): H41-O4=1.95A; N3-H3=2.02A
MODEL       10
ATOM      1 C1'  URA     1       4.425  -1.956  -0.482
ATOM      2 H1'1 URA     1       4.103  -2.804   0.123
ATOM      3 N1   URA     1       3.633  -0.777  -0.149
ATOM      4 C6   URA     1       4.211   0.400   0.243
ATOM      5 H6   URA     1       5.294   0.385   0.314
ATOM      6 C5   URA     1       3.487   1.512   0.522
ATOM      7 H5   URA     1       3.962   2.435   0.825
ATOM      8 C4   URA     1       2.039   1.476   0.405
ATOM      9 O4   URA     1       1.296   2.435   0.602
ATOM     10 H1'2 URA     1       5.473  -1.732  -0.281
ATOM     11 H1'3 URA     1       4.297  -2.215  -1.535
ATOM     12 N3   URA     1       1.532   0.230   0.039
ATOM     13 H3   URA     1       0.504   0.143   0.011
ATOM     14 C2   URA     1       2.244  -0.910  -0.294
ATOM     15 O2   URA     1       1.743  -1.948  -0.679
TER
ATOM     16 C1'  CYT     2      -4.282  -2.106   0.381
ATOM     17 H1'1 CYT     2      -3.841  -2.910  -0.209
ATOM     18 N1   CYT     2      -3.585  -0.855   0.104
ATOM     19 C2   CYT     2      -2.180  -0.851   0.349
ATOM     20 O2   CYT     2      -1.662  -1.866   0.784
ATOM     21 N3   CYT     2      -1.503   0.315   0.072
ATOM     22 C4   CYT     2      -2.152   1.395  -0.333
ATOM     23 N4   CYT     2      -1.419   2.508  -0.594
ATOM     24 C5   CYT     2      -3.569   1.414  -0.558
ATOM     25 H5   CYT     2      -4.087   2.299  -0.906
ATOM     26 C6   CYT     2      -4.239   0.250  -0.327
ATOM     27 H6   CYT     2      -5.311   0.152  -0.472
ATOM     28 H42  CYT     2      -1.914   3.383  -0.647
ATOM     29 H41  CYT     2      -0.485   2.538  -0.185
ATOM     30 H1'2 CYT     2      -5.335  -1.981   0.122
ATOM     31 H1'3 CYT     2      -4.181  -2.364   1.437
ENDMDL
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```
TITLE      G:C   1-methyl-guanine:1-methyl-cytosine BP
REMARK     6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK     Delta E = -24.9 kcal/mol
REMARK     H-Bonds (G->C) O6-H41=1.86A; H1-N3=1.98A; H21-O2=2.01A
MODEL       11
ATOM      1 C1'  CYT     1      -5.159  -1.905   0.335
ATOM      2 H1'1 CYT     1      -4.979  -2.572  -0.510
ATOM      3 N1   CYT     1      -4.388  -0.677   0.168
ATOM      4 C2   CYT     1      -2.985  -0.815   0.064
ATOM      5 O2   CYT     1      -2.505  -1.946   0.127
ATOM      6 N3   CYT     1      -2.241   0.319  -0.097
ATOM      7 C4   CYT     1      -2.820   1.516  -0.135
ATOM      8 N4   CYT     1      -2.031   2.590  -0.320
ATOM      9 C5   CYT     1      -4.243   1.678  -0.028
ATOM     10 H5   CYT     1      -4.717   2.651  -0.068
ATOM     11 C6   CYT     1      -4.981   0.544   0.122
ATOM     12 H6   CYT     1      -6.063   0.557   0.211
ATOM     13 H42  CYT     1      -2.421   3.506  -0.176
ATOM     14 H41  CYT     1      -1.017   2.476  -0.220
ATOM     15 H1'2 CYT     1      -6.216  -1.645   0.390
ATOM     16 H1'3 CYT     1      -4.849  -2.416   1.248
TER
ATOM     17 C1'  GUA     2       5.562  -1.450   0.127
ATOM     18 H1'1 GUA     2       5.186  -2.206  -0.562
