Supporting Information

Deprotonated Guanine·Cytosine and 9-Methylguanine·Cytosine Base Pairs and Their ″Non-Statistical″ Kinetics: A Combined Guided-Ion Beam and Computational Study

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Table of Contents

References

[S1] W. Lu and J. Liu, *Chem. Eur. J.*, 2016, **22**, 3127-3138.

[S2] W. Lu, H. Teng and J. Liu, *Phys. Chem. Chem. Phys.*, 2016, **18**, 15223-15234.

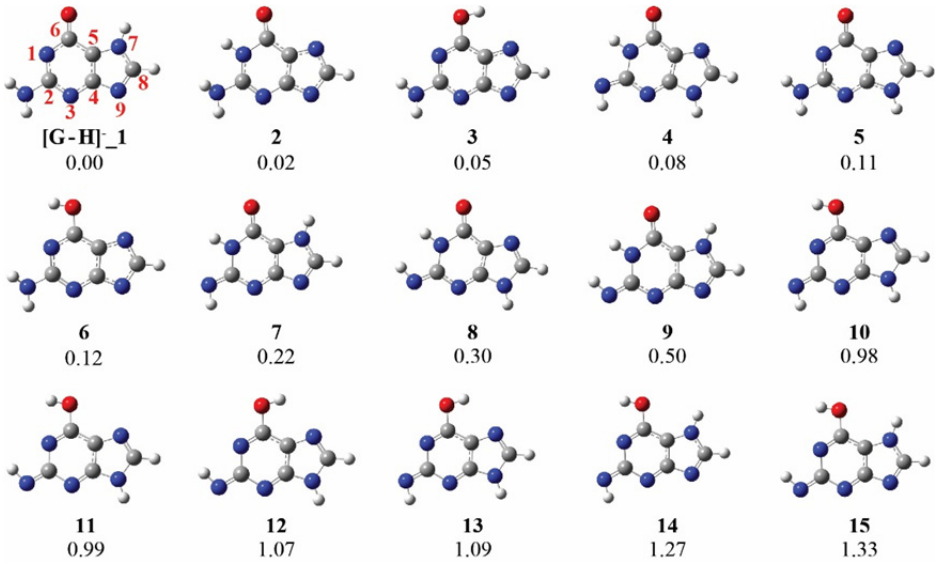

Fig. S1 Stable tautomers/rotamers of $[G - H]^-$. Relative energies (eV, including thermal corrections at 298 K) were calculated at B3LYP/6-311++G(d,p). See ref [S1] for their Cartesian coordinates.

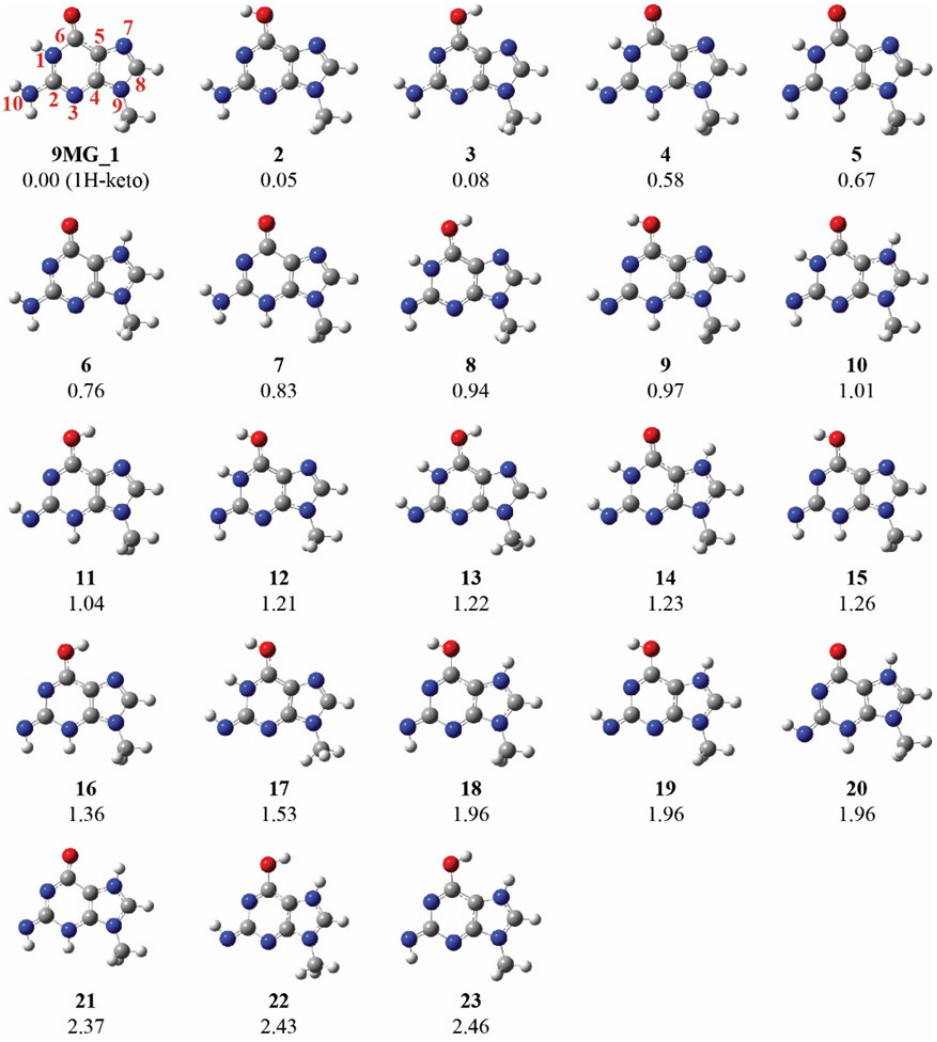

Fig. S2 Stable tautomers/rotamers of 9MG. Relative energies (eV, including thermal corrections at 298 K) were calculated at B3LYP/6-311++G(d,p). See ref [S2] for their Cartesian coordinates.

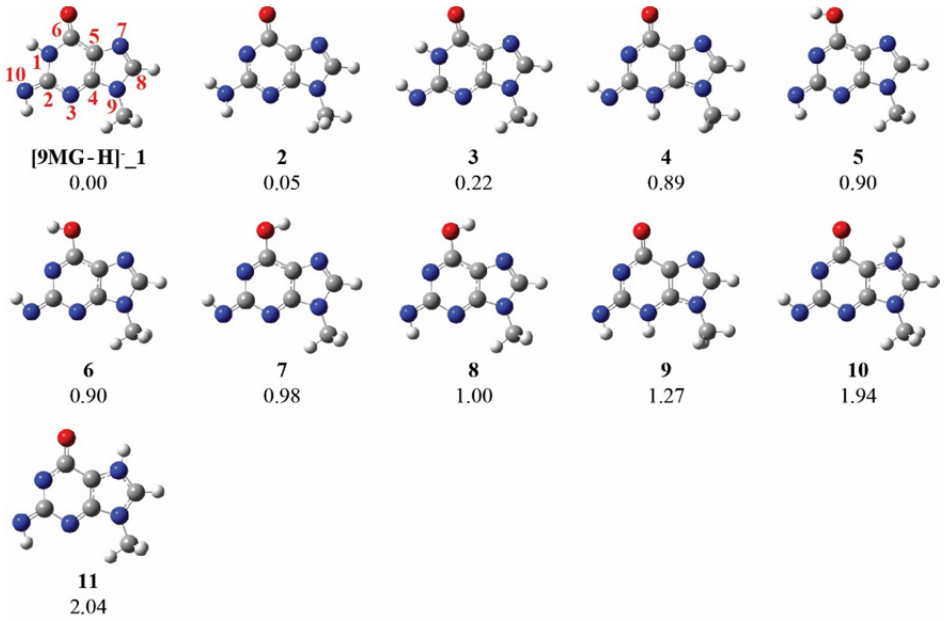

Fig. S3 Stable tautomers/rotamers of [9MG – H]$^-$. Relative energies (eV, including thermal corrections at 298 K) were calculated at B3LYP/6-311++G(d,p). See ref [S2] for their Cartesian coordinates.

