

Supporting Information

How Protonation and Deprotonation of 9-Methylguanine Alter Its Singlet O₂ Addition

Path: About the Initial Stage of Guanine Nucleoside Oxidation

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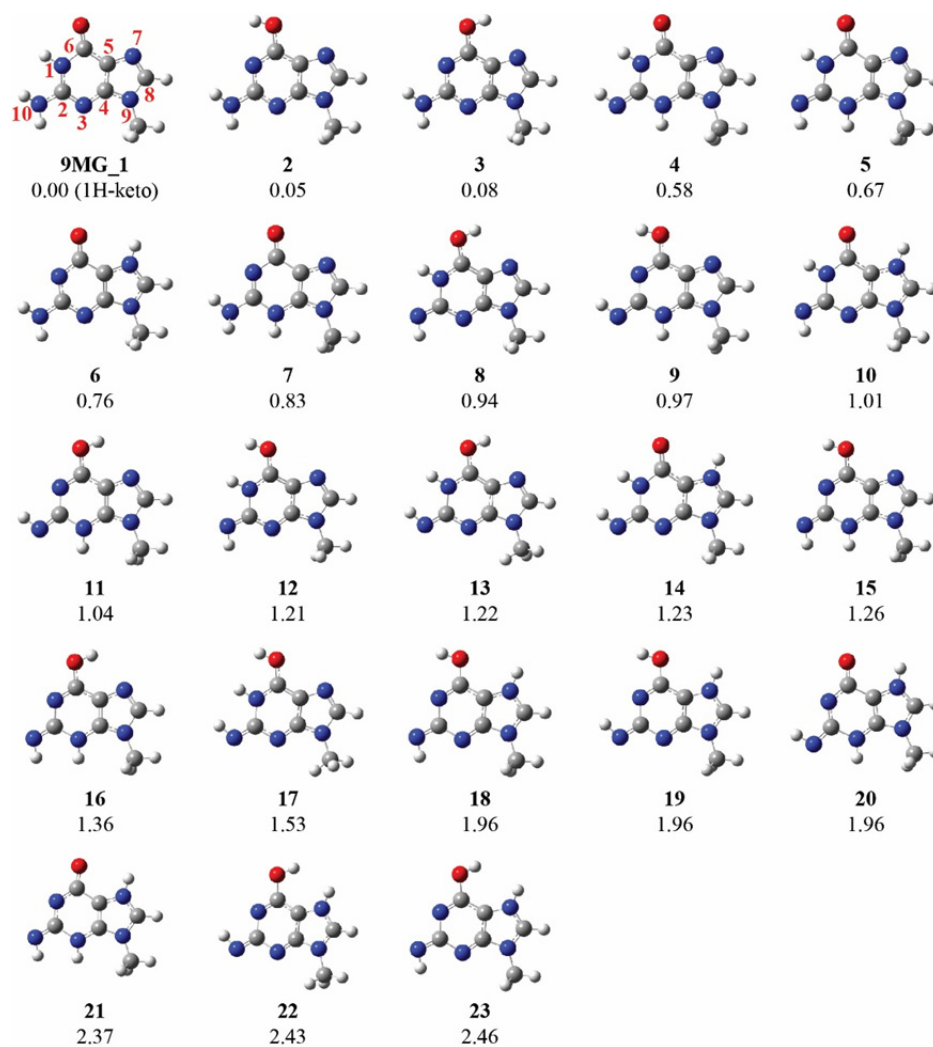


Fig. S1 Stable tautomers of 9MG. Relative energies (eV, including thermal corrections at 298 K) were calculated at B3LYP/6-311++G**.

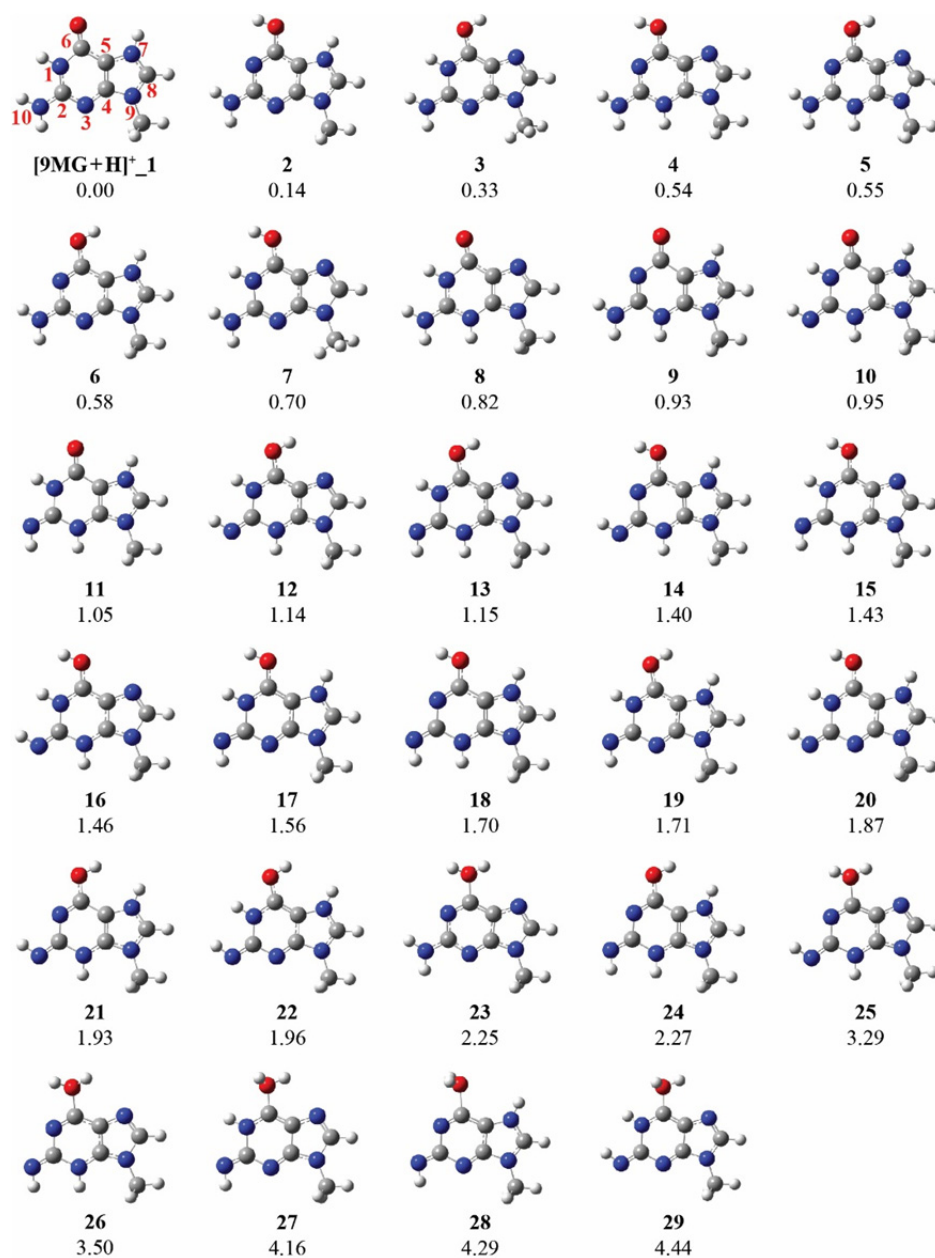


Fig. S2 Stable tautomers of $[9\text{MG} + \text{H}]^+$. Relative energies (eV, including thermal corrections at 298 K) were calculated at B3LYP/6-311++G**.

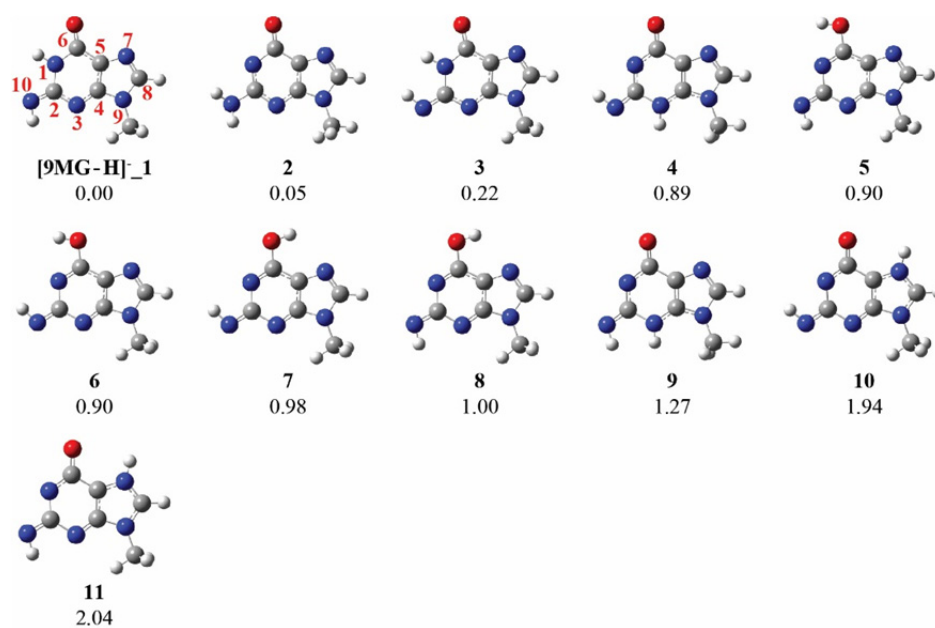


Fig. S3 Stable tautomers of $[9\text{MG} - \text{H}]^-$. Relative energies (eV, including thermal corrections at 298 K) were calculated at B3LYP/6-311++G**.