ATOM     19 N9   GUA     2       4.654  -0.318   0.109
ATOM     20 C8   GUA     2       4.954   1.018   0.256
ATOM     21 H8   GUA     2       5.977   1.353   0.364
ATOM     22 N7   GUA     2       3.889   1.806   0.238
ATOM     23 C5   GUA     2       2.842   0.927   0.077
ATOM     24 C6   GUA     2       1.427   1.166  -0.017
ATOM     25 O6   GUA     2       0.813   2.230   0.031
ATOM     26 N1   GUA     2       0.736  -0.052  -0.187
ATOM     27 C2   GUA     2       1.292  -1.305  -0.257
ATOM     28 N2   GUA     2       0.425  -2.332  -0.508
ATOM     29 N3   GUA     2       2.584  -1.543  -0.165
ATOM     30 C4   GUA     2       3.290  -0.394  -0.004
ATOM     31 H1   GUA     2      -0.289   0.034  -0.223
ATOM     32 H22  GUA     2       0.827  -3.237  -0.317
ATOM     33 H21  GUA     2      -0.549  -2.215  -0.237
ATOM     34 H1'2 GUA     2       6.550  -1.116  -0.193
ATOM     35 H1'3 GUA     2       5.626  -1.881   1.130
TER
ENDMDL
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TITLE      G:5HOdU   1-methyl-guanine:1-methyl-5-hydroxy-uracil BP
REMARK     6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK     Delta E = -14.9 kcal/mol
REMARK     H-Bonds (G->U) O6-H3=1.88 and H1-O2=1.86A
MODEL       12
ATOM      1 C1'  HOU     1       3.908   2.749   0.073
ATOM      2 H1'1 HOU     1       3.350   3.211  -0.742
ATOM      3 N1   HOU     1       3.743   1.299   0.027
ATOM      4 C6   HOU     1       4.851   0.457   0.030
ATOM      5 H6   HOU     1       5.824   0.931   0.045
ATOM      6 C5   HOU     1       4.699  -0.888   0.007
ATOM      7 O5   HOU     1       5.732  -1.759   0.003
ATOM      8 HO5  HOU     1       5.297  -2.628  -0.016
ATOM      9 C4   HOU     1       3.359  -1.474  -0.016
ATOM     10 O4   HOU     1       3.196  -2.689  -0.039
ATOM     11 N3   HOU     1       2.328  -0.549  -0.010
ATOM     12 H3   HOU     1       1.364  -0.916  -0.021
ATOM     13 C2   HOU     1       2.454   0.828   0.019
ATOM     14 O2   HOU     1       1.485   1.591   0.037
ATOM     15 H1'2 HOU     1       4.969   2.974  -0.031
ATOM     16 H1'3 HOU     1       3.537   3.147   1.020
TER
ATOM     17 C1'  GUA     2      -6.258   0.148   0.088
ATOM     18 H1'1 GUA     2      -6.191   1.052  -0.519
ATOM     19 N9   GUA     2      -4.983  -0.545   0.026
ATOM     20 C8   GUA     2      -4.752  -1.902   0.042
ATOM     21 H8   GUA     2      -5.571  -2.609   0.063
ATOM     22 N7   GUA     2      -3.466  -2.221   0.021
ATOM     23 C5   GUA     2      -2.832  -1.003  -0.006
ATOM     24 C6   GUA     2      -1.430  -0.679  -0.038
ATOM     25 O6   GUA     2      -0.451  -1.419  -0.038
ATOM     26 N1   GUA     2      -1.261   0.723  -0.075
ATOM     27 C2   GUA     2      -2.251   1.668  -0.059
ATOM     28 N2   GUA     2      -1.826   2.977  -0.168
ATOM     29 N3   GUA     2      -3.533   1.396  -0.017
ATOM     30 C4   GUA     2      -3.751   0.052  -0.002
ATOM     31 H1   GUA     2      -0.285   1.038  -0.097
ATOM     32 H42  GUA     2      -2.540   3.633   0.116