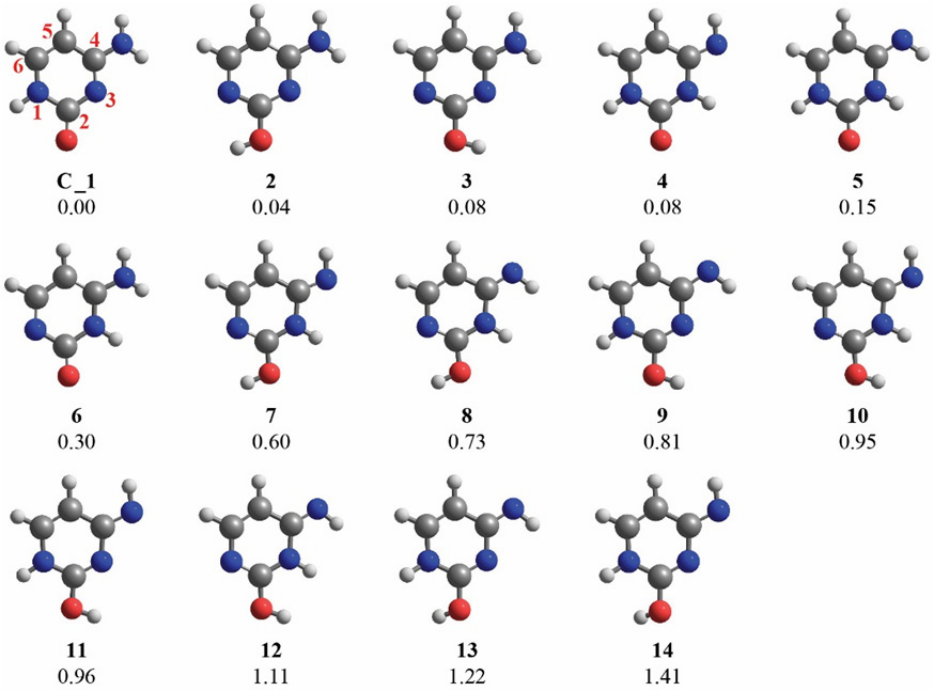

Fig. S4 Stable tautomers/rotamers of cytosine. Relative energies (eV, including thermal corrections at 298 K) were calculated at B3LYP/6-311++G(d,p).

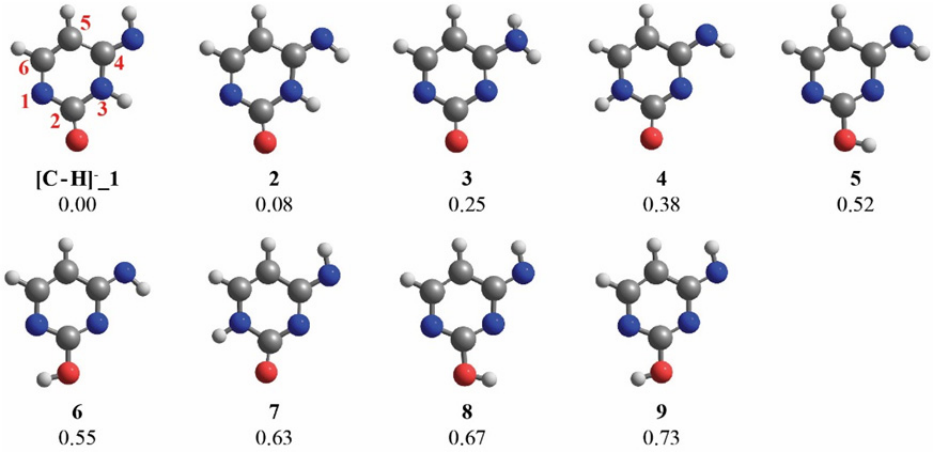

Fig. S5 Stable tautomers/rotamers of $[C - H]^-$. Relative energies (eV, including thermal corrections at 298 K) were calculated at B3LYP/6-311++G(d,p).

Cartesian coordinates for the $[G{\cdot}C - H]^-$ structures in Fig. 2, optimized at B3LYP/6-311++G(d,p) with BSSE correction

7HG·[C – H1]$^-$_PT1

C1 -1.357816 -0.850521 0.046725
C2 -2.763907 -0.642538 -0.034803
H3 1.219002 0.130673 0.091085
C4 -1.251786 1.503862 0.174695
C5 -4.953162 -0.723036 -0.203364
N6 -0.626968 0.294288 0.149085
N7 -3.837138 -1.508620 -0.154160
N8 -4.691319 0.564904 -0.126588
N9 -2.562372 1.756245 0.086212
C10 -3.308400 0.638518 -0.018927
N11 -0.426566 2.591341 0.344982
H12 -0.853241 3.477166 0.127677
H13 0.563916 2.489227 0.133223
O14 -0.828853 -2.004268 0.021927
H15 -5.942934 -1.148021 -0.296115
H16 -3.778898 -2.512841 -0.195438
C17 3.067429 1.116896 -0.140562
N18 2.254786 -0.026928 0.028075
C19 2.731758 -1.293749 0.103042
C20 4.881750 -0.305044 -0.156691
N21 4.424256 0.935943 -0.231750
H22 5.965383 -0.406412 -0.234081
O23 2.517338 2.217000 -0.198467
N24 1.852963 -2.293881 0.281150
H25 0.814292 -2.150059 0.194121
H26 2.208678 -3.233673 0.234249
C27 4.122468 -1.460745 0.006307
H28 4.572422 -2.442821 0.060021

9HG·[C – H1]$^-$_PT1

C1 -1.360309 -0.898887 0.046275
C2 -2.786662 -0.718006 -0.038281
H3 1.217296 0.116809 0.088318
C4 -1.234170 1.470668 0.165955
H5 -5.281215 1.248448 -0.131236
C6 -4.913196 -0.877420 -0.196229
N7 -0.629618 0.264935 0.143275
N8 -3.839695 -1.617755 -0.150148
N9 -4.631159 0.479563 -0.121454
N10 -2.554664 1.725441 0.079800
C11 -3.260118 0.593230 -0.018076
N12 -0.418016 2.562012 0.324859
H13 -0.844444 3.447909 0.109127
H14 0.578898 2.463002 0.135674
O15 -0.788149 -2.018851 0.031226
H16 -5.927414 -1.240331 -0.283174
C17 3.056935 1.125700 -0.126732
N18 2.256081 -0.026306 0.027847
C19 2.745729 -1.290010 0.092316
C20 4.885854 -0.275737 -0.154339
N21 4.414576 0.962013 -0.217847
H22 5.970619 -0.364068 -0.231310
O23 2.495373 2.222686 -0.173388
N24 1.876217 -2.297035 0.257900
H25 0.832348 -2.156077 0.183246
H26 2.237798 -3.234628 0.210923
C27 4.139643 -1.440200 -0.003461
H28 4.600038 -2.417849 0.041527

9HG·[C – H1]$^-$

C1 -1.421001 -1.004631 -0.030633
C2 -2.831258 -0.726819 -0.059378
H3 0.379916 0.067589 0.087369
C4 -1.177904 1.455000 0.123278
H5 -5.218778 1.361392 -0.016362
C6 -4.962831 -0.778999 -0.132994
N7 -0.666603 0.179667 0.062440
N8 -3.927260 -1.571024 -0.145025
N9 -4.609071 0.559996 -0.042740
N10 -2.487486 1.718033 0.094126
C11 -3.234573 0.607298 0.005478
N12 -0.293698 2.455281 0.231534
H13 -0.682425 3.382743 0.193846
H14 0.747629 2.315400 0.111080
O15 -0.860387 -2.100239 -0.076561
H16 -5.996039 -1.089697 -0.185570
C17 2.958005 1.086035 -0.081541
N18 2.218469 -0.074753 0.082996
C19 2.848299 -1.250205 0.122734
C20 4.908920 -0.128400 -0.186830
N21 4.327637 1.062918 -0.222603
H22 5.994934 -0.128274 -0.302010
O23 2.348536 2.188153 -0.107192
N24 2.082530 -2.373420 0.343473
H25 1.076884 -2.296580 0.190092
H26 2.493057 -3.254010 0.078326
C27 4.248128 -1.338236 -0.016262
H28 4.773285 -2.285016 0.020728