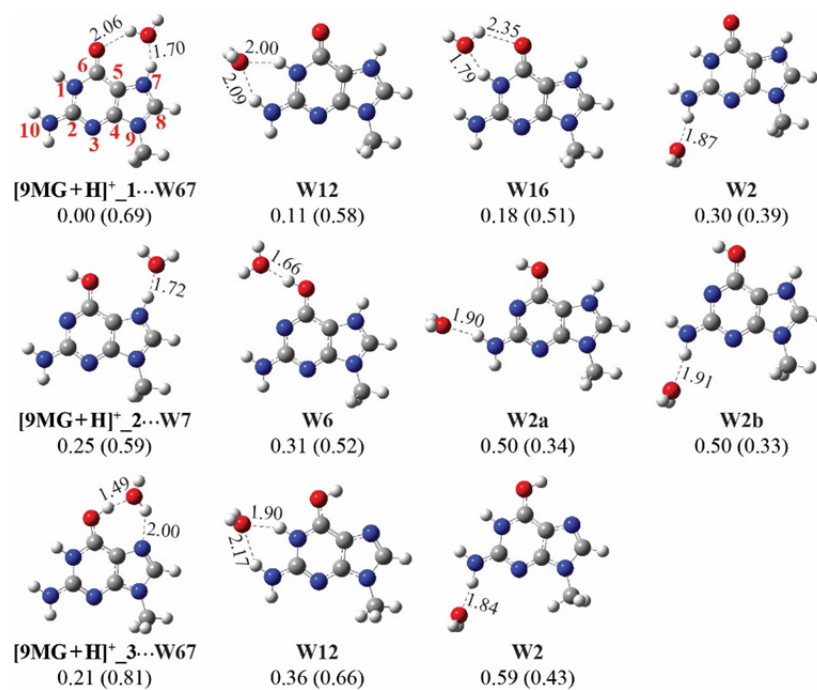


Fig. S4 Stable tautomers of $[9\text{MG} + \text{H}]^+(\text{H}_2\text{O})$. Dashed lines indicate hydrogen bonds. Bond distances are shown in Å. Relative energies (eV, including thermal corrections at 298 K) and hydration energies (presented in parentheses) were calculated at B3LYP/6-311++G**.

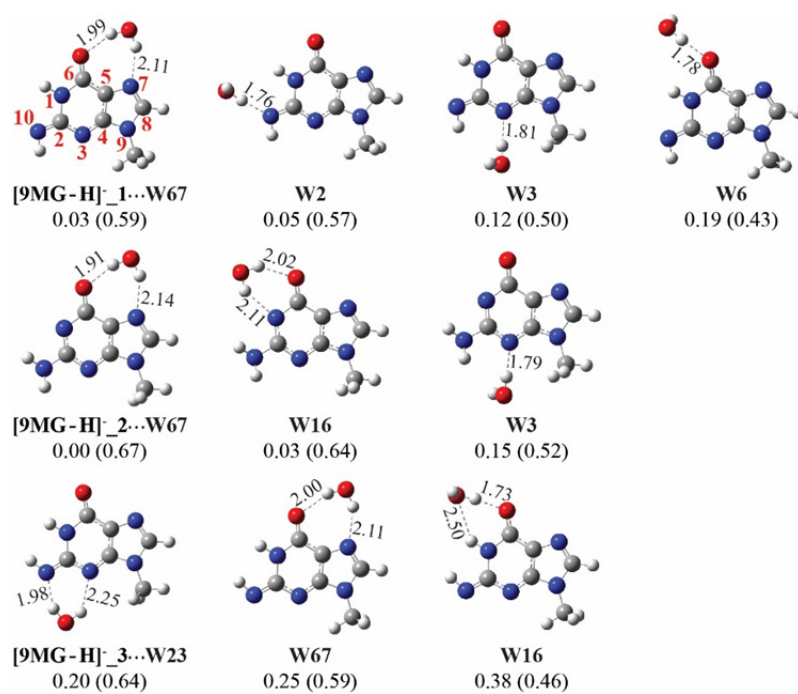


Fig. S5 Stable tautomers of $[9\text{MG} - \text{H}]^-(\text{H}_2\text{O})$. Dashed lines indicate hydrogen bonds. Bond distances are shown in Å. Relative energies (eV, including thermal corrections at 298 K) and hydration energies (presented in parentheses) were calculated at B3LYP/6-311++G**.

**Cartesian coordinates for neutral
9-methylguanine tautomers in Fig. S1,
optimized at B3LYP/6-311++G****

9MG_1

C1 -1.131953 1.411029 0.002092
C2 0.250552 1.017026 0.008669
H3 -2.953631 0.444518 -0.075120
C4 -1.539649 -1.064977 -0.002015
C5 2.370540 0.905150 0.002331
N6 -1.965683 0.236805 -0.003787
N7 1.399169 1.777857 0.008326
N8 1.929317 -0.407996 -0.002617
N9 -0.277730 -1.409475 0.009469
C10 0.561319 -0.342177 0.001376
N11 -2.510758 -2.038509 -0.064996
H12 -2.160141 -2.970615 0.099750
H13 -3.404184 -1.845254 0.362160
O14 -1.654728 2.506416 -0.005271
H15 3.425606 1.137894 0.000295
C16 2.735046 -1.618839 -0.004474
H17 2.559640 -2.197423 0.904386
H18 2.488650 -2.237347 -0.868939
H19 3.786550 -1.337149 -0.053021

9MG_2

C1 -1.201472 1.174759 0.000910
C2 0.185703 0.982777 -0.003785
H3 -2.693473 2.294871 0.005302
C4 -1.504506 -1.112407 -0.006228
C5 2.305531 1.006466 -0.001743
N6 -2.027010 0.136587 0.000518
N7 1.286833 1.820974 -0.003060
N8 1.955344 -0.336494 -0.002660
N9 -0.207012 -1.438811 -0.000048
C10 0.583249 -0.364712 -0.002465
N11 -2.410933 -2.138882 -0.055672
H12 -2.069476 -3.058607 0.170721
H13 -3.364005 -1.919457 0.182543
O14 -1.731437 2.404810 0.008828
H15 3.343997 1.306370 -0.002696
C16 2.839610 -1.490221 0.008653
H17 2.742293 -2.041610 0.946214
H18 2.595206 -2.158420 -0.818462
H19 3.867713 -1.145212 -0.099848

9MG_3

C1 -1.194078 1.188443 0.000394
C2 0.186519 0.947404 -0.005615
H3 -0.968701 3.059869 0.010056
C4 -1.549900 -1.078618 -0.005625
C5 2.305582 0.948795 -0.002069
N6 -2.046141 0.181827 0.000936
N7 1.293333 1.776424 -0.004454
N8 1.936053 -0.387395 -0.001903
N9 -0.259342 -1.449573 0.000466

C10 0.560333 -0.399871 -0.002755
N11 -2.483191 -2.077729 -0.051787
H12 -2.174414 -3.011131 0.163391
H13 -3.434425 -1.826326 0.160546
O14 -1.704624 2.431731 0.009786
H15 3.347346 1.235734 -0.002418
C16 2.806432 -1.552335 0.008753
H17 2.686791 -2.112113 0.938489
H18 2.565648 -2.207891 -0.829474
H19 3.840437 -1.219778 -0.080183

9MG_4

C1 -1.207172 1.350021 0.000014
C2 0.199007 1.006263 -0.000032
H3 -3.014366 0.382459 0.000165
C4 -1.666035 -1.167894 0.000007
C5 2.328296 0.993568 -0.000056
N6 -2.024136 0.178598 0.000029
N7 1.318455 1.812568 -0.000072
N8 1.939085 -0.348425 0.000001
N9 -0.285322 -1.382030 0.000114
C10 0.576821 -0.322622 0.000010
N11 -2.433894 -2.189121 -0.000092
H12 -3.417904 -1.937565 -0.000240
O13 -1.729099 2.443698 0.000047
H14 3.373549 1.264643 -0.000089
C15 2.800217 -1.520616 0.000046
H16 2.631913 -2.128232 0.892883
H17 2.632155 -2.128144 -0.892897
H18 3.837325 -1.187978 0.000204
H19 0.004001 -2.348215 -0.000187

9MG_5

C1 -1.215551 -1.347282 -0.003317
C2 0.196221 -1.004452 0.003300
H3 -3.023119 -0.352111 -0.012722
C4 -1.675907 1.160965 -0.001576
C5 2.325984 -0.996040 0.010448
N6 -2.025414 -0.183454 -0.018580
N7 1.313249 -1.812411 0.011309
N8 1.939692 0.345768 0.000545
N9 -0.289571 1.386409 -0.026615
C10 0.576211 0.320526 -0.001734
N11 -2.587507 2.055159 0.025474
H12 -2.213155 3.000071 0.024004
O13 -1.725963 -2.446406 -0.000165
H14 3.370533 -1.269774 0.017994
C15 2.804329 1.514711 -0.007104
H16 2.623346 2.127657 -0.893981
H17 2.657025 2.118250 0.892637
H18 3.840203 1.178907 -0.028167
H19 0.031992 2.337371 0.056520

9MG_6

C1 -1.235045 1.343639 0.001367
C2 0.161519 0.937752 -0.006251

C3 -1.625829 -0.983705 -0.006077
 C4 2.374856 0.812563 -0.000776
 N5 -2.088395 0.266691 0.002165
 N6 1.338084 1.653981 -0.004393
 N7 1.901452 -0.452802 0.000609
 N8 -0.332474 -1.429460 0.000717
 C9 0.502749 -0.403720 -0.001543
 N10 -2.569856 -1.975661 -0.053637
 H11 -2.276546 -2.909222 0.181641
 H12 -3.517418 -1.702505 0.149448
 O13 -1.571918 2.529260 0.010168
 H14 3.414794 1.087726 -0.001510
 C15 2.687047 -1.681039 0.006086
 H16 2.479448 -2.244841 0.916092
 H17 2.410586 -2.290558 -0.854366
 H18 3.746197 -1.431160 -0.041332
 H19 1.384824 2.664295 -0.006384