ATOM     33 H41  GUA     2      -0.913   3.169   0.222
ATOM     34 H1'2 GUA     2      -7.035  -0.506  -0.309
ATOM     35 H1'3 GUA     2      -6.499   0.424   1.118
TER
ENDMDL
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TITLE      G:5HOdC   1-methyl-guanine:1-methyl-5-hydroxy-cytosine BP
REMARK     6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK     Delta E = -24.7 kcal/mol
REMARK     H-Bonds 1.87, 1.97 and 2.01 angstrom
MODEL       13
ATOM      1 C1'  HOC     1      -4.756   2.382   0.422
ATOM      2 H1'1 HOC     1      -4.375   2.862   1.326
ATOM      3 N1   HOC     1      -4.070   1.111   0.210
ATOM      4 C2   HOC     1      -2.674   1.164   0.048
ATOM      5 O2   HOC     1      -2.115   2.260   0.082
ATOM      6 N3   HOC     1      -2.006  -0.022  -0.123
ATOM      7 C4   HOC     1      -2.655  -1.176  -0.128
ATOM      8 N7   HOC     1      -1.969  -2.327  -0.303
ATOM      9 C5   HOC     1      -4.088  -1.241  -0.022
ATOM     10 C6   HOC     1      -4.753  -0.068   0.158
ATOM     11 H6   HOC     1      -5.831  -0.036   0.270
ATOM     12 H71  HOC     1      -2.428  -3.165   0.021
ATOM     13 H72  HOC     1      -0.949  -2.286  -0.201
ATOM     14 H1'2 HOC     1      -5.825   2.187   0.523
ATOM     15 H1'3 HOC     1      -4.572   3.047  -0.423
ATOM     16 O8   HOC     1      -4.749  -2.452  -0.023
ATOM     17 HO8  HOC     1      -4.625  -2.832  -0.899
TER
ATOM     18 C1'  GUA     2       5.906   1.182   0.103
ATOM     19 H1'1 GUA     2       5.374   2.119  -0.064
ATOM     20 N9   GUA     2       4.912   0.124   0.134
ATOM     21 C8   GUA     2       5.112  -1.228   0.297
ATOM     22 H8   GUA     2       6.106  -1.637   0.427
ATOM     23 N7   GUA     2       3.992  -1.936   0.277
ATOM     24 C5   GUA     2       3.014  -0.987   0.090
ATOM     25 C6   GUA     2       1.587  -1.124  -0.012
ATOM     26 O6   GUA     2       0.897  -2.141   0.046
ATOM     27 N1   GUA     2       0.987   0.137  -0.205
ATOM     28 C2   GUA     2       1.632   1.347  -0.285
ATOM     29 N2   GUA     2       0.843   2.430  -0.557
ATOM     30 N3   GUA     2       2.937   1.490  -0.185
ATOM     31 C4   GUA     2       3.558   0.297  -0.002
ATOM     32 H1   GUA     2      -0.041   0.125  -0.249
ATOM     33 H21  GUA     2       1.307   3.306  -0.374
ATOM     34 H22  GUA     2      -0.139   2.387  -0.293
ATOM     35 H1'2 GUA     2       6.442   1.231   1.054
ATOM     36 H1'3 GUA     2       6.615   1.015  -0.712
ENDMDL
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TITLE      G:U   1-methyl-guanine:1-methyl-uracil base pair
REMARK     6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK     Delta E = -13.4 kcal/mol
REMARK     H-Bonds (G->U) O6-H3=1.94A and H1-O2=1.87A
MODEL       14
ATOM      1 C1'  URA     1       4.348   2.408   0.069
ATOM      2 H1'1 URA     1       3.880   2.882  -0.796
ATOM      3 N1   URA     1       4.119   0.967   0.037
ATOM      4 C6   URA     1       5.161   0.066   0.021
ATOM      5 H6   URA     1       6.152   0.508   0.032
ATOM      6 C5   URA     1       4.965  -1.272  -0.008