7HG·[C – H1]$^-$

C1 -1.405281 -0.948978 -0.038530
C2 -2.795426 -0.652644 -0.060607
H3 0.395980 0.107707 0.088115
C4 -1.193964 1.491181 0.137049
C5 -4.986516 -0.633367 -0.129862
N6 -0.654523 0.216730 0.064364
N7 -3.908574 -1.468176 -0.151392
N8 -4.662912 0.639318 -0.034211
N9 -2.496594 1.749026 0.109234
C10 -3.278545 0.652656 0.011482
N11 -0.306993 2.493278 0.261471
H12 -0.697901 3.419520 0.217348
H13 0.722859 2.352953 0.114951
O14 -0.887891 -2.076120 -0.099380
H15 -5.997535 -1.010858 -0.187554

H16 -3.900087 -2.473264 -0.215402
C17 2.955805 1.076535 -0.102123
N18 2.209160 -0.079823 0.079912
C19 2.831919 -1.257297 0.138154
C20 4.899636 -0.154173 -0.186084
N21 4.326884 1.039364 -0.242057
H22 5.985839 -0.163540 -0.299994
O23 2.353739 2.178839 -0.144998
N24 2.057401 -2.374851 0.374565
H25 1.056053 -2.291394 0.200981
H26 2.463882 -3.257501 0.108715
C27 4.230373 -1.357631 0.003477
H28 4.749176 -2.307129 0.056923

[7HG – H1]$^{-}$·C
C1 -1.961793 -1.094728 0.137816
C2 -3.270596 -0.538051 -0.041755
C3 -1.306605 1.184797 0.265944
C4 -5.398381 -0.092376 -0.371342
N5 -0.995104 -0.131965 0.293808
N6 -4.509673 -1.120748 -0.238913
N7 -4.837602 1.095974 -0.277667
N8 -2.503099 1.749512 0.083842
C9 -3.488933 0.835988 -0.069307
N10 -0.241990 2.043446 0.490267
H11 -0.404397 2.990270 0.185789
H12 0.687937 1.676809 0.317228
O13 -1.709027 -2.322524 0.147236
H14 -6.452581 -0.268257 -0.534732
H15 -4.688550 -2.111011 -0.274718
C16 3.966875 1.049482 -0.142469
N17 2.764734 0.456115 0.057465
C18 2.654297 -0.876900 0.116609
C19 5.006107 -1.168248 -0.229676
N20 5.100064 0.187119 -0.283359
H21 5.925979 -1.728779 -0.352333
O22 4.173582 2.255556 -0.214781
N23 1.453194 -1.407062 0.326601
H24 0.561594 -0.830998 0.353608
H25 1.325439 -2.406379 0.302452
C26 3.804353 -1.752976 -0.033196
H27 3.700969 -2.828125 0.014088
H28 5.981556 0.653561 -0.431085

7HG·[C – H4b]$^{-}$
C1 1.503858 -0.995803 0.077770
C2 2.888081 -0.650634 0.052228
H3 -0.326959 0.017799 -0.007276
C4 1.222089 1.438127 -0.133449
C5 5.078636 -0.572949 0.058399
N6 0.714760 0.156083 -0.021511
N7 4.023611 -1.434238 0.123915
N8 4.716878 0.689543 -0.048165
N9 2.513172 1.735505 -0.147051
C10 3.332828 0.662413 -0.054259
N11 0.312792 2.428969 -0.262187
H12 0.696136 3.358406 -0.217798
H13 -0.692173 2.290516 -0.047711
O14 1.028766 -2.128340 0.171650
H15 6.100600 -0.922440 0.092822
H16 4.040237 -2.438369 0.203985
C17 -2.895389 0.992267 0.160892
N18 -2.215593 -0.145345 0.025166
C19 -2.870382 -1.375879 -0.115481
C20 -5.004355 -0.212133 -0.025113
N21 -4.306360 0.957854 0.180580
H22 -6.085467 -0.130452 -0.044691
O23 -2.382323 2.133734 0.279648
N24 -2.263858 -2.513947 -0.200144
H25 -1.252804 -2.383532 -0.126336
C26 -4.339304 -1.368841 -0.174615
H27 -4.852115 -2.308848 -0.321632
H28 -4.763188 1.853376 0.225794

[7HG – H7]$^{-}$·C
C1 -1.495840 -0.913908 0.111133
C2 -2.887601 -0.739787 -0.019964
H3 0.201087 0.264139 0.254264
C4 -1.419450 1.551741 0.174797
C5 -4.975128 -0.850510 -0.253432
N6 -0.817757 0.315525 0.214761
N7 -3.913115 -1.649932 -0.150095
N8 -4.768806 0.498171 -0.207829
N9 -2.697525 1.737994 0.036980
C10 -3.433342 0.578561 -0.057909
N11 -0.563242 2.634893 0.357927
H12 -0.984390 3.500994 0.057142
H13 0.405925 2.521880 0.075823
O14 -0.810835 -1.972365 0.143767
H15 -5.976453 -1.252927 -0.370172
C16 3.022633 1.069714 -0.110074
N17 2.210435 -0.002434 0.043326
C18 2.692596 -1.248788 0.072794
C19 4.933730 -0.446703 -0.166153
N20 4.418008 0.811392 -0.207095
H21 6.010428 -0.534752 -0.250772
O22 2.648810 2.237278 -0.171722
N23 1.827566 -2.252943 0.204256
H24 0.772265 -2.089219 0.199735
H25 2.171774 -3.198877 0.190367
C26 4.114766 -1.513836 -0.028642
H27 4.505810 -2.521178 0.003471
H28 5.006629 1.623061 -0.317140

[9HG – H1]$^{-}$·C
C1 -1.963738 -1.150602 0.127232
C2 -3.297651 -0.607852 -0.049307
C3 -1.270423 1.137825 0.257176
C4 -5.384458 -0.232303 -0.347415
N5 -0.987069 -0.171183 0.279353

N6 -4.533362 -1.215775 -0.232019
N7 -4.776481 1.011086 -0.252419
N8 -2.475011 1.713219 0.083441
C9 -3.429397 0.780565 -0.059079
N10 -0.207194 1.995218 0.470539
H11 -0.362193 2.942968 0.166242
H12 0.725069 1.623518 0.315110
O13 -1.659023 -2.354278 0.142857
H14 -6.449729 -0.331892 -0.500618
H15 -5.210002 1.918381 -0.303743
C16 3.925248 1.068606 -0.127112
N17 2.733074 0.452756 0.058863
C18 2.643917 -0.884342 0.103730
C19 5.003685 -1.129152 -0.228700
N20 5.074263 0.228674 -0.268036
H21 5.934266 -1.671904 -0.350474
O22 4.110304 2.279720 -0.186722
N23 1.451486 -1.435138 0.297899
H24 0.547208 -0.871089 0.329566
H25 1.339662 -2.436417 0.269735
C26 3.811530 -1.737175 -0.046743
H27 3.726975 -2.814396 -0.011413
H28 5.948265 0.711893 -0.405514

9HG·[C – H4b]$^-$
C1 -1.529968 -1.057333 -0.059191
C2 -2.934858 -0.728017 -0.046299
H3 0.302031 -0.028088 0.009088
C4 -1.212674 1.399406 0.104110
C5 -5.068960 -0.715720 -0.059755
N6 -0.734587 0.116256 0.018912
N7 -4.057605 -1.537825 -0.105564
N8 -4.672043 0.611022 0.027673
N9 -2.511005 1.702573 0.112134
C10 -3.295986 0.614104 0.037322
N11 -0.309014 2.391318 0.204870
H12 -0.689022 3.322038 0.165971
H13 0.710365 2.251913 0.041747
O14 -1.007661 -2.159584 -0.125345
H15 -6.112124 -0.995037 -0.084825
H16 -5.255654 1.430431 0.077940
C17 2.904724 1.004526 -0.121505
N18 2.234997 -0.140000 -0.016243
C19 2.902494 -1.368651 0.088122
C20 5.025999 -0.183370 0.012758
N21 4.315070 0.986614 -0.146659
H22 6.106443 -0.092207 0.024791
O23 2.381358 2.147143 -0.206564
N24 2.308222 -2.513346 0.152687
H25 1.294421 -2.393942 0.098553
C26 4.372271 -1.349858 0.130790
H27 4.894336 -2.289517 0.243513
H28 4.763122 1.887130 -0.174282