9MG_7

C1 -1.171003 1.401710 -0.003361
 C2 0.239059 1.002977 0.006813
 C3 -1.688857 -0.920917 0.011660
 C4 2.371362 0.900563 0.014055
 N5 -2.075892 0.305521 0.040384
 N6 1.393432 1.760830 0.020684
 N7 1.933658 -0.421550 0.000992
 N8 -0.359760 -1.348201 0.016966
 C9 0.571210 -0.332104 -0.011017
 N10 -2.608426 -1.953217 -0.069720
 H11 -2.418667 -2.774529 0.488631
 H12 -3.557480 -1.617474 0.022771
 O13 -1.577655 2.543386 -0.034963
 H14 3.426711 1.131136 0.013474
 C15 2.748260 -1.625042 -0.008348
 H16 2.487455 -2.274818 0.830937
 H17 2.632360 -2.175673 -0.946253
 H18 3.793845 -1.336607 0.092506
 H19 -0.144253 -2.265911 -0.346318

9MG_8

C1 -1.228742 -1.139003 0.000002
 C2 0.131013 -0.949485 -0.000001
 H3 -3.009014 -0.130865 0.000005
 C4 -1.512773 1.316783 -0.000001
 C5 2.242988 -1.062288 -0.000005
 N6 -2.001245 -0.038297 0.000004
 N7 1.197503 -1.837578 -0.000002
 N8 1.946318 0.297376 -0.000010
 N9 -0.143631 1.500643 -0.000001
 C10 0.570026 0.403115 -0.000004
 N11 -2.426667 2.213414 -0.000003
 H12 -1.994859 3.133801 -0.000009
 O13 -1.862119 -2.314712 0.000005
 H14 3.268785 -1.402880 -0.000009
 C15 2.877145 1.414012 0.000012
 H16 2.725718 2.032568 -0.886497

H17 2.726010 2.032319 0.886748
 H18 3.895177 1.024947 -0.000210
 H19 -1.198743 -3.019904 0.000003

9MG_9

C1 1.276527 -1.109952 0.000003
 C2 -0.140944 -0.961425 -0.000004
 H3 2.754546 -2.243970 0.000011
 C4 1.629513 1.218654 0.000000
 C5 -2.263587 -1.089371 -0.000008
 N6 2.089758 -0.090139 0.000006
 N7 -1.204292 -1.843779 -0.000010
 N8 -1.963322 0.279016 -0.000001
 N9 0.221317 1.416864 0.000020
 C10 -0.603622 0.344522 0.000000
 N11 2.348782 2.276554 -0.000016
 H12 3.331801 2.017971 -0.000027
 O13 1.790575 -2.344953 0.000006
 H14 -3.289248 -1.426917 -0.000015
 C15 -2.900842 1.390755 0.000005
 H16 -2.772170 2.008407 0.892398
 H17 -2.772266 2.008345 -0.892445
 H18 -3.913752 0.990232 0.000075
 H19 -0.091474 2.376844 -0.000014

9MG_10

C1 1.279461 1.290074 -0.000030
 C2 -0.115325 0.940579 0.000304
 H3 3.043509 0.246919 -0.000731
 C4 1.597219 -1.228433 0.000046
 C5 -2.327492 0.919321 0.000065
 N6 2.037964 0.132650 -0.000108
 N7 -1.256487 1.712328 0.000246
 N8 -1.916135 -0.368092 -0.000023
 N9 0.230663 -1.478595 -0.000042
 C10 -0.507234 -0.399774 0.000072
 N11 2.527133 -2.110143 0.000236
 H12 2.106432 -3.036258 0.000130
 O13 1.744185 2.425528 -0.000272
 H14 -3.352066 1.247308 0.000094
 C15 -2.754918 -1.559267 -0.000253
 H16 -2.536515 -2.157099 -0.885716
 H17 -2.536567 -2.157397 0.885019
 H18 -3.803098 -1.262655 -0.000235
 H19 -1.267414 2.722916 0.000244

9MG_11

C1 1.274340 1.124239 0.000014
 C2 -0.139606 0.923932 -0.000015
 C3 1.677688 -1.182449 0.000004
 C4 -2.262361 1.036906 -0.000039
 N5 2.112925 0.135458 0.000033
 N6 -1.204801 1.800322 -0.000044
 N7 -1.946912 -0.326017 -0.000004
 N8 0.270229 -1.429505 0.000089
 C9 -0.584083 -0.382046 0.000007

N10 2.422378 -2.221674 -0.000081
 H11 3.397851 -1.935160 -0.000117
 O12 1.766729 2.374097 0.000026
 H13 -3.290286 1.366094 -0.000064
 C14 -2.875947 -1.445857 0.000020
 H15 -2.740509 -2.061717 -0.892310
 H16 -2.740450 -2.061720 0.892339
 H17 -3.892357 -1.054466 0.000054
 H18 1.024414 2.995309 0.000011
 H19 -0.009421 -2.399556 -0.000022

9MG_12

C1 1.240758 -1.131007 -0.000049
 C2 -0.124054 -0.975569 0.000081
 C3 1.465394 1.347450 0.000030
 C4 -2.237225 -1.106711 0.000059
 N5 1.983030 0.002039 -0.000063
 N6 -1.187137 -1.869950 0.000110
 N7 -1.957448 0.258163 0.000014
 N8 0.098825 1.494373 0.000005
 C9 -0.586739 0.376811 0.000014
 N10 2.367163 2.257929 0.000084
 H11 1.924581 3.172956 0.000103
 O12 1.835331 -2.328069 -0.000197
 H13 -3.259763 -1.457986 0.000077
 C14 -2.899230 1.364970 -0.000108
 H15 -2.755141 1.985713 0.886181
 H16 -2.755781 1.985043 -0.886975
 H17 -3.912751 0.964228 0.000406
 H18 2.797009 -2.250595 0.000945
 H19 2.994747 -0.028339 -0.000379

9MG_13

C1 -1.210644 1.146754 -0.003352
 C2 0.142793 0.952025 0.000652
 H3 -2.994476 0.187782 -0.006950
 C4 -1.511485 -1.330369 0.001742
 C5 2.255694 1.044660 0.007382
 N6 -1.994015 0.043879 -0.004717
 N7 1.217973 1.831249 0.003470
 N8 1.949735 -0.311057 0.012603
 N9 -0.144128 -1.497336 0.000697
 C10 0.570049 -0.407445 0.002955
 N11 -2.320344 -2.323161 0.006671
 H12 -3.294840 -2.029706 0.007046
 O13 -1.847898 2.322831 -0.006485
 H14 3.283646 1.379336 0.012306
 C15 2.873385 -1.435049 -0.015239
 H16 2.327132 -2.322774 0.301364
 H17 3.262182 -1.601099 -1.023222
 H18 3.702876 -1.254736 0.670331
 H19 -1.186638 3.030067 -0.004907

9MG_14

C1 -1.260587 1.297228 0.000022
 C2 0.127510 0.945678 -0.000068

H3 -3.024341 0.295980 0.000200
 C4 -1.591546 -1.243730 -0.000013
 C5 2.339565 0.902126 -0.000044
 N6 -2.026048 0.133795 0.000052
 N7 1.277837 1.707506 -0.000069
 N8 1.918569 -0.379930 -0.000029
 N9 -0.226332 -1.475870 0.000018
 C10 0.506873 -0.400553 -0.000018
 N11 -2.424792 -2.218252 -0.000086
 H12 -3.388507 -1.889541 -0.000138
 O13 -1.737888 2.427699 0.000081
 H14 3.367215 1.221006 -0.000073
 C15 2.742851 -1.581639 0.000103
 H16 2.515227 -2.176421 0.885187
 H17 2.513778 -2.177473 -0.883891
 H18 3.794701 -1.298103 -0.000923
 H19 1.302406 2.717554 -0.000098

9MG_15

C1 1.277406 -1.117049 0.000001
 C2 -0.142869 -0.966841 -0.000002
 C3 1.657331 1.208068 0.000000
 C4 -2.266139 -1.086448 -0.000004
 N5 2.092084 -0.104614 0.000003
 N6 -1.209026 -1.844711 -0.000005
 N7 -1.959951 0.279754 0.000000
 N8 0.234653 1.412010 0.000010
 C9 -0.598572 0.337981 0.000001
 N10 2.494953 2.176094 -0.000009
 H11 2.030034 3.082697 -0.000009
 O12 1.787050 -2.354181 0.000003
 H13 -3.293114 -1.420012 -0.000007
 C14 -2.893936 1.393723 0.000003
 H15 -2.765532 2.011047 0.892970
 H16 -2.765541 2.011045 -0.892967
 H17 -3.908026 0.996189 0.000008
 H18 2.751488 -2.252337 0.000004
 H19 -0.114021 2.358473 -0.000008

9MG_16

C1 -1.273332 -1.133968 0.000017
 C2 0.142722 -0.929108 -0.000007
 C3 -1.709444 1.167826 0.000001
 C4 2.266342 -1.030122 -0.000049
 N5 -2.115796 -0.154209 0.000030
 N6 1.212448 -1.799199 -0.000047
 N7 1.942732 0.330026 -0.000008
 N8 -0.286189 1.423569 0.000112
 C9 0.578264 0.376539 0.000013
 N10 -2.568236 2.116144 -0.000092
 H11 -2.124504 3.033480 -0.000105
 O12 -1.756836 -2.388153 0.000025
 H13 3.296113 -1.353568 -0.000082
 C14 2.866345 1.453643 0.000024
 H15 2.729986 2.068982 -0.892804
 H16 2.729998 2.068917 0.892898

H17 3.884547 1.066931 0.000002
 H18 -1.010564 -3.004310 0.000013
 H19 0.029020 2.381613 -0.000077

9MG_17

C1 -1.222121 1.141225 0.006499
 C2 0.135705 0.977083 -0.003306
 H3 -2.983400 0.092904 0.072501
 C4 -1.467873 -1.360329 -0.004534
 C5 2.249985 1.086336 -0.012364
 N6 -1.979053 0.006490 0.003259
 N7 1.208194 1.861790 -0.012676
 N8 1.959936 -0.274552 -0.010223
 N9 -0.102881 -1.490896 0.000314
 C10 0.585590 -0.382870 -0.000119
 N11 -2.258874 -2.368470 -0.012092
 H12 -3.239664 -2.096644 -0.021558
 O13 -1.813210 2.343109 0.027337
 H14 3.274985 1.430912 -0.019992
 C15 2.894941 -1.388419 0.019324
 H16 3.286157 -1.548383 1.027474
 H17 2.359408 -2.283063 -0.295961
 H18 3.722590 -1.199189 -0.666154
 H19 -2.763003 2.279901 -0.128076