ATOM      7 H5   URA     1       5.799  -1.962  -0.021
ATOM      8 C4   URA     1       3.611  -1.816  -0.022
ATOM      9 O4   URA     1       3.316  -2.995  -0.048
ATOM     10 N3   URA     1       2.617  -0.813  -0.002
ATOM     11 H3   URA     1       1.640  -1.135  -0.010
ATOM     12 C2   URA     1       2.797   0.546   0.028
ATOM     13 O2   URA     1       1.879   1.366   0.047
ATOM     14 H1'2 URA     1       5.424   2.582   0.048
ATOM     15 H1'3 URA     1       3.922   2.840   0.977
TER
ATOM     16 C1'  GUA     2      -5.952   0.420   0.075
ATOM     17 H1'1 GUA     2      -5.824   1.318  -0.530
ATOM     18 N9   GUA     2      -4.725  -0.355   0.020
ATOM     19 C8   GUA     2      -4.582  -1.723   0.042
ATOM     20 H8   GUA     2      -5.445  -2.376   0.061
ATOM     21 N7   GUA     2      -3.320  -2.125   0.027
ATOM     22 C5   GUA     2      -2.608  -0.950  -0.001
ATOM     23 C6   GUA     2      -1.186  -0.719  -0.029
ATOM     24 O6   GUA     2      -0.257  -1.518  -0.023
ATOM     25 N1   GUA     2      -0.928   0.672  -0.069
ATOM     26 C2   GUA     2      -1.856   1.677  -0.060
ATOM     27 N2   GUA     2      -1.348   2.957  -0.171
ATOM     28 N3   GUA     2      -3.153   1.489  -0.023
ATOM     29 C4   GUA     2      -3.457   0.161  -0.004
ATOM     30 H1   GUA     2       0.065   0.922  -0.090
ATOM     31 H21  GUA     2      -2.021   3.656   0.107
ATOM     32 H22  GUA     2      -0.429   3.091   0.228
ATOM     33 H1'2 GUA     2      -6.768  -0.182  -0.326
ATOM     34 H1'3 GUA     2      -6.181   0.711   1.104
ENDMDL
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Supplementary Material for Organic & Biomolecular Chemistry


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TITLE   T:FOU(conformation 1) 1-methyl-thymine:1-methyl-5-formyl uracil
REMARK    6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK    Delta E = -10.3 kcal/mol
REMARK    H-bonds (T > FoU) = O4-H3=1.91A,H3-O2=1.97A
MODEL       15
ATOM      1 C1'  FOU     1       5.189  -1.848   0.000
ATOM      2 H1'1 FOU     1       4.838  -2.877  -0.002
ATOM      3 N1   FOU     1       4.011  -0.980  -0.000
ATOM      4 C6   FOU     1       4.158   0.369  -0.000
ATOM      5 H6   FOU     1       5.178   0.747  -0.000
ATOM      6 C5   FOU     1       3.113   1.244  -0.000
ATOM      7 C7   FOU     1       3.374   2.699  -0.000
ATOM      8 H7   FOU     1       2.468   3.329  -0.000
ATOM      9 O8   FOU     1       4.494   3.181  -0.001
ATOM     10 C4   FOU     1       1.753   0.719  -0.000
ATOM     11 O4   FOU     1       0.735   1.402  -0.000
ATOM     12 N3   FOU     1       1.692  -0.674  -0.000
ATOM     13 H3   FOU     1       0.751  -1.084  -0.000
ATOM     14 C2   FOU     1       2.734  -1.583  -0.000
ATOM     15 O2   FOU     1       2.580  -2.787   0.000
ATOM     16 H1'2 FOU     1       5.786  -1.664   0.896
ATOM     17 H1'3 FOU     1       5.789  -1.661  -0.893
TER
ATOM     18 C1'  THY     2      -3.510  -2.911   0.000
ATOM     19 H1'1 THY     2      -2.504  -3.327   0.001