7HG·[C – H4b]$^-$_PT1
C1 -1.382292 -0.861317 -0.008722
C2 -2.797538 -0.655576 -0.048486
C3 -1.307091 1.492393 0.199101
C4 -4.989301 -0.763349 -0.162288
N5 -0.663388 0.300627 0.114206
N6 -3.860671 -1.531748 -0.170014
N7 -4.742166 0.525861 -0.046774
N8 -2.619656 1.738343 0.154220
C9 -3.358090 0.613677 0.027463
N10 -0.490275 2.595596 0.392533
H11 -0.941061 3.469538 0.170611
H12 0.474247 2.504104 0.091515
O13 -0.847304 -1.995356 -0.082305
H14 -5.975245 -1.199300 -0.244087
H15 -3.784543 -2.533112 -0.245289
C16 2.928536 1.044224 -0.204976
N17 2.215067 -0.102686 -0.031389
C18 2.758784 -1.410068 0.127454
C19 4.940864 -0.328220 -0.008008
N20 4.316148 0.890174 -0.211441
H21 6.023741 -0.306380 -0.002996
O22 2.442215 2.163020 -0.351738
N23 2.071578 -2.477076 0.232615
H24 1.055966 -2.308893 0.163626
C25 4.223198 -1.447831 0.161012
H26 4.691812 -2.409132 0.310285
H27 4.837695 1.744839 -0.314163
H28 1.169221 0.019797 0.009861

[7HG – H7]$^-$·C_PT4
C1 -1.493969 -0.907888 0.043350
C2 -2.861727 -0.704114 -0.021548
H3 0.314473 0.144842 0.118128
C4 -1.268542 1.501217 0.138227
C5 -4.954705 -0.714872 -0.160763
N6 -0.724742 0.231468 0.124389
N7 -3.933114 -1.566320 -0.114433
N8 -4.686506 0.625448 -0.109417
N9 -2.549152 1.750215 0.060673
C10 -3.347437 0.646653 -0.019413
N11 -0.369636 2.529329 0.295399
H12 -0.758849 3.434226 0.085305
H13 0.617186 2.397623 0.070618
O14 -0.905672 -2.079025 0.030886
H15 -5.977858 -1.067767 -0.236958
C16 2.959084 1.055404 -0.109681
N17 2.136121 0.002830 0.003286
C18 2.592812 -1.283753 0.062746
C19 4.862922 -0.464730 -0.068854
N20 4.354315 0.801148 -0.149358
H21 5.942900 -0.554753 -0.098960
O22 2.598060 2.238891 -0.182583
N23 1.705482 -2.245476 0.133736
H24 2.138627 -3.162144 0.182853
C25 4.035852 -1.524327 0.040585

H26 4.427206 -2.531229 0.100506
H27 4.947458 1.611697 -0.228223
H28 0.134640 -2.073469 0.082486

9HG·[C – H4b]$^-$_PT1
C1 -1.383451 -0.911628 -0.016535
C2 -2.820098 -0.734925 -0.061009
C3 -1.290828 1.458366 0.200713
C4 -4.949806 -0.914974 -0.171712
N5 -0.666773 0.272804 0.110477
N6 -3.865577 -1.641494 -0.185993
N7 -4.681406 0.440795 -0.043494
N8 -2.614324 1.704438 0.161150
C9 -3.309045 0.565695 0.030045
N10 -0.485694 2.567281 0.391376
H11 -0.937103 3.439734 0.165898
H12 0.483858 2.479277 0.102919
O13 -0.798246 -2.007391 -0.085666
H14 -5.961625 -1.286953 -0.249212
H15 -5.339850 1.201204 0.000517
C16 2.915381 1.050584 -0.204758
N17 2.216635 -0.104012 -0.032959
C18 2.778976 -1.405061 0.127914
C19 4.946647 -0.293881 -0.009485
N20 4.304420 0.915994 -0.213893
H21 6.029103 -0.256800 -0.005460
O22 2.415811 2.165605 -0.348409
N23 2.106756 -2.480196 0.235047
H24 1.088554 -2.325102 0.165375
C25 4.244109 -1.422437 0.161023
H26 4.725250 -2.377462 0.310883
H27 4.813687 1.778233 -0.314148
H28 1.168041 0.002449 0.006673

7HG·[C – H4a]$^-$
C1 1.543619 -1.002101 -0.400400
C2 2.916125 -0.635503 -0.232280
C3 1.179730 1.299386 0.388707
C4 5.103291 -0.501195 -0.152773
N5 0.716110 0.059494 -0.005906
N6 4.077946 -1.344344 -0.466126
N7 4.697254 0.685551 0.250809
N8 2.456288 1.624398 0.509368
C9 3.315045 0.620885 0.205987
N10 0.227382 2.222528 0.685186
H11 0.601641 3.149539 0.811781
H12 -0.696963 2.153326 0.233275
O13 1.119754 -2.072896 -0.827019
H14 6.136544 -0.806510 -0.235971
C15 -2.832668 0.971042 -0.356411
N16 -2.228533 -0.071797 0.205367
C17 -2.933649 -1.200464 0.599943
C18 -4.936338 -0.251349 -0.412616
N19 -4.222366 0.898795 -0.633785
H20 -5.974106 -0.246291 -0.728650
O21 -2.270916 2.046866 -0.670266
N22 -2.330694 -2.105648 1.308370
H23 -2.978428 -2.873168 1.488080
C24 -4.343769 -1.303832 0.180180
H25 -4.899717 -2.212527 0.375503
H26 -0.314886 -0.110670 0.040791
H27 4.127899 -2.299041 -0.783849
H28 -4.614712 1.689538 -1.117684

9HG·[C – H4a]$^-$
C1 1.568972 -1.060896 -0.420680
C2 2.963453 -0.709403 -0.266408
C3 1.171327 1.257350 0.379019
C4 5.096561 -0.638993 -0.209086
N5 0.735799 0.018901 -0.011613
N6 4.113569 -1.442900 -0.508779
N7 4.654036 0.603339 0.220322
N8 2.455913 1.585583 0.499002
C9 3.278532 0.568406 0.184958
N10 0.227143 2.182098 0.671301
H11 0.598199 3.108920 0.806134
H12 -0.711158 2.111170 0.241294
O13 1.091657 -2.101360 -0.836593
H14 6.148632 -0.875821 -0.272194
C15 -2.841515 0.987822 -0.331399
N16 -2.253530 -0.053534 0.245800
C17 -2.971816 -1.181669 0.619371
C18 -4.937638 -0.238003 -0.466861
N19 -4.222512 0.919428 -0.648041
H20 -5.961830 -0.236045 -0.824367
O21 -2.268997 2.065188 -0.628701
N22 -2.396525 -2.078937 1.359027
H23 -3.046873 -2.849521 1.514663
C24 -4.362899 -1.291550 0.140979
H25 -4.920252 -2.205333 0.306315
H26 -0.288359 -0.160710 0.036128
H27 5.208397 1.395765 0.501767
H28 -4.595150 1.704729 -1.155874

[9HG – H2b]$^-$·C
C1 1.512868 -0.764789 0.000087
C2 2.932671 -0.739340 0.000011
H3 -0.046730 0.552699 -0.000031
C4 1.658117 1.777324 -0.000304
C5 5.027962 -1.150663 -0.000031
N6 0.969170 0.515640 -0.000078
N7 3.876449 -1.759785 0.000118
N8 4.903853 0.234646 -0.000236
N9 3.030477 1.741875 -0.000369
C10 3.549037 0.530116 -0.000212
N11 1.007230 2.897232 -0.000441
H12 0.001800 2.731695 -0.000363
O13 0.766816 -1.772652 0.000276
H14 5.995171 -1.633230 -0.000006
H15 5.637358 0.924213 -0.000374

C16 -3.394175 1.091502 0.000001
N17 -2.471046 0.092584 0.000119
C18 -2.845856 -1.185421 0.000259
C19 -5.165329 -0.602566 0.000170
N20 -4.770362 0.696021 0.000030
H21 -6.232819 -0.791292 0.000180
O22 -3.155644 2.288912 -0.000127
N23 -1.896576 -2.126415 0.000380
H24 -0.873038 -1.889715 0.000335
H25 -2.163557 -3.096187 0.000460
C26 -4.240067 -1.588544 0.000289
H27 -4.527808 -2.630760 0.000404
H28 -5.435476 1.454199 -0.000060