9MG_18

C1 1.342448 -1.060465 -0.000001
 C2 -0.066221 -0.927036 0.000080
 C3 1.564003 1.293333 0.000001
 C4 -2.282112 -1.018720 0.000000
 N5 2.100788 -0.023468 -0.000038
 N6 -1.169472 -1.758721 0.000058
 N7 -1.941215 0.288505 -0.000022
 N8 0.159640 1.492670 -0.000028
 C9 -0.532740 0.397832 0.000017
 N10 2.402188 2.265761 0.000047
 H11 1.875421 3.138520 0.000067
 O12 1.867434 -2.311990 -0.000042
 H13 -3.286977 -1.402487 -0.000013
 C14 -2.840968 1.432725 -0.000035
 H15 -2.654045 2.041889 0.885169
 H16 -2.653656 2.042140 -0.884982
 H17 -3.872593 1.082359 -0.000310
 H18 2.830370 -2.198095 -0.000133
 H19 -1.147958 -2.767649 0.000044

9MG_19

C1 -1.328185 1.061404 0.000025
 C2 0.076759 0.923539 0.000057
 H3 -2.816300 2.202914 -0.000018
 C4 -1.544728 -1.306911 -0.000013
 C5 2.293070 1.002472 -0.000051
 N6 -2.087069 0.020103 -0.000010
 N7 1.185535 1.750221 0.000034
 N8 1.947957 -0.301593 -0.000130
 N9 -0.149100 -1.499570 -0.000014

C10 0.537127 -0.405621 -0.000007
 N11 -2.317905 -2.331568 -0.000013
 H12 -3.283256 -2.006928 -0.000007
 O13 -1.853489 2.313021 0.000018
 H14 3.299792 1.381836 -0.000103
 C15 2.838910 -1.453313 0.000089
 H16 2.646795 -2.059400 0.886180
 H17 2.641900 -2.063003 -0.882416
 H18 3.873373 -1.111290 -0.003451
 H19 1.171965 2.759137 0.000003

9MG_20

C1 -1.322880 1.274532 0.009722
 C2 0.109807 0.904980 -0.010018
 C3 -1.770267 -1.077460 0.003573
 C4 2.329365 0.907930 -0.020246
 N5 -2.163348 0.224325 0.018838
 N6 1.239738 1.678684 -0.023229
 N7 1.916499 -0.391342 -0.001830
 N8 -0.346688 -1.409198 0.052971
 C9 0.534176 -0.399271 0.002238
 N10 -2.506904 -2.129151 -0.045359
 H11 -3.482372 -1.842259 -0.072146
 O12 -1.613595 2.476601 0.016030
 H13 3.353458 1.233599 -0.037242
 C14 2.781308 -1.567448 0.012627
 H15 2.565145 -2.174477 0.893356
 H16 2.623223 -2.160407 -0.889879
 H17 3.820300 -1.244861 0.049441
 H18 1.206571 2.691379 -0.032486
 H19 -0.121711 -2.388589 -0.036384

9MG_21

C1 1.316075 1.286766 -0.011436
 C2 -0.113516 0.905836 0.004603
 C3 1.815264 -1.055263 -0.002296
 C4 -2.332160 0.897516 0.029973
 N5 2.165880 0.249940 -0.022358
 N6 -1.246783 1.674305 0.027850
 N7 -1.912155 -0.397905 0.002812
 N8 0.360280 -1.410297 -0.090413
 C9 -0.527950 -0.398569 -0.006014
 N10 2.663083 -2.017399 0.067554
 H11 2.211708 -2.930090 0.045142
 O12 1.589651 2.493317 -0.014908
 H13 -3.357942 1.217468 0.058574
 C14 -2.772519 -1.576928 -0.014864
 H15 -2.517834 -2.203435 -0.871271
 H16 -2.652550 -2.147741 0.907798
 H17 -3.809997 -1.259658 -0.103937
 H18 -1.216064 2.687247 0.041187
 H19 0.102167 -2.356985 0.143856

9MG_22

C1 -1.349723 1.060093 -0.019133
 C2 0.065965 0.924659 0.037097

C3 -1.549739 -1.307226 0.007474
C4 2.294151 0.984588 0.042286
N5 -2.091849 0.014018 -0.035664
N6 1.190278 1.741474 0.063697
N7 1.939183 -0.312605 -0.008109
N8 -0.154127 -1.501150 -0.036466
C9 0.527441 -0.407410 -0.008117
N10 -2.320551 -2.330939 0.071329
H11 -3.285153 -2.004193 0.087774
O12 -1.967434 2.282800 -0.024946
H13 3.302511 1.357925 0.077417
C14 2.818804 -1.472252 -0.054511
H15 2.565173 -2.144350 0.765632
H16 2.670185 -2.006266 -0.994019
H17 3.854584 -1.145435 0.031709
H18 -1.363772 2.964209 -0.338315
H19 1.214015 2.745409 0.155281

9MG_23

C1 1.365305 1.058679 0.016597
C2 -0.054619 0.927881 -0.016041
C3 1.568901 -1.295244 -0.007709
C4 -2.281853 1.001994 -0.044688
N5 2.107470 0.017005 0.022306
N6 -1.172198 1.750189 -0.058845
N7 -1.932230 -0.298704 0.011881
N8 0.164473 -1.494356 0.040050
C9 -0.523010 -0.399439 0.020016
N10 2.402072 -2.269717 -0.065428
H11 1.871706 -3.140504 -0.072884
O12 1.976314 2.286068 0.005574
H13 -3.288017 1.380516 -0.081501
C14 -2.821744 -1.450642 0.042534
H15 -2.600049 -2.099581 -0.805426
H16 -2.656221 -2.014544 0.961403
H17 -3.855886 -1.111271 -0.005902
H18 1.397996 2.951762 0.392403
H19 -1.185032 2.754790 -0.146676

**Cartesian coordinates for protonated
9-methylguanine tautomers in Fig. S2,
optimized at B3LYP/6-311++G****

[9MG + H]⁺_1

C1 -1.156239 1.403566 -0.000003
C2 0.214431 0.967273 -0.000006
H3 -2.991346 0.481236 0.000035
C4 -1.590709 -1.057113 -0.000003
C5 2.411459 0.791130 0.000002
N6 -2.001855 0.258060 -0.000003
N7 1.405678 1.665234 0.000000
N8 1.917983 -0.459066 0.000000
N9 -0.313970 -1.414381 -0.000011
C10 0.527429 -0.377755 -0.000005
N11 -2.535088 -2.010797 0.000045
H12 -2.237834 -2.974369 -0.000069
H13 -3.521739 -1.810584 -0.000161
O14 -1.591262 2.530198 0.000003
H15 3.459036 1.044271 0.000006
C16 2.690661 -1.709218 0.000003
H17 2.440199 -2.285133 0.889858
H18 2.440220 -2.285125 -0.889863
H19 3.751417 -1.466866 0.000017
H20 1.498717 2.674340 0.000001

[9MG + H]⁺_2

C1 1.241258 1.169552 0.000000
C2 -0.148202 0.943944 0.000000
C3 1.543743 -1.122439 0.000000
C4 -2.355629 0.898679 0.000000
N5 2.055428 0.143230 0.000000
N6 -1.301057 1.715534 0.000001
N7 -1.947387 -0.378615 0.000000
N8 0.233057 -1.447901 0.000000
C9 -0.549919 -0.389269 0.000000
N10 2.436666 -2.122007 0.000001
H11 2.120704 -3.078299 0.000001
H12 3.422293 -1.915651 0.000001
O13 1.697527 2.417704 -0.000001
H14 -3.385399 1.217968 0.000000
C15 -2.796612 -1.577461 -0.000001
H16 -2.580758 -2.167866 -0.889512
H17 -2.580777 -2.167854 0.889523
H18 -3.840578 -1.270466 -0.000014
H19 2.668169 2.404275 -0.000001
H20 -1.348653 2.726536 0.000001

[9MG + H]⁺_3

C1 1.124359 1.242626 -0.002603
C2 -0.222851 0.970946 -0.000341
C3 1.507991 -1.147953 0.001555
C4 -2.329999 0.959923 0.006622
N5 1.964948 0.163679 -0.002462
N6 -1.327903 1.792789 0.002240
N7 -1.953614 -0.383378 0.010357

N8 0.223453 -1.447252 0.003160
C9 -0.595628 -0.394169 0.002554
N10 2.429628 -2.124460 0.002568
H11 2.103858 -3.079215 0.004858
H12 3.422398 -1.956726 0.005377
O13 1.723497 2.413495 -0.005410
H14 -3.373268 1.242393 0.011362
C15 -2.843028 -1.548845 -0.013787
H16 -3.188382 -1.740522 -1.030610
H17 -2.289822 -2.412193 0.350409
H18 -3.695647 -1.363486 0.638114
H19 1.072345 3.134102 -0.005050
H20 2.959892 0.362883 -0.006215

[9MG + H]⁺_4

C1 1.170802 1.221678 0.000001
C2 -0.219333 0.982880 0.000001
C3 1.617975 -1.050581 0.000000
C4 -2.337338 0.991203 -0.000003
N5 2.038082 0.205730 0.000001
N6 -1.323453 1.803208 -0.000002
N7 -1.970693 -0.362083 0.000000
N8 0.281584 -1.380276 0.000005
C9 -0.619006 -0.349516 0.000002
N10 2.522109 -2.039812 -0.000006
H11 2.281399 -3.017827 0.000004
H12 3.498592 -1.785136 -0.000003
O13 1.628858 2.448999 0.000001
H14 -3.379580 1.275699 -0.000005
C15 -2.867356 -1.519400 0.000001
H16 -2.714758 -2.122918 -0.896864
H17 -2.714800 -2.122885 0.896895
H18 -3.893260 -1.156109 -0.000031
H19 2.599993 2.440203 0.000000
H20 -0.016310 -2.347960 -0.000002