ATOM     20 N1   THY     2      -3.387  -1.457   0.000
ATOM     21 C2   THY     2      -2.122  -0.891   0.000
ATOM     22 O2   THY     2      -1.096  -1.564   0.000
ATOM     23 N3   THY     2      -2.119   0.486   0.000
ATOM     24 H3   THY     2      -1.189   0.914   0.000
ATOM     25 C4   THY     2      -3.218   1.358   0.001
ATOM     26 O4   THY     2      -3.068   2.569  -0.000
ATOM     27 C5   THY     2      -4.514   0.677   0.000
ATOM     28 C7   THY     2      -5.751   1.523  -0.000
ATOM     29 C6   THY     2      -4.528  -0.678   0.000
ATOM     30 H6   THY     2      -5.459  -1.240   0.000
ATOM     31 H71  THY     2      -5.766   2.173   0.879
ATOM     32 H72  THY     2      -5.765   2.173  -0.879
ATOM     33 H73  THY     2      -6.651   0.903  -0.001
ATOM     34 H1'2 THY     2      -4.042  -3.243  -0.895
ATOM     35 H1'3 THY     2      -4.044  -3.244   0.894
ENDMDL
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TITLE  T-FoU(conformation 2)   1-methyl-thymine:1-methyl-5-formyl-uracil
REMARK    6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK    Delta E = -10.1 kcal/mol
REMARK    H-bonds (T > FoU) = O4-H3=1.92A,H3-O2=1.97A
MODEL       16
ATOM      1 C1'  FOU     1       2.875  -3.063   0.003
ATOM      2 H1'1 FOU     1       1.845  -3.412  -0.004
ATOM      3 N1   FOU     1       2.848  -1.600   0.001
ATOM      4 C6   FOU     1       4.013  -0.896   0.001
ATOM      5 H6   FOU     1       4.931  -1.479   0.002
ATOM      6 C5   FOU     1       4.072   0.463   0.000
ATOM      7 C7   FOU     1       5.388   1.139   0.001
ATOM      8 O8   FOU     1       6.451   0.542   0.002
ATOM      9 H7   FOU     1       5.338   2.241  -0.000
ATOM     10 C4   FOU     1       2.830   1.235  -0.001
ATOM     11 O4   FOU     1       2.746   2.450  -0.002
ATOM     12 N3   FOU     1       1.681   0.424  -0.002
ATOM     13 H3   FOU     1       0.773   0.902  -0.002
ATOM     14 C2   FOU     1       1.605  -0.948  -0.000
ATOM     15 O2   FOU     1       0.552  -1.568  -0.000
ATOM     16 H1'2 FOU     1       3.380  -3.424   0.901
ATOM     17 H1'3 FOU     1       3.392  -3.426  -0.888
TER
ATOM     18 C1'  THY     2      -5.817  -1.213  -0.000
ATOM     19 H1'1 THY     2      -5.589  -2.277  -0.019
ATOM     20 N1   THY     2      -4.547  -0.492  -0.003
ATOM     21 C2   THY     2      -3.364  -1.230  -0.001
ATOM     22 O2   THY     2      -3.327  -2.447  -0.000
ATOM     23 N3   THY     2      -2.224  -0.439  -0.001
ATOM     24 H3   THY     2      -1.338  -0.949  -0.000
ATOM     25 C4   THY     2      -2.135   0.948   0.000
ATOM     26 O4   THY     2      -1.048   1.523   0.002
ATOM     27 C5   THY     2      -3.419   1.640   0.000
ATOM     28 C7   THY     2      -3.417   3.138   0.001
ATOM     29 C6   THY     2      -4.547   0.885  -0.001
ATOM     30 H6   THY     2      -5.534   1.339  -0.001
ATOM     31 H71  THY     2      -2.889   3.520  -0.877
ATOM     32 H72  THY     2      -4.437   3.531   0.001
ATOM     33 H73  THY     2      -2.890   3.519   0.881
ATOM     34 H1'2 THY     2      -6.401  -0.948  -0.885