[7HG – H2b]$^{-}$·C
C1 1.514767 -0.703958 0.000121
C2 2.915546 -0.669344 -0.000019
H3 -0.031757 0.626663 0.000015
C4 1.713188 1.821092 -0.000382
C5 5.080447 -1.036478 -0.000145
N6 0.982873 0.570353 -0.000072
N7 3.876421 -1.676883 0.000086
N8 4.993642 0.272605 -0.000389
N9 3.080859 1.762931 -0.000499
C10 3.617765 0.553609 -0.000317
N11 1.073972 2.950098 -0.000540
H12 0.066832 2.795456 -0.000412
O13 0.789194 -1.740689 0.000387
H14 6.009853 -1.591035 -0.000123
C15 -3.427530 1.085328 0.000073
N16 -2.489382 0.099127 0.000237
C17 -2.846406 -1.182611 0.000345
C18 -5.173891 -0.634766 0.000115
N19 -4.797943 0.668961 0.000014
H20 -6.238466 -0.839262 0.000056
O21 -3.206867 2.285302 -0.000029
N22 -1.883386 -2.111847 0.000534
H23 -0.864367 -1.863196 0.000483
H24 -2.139234 -3.084487 0.000521
C25 -4.233939 -1.607103 0.000281
H26 -4.506376 -2.653434 0.000369
H27 -5.474103 1.417411 -0.000111
H28 3.699917 -2.667050 0.000301

Cartesian coordinates for the [9MG·C – H]$^-$ structures in Fig. 3, optimized at B3LYP/6-311++G(d,p) with BSSE correction

9MG·[C – H1]$^-$_PT1

C1 -0.978794 -1.059959 0.056176
C2 -2.413059 -0.967076 -0.025864
C3 -0.997055 1.313066 0.181051
C4 -4.523956 -1.243488 -0.185533
N5 -0.320353 0.146873 0.154915
N6 -3.410285 -1.924795 -0.141519
N7 -4.330849 0.129421 -0.114198
N8 -2.331096 1.486595 0.098542
C9 -2.966677 0.312743 -0.002876
N10 -0.248473 2.452209 0.341495
H11 -0.727892 3.310720 0.126292
H12 0.752139 2.414042 0.149594
O13 -0.337470 -2.142049 0.037828
H14 -5.517264 -1.661285 -0.278655
C15 -5.332681 1.171990 -0.080024
H16 -5.580362 1.462221 0.947016
H17 -4.950379 2.051668 -0.599815
H18 -6.239350 0.822788 -0.579113
C19 3.306124 1.231154 -0.125943
N20 2.577477 0.032152 0.028172
C21 3.143240 -1.199869 0.084218
C22 5.216520 -0.056330 -0.169600
N23 4.670654 1.150849 -0.224981
H24 6.304196 -0.078395 -0.252799
O25 2.678607 2.292187 -0.165102
N26 2.337560 -2.258440 0.249948
H27 1.286117 -2.180711 0.181386
H28 2.755413 -3.172006 0.196074
C29 4.543205 -1.264466 -0.019982
H30 5.062495 -2.212483 0.017983
H31 1.532132 0.111710 0.093868

9MG·[C – H1]$^-$

C1 1.034912 1.181384 -0.031902
C2 2.459532 0.995282 -0.060199
H3 -0.692880 -0.005449 0.083954
C4 0.949682 -1.289911 0.117409
C5 4.580373 1.172083 -0.134739
N6 0.358175 -0.050080 0.058779
N7 3.499956 1.903995 -0.145224
N8 4.319429 -0.189119 -0.051983
N9 2.273431 -1.468183 0.088752
C10 2.948757 -0.310563 0.001086
N11 0.130790 -2.345105 0.223817
H12 0.577636 -3.245884 0.184641
H13 -0.917411 -2.271990 0.105041
O14 0.402715 2.237714 -0.075939
H15 5.594790 1.541769 -0.189999
C16 5.271295 -1.278769 0.015661
H17 5.341259 -1.682396 1.030189
H18 4.959216 -2.083184 -0.652369
H19 6.252591 -0.914001 -0.292496
C20 -3.203648 -1.188909 -0.080704
N21 -2.539688 0.016908 0.081242
C22 -3.243436 1.149567 0.122626
C23 -5.228955 -0.102260 -0.179225
N24 -4.572587 -1.253899 -0.216475
H25 -6.313184 -0.172209 -0.290169
O26 -2.524749 -2.249647 -0.108742
N27 -2.550526 2.319412 0.341053
H28 -1.541943 2.306957 0.187488
H29 -3.016915 3.172231 0.077647
C30 -4.646592 1.147644 -0.012118
H31 -5.231268 2.058825 0.026425

9MG·[C – H1]$^-$_PT2

C1 -1.071975 1.212877 0.001329
C2 -2.488533 0.996912 -0.018858
C3 -0.903337 -1.286961 0.041643
C4 -4.616988 1.117096 -0.057262
N5 -0.380050 0.004740 0.033864
N6 -3.556466 1.877813 -0.052632
N7 -4.317306 -0.239475 -0.030639
N8 -2.245317 -1.475181 0.026029
C9 -2.937795 -0.332866 -0.003445
N10 -0.015016 -2.261570 0.063897
H11 -0.485345 -3.159663 0.069198
O12 -0.445343 2.285749 -0.006436
H13 -5.640970 1.463603 -0.081850
C14 3.217807 -1.156163 -0.005157
N15 2.533369 0.007016 0.064309
C16 3.213919 1.161212 0.045239
C17 5.219688 -0.091760 -0.109751
N18 4.563333 -1.253849 -0.088513
H19 6.304588 -0.165885 -0.179219
O20 2.545860 -2.272896 0.006227
N21 2.493943 2.310298 0.147119
H22 1.468841 2.292142 0.086902
H23 2.957017 3.186070 -0.023096
C24 4.623736 1.155531 -0.051274
H25 5.203059 2.070555 -0.066782
C26 -5.235516 -1.358013 -0.011982
H27 -5.933230 -1.305351 -0.853298
H28 -4.642671 -2.269036 -0.095006
H29 -5.806176 -1.391745 0.922186
H30 0.648082 0.060300 0.055096
H31 1.461187 -2.179540 0.040609

[9MG – H1]$^-$·C

C1 1.567221 -1.404157 -0.130394
C2 2.934950 -0.947644 0.025318
C3 1.024642 0.922302 -0.306053
C4 5.040582 -0.693704 0.294430
N5 0.655602 -0.364802 -0.296713
N6 4.129775 -1.627445 0.209674

N7 4.521800 0.587127 0.168735
N8 2.266284 1.420240 -0.152914
C9 3.159208 0.429081 0.001760
N10 0.018589 1.843983 -0.531484
H11 0.238079 2.784858 -0.245962
H12 -0.934736 1.538097 -0.360501
O13 1.181635 -2.584552 -0.118148
H14 6.101025 -0.854131 0.435444
C15 -4.157378 1.210378 0.116677
N16 -3.010923 0.511819 -0.064088
C17 -3.012266 -0.828994 -0.081316
C18 -5.380514 -0.907015 0.271588
N19 -5.359193 0.452986 0.282466
H20 -6.344540 -1.383109 0.410898
O21 -4.260027 2.432221 0.152207
N22 -1.861225 -1.462745 -0.271767
H23 -0.920979 -0.961635 -0.321320
H24 -1.816896 -2.468543 -0.223973
C25 -4.233495 -1.597777 0.094804
H26 -4.222039 -2.678726 0.081583
C27 5.222529 1.848031 0.261727
H28 4.751074 2.567336 -0.409678
H29 5.189896 2.257331 1.277966
H30 6.265958 1.709197 -0.031066
H31 -6.197537 0.996830 0.415517