[9MG + H]⁺_5

C1 -1.162467 1.234388 0.000000
C2 0.220095 0.951171 -0.000001
C3 -1.654531 -1.017435 0.000000
C4 2.337506 0.942850 -0.000001
N5 -2.050471 0.245265 0.000000
N6 1.327883 1.764854 -0.000001
N7 1.955956 -0.403645 0.000000
N8 -0.323159 -1.388286 -0.000001
C9 0.601596 -0.380944 0.000000
N10 -2.582461 -1.983412 0.000002
H11 -2.369719 -2.967871 -0.000017
H12 -3.551048 -1.698027 -0.000002
O13 -1.641256 2.457114 0.000001
H14 3.382023 1.217955 0.000000
C15 2.842758 -1.569643 0.000001
H16 2.682956 -2.171114 0.896740
H17 2.682930 -2.171133 -0.896721
H18 3.872110 -1.216375 -0.000018
H19 -0.920312 3.107840 0.000001

H20 -0.052861 -2.363940 0.000012

[9MG + H]⁺₆

C1 1.259595 1.172620 0.000000
 C2 -0.140391 0.952789 -0.000001
 C3 1.542434 -1.124263 0.000000
 C4 -2.359730 0.885381 0.000000
 N5 2.053421 0.134145 0.000000
 N6 -1.311059 1.712716 -0.000001
 N7 -1.941786 -0.384227 0.000001
 N8 0.228449 -1.447408 0.000000
 C9 -0.543371 -0.385714 0.000000
 N10 2.432365 -2.125319 -0.000001
 H11 2.117683 -3.081974 0.000000
 H12 3.417746 -1.915389 0.000000
 O13 1.855759 2.368565 0.000000
 H14 -3.391384 1.198864 -0.000001
 C15 -2.778364 -1.592254 0.000001
 H16 -2.554686 -2.179974 -0.889303
 H17 -2.554709 -2.179960 0.889320
 H18 -3.825534 -1.296356 -0.000015
 H19 -1.401263 2.719510 -0.000002
 H20 1.235296 3.106059 0.000009

[9MG + H]⁺₇

C1 -1.139485 1.238799 0.002403
 C2 0.214416 0.988178 -0.001988
 H3 -2.963151 0.274288 0.039839
 C4 -1.477785 -1.174217 -0.003635
 C5 2.323277 0.993939 -0.007058
 N6 -1.960631 0.133214 0.003352
 N7 1.315751 1.815931 -0.005535
 N8 1.960996 -0.355433 -0.008322
 N9 -0.193070 -1.446230 -0.007115
 C10 0.606840 -0.376174 -0.002238
 N11 -2.385702 -2.166938 0.012277
 H12 -2.039704 -3.114265 -0.020037
 H13 -3.376646 -2.021346 -0.089935
 O14 -1.639180 2.455938 0.008766
 H15 3.364013 1.286266 -0.010867
 C16 2.861744 -1.511390 0.014747
 H17 3.264008 -1.656636 1.018265
 H18 2.297727 -2.393525 -0.281171
 H19 3.676154 -1.348261 -0.690181
 H20 -2.604413 2.507350 -0.012035

[9MG + H]⁺₈

C1 1.077242 1.473278 -0.000003
 C2 -0.293206 1.029647 0.000000
 H3 2.962226 0.557843 -0.000073
 C4 1.659551 -1.004799 -0.000022
 C5 -2.410031 0.882740 0.000013
 N6 1.982541 0.292261 -0.000075
 N7 -1.450380 1.763169 0.000015
 N8 -1.947275 -0.431796 -0.000008
 N9 0.348979 -1.337828 -0.000035

C10 -0.594898 -0.318731 -0.000008
 N11 2.595700 -1.961574 0.000175
 H12 2.359937 -2.942183 -0.000454
 H13 3.577467 -1.729291 -0.000217
 O14 1.576938 2.556113 0.000024
 H15 -3.468899 1.095641 0.000026
 C16 -2.755252 -1.651879 -0.000009
 H17 -2.561380 -2.243083 -0.897482
 H18 -2.561496 -2.243016 0.897535
 H19 -3.805082 -1.365035 -0.000089
 H20 0.074341 -2.310933 0.000220

[9MG + H]⁺₉

C1 -1.199089 1.389937 -0.003348
 C2 0.201331 0.939140 0.003363
 C3 -1.742790 -0.911160 0.009934
 C4 2.407358 0.791152 0.005681
 N5 -2.100701 0.335591 0.022049
 N6 1.385653 1.642626 0.010592
 N7 1.922718 -0.471483 -0.000819
 N8 -0.403627 -1.363243 0.015316
 C9 0.544688 -0.381553 -0.007505
 N10 -2.673570 -1.888801 -0.036467
 H11 -2.471902 -2.840504 0.226535
 H12 -3.635889 -1.586494 0.015546
 O13 -1.494058 2.564056 -0.019419
 H14 3.453349 1.049277 0.004852
 C15 2.727138 -1.702366 -0.003508
 H16 2.465669 -2.311221 0.862473
 H17 2.555440 -2.255699 -0.927530
 H18 3.779299 -1.432572 0.057891
 H19 -0.184743 -2.325037 -0.203299
 H20 1.446100 2.656081 0.016489

[9MG + H]⁺₁₀

C1 -1.239268 1.338404 0.000045
 C2 0.160185 0.940757 -0.000019
 H3 -3.059470 0.419191 0.000125
 C4 -1.721320 -1.156710 0.000015
 C5 2.365749 0.887635 -0.000111
 N6 -2.067903 0.208851 0.000174
 N7 1.312443 1.696384 -0.000108
 N8 1.933010 -0.395858 -0.000013
 N9 -0.322305 -1.400010 0.000304
 C10 0.551926 -0.372778 0.000030
 N11 -2.479257 -2.163886 -0.000279
 H12 -3.473059 -1.954240 -0.000444
 O13 -1.647755 2.475180 0.000013
 H14 3.399579 1.190810 -0.000189
 C15 2.783852 -1.596185 0.000049
 H16 2.586006 -2.185279 0.896119
 H17 2.586196 -2.185258 -0.896078
 H18 3.826447 -1.285552 0.000164
 H19 1.339198 2.710763 -0.000167
 H20 -0.061523 -2.376981 -0.000225

[9MG + H]⁺_11

C1 1.243184 1.335814 -0.000018
 C2 -0.160128 0.934621 0.000018
 H3 3.065190 0.388789 -0.000074
 C4 1.731082 -1.151057 -0.000004
 C5 -2.365455 0.887522 0.000051
 N6 2.065137 0.214619 -0.000097
 N7 -1.308807 1.692669 0.000052
 N8 -1.934990 -0.396603 0.000007
 N9 0.326899 -1.408774 -0.000150
 C10 -0.553408 -0.375406 -0.000005
 N11 2.652159 -2.010468 0.000138
 H12 2.348188 -2.979485 0.000144
 O13 1.636059 2.478790 -0.000004
 H14 -3.398511 1.193271 0.000087
 C15 -2.791392 -1.592468 -0.000035
 H16 -2.598491 -2.182361 -0.896765
 H17 -2.598655 -2.182323 0.896756
 H18 -3.832534 -1.276950 -0.000137
 H19 -1.329442 2.707513 0.000077
 H20 0.029707 -2.373029 0.000250

[9MG + H]⁺_12

C1 1.193174 1.188352 0.000001
 C2 -0.172193 0.948522 0.000001
 C3 1.631377 -1.250963 0.000000
 C4 -2.283348 1.045344 -0.000003
 N5 2.022900 0.119861 0.000005
 N6 -1.243189 1.818224 -0.000002
 N7 -1.960458 -0.326676 -0.000001
 N8 0.231635 -1.431541 0.000006
 C9 -0.612413 -0.380074 0.000002
 N10 2.376455 -2.263528 -0.000007
 H11 3.375457 -2.082809 -0.000010
 O12 1.773545 2.361982 0.000000
 H13 -3.315149 1.365014 -0.000006
 C14 -2.900716 -1.452131 0.000001
 H15 -2.764252 -2.059876 -0.895994
 H16 -2.764268 -2.059861 0.896008
 H17 -3.912879 -1.052611 -0.000012
 H18 1.114641 3.077098 -0.000003
 H19 3.019456 0.307868 -0.000005
 H20 -0.068059 -2.399364 0.000001

[9MG + H]⁺_13

C1 -1.198110 -1.185785 0.000003
 C2 0.174073 -0.943608 0.000001
 C3 -1.636124 1.247070 0.000000
 C4 2.285052 -1.043966 -0.000007
 N5 -2.017894 -0.122753 0.000009
 N6 1.241523 -1.814290 -0.000006
 N7 1.962949 0.326402 -0.000001
 N8 -0.234373 1.440664 0.000015
 C9 0.613568 0.379560 0.000004
 N10 -2.553651 2.106847 -0.000015
 H11 -2.252738 3.076745 -0.000019

O12 -1.768788 -2.362489 0.000000
 H13 3.316081 -1.365691 -0.000012
 C14 2.905387 1.449330 0.000001
 H15 2.772363 2.057256 -0.896570
 H16 2.772373 2.057243 0.896583
 H17 3.916686 1.047582 -0.000008
 H18 -1.104177 -3.072180 -0.000003
 H19 -3.023587 -0.269415 -0.000003
 H20 0.100350 2.394674 -0.000001