ATOM     35 H1'3 THY     2      -6.384  -0.976   0.904
ENDMDL
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TITLE   T(1):5HOdU   1-methyl-5-hydroxy-uracil:T1 base pair
REMARK   6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK   Delta E = -10.2 kcal/mol
REMARK   H-Bonds(T->U) = H3-O4=1.98; O2-H3=1.92
MODEL       17
ATOM      1 C1'  HOU     1       5.534   1.203   0.000
ATOM      2 H1'1 HOU     1       5.302   2.266   0.000
ATOM      3 N1   HOU     1       4.269   0.477   0.000
ATOM      4 C6   HOU     1       4.298  -0.911   0.000
ATOM      5 H6   HOU     1       5.279  -1.372   0.000
ATOM      6 C5   HOU     1       3.158  -1.644   0.000
ATOM      7 O5   HOU     1       3.134  -2.996   0.000
ATOM      8 HO5  HOU     1       2.188  -3.211   0.000
ATOM      9 C4   HOU     1       1.871  -0.962  -0.000
ATOM     10 O4   HOU     1       0.815  -1.603  -0.000
ATOM     11 N3   HOU     1       1.942   0.408  -0.000
ATOM     12 H3   HOU     1       1.049   0.914  -0.000
ATOM     13 C2   HOU     1       3.090   1.206   0.000
ATOM     14 O2   HOU     1       3.034   2.422  -0.000
ATOM     15 H1'2 HOU     1       6.111   0.953  -0.894
ATOM     16 H1'3 HOU     1       6.111   0.953   0.894
TER
ATOM     17 C1'  THY     2      -3.091   3.025   0.000
ATOM     18 H1'1 THY     2      -2.058   3.367  -0.002
ATOM     19 N1   THY     2      -3.074   1.565  -0.000
ATOM     20 C2   THY     2      -1.853   0.910   0.000
ATOM     21 O2   THY     2      -0.781   1.506   0.000
ATOM     22 N3   THY     2      -1.950  -0.464   0.000
ATOM     23 H3   THY     2      -1.053  -0.959   0.000
ATOM     24 C4   THY     2      -3.108  -1.254  -0.000
ATOM     25 O4   THY     2      -3.047  -2.473   0.000
ATOM     26 C5   THY     2      -4.352  -0.482  -0.000
ATOM     27 C7   THY     2      -5.647  -1.235  -0.000
ATOM     28 C6   THY     2      -4.268   0.872  -0.000
ATOM     29 H6   THY     2      -5.156   1.499  -0.000
ATOM     30 H71  THY     2      -5.709  -1.883  -0.879
ATOM     31 H72  THY     2      -5.709  -1.883   0.879
ATOM     32 H73  THY     2      -6.500  -0.551  -0.000
ATOM     33 H1'2 THY     2      -3.597   3.395   0.896
ATOM     34 H1'3 THY     2      -3.601   3.395  -0.893
ENDMDL
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TITLE   T(2):5HOdU   1-methyl-5-hydroxy-uracil:T2 base pair
REMARK   6-311G(d,p)/MP2-BSSE Optimized Geometry
REMARK   Delta E = -10.9 kcal/mol
REMARK   H-Bonds (T2->5HOU) H3-O2=1.94; O4-H3=1.91
MODEL       18
ATOM      1 C1'  HOU     1      -3.185  -2.997   0.001
ATOM      2 H1'1 HOU     1      -2.163  -3.369   0.000
ATOM      3 N1   HOU     1      -3.128  -1.539   0.000
ATOM      4 C6   HOU     1      -4.322  -0.826   0.001
ATOM      5 H6   HOU     1      -5.233  -1.413   0.001
ATOM      6 C5   HOU     1      -4.332   0.528   0.001
ATOM      7 O5   HOU     1      -5.460   1.273   0.001
ATOM      8 HO5  HOU     1      -5.129   2.186   0.001
ATOM      9 C4   HOU     1      -3.069   1.265   0.000
ATOM     10 O4   HOU     1      -3.045   2.491  -0.001