9MG·[C – H4b]$^-$
C1 1.140343 1.245288 -0.062960
C2 2.562663 1.005347 -0.057709
C3 0.978433 -1.228086 0.092169
C4 4.689888 1.115212 -0.084609
N5 0.420748 0.022539 0.013966
N6 3.632656 1.879984 -0.121500
N7 4.383796 -0.236389 -0.004116
N8 2.293242 -1.448861 0.093925
C9 3.008895 -0.312021 0.018110
N10 0.138656 -2.275312 0.194013
H11 0.575977 -3.180112 0.146679
H12 -0.887295 -2.199749 0.030626
O13 0.547037 2.311662 -0.121895
H14 5.716394 1.452802 -0.117921
C15 5.298468 -1.355060 0.089803
H16 5.333874 -1.755525 1.107530
H17 4.976285 -2.153036 -0.581301
H18 6.297492 -1.023276 -0.198271
H19 -0.622490 0.101404 0.008596
C20 -3.157530 -1.095877 -0.126672
N21 -2.562175 0.088167 -0.012956
C22 -3.306606 1.270760 0.101574
C23 -5.350217 -0.047153 0.019220
N24 -4.566338 -1.167824 -0.152462
H25 -6.422630 -0.207176 0.031887
O26 -2.562433 -2.202225 -0.219774
N27 -2.786575 2.450628 0.173409
H28 -1.767344 2.396582 0.115843
C29 -4.772094 1.157615 0.146886
H30 -5.352898 2.061021 0.268349
H31 -4.955726 -2.095110 -0.183494

9MG·[C – H4b]$^-$_PT1
C1 -1.001159 -1.067039 -0.014104
C2 -2.444846 -0.975012 -0.064003
C3 -1.046900 1.305769 0.195184
C4 -4.558111 -1.266618 -0.181269
N5 -0.355100 0.158481 0.110858
N6 -3.436790 -1.936754 -0.190204
N7 -4.374894 0.104523 -0.061026
N8 -2.382770 1.474191 0.151591
C9 -3.009639 0.295491 0.020592
N10 -0.307981 2.460523 0.384884
H11 -0.807976 3.304369 0.153072
H12 0.666059 2.427413 0.099972
O13 -0.350977 -2.126150 -0.076697
H14 -5.550252 -1.689644 -0.264344
C15 -5.383595 1.135924 0.024913
H16 -5.467479 1.529698 1.043314
H17 -5.127553 1.964862 -0.638603
H18 -6.347361 0.719541 -0.275809
C19 3.177399 1.139909 -0.201728
N20 2.546341 -0.052880 -0.029438
C21 3.182706 -1.319690 0.129897
C22 5.282927 -0.086153 -0.011773
N23 4.571866 1.085364 -0.212002
H24 6.361500 0.012859 -0.010574
O25 2.614622 2.224521 -0.344829
N26 2.573337 -2.431415 0.238778
H27 1.547654 -2.334586 0.171778
C28 4.646591 -1.253321 0.158628
H29 5.181863 -2.179545 0.305638
H30 1.493378 -0.006878 0.010418
H31 5.030711 1.975157 -0.314748

9MG·[C – H4a]$^-$
C1 1.179569 1.259031 -0.441442
C2 2.594483 0.986604 -0.323468
C3 0.933892 -1.106058 0.281469
C4 4.725170 1.029636 -0.303651
N5 0.419287 0.117193 -0.056114
N6 3.695071 1.790669 -0.559516
N7 4.371158 -0.254567 0.084120
N8 2.237690 -1.360678 0.368367
C9 2.993899 -0.285433 0.076193
N10 0.051062 -2.095280 0.555998
H11 0.478267 -3.002730 0.649975
H12 -0.897471 -2.065248 0.144205
O13 0.631642 2.282101 -0.811542
H14 5.762982 1.323226 -0.378475
C15 -3.102649 -1.055058 -0.349796
N16 -2.567434 -0.003195 0.258733
C17 -3.344514 1.065155 0.686096

C18 -5.269534 0.047891 -0.406770
N19 -4.490682 -1.057402 -0.642750
H20 -6.297699 -0.001486 -0.749180
O21 -2.472685 -2.084227 -0.697500
N22 -2.810701 1.966868 1.451147
H23 -3.502742 2.690944 1.645503
C24 -4.747659 1.110028 0.232959
H25 -5.354935 1.982231 0.441499
C26 5.242977 -1.342987 0.473602
H27 5.284585 -1.452126 1.561925
H28 4.871417 -2.277182 0.049685
H29 6.248655 -1.149530 0.095845
H30 -0.612027 0.234041 0.016299
H31 -4.824650 -1.843250 -1.176001

[9MG – H2b]$^{-}$·C
C1 1.134300 -0.894298 -0.000199
C2 2.553784 -0.928356 -0.000032
C3 1.383872 1.639333 -0.000011
C4 4.630217 -1.414770 0.000096
N5 0.643540 0.408052 -0.000159
N6 3.455872 -1.982908 -0.000055
N7 4.570628 -0.025195 0.000259
N8 2.752890 1.545400 0.000170
C9 3.222817 0.312875 0.000148
N10 0.781117 2.786181 -0.000047
H11 -0.230418 2.663360 -0.000197
O12 0.346058 -1.869679 -0.000364
H13 5.579141 -1.934082 0.000150
C14 5.662514 0.921419 0.000198
H15 5.221121 1.918962 -0.000030
H16 6.289460 0.808430 0.891623
H17 6.289642 0.808058 -0.891046
H18 -0.369957 0.487102 -0.000280
C19 -3.686388 1.172169 -0.000163
N20 -2.807252 0.134373 -0.000298
C21 -3.236879 -1.126357 -0.000076
C22 -5.529061 -0.443800 0.000534
N23 -5.078373 0.836514 0.000403
H24 -6.603708 -0.586213 0.000847
O25 -3.396436 2.358218 -0.000462
N26 -2.329230 -2.107471 -0.000247
H27 -1.296075 -1.915538 -0.000331
C28 -4.647258 -1.468787 0.000311
H29 -4.979872 -2.497568 0.000440
H30 -5.710091 1.622736 0.000406
H31 -2.638078 -3.064734 0.000006

Cartesian coordinates for TS structures in Fig. 6, optimized at B3LYP/6-311++G(d,p)

proton transfer TS of 7HG·[C – H1]$^-$

C1 -1.291206 -0.883626 -0.187144
C2 -2.688354 -0.622735 -0.143344
H3 0.760780 0.105156 0.003720
C4 -1.104913 1.468892 0.262248
C5 -4.882249 -0.642317 -0.133673
N6 -0.526028 0.242888 0.023939
N7 -3.790325 -1.445208 -0.293607
N8 -4.577480 0.615727 0.108288
N9 -2.410299 1.729656 0.313123
C10 -3.190941 0.649352 0.107573
N11 -0.239960 2.494874 0.497022
H12 -0.678247 3.402051 0.486257
H13 0.717808 2.424906 0.118918
O14 -0.792782 -2.018242 -0.387738
H15 -5.888142 -1.031452 -0.205425
H16 -3.764818 -2.432848 -0.488473
C17 2.877093 1.056488 -0.311406
N18 2.079960 -0.055208 -0.007618
C19 2.642558 -1.246016 0.266046
C20 4.765575 -0.241337 -0.069664
N21 4.248263 0.944286 -0.348579
H22 5.855175 -0.300908 -0.104441
O23 2.315420 2.142991 -0.544926
N24 1.816175 -2.287201 0.582780
H25 0.843026 -2.243625 0.244327
H26 2.242318 -3.199845 0.562436
C27 4.040801 -1.383664 0.250635
H28 4.518659 -2.330358 0.468929

proton transfer TS of 9HG·[C – H1]$^-$

C1 -1.293986 -0.929678 -0.194231
C2 -2.713208 -0.698074 -0.154338
H3 0.770217 0.087122 -0.002711
C4 -1.092382 1.437330 0.255604
H5 -5.148572 1.298877 0.244545
C6 -4.846382 -0.799500 -0.163512
N7 -0.530116 0.217044 0.018453
N8 -3.793621 -1.554820 -0.313990
N9 -4.521545 0.525618 0.092338
N10 -2.406977 1.697181 0.309221
C11 -3.145797 0.600442 0.100560
N12 -0.239545 2.469980 0.485029
H13 -0.680709 3.375524 0.476368
H14 0.726204 2.403085 0.118404
O15 -0.748702 -2.031680 -0.388384
H16 -5.873668 -1.128760 -0.224028
C17 2.871588 1.066802 -0.303230
N18 2.082637 -0.052162 -0.009252
C19 2.654613 -1.241095 0.260991
C20 4.769867 -0.215872 -0.067445
N21 4.242144 0.967599 -0.340483
H22 5.859872 -0.265644 -0.102387
O23 2.301745 2.152874 -0.528343
N24 1.837832 -2.287623 0.570417
H25 0.860418 -2.247055 0.237105
H26 2.269101 -3.197818 0.555269
C27 4.055111 -1.364704 0.247002
H28 4.540583 -2.308514 0.460714