[9MG + H]⁺_14

C1 1.319578 1.104848 -0.000009
 C2 -0.103934 0.911643 -0.000005
 C3 1.675650 -1.224069 -0.000003
 C4 -2.312786 0.987251 0.000022
 N5 2.122605 0.101059 -0.000010
 N6 -1.213387 1.735359 0.000014
 N7 -1.956360 -0.319933 0.000008
 N8 0.247677 -1.436615 -0.000052
 C9 -0.577173 -0.381578 -0.000008
 N10 2.385812 -2.267915 0.000040
 H11 3.377961 -2.044262 0.000066
 O12 1.743063 2.367224 -0.000008
 H13 -3.326620 1.351171 0.000039
 C14 -2.875514 -1.468036 -0.000008
 H15 -2.711437 -2.067988 -0.895651
 H16 -2.711420 -2.068029 0.895604
 H17 -3.898399 -1.097558 0.000011
 H18 2.714420 2.379260 -0.000008
 H19 -1.195749 2.748447 0.000029
 H20 -0.052616 -2.402871 0.000024

[9MG + H]⁺_15

C1 -1.212715 -1.178024 0.000002
 C2 0.165683 -0.966298 0.000000
 C3 -1.595250 1.279863 0.000000
 C4 2.277857 -1.082895 -0.000007
 N5 -2.006750 -0.084742 0.000012
 N6 1.230773 -1.842724 -0.000007
 N7 1.970377 0.293533 -0.000001
 N8 -0.197240 1.439047 0.000015
 C9 0.624743 0.356045 0.000003
 N10 -2.502556 2.151628 -0.000016
 H11 -2.189945 3.117739 -0.000022
 O12 -1.707469 -2.389196 -0.000001
 H13 3.306355 -1.413363 -0.000012
 C14 2.921594 1.407889 0.000002
 H15 2.795445 2.017434 -0.896692
 H16 2.795453 2.017422 0.896706
 H17 3.929181 0.996838 -0.000005
 H18 -2.674929 -2.434412 0.000013
 H19 -3.018672 -0.168528 -0.000009
 H20 0.163167 2.383771 0.000000

[9MG + H]⁺_16

C1 -1.207276 -1.182989 0.000000

C2 0.163666 -0.970261 0.000001
 C3 -1.593867 1.283031 0.000000
 C4 2.276132 -1.081968 -0.000001
 N5 -2.013856 -0.084211 0.000002
 N6 1.232870 -1.845040 -0.000001
 N7 1.966790 0.295993 0.000000
 N8 -0.197207 1.429515 0.000003
 C9 0.622510 0.357696 0.000002
 N10 -2.323178 2.307646 -0.000003
 H11 -3.325605 2.148530 -0.000005
 O12 -1.703536 -2.395495 -0.000001
 H13 3.305652 -1.409652 -0.000002
 C14 2.915007 1.413639 -0.000001
 H15 2.784862 2.022920 -0.896103
 H16 2.784880 2.022907 0.896112
 H17 3.923793 1.005596 -0.000014
 H18 -2.670130 -2.445435 0.000001
 H19 -3.018308 -0.212179 -0.000004
 H20 0.128166 2.389055 0.000002

[9MG + H]⁺_17

C1 -1.285327 -1.122953 0.000001
 C2 0.084533 -0.933729 -0.000008
 C3 -1.502088 1.363302 0.000001
 C4 2.290745 -1.001572 -0.000004
 N5 -2.020966 -0.005059 0.000017
 N6 1.202147 -1.765951 -0.000008
 N7 1.960923 0.295560 0.000000
 N8 -0.119467 1.503280 0.000004
 C9 0.553763 0.402947 -0.000002
 N10 -2.396738 2.254475 -0.000014
 H11 -1.995928 3.188914 -0.000022
 O12 -1.804825 -2.341077 0.000001
 H13 3.301560 -1.378759 -0.000006
 C14 2.872440 1.446609 0.000009
 H15 2.685475 2.048355 -0.888701
 H16 2.685463 2.048351 0.888719
 H17 3.899198 1.085895 0.000015
 H18 -2.772774 -2.355943 0.000029
 H19 -3.035861 -0.034399 -0.000004
 H20 1.205775 -2.777554 -0.000015

[9MG + H]⁺_18

C1 -1.314497 -1.113773 -0.000014
 C2 0.109862 -0.913836 -0.000016
 C3 -1.706813 1.211885 0.000002
 C4 2.318804 -0.978411 0.000043
 N5 -2.121199 -0.119047 -0.000010
 N6 1.222450 -1.731596 0.000024
 N7 1.954147 0.326272 0.000014
 N8 -0.262146 1.435417 -0.000113
 C9 0.573755 0.379720 -0.000020
 N10 -2.554770 2.147139 0.000077
 H11 -2.152470 3.082078 0.000068
 O12 -1.730066 -2.379679 -0.000013
 H13 3.334625 -1.336702 0.000080

C14 2.869476 1.476722 -0.000012
 H15 2.705626 2.076009 -0.896253
 H16 2.705614 2.076066 0.896189
 H17 3.893557 1.109509 0.000008
 H18 -2.701886 -2.393429 -0.000006
 H19 1.207782 -2.744882 0.000047
 H20 0.074776 2.387648 0.000118

[9MG + H]⁺_19

C1 -1.293284 -1.122157 -0.000001
 C2 0.084551 -0.951850 0.000002
 C3 -1.503416 1.359339 0.000000
 C4 2.301810 -0.994189 0.000001
 N5 -2.014835 0.001416 -0.000001
 N6 1.219839 -1.772057 0.000002
 N7 1.961409 0.295204 0.000000
 N8 -0.115203 1.492447 -0.000001
 C9 0.550992 0.392573 0.000000
 N10 -2.384253 2.263535 0.000002
 H11 -1.967674 3.191153 0.000002
 O12 -2.001526 -2.244304 -0.000001
 H13 3.315246 -1.364721 0.000002
 C14 2.860165 1.456562 -0.000002
 H15 2.664689 2.055853 -0.888507
 H16 2.664689 2.055855 0.888502
 H17 3.890956 1.107535 -0.000002
 H18 -1.467348 -3.047275 -0.000010
 H19 -3.028461 -0.068099 -0.000002
 H20 1.266496 -2.781352 0.000005

[9MG + H]⁺_20

C1 1.268636 1.136750 -0.000003
 C2 -0.093339 0.940087 0.000004
 C3 1.505526 -1.376425 0.000003
 C4 -2.301239 0.981559 0.000006
 N5 2.019345 0.016473 0.000008
 N6 -1.221680 1.760585 0.000011
 N7 -1.960640 -0.309969 -0.000002
 N8 0.123628 -1.496453 -0.000005
 C9 -0.549577 -0.403738 -0.000002
 N10 2.269510 -2.380135 0.000007
 H11 3.264140 -2.169898 0.000018
 O12 1.783014 2.359659 -0.000019
 H13 -3.315967 1.348761 0.000008
 C14 -2.856388 -1.473903 -0.000007
 H15 -2.658527 -2.073194 -0.887990
 H16 -2.658514 -2.073211 0.887963
 H17 -3.888103 -1.127578 0.000004
 H18 2.750160 2.383372 0.000061
 H19 3.028342 0.103167 -0.000058
 H20 -1.238488 2.771835 0.000014

[9MG + H]⁺_21

C1 1.344600 1.105612 0.015192
 C2 -0.093954 0.923539 -0.002459
 C3 1.666849 -1.232366 -0.006170

C4 -2.316291 0.980565 -0.031210
 N5 2.118515 0.083681 0.012690
 N6 -1.220402 1.736963 -0.035807
 N7 -1.951013 -0.319551 0.004876
 N8 0.238149 -1.434935 0.041034
 C9 -0.571705 -0.373002 0.020426
 N10 2.368805 -2.280927 -0.049170
 H11 3.361753 -2.060154 -0.070172
 O12 1.918742 2.316348 0.002653
 H13 -3.331463 1.340092 -0.055293
 C14 -2.859998 -1.476159 0.016457
 H15 -2.678285 -2.091672 -0.865180
 H16 -2.700953 -2.056525 0.925782
 H17 -3.886112 -1.115300 -0.003582
 H18 1.309531 3.037075 0.197628
 H19 -1.245396 2.747430 -0.080724
 H20 -0.074398 -2.397482 0.041534

[9MG + H]⁺_22

C1 1.275187 1.134539 0.000044
 C2 -0.094549 0.958810 -0.000155
 C3 1.506104 -1.369088 -0.000032
 C4 -2.313185 0.974342 -0.000095
 N5 2.010745 0.008272 0.000123
 N6 -1.240439 1.767050 -0.000181
 N7 -1.962245 -0.309328 0.000033
 N8 0.118708 -1.485580 0.000082
 C9 -0.547963 -0.393275 -0.000007
 N10 2.258402 -2.381903 -0.000207
 H11 3.254056 -2.174787 -0.000295
 O12 1.985710 2.257506 0.000106
 H13 -3.330488 1.334832 -0.000149
 C14 -2.845066 -1.483458 0.000171
 H15 -2.638558 -2.080273 -0.887486
 H16 -2.638565 -2.080065 0.887969
 H17 -3.880664 -1.148932 0.000129
 H18 1.451917 3.061044 0.000616
 H19 3.017137 0.131839 0.000288
 H20 -1.299881 2.775481 -0.000438

[9MG + H]⁺_23

C1 -1.192497 -1.001802 0.018499
 C2 0.170830 -0.953883 0.016974
 C3 -1.458849 1.234268 -0.000496
 C4 2.271197 -1.067902 -0.006649
 N5 -2.019528 -0.020486 0.003072
 N6 1.216574 -1.844215 0.004941
 N7 1.986740 0.289003 -0.005218
 N8 -0.137105 1.476916 0.002127
 C9 0.622504 0.395774 0.006146
 N10 -2.307515 2.275104 -0.012310
 H11 -1.940394 3.212986 -0.001450
 H12 -3.302401 2.125695 0.012910
 O13 -1.855986 -2.348909 0.062149
 H14 3.292986 -1.419540 -0.018432
 C15 2.942620 1.399149 -0.005143

H16 2.739455 2.059114 -0.848086
 H17 2.861706 1.961629 0.925218
 H18 3.947669 0.991550 -0.097562
 H19 -2.759643 -2.328978 -0.313648
 H20 -1.300477 -3.079069 -0.280398