ATOM     11 N3   HOU     1      -1.944   0.463  -0.000
ATOM     12 H3   HOU     1      -1.027   0.926  -0.001
ATOM     13 C2   HOU     1      -1.895  -0.924  -0.000
ATOM     14 O2   HOU     1      -0.832  -1.539  -0.001
ATOM     15 H1'2 HOU     1      -3.705  -3.351   0.895
ATOM     16 H1'3 HOU     1      -3.706  -3.351  -0.893
TER
ATOM     17 C1'  THY     2       5.487  -1.290   0.001
ATOM     18 H1'1 THY     2       5.235  -2.349  -0.007
ATOM     19 N1   THY     2       4.233  -0.542  -0.001
ATOM     20 C2   THY     2       3.033  -1.256  -0.001
ATOM     21 O2   THY     2       2.973  -2.471   0.000
ATOM     22 N3   THY     2       1.910  -0.441  -0.001
ATOM     23 H3   THY     2       1.011  -0.933  -0.001
ATOM     24 C4   THY     2       1.853   0.946  -0.000
ATOM     25 O4   THY     2       0.779   1.547   0.000
ATOM     26 C5   THY     2       3.150   1.612  -0.000
ATOM     27 C7   THY     2       3.179   3.110   0.000
ATOM     28 C6   THY     2       4.262   0.834  -0.000
ATOM     29 H6   THY     2       5.259   1.267  -0.000
ATOM     30 H71  THY     2       2.660   3.502  -0.879
ATOM     31 H72  THY     2       2.660   3.501   0.880
ATOM     32 H73  THY     2       4.208   3.481   0.001
ATOM     33 H1'2 THY     2       6.064  -1.058   0.899
ATOM     34 H1'3 THY     2       6.072  -1.047  -0.889
ENDMDL
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TITLE      T(1):U  1-methyl-uracil:1-methyl-thymine(conformation 1)
REMARK     6-311G(d,p) MP2-BSSE Optimized Geometry
REMARK     Delta E = -9.9 kcal/mol
REMARK     H-Bonds (T1->U):  H3-O4=1.96; O2-H3=1.94
MODEL       19
ATOM      1 C1'  URA     1      -5.756   0.728   0.000
ATOM      2 H1'1 URA     1      -5.564   1.799  -0.004
ATOM      3 N1   URA     1      -4.462   0.051  -0.000
ATOM      4 C6   URA     1      -4.408  -1.320  -0.000
ATOM      5 H6   URA     1      -5.375  -1.815  -0.000
ATOM      6 C5   URA     1      -3.246  -2.017  -0.000
ATOM      7 H5   URA     1      -3.232  -3.098  -0.000
ATOM      8 C4   URA     1      -1.983  -1.297  -0.000
ATOM      9 O4   URA     1      -0.873  -1.819  -0.000
ATOM     10 N3   URA     1      -2.132   0.090  -0.000
ATOM     11 H3   URA     1      -1.265   0.636  -0.000
ATOM     12 C2   URA     1      -3.300   0.834  -0.000
ATOM     13 O2   URA     1      -3.318   2.050   0.000
ATOM     14 H1'2 URA     1      -6.321   0.461   0.897
ATOM     15 H1'3 URA     1      -6.325   0.455  -0.892
TER
ATOM     16 C1'  THY     2       2.753   3.014   0.000
ATOM     17 H1'1 THY     2       1.702   3.295   0.002
ATOM     18 N1   THY     2       2.821   1.556   0.000
ATOM     19 C2   THY     2       1.638   0.831   0.000
ATOM     20 O2   THY     2       0.535   1.366   0.000
ATOM     21 N3   THY     2       1.813  -0.536   0.000
ATOM     22 H3   THY     2       0.945  -1.080   0.000
ATOM     23 C4   THY     2       3.015  -1.257   0.000
ATOM     24 O4   THY     2       3.027  -2.477  -0.000
ATOM     25 C5   THY     2       4.213  -0.414   0.000