proton transfer TS of 9MG·[C – H1]$^-$

C1 -0.911585 -1.096507 -0.209341
C2 -2.342728 -0.958538 -0.188895
C3 -0.870296 1.284631 0.209930
C4 -4.461987 -1.187555 -0.221288
N5 -0.226862 0.101205 -0.003650
N6 -3.363669 -1.881988 -0.349554
N7 -4.233909 0.161924 0.012988
N8 -2.199677 1.458396 0.245456
C9 -2.863495 0.312330 0.041677
N10 -0.088923 2.373994 0.435462
H11 -0.587621 3.248751 0.407270
H12 0.882942 2.365125 0.079291
O13 -0.290949 -2.162156 -0.381365
H14 -5.468109 -1.577472 -0.292346
C15 -5.209024 1.204686 0.251122
H16 -5.333275 1.402090 1.320990
H17 -4.878034 2.126074 -0.230211
H18 -6.170272 0.902819 -0.169542
C19 3.115676 1.167405 -0.305631
N20 2.398015 0.004143 -0.000941
C21 3.042747 -1.141856 0.290440
C22 5.090350 0.012526 -0.038978
N23 4.490023 1.155852 -0.332580
H24 6.181535 0.032184 -0.066385
O25 2.478863 2.211341 -0.549836
N26 2.292119 -2.234010 0.609078
H27 1.317000 -2.261014 0.266345
H28 2.781167 -3.114668 0.609738
C29 4.448445 -1.175163 0.287855
H30 4.991836 -2.082814 0.518179
H31 1.081068 0.057070 -0.008877

Cartesian coordinates for neutral cytosine structures in Fig. S4, optimized at B3LYP/6-311++G(d,p)

C_1
C1 1.185789 -0.530607 0.000100
N2 -0.081850 -1.048529 0.002049
C3 -1.130136 -0.251582 -0.002085
C4 -1.047621 1.185675 -0.000972
C5 0.202506 1.712032 0.001138
N6 1.281556 0.894122 0.001665
H7 -1.925395 1.815585 -0.009261
H8 0.394746 2.778146 0.001544
O9 2.215318 -1.177607 0.000610
N10 -2.355667 -0.841873 -0.029867
H11 -2.390703 -1.844524 0.068019
H12 -3.194469 -0.310380 0.125813
H13 2.221787 1.262886 0.002996

C_2
C1 1.105001 -0.339355 -0.000084
N2 -0.046504 -0.997948 -0.000334
C3 -1.155166 -0.247909 -0.004076
C4 -1.091085 1.162250 -0.001676
C5 0.173428 1.713743 0.002332
N6 1.297205 0.980436 0.002459
H7 -1.980772 1.778152 -0.008520
H8 0.307349 2.791482 0.005015
O9 2.207910 -1.110287 0.001541
N10 -2.341228 -0.919437 -0.039120
H11 -2.309873 -1.916440 0.105133
H12 -3.201547 -0.439353 0.162118
H13 2.962187 -0.505281 0.003911

C_3
C1 1.136064 -0.274472 0.000666
N2 -0.002823 -0.970469 0.000605
C3 -1.138936 -0.260921 -0.004559
C4 -1.112135 1.147500 -0.002467
C5 0.139109 1.733729 0.002625
N6 1.288203 1.043296 0.003535
H7 -2.018542 1.738566 -0.010319
H8 0.237278 2.815667 0.005779
O9 2.273108 -0.994468 0.001315
N10 -2.305298 -0.969247 -0.042966
H11 -2.247744 -1.961770 0.121648
H12 -3.174967 -0.511379 0.171074
H13 2.013918 -1.925416 -0.004511

C_4
C1 -1.224811 -0.423506 0.000006
N2 0.031824 -0.985612 0.000193
C3 1.274839 -0.326310 0.000043
C4 1.165314 1.128289 0.000068
C5 -0.046818 1.712445 -0.000004
N6 -1.207804 0.970942 -0.000020
H7 2.066621 1.723821 0.000124
H8 -0.178837 2.786918 0.000036
O9 -2.257589 -1.061583 -0.000131
N10 2.325773 -1.056213 0.000025
H11 0.061690 -1.997149 0.000287
H12 -2.114299 1.412336 -0.000122
H13 3.165846 -0.482586 -0.001343

C_5
C1 1.218807 -0.431894 -0.000019
N2 -0.053650 -0.978165 -0.000361
C3 -1.290282 -0.292879 -0.000048
C4 -1.147625 1.156562 -0.000066
C5 0.072013 1.718877 -0.000024
N6 1.225274 0.954825 0.000004
H7 -2.048313 1.750723 -0.000060
H8 0.224610 2.790106 -0.000137
O9 2.233378 -1.099585 0.000214
N10 -2.438099 -0.857416 0.000475
H11 -2.372616 -1.875603 -0.001238
H12 -0.061306 -1.989397 -0.000356
H13 2.138442 1.382153 0.000189

C_6
C1 1.299593 -0.376917 0.001945
N2 -0.031102 -0.917773 0.001151
C3 -1.167589 -0.177992 -0.003544
C4 -1.029303 1.197481 0.000510
C5 0.286627 1.698625 0.002251
N6 1.395604 0.992914 0.006335
H7 -1.888946 1.851892 0.001028
H8 0.420501 2.779498 0.005101
O9 2.224756 -1.163088 -0.001531
N10 -2.364209 -0.839377 -0.056072
H11 -2.406367 -1.797283 0.256571
H12 -3.195548 -0.298434 0.121552
H13 -0.065700 -1.928498 -0.038887

C_7
C1 -1.137175 -0.233521 0.000000
N2 0.009924 -0.944846 0.000001
C3 1.288992 -0.343033 0.000000
C4 1.204697 1.106581 0.000001
C5 -0.005479 1.719414 0.000000
N6 -1.216676 1.060259 0.000000
H7 2.122587 1.679265 0.000000
H8 -0.077315 2.801597 -0.000001
O9 -2.243845 -0.991020 0.000000
N10 2.299248 -1.130721 -0.000001
H11 -2.996149 -0.382136 0.000000
H12 -0.020639 -1.957019 0.000001
H13 3.168601 -0.603045 -0.000001

C_8

C1 1.135462 -0.236132 0.000000
N2 -0.025242 -0.941397 -0.000001
C3 -1.302571 -0.318314 0.000000
C4 -1.193359 1.128325 0.000000
C5 0.020163 1.727420 0.000000
N6 1.228050 1.050419 0.000000
H7 -2.113544 1.694760 0.000000
H8 0.106514 2.807917 -0.000001
O9 2.229716 -1.015559 0.000000
N10 -2.418960 -0.945424 0.000000
H11 -2.302004 -1.958680 0.000000
H12 2.993620 -0.421216 0.000002
H13 0.032572 -1.951288 0.000001

C_9
C1 1.057694 -0.347676 0.000000
N2 -0.018991 -1.041642 0.000000
C3 -1.269184 -0.378172 0.000000
C4 -1.233636 1.088375 0.000000
C5 -0.059832 1.737188 0.000000
N6 1.129881 1.015008 0.000000
H7 -2.171481 1.624820 0.000000
H8 0.042381 2.813486 0.000000
O9 2.272855 -0.929206 0.000000
N10 -2.389958 -0.998701 0.000000
H11 -2.222295 -2.005605 0.000000
H12 2.031503 1.464808 0.000000
H13 2.120277 -1.884810 -0.000001

C_10
C1 -1.162835 -0.177742 0.000000
N2 -0.024035 -0.924106 0.000001
C3 1.276544 -0.362402 0.000000
C4 1.237848 1.084956 0.000000
C5 0.042623 1.728602 0.000000
N6 -1.187669 1.112968 0.000000
H7 2.171526 1.631522 0.000000
H8 0.003617 2.812793 -0.000001
O9 -2.340484 -0.830259 0.000000
N10 2.254048 -1.191317 -0.000001
H11 -0.038292 -1.937102 0.000002
H12 -2.219840 -1.786335 0.000000
H13 3.145373 -0.702108 -0.000001