[9MG + H]⁺_24

C1 1.341595 1.112916 0.026170
 C2 -0.097375 0.924321 -0.003738
 C3 1.696641 -1.222179 -0.012761
 C4 -2.318682 0.973477 -0.060914
 N5 2.119152 0.099586 0.024811
 N6 -1.224486 1.732786 -0.068728
 N7 -1.948082 -0.323865 0.006980
 N8 0.252376 -1.433388 0.082792
 C9 -0.568043 -0.370929 0.038254
 N10 2.531128 -2.165253 -0.101255
 H11 2.116654 -3.094760 -0.124376
 O12 1.901989 2.332220 0.015901
 H13 -3.334851 1.328284 -0.104506
 C14 -2.855767 -1.480546 0.032594
 H15 -2.662689 -2.116018 -0.832423
 H16 -2.711685 -2.039315 0.957892
 H17 -3.881874 -1.121695 -0.011042
 H18 1.302966 3.033618 0.295676
 H19 -1.247953 2.741645 -0.144489
 H20 -0.097309 -2.380946 0.106230

[9MG + H]⁺_25

C1 -1.255315 -0.937364 0.017146
 C2 0.129578 -0.918776 0.018901
 C3 -1.585484 1.341454 -0.002349
 C4 2.226275 -1.145200 -0.007695
 N5 -2.080528 0.012904 -0.000745
 N6 1.135653 -1.856345 0.002643
 N7 1.990498 0.239104 -0.002067
 N8 -0.156003 1.466590 0.006529
 C9 0.643125 0.382344 0.009950
 N10 -2.265054 2.402531 -0.010754
 H11 -3.265626 2.225933 -0.012582
 O12 -1.890576 -2.307482 0.061667
 H13 3.234417 -1.531567 -0.020024
 C14 2.999047 1.302695 -0.008211
 H15 2.887045 1.925515 -0.897218
 H16 2.912635 1.912038 0.892871
 H17 3.984630 0.841690 -0.025997
 H18 -1.327474 -3.031490 -0.282581
 H19 0.187956 2.419207 0.005791
 H20 -2.804293 -2.305875 -0.289289

[9MG + H]⁺_26

C1 -1.254460 -0.941013 0.017045
 C2 0.134858 -0.927144 0.013634
 C3 -1.600971 1.339459 -0.002756
 C4 2.232279 -1.148073 -0.011640
 N5 -2.071431 0.008820 0.002791

N6 1.142428 -1.861235 -0.003983
 N7 1.992202 0.234308 -0.001964
 N8 -0.159769 1.464500 0.012263
 C9 0.643266 0.372335 0.009452
 N10 -2.424532 2.293710 -0.020039
 H11 -2.000817 3.218807 -0.025535
 O12 -1.910575 -2.301588 0.067238
 H13 3.241282 -1.532059 -0.024520
 C14 2.998749 1.298832 -0.002361
 H15 2.889833 1.924496 -0.889964
 H16 2.911781 1.904731 0.901197
 H17 3.985074 0.839344 -0.019743
 H18 -1.395276 -3.031443 -0.332891
 H19 0.222959 2.400296 0.015052
 H20 -2.844851 -2.258557 -0.225222

[9MG + H]⁺_27

C1 -1.237407 -0.973962 0.035604
 C2 0.096997 -0.928144 0.047324
 C3 -1.427700 1.459301 -0.016220
 C4 2.188825 -1.147925 0.003498
 N5 -2.021484 0.106974 -0.026460
 N6 1.101782 -1.874084 0.017521
 N7 1.987663 0.222159 0.006848
 N8 -0.036123 1.534304 -0.032317
 C9 0.623080 0.428230 0.022400
 N10 -2.273906 2.392635 0.021725
 H11 -1.826076 3.305240 0.046360
 O12 -1.912553 -2.289352 0.019280
 H13 3.190035 -1.556827 -0.009726
 C14 3.004161 1.276373 -0.029654
 H15 2.880619 1.878046 -0.930366
 H16 2.905168 1.914718 0.848331
 H17 3.988448 0.811464 -0.032789
 H18 -1.256257 -2.990792 0.240258
 H19 -2.369034 -2.500291 -0.824422
 H20 -3.005740 0.096103 0.219191

[9MG + H]⁺_28

C1 1.348248 -0.806620 0.000140
 C2 -0.024389 -0.937209 0.001491
 C3 1.387598 1.528249 -0.000056
 C4 -2.220184 -1.184593 -0.000741
 N5 2.033709 0.215984 -0.000531
 N6 -1.066497 -1.855593 -0.000279
 N7 -1.999067 0.135272 0.000213
 N8 -0.024972 1.517910 0.000390
 C9 -0.606544 0.371095 0.001074
 N10 2.144002 2.538116 -0.000111
 H11 1.594861 3.395890 0.000355
 O12 2.227425 -2.224218 -0.001649
 H13 -3.193712 -1.647925 -0.001592
 C14 -3.005277 1.203337 -0.000375
 H15 -2.870720 1.819143 0.888256
 H16 -2.868637 1.820028 -0.888076
 H17 -3.997687 0.756422 -0.001749

H18 2.803953 -2.205034 0.786983
 H19 2.821380 -2.188535 -0.776815
 H20 -0.995777 -2.863607 -0.001145

[9MG + H]⁺_29

C1 -1.230447 -0.977400 0.065771
 C2 0.098931 -0.932128 0.017896
 C3 -1.416816 1.482047 -0.020957
 C4 2.192204 -1.138056 -0.050896
 N5 -2.031904 0.103114 0.050067
 N6 1.107394 -1.870482 -0.068702
 N7 1.990627 0.226598 0.023010
 N8 -0.029454 1.533212 0.023264
 C9 0.623419 0.429020 0.044859
 N10 -2.127938 2.517035 -0.095392
 H11 -3.128606 2.356024 -0.171875
 O12 -1.906166 -2.309582 0.036401
 H13 3.194017 -1.544451 -0.089415
 C14 3.001683 1.287448 0.018393
 H15 2.862645 1.924947 -0.854965
 H16 2.907680 1.888990 0.922343
 H17 3.988199 0.828423 -0.014627
 H18 -1.240339 -3.013013 0.216655
 H19 -2.382819 -2.498244 -0.801010
 H20 -2.926365 0.062048 0.525553

**Cartesian coordinates for deprotonated
9-methylguanine tautomers in Fig. S3,
optimized at B3LYP/6-311++G****

[9MG – H]⁻_1

C1 -1.250962 -1.299424 0.001295
C2 0.154814 -1.002150 0.000302
H3 -3.002916 -0.226820 0.001424
C4 -1.551534 1.229012 -0.000698
C5 2.289585 -1.020819 -0.002462
N6 -1.999426 -0.112028 0.000911
N7 1.265198 -1.830069 -0.000768
N8 1.922991 0.320947 -0.004811
N9 -0.201299 1.458940 -0.000741
C10 0.536274 0.350555 -0.001071
N11 -2.485020 2.138512 -0.001624
H12 -2.024164 3.046273 -0.002393
O13 -1.819863 -2.393938 0.002405
H14 3.329387 -1.318343 -0.004679
C15 2.782251 1.482570 0.005277
H16 2.140689 2.360945 -0.073263
H17 3.359535 1.548394 0.934656
H18 3.476692 1.468477 -0.841610

[9MG – H]⁻_2

C1 -1.215741 1.349489 0.002854
C2 0.199142 0.997443 -0.004794
C3 -1.575130 -0.992345 -0.019999
C4 2.339021 0.920473 -0.002249
N5 -2.063336 0.239389 -0.003031
N6 1.349304 1.774809 0.000900
N7 1.916554 -0.401424 -0.017656
N8 -0.292521 -1.413890 -0.015404
C9 0.534460 -0.354985 -0.011446
N10 -2.530246 -2.026166 -0.077554
H11 -2.196488 -2.887764 0.331510
H12 -3.427070 -1.724106 0.276058
O13 -1.657698 2.504770 0.020725
H14 3.392157 1.168766 -0.005602
C15 2.724184 -1.597864 0.024555
H16 2.821923 -1.988549 1.044487
H17 2.256312 -2.369390 -0.589789
H18 3.720857 -1.379401 -0.366779

[9MG – H]⁻_3

C1 -1.230525 1.304491 0.000026
C2 0.168580 1.003050 -0.000002
H3 -2.982104 0.271680 0.000041
C4 -1.543002 -1.245515 -0.000015
C5 2.302475 1.004140 -0.000047
N6 -1.984697 0.112036 0.000027
N7 1.285978 1.823096 -0.000020
N8 1.926545 -0.334013 -0.000090
N9 -0.195551 -1.460362 -0.000017
C10 0.538488 -0.355163 -0.000025
N11 -2.395960 -2.233169 -0.000039

H12 -3.347986 -1.868033 -0.000032
O13 -1.808705 2.395014 0.000049
H14 3.344583 1.293867 -0.000086
C15 2.774227 -1.504652 0.000105
H16 3.409722 -1.537253 0.892036
H17 2.117846 -2.375794 -0.001344
H18 3.411923 -1.535798 -0.890289

[9MG – H]⁻_4

C1 -1.307701 1.277587 0.021743
C2 0.146099 0.982830 -0.023077
C3 -1.706101 -1.097251 0.007374
C4 2.292566 1.010127 -0.055615
N5 -2.133148 0.181923 0.031125
N6 1.258538 1.807164 -0.065560
N7 1.926321 -0.336917 -0.001474
N8 -0.300862 -1.383383 0.125136
C9 0.554537 -0.331096 0.011219
N10 -2.434241 -2.175648 -0.102283
H11 -3.404071 -1.875350 -0.170526
O12 -1.731817 2.439371 0.044872
H13 3.333404 1.298853 -0.096119
C14 2.795671 -1.490721 0.033137
H15 2.575746 -2.119338 0.902051
H16 2.696587 -2.098597 -0.873162
H17 3.829709 -1.150138 0.106835
H18 -0.043524 -2.331238 -0.105343