ATOM     26 C7   THY     2       5.548  -1.093   0.000
ATOM     27 C6   THY     2       4.052   0.932   0.000
ATOM     28 H6   THY     2       4.903   1.609   0.000
ATOM     29 H71  THY     2       5.648  -1.736   0.879
ATOM     30 H72  THY     2       5.647  -1.736  -0.879
ATOM     31 H73  THY     2       6.361  -0.361  -0.000
ATOM     32 H1'2 THY     2       3.237   3.413  -0.895
ATOM     33 H1'3 THY     2       3.240   3.413   0.894
ENDMDL
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TITLE     T(2):U   (1-me-thymine:1-methyl-uracil)
REMARK    6-311G(d,p) MP2-BSSE Optimized Geometry
REMARK    Delta E = -9.8 kcal/mol
REMARK    H-Bonds (T->U) = O4-H3=1.95A; H3-O2=1.95A
MODEL       20
ATOM      1  C1' URU     1       0.259  -2.149   0.105  1.00  0.00
ATOM      2 1H1' URU     1      -0.622  -2.613  -0.334  1.00  0.00
ATOM      3  N1  URU     1       0.079  -0.702   0.032  1.00  0.00
ATOM      4  C6  URU     1       1.056   0.134   0.521  1.00  0.00
ATOM      5 6H   URU     1       1.920  -0.373   0.941  1.00  0.00
ATOM      6  C5  URU     1       0.958   1.484   0.487  1.00  0.00
ATOM      7 5H   URU     1       1.744   2.115   0.880  1.00  0.00
ATOM      8  C4  URU     1      -0.226   2.111  -0.090  1.00  0.00
ATOM      9  O4  URU     1      -0.430   3.309  -0.177  1.00  0.00
ATOM     10  N3  URU     1      -1.164   1.174  -0.561  1.00  0.00
ATOM     11 3H   URU     1      -2.023   1.548  -0.978  1.00  0.00
ATOM     12  C2  URU     1      -1.088  -0.199  -0.538  1.00  0.00
ATOM     13  O2  URU     1      -1.968  -0.929  -0.978  1.00  0.00
ATOM     14 2H1' URU     1       0.358  -2.463   1.147  1.00  0.00
ATOM     15 3H1' URU     1       1.148  -2.447  -0.457  1.00  0.00
TER
ATOM      1  C1' THY     2      -7.636  -1.399  -3.768  1.00  0.00
ATOM      2  N1  THY     2      -6.597  -0.515  -3.248  1.00  0.00
ATOM      3  C2  THY     2      -5.454  -1.087  -2.692  1.00  0.00
ATOM      4  O2  THY     2      -5.271  -2.288  -2.616  1.00  0.00
ATOM      5  N3  THY     2      -4.540  -0.151  -2.232  1.00  0.00
ATOM      6 3H   THY     2      -3.686  -0.537  -1.817  1.00  0.00
ATOM      7  C4  THY     2      -4.635   1.235  -2.262  1.00  0.00
ATOM      8  O4  THY     2      -3.742   1.951  -1.814  1.00  0.00
ATOM      9  C5  THY     2      -5.863   1.748  -2.859  1.00  0.00
ATOM     10  C7  THY     2      -6.049   3.234  -2.932  1.00  0.00
ATOM     11 1H7  THY     2      -5.240   3.691  -3.508  1.00  0.00
ATOM     12 2H7  THY     2      -7.005   3.486  -3.399  1.00  0.00
ATOM     13 3H7  THY     2      -6.016   3.672  -1.931  1.00  0.00
ATOM     14  Q7  THY     2      -6.087   3.616  -2.946  1.00  0.00
ATOM     15  C6  THY     2      -6.771   0.850  -3.316  1.00  0.00
ATOM     16 6H   THY     2      -7.705   1.167  -3.771  1.00  0.00
ATOM     17 1H1' THY     2      -7.295  -2.423  -3.623  1.00  0.00
ATOM     18 2H1' THY     2      -7.793  -1.212  -4.833  1.00  0.00
ATOM     19 3H1' THY     2      -8.571  -1.246  -3.222  1.00  0.00
TER
ENDMDL
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