C_11
C1 -1.068459 -0.340591 0.000000
N2 -0.007706 -1.051420 0.000000
C3 1.254057 -0.421979 0.000000
C4 1.239595 1.051213 0.000001
C5 0.076997 1.723426 0.000000
N6 -1.121877 1.027819 -0.000001
H7 2.176583 1.592664 0.000002
H8 -0.000848 2.802215 -0.000001
O9 -2.294029 -0.900146 0.000000
N10 2.300122 -1.164431 -0.000001
H11 -2.015499 1.493396 0.000000
H12 -2.154216 -1.858227 0.000002
H13 3.139301 -0.585081 0.000000

C_12
C1 1.162575 -0.181317 0.000358
N2 0.009585 -0.924133 0.005446
C3 -1.291330 -0.341077 -0.001587
C4 -1.227548 1.104613 -0.001887
C5 -0.029814 1.735794 0.001412
N6 1.197854 1.102757 -0.004160
H7 -2.163881 1.643991 -0.001731
H8 0.023017 2.818757 0.004870
O9 2.333759 -0.851160 0.009116
N10 -2.384406 -1.008637 -0.002781
H11 -2.235071 -2.017776 -0.001927
H12 0.053774 -1.933808 0.046750
H13 2.207564 -1.799871 -0.100208

C_13
C1 1.042822 -0.390112 0.001521
N2 -0.044614 -1.053105 0.017910
C3 -1.281836 -0.368594 0.000871
C4 -1.231556 1.096854 0.007540
C5 -0.050262 1.727536 0.000875
N6 1.135827 0.988341 0.021427
H7 -2.162344 1.645764 0.011699
H8 0.068731 2.802406 -0.004095
O9 2.220190 -1.060372 -0.042055
N10 -2.409046 -0.976014 -0.010257
H11 -2.249053 -1.984404 -0.014511
H12 1.996483 1.438076 -0.250958
H13 2.934477 -0.527516 0.325902

C_14
C1 -1.054375 -0.384539 -0.001134
N2 0.017436 -1.065261 -0.022609
C3 1.267372 -0.413957 -0.002897
C4 1.237637 1.058450 -0.018469
C5 0.067718 1.712991 -0.000160
N6 -1.127723 1.000490 -0.012548
H7 2.167549 1.612196 -0.031192
H8 -0.026369 2.790792 0.007683
O9 -2.247402 -1.028597 0.042460
N10 2.323860 -1.140346 0.018537
H11 -1.978619 1.463613 0.268234
H12 -2.942695 -0.491763 -0.354883
H13 3.154230 -0.547910 0.022786

Cartesian coordinates for the [C – H]$^-$ structures in Fig. S5, optimized at B3LYP/6-311++G(d,p)

[C – H]$^-$_1
C1 1.264808 -0.315992 -0.000004
N2 -0.004434 -0.933907 0.000093
C3 -1.248730 -0.312941 0.000046
C4 -1.138659 1.119604 0.000080
C5 0.120442 1.683863 -0.000011
N6 1.302524 1.048223 -0.000075
H7 -2.034075 1.729575 0.000106
H8 0.192703 2.774253 -0.000060
O9 2.260249 -1.050898 -0.000009
N10 -2.310673 -1.074265 -0.000129
H11 -3.138063 -0.479899 0.000021
H12 -0.001639 -1.944312 0.000121

[C – H]$^-$_2
C1 1.258067 -0.327439 -0.000017
N2 -0.032147 -0.920728 -0.000061
C3 -1.268695 -0.269940 0.000016
C4 -1.119030 1.157052 0.000036
C5 0.149695 1.690088 0.000007
N6 1.323603 1.027957 -0.000037
H7 -2.006005 1.775694 0.000003
H8 0.247372 2.777757 0.000005
O9 2.229211 -1.096436 0.000033
N10 -2.420220 -0.886006 0.000019
H11 -2.276535 -1.897863 -0.000243
H12 -0.017404 -1.931227 0.000271

[C – H]$^-$_3
C1 1.230574 -0.432137 0.001732
N2 -0.047267 -1.007362 0.000965
C3 -1.102487 -0.222224 -0.019959
C4 -1.030241 1.183027 -0.021924
C5 0.271526 1.688832 0.008002
N6 1.373399 0.963270 0.022906
H7 -1.904933 1.821466 -0.063615
H8 0.415344 2.773804 0.019523
O9 2.231712 -1.160084 -0.004773
N10 -2.359172 -0.868682 -0.076649
H11 -3.084336 -0.391988 0.443238
H12 -2.264730 -1.838178 0.201368

[C – H]$^-$_4
C1 1.141223 -0.506669 0.001680
N2 -0.065795 -1.081458 -0.001811
C3 -1.228998 -0.338732 -0.000714
C4 -1.142975 1.128613 -0.015787
C5 0.072775 1.707310 -0.003633
N6 1.201104 0.929017 0.030907
H7 -2.054000 1.711128 -0.032992
H8 0.223695 2.782717 -0.011581
O9 2.242421 -1.083741 -0.013762
N10 -2.420709 -0.876275 0.008191
H11 -2.289259 -1.890222 0.016521
H12 2.125850 1.324189 -0.012139

[C – H]$^-$_5
C1 1.090121 -0.229643 -0.000025
N2 0.012027 -0.991947 -0.000059
C3 -1.234526 -0.365765 0.000037
C4 -1.202981 1.085795 0.000199
C5 0.003804 1.722264 -0.000046
N6 1.214801 1.092162 -0.000148
H7 -2.138871 1.631600 0.000512
H8 0.049806 2.811003 -0.000115
O9 2.282052 -0.922847 0.000084
N10 -2.364857 -1.024193 -0.000179
H11 -2.139399 -2.020889 0.000371
H12 1.999750 -1.847002 0.000265

[C – H]$^-$_6
C1 1.050965 -0.320692 -0.000002
N2 -0.047280 -1.030931 -0.000264
C3 -1.260790 -0.337979 -0.000008
C4 -1.172054 1.112587 0.000030
C5 0.058402 1.699960 -0.000026
N6 1.233501 1.007525 0.000060
H7 -2.085225 1.695417 0.000197
H8 0.155464 2.785095 -0.000079
O9 2.228318 -1.040840 0.000103
N10 -2.418960 -0.944090 -0.000042
H11 -2.235486 -1.949275 0.000956
H12 2.908737 -0.355299 -0.000142

[C – H]$^-$_7
C1 1.160029 -0.492813 0.002782
N2 -0.026121 -1.101494 -0.007457
C3 -1.209117 -0.402101 -0.002259
C4 -1.157102 1.075283 -0.037333
C5 0.040610 1.692737 -0.006972
N6 1.185298 0.950058 0.063506
H7 -2.073561 1.652964 -0.078071
H8 0.156442 2.772972 -0.022974
O9 2.279989 -1.031174 -0.027351
N10 -2.348061 -1.051004 0.025178
H11 -3.105857 -0.366289 0.018518
H12 2.098732 1.368198 -0.004566

[C – H]$^-$_8
C1 1.101273 -0.221517 0.000064
N2 0.045062 -1.006344 0.000299
C3 -1.213780 -0.416571 -0.000060
C4 -1.210367 1.040697 -0.000404
C5 -0.017652 1.708001 0.000085
N6 1.202305 1.107768 0.000297
H7 -2.151593 1.582465 -0.000883
H8 0.000133 2.798208 0.000331

O9 2.308204 -0.885898 -0.000284
N10 -2.277872 -1.181922 0.000058
H11 -3.101359 -0.577716 0.000463
H12 2.043873 -1.815948 -0.000327

[C – H]$^{-}$_9
C1 1.064115 -0.312927 0.000014
N2 -0.012363 -1.048520 0.000501
C3 -1.241124 -0.393059 0.000116
C4 -1.182154 1.064817 0.000132
C5 0.034158 1.685659 -0.000003
N6 1.220659 1.024283 -0.000193
H7 -2.101561 1.642699 0.000017
H8 0.101434 2.773692 -0.000007
O9 2.260215 -1.000832 -0.000113
N10 -2.339865 -1.106529 -0.000520
H11 -3.133362 -0.463033 0.000896
H12 2.922781 -0.298286 -0.000078