[9MG – H]⁻_5

C1 -1.300100 -1.069743 -0.000012
C2 0.105426 -0.973887 -0.000002
C3 -1.530008 1.279364 0.000007
C4 2.233063 -1.114036 0.000028
N5 -2.072063 -0.021362 -0.000010
N6 1.165314 -1.868464 0.000008
N7 1.947635 0.248615 0.000057
N8 -0.141308 1.472638 0.000008
C9 0.560534 0.361048 0.000013
N10 -2.369212 2.278488 0.000018
H11 -1.807128 3.129952 0.000027
O12 -1.907595 -2.294425 -0.000027
H13 3.253668 -1.471945 0.000051
C14 2.873057 1.356704 -0.000062
H15 2.278869 2.271685 0.000729
H16 3.511864 1.347050 0.890567
H17 3.510719 1.347910 -0.891530
H18 -2.851619 -2.075357 -0.000032

[9MG – H]⁻_6

C1 1.282991 1.070388 0.000000
C2 -0.118765 0.967770 0.000001
C3 1.509486 -1.293271 0.000000
C4 -2.246457 1.095985 0.000000
N5 2.055231 0.018090 -0.000001
N6 -1.183676 1.857449 0.000000
N7 -1.955297 -0.264320 0.000001

N8 0.130044 -1.482744 0.000002
 C9 -0.566943 -0.371865 0.000002
 N10 2.300163 -2.331429 -0.000001
 H11 3.255294 -1.975553 -0.000002
 O12 1.889626 2.296083 -0.000001
 H13 -3.268785 1.449240 -0.000001
 C14 -2.872506 -1.379746 -0.000002
 H15 -3.510427 -1.375224 -0.891245
 H16 -2.268986 -2.288798 -0.000021
 H17 -3.510406 -1.375249 0.891256
 H18 2.834217 2.082037 -0.000001

[9MG – H]₇

C1 -1.286329 1.079847 -0.000007
 C2 0.115118 0.927721 0.000119
 C3 -1.561627 -1.263861 0.000009
 C4 2.242937 1.041385 0.000034
 N5 -2.086394 0.061494 -0.000078
 N6 1.180980 1.811550 0.000070
 N7 1.934641 -0.315078 0.000073
 N8 -0.184232 -1.500404 0.000030
 C9 0.542556 -0.410196 0.000063
 N10 -2.378190 -2.279933 0.000024
 H11 -3.322463 -1.896518 -0.000006
 O12 -1.833502 2.341494 0.000039
 H13 3.267679 1.385582 0.000027
 C14 2.840565 -1.440161 -0.000133
 H15 3.478761 -1.442428 0.890760
 H16 2.226972 -2.342533 0.000735
 H17 3.477392 -1.443293 -0.892014
 H18 -1.087272 2.955422 -0.001149

[9MG – H]₈

C1 1.301584 1.082521 0.000001
 C2 -0.103575 0.933816 0.000000
 C3 1.585979 -1.245654 0.000000
 C4 -2.231815 1.054887 -0.000002
 N5 2.103880 0.069757 0.000001
 N6 -1.166447 1.820248 0.000000
 N7 -1.926427 -0.303344 -0.000003
 N8 0.198974 -1.489244 -0.000001
 C9 -0.535375 -0.400503 -0.000001
 N10 2.448565 -2.223041 -0.000001
 H11 1.906718 -3.087780 -0.000001
 O12 1.844570 2.346212 0.000001
 H13 -3.255590 1.401660 -0.000003
 C14 -2.838398 -1.423030 0.000003
 H15 -2.232275 -2.330235 -0.000043
 H16 -3.476252 -1.422256 0.891208
 H17 -3.476319 -1.422206 -0.891153
 H18 1.096934 2.958252 0.000001

[9MG – H]₉

C1 1.306707 1.288626 -0.017289
 C2 -0.146999 0.987724 0.019790
 C3 1.746020 -1.077687 -0.003911

C4 -2.293012 1.005162 0.049332
 N5 2.139785 0.203291 -0.030526
 N6 -1.262944 1.807832 0.057166
 N7 -1.920385 -0.338393 0.000318
 N8 0.312267 -1.384839 -0.129663
 C9 -0.546720 -0.325585 -0.007249
 N10 2.570707 -2.086188 0.101933
 H11 2.054121 -2.965059 0.046671
 O12 1.718380 2.454457 -0.035127
 H13 -3.335111 1.289656 0.090231
 C14 -2.784771 -1.495686 -0.033401
 H15 -2.523530 -2.148909 -0.871947
 H16 -2.726052 -2.075667 0.894993
 H17 -3.815589 -1.162379 -0.163910
 H18 0.035772 -2.280545 0.246754

[9MG – H]₁₀

C1 -1.342908 1.226484 0.004925
 C2 0.080214 0.907175 -0.033829
 C3 -1.640563 -1.173006 -0.001208
 C4 2.309615 0.932041 0.006255
 N5 -2.130246 0.142422 0.015699
 N6 1.196207 1.687520 -0.016108
 N7 1.907055 -0.377371 -0.006586
 N8 -0.255401 -1.489932 -0.002403
 C9 0.493433 -0.429767 -0.017078
 N10 -2.463634 -2.185477 -0.011855
 H11 -3.401667 -1.784403 -0.007061
 O12 -1.703277 2.433061 0.024598
 H13 3.323359 1.284838 -0.034767
 C14 2.753448 -1.550098 0.025490
 H15 2.084306 -2.411736 0.001674
 H16 3.419239 -1.583313 -0.843083
 H17 3.352034 -1.583995 0.941796
 H18 1.151640 2.697011 -0.013903

[9MG – H]₁₁

C1 1.352759 1.233885 -0.008128
 C2 -0.070765 0.911485 0.052891
 C3 1.674284 -1.146876 0.001125
 C4 -2.300233 0.939456 -0.009302
 N5 2.149792 0.159888 -0.024815
 N6 -1.184945 1.692257 0.026704
 N7 -1.897555 -0.371749 0.011252
 N8 0.275444 -1.478072 0.002073
 C9 -0.485162 -0.423958 0.026694
 N10 2.539284 -2.124778 0.018288
 H11 1.997820 -2.989846 0.032180
 O12 1.698877 2.444422 -0.039468
 H13 -3.312540 1.291825 0.063793
 C14 -2.748575 -1.539833 -0.042124
 H15 -3.313798 -1.579209 -0.979346
 H16 -2.088569 -2.406664 0.012617
 H17 -3.446378 -1.561019 0.801278
 H18 -1.135546 2.701764 0.023760

**Cartesian coordinates for mono-hydrated
protonated 9-methylguanine tautomers
in Fig. S4, optimized at B3LYP/6-311++G****

[9MG + H]⁺_1^{...}W67

C1 0.455103 -1.470925 -0.000032
C2 0.542034 -0.039416 -0.000026
H3 -1.048540 -2.862505 -0.000014
C4 -1.993401 -1.006836 0.000014
C5 1.164301 2.061257 -0.000037
N6 -0.907183 -1.858224 -0.000010
N7 1.623245 0.817759 -0.000050
N8 -0.185927 2.054926 -0.000004
N9 -1.875395 0.310779 0.000022
C10 -0.606226 0.731419 0.000001
N11 -3.218914 -1.557448 0.000030
H12 -4.016206 -0.940312 0.000049
H13 -3.378137 -2.551302 0.000023
O14 1.349941 -2.295791 -0.000052
H15 1.772530 2.951000 -0.000049
C16 -1.071743 3.225980 0.000023
H17 -1.699744 3.203797 -0.889698
H18 -1.699671 3.203812 0.889795
H19 -0.461810 4.127116 -0.000010
H20 2.610312 0.480594 -0.000074
O21 3.765111 -0.761158 0.000062
H22 4.712420 -0.927493 0.000339
H23 3.297232 -1.612519 -0.000009

[9MG + H]⁺_1^{...}W12

C1 0.619667 1.419191 0.000001
C2 -0.746441 0.963789 0.000001
H3 2.481712 0.498242 0.000000
C4 1.087435 -1.025181 0.000002
C5 -2.942082 0.757839 -0.000001
N6 1.479354 0.295842 0.000002
N7 -1.947449 1.644688 0.000000
N8 -2.430949 -0.485703 -0.000001
N9 -0.185727 -1.409854 0.000001
C10 -1.040448 -0.386272 0.000000
N11 2.059178 -1.947069 0.000003
H12 1.794998 -2.919327 0.000002
H13 3.035698 -1.679040 0.000007
O14 1.027040 2.559655 0.000001
H15 -3.992777 0.996589 -0.000002
C16 -3.184747 -1.745802 -0.000002
H17 -2.925714 -2.318855 -0.889339
H18 -2.925718 -2.318854 0.889338
H19 -4.249213 -1.519892 -0.000004
H20 -2.052809 2.652219 0.000000
O21 4.393805 -0.085544 -0.000004
H22 4.942952 0.114669 0.768085
H23 4.942946 0.114658 -0.768100

[9MG + H]⁺_1^{...}W16

C1 -0.973083 -1.006255 0.000080

C2 0.461623 -0.924062 0.000050
H3 -2.550028 0.305912 0.000183
C4 -0.801695 1.465157 0.000055
C5 2.636745 -1.286525 -0.000035
N6 -1.518749 0.295114 0.000117
N7 1.448563 -1.890086 0.000011
N8 2.461803 0.046068 -0.000031
N9 0.527269 1.512741 0.000011
C10 1.092358 0.305769 0.000019
N11 -1.492806 2.616019 0.000071
H12 -0.979760 3.483472 -0.000085
H13 -2.499310 2.643553 -0.000153
O14 -1.663570 -2.007529 0.000078
H15 3.591300 -1.786589 -0.000071
C16 3.513470 1.071549 -0.000081
H17 3.409399 1.691457 -0.889585
H18 3.409490 1.691452 0.889438
H19 4.484488 0.580450 -0.000132
H20 1.294346 -2.891280 0.000017
O21 -4.168402 -0.459588 -0.000356
H22 -3.934732 -1.398218 -0.000170
H23 -5.128484 -0.396060 0.001005

[9MG + H]⁺_1^{...}W2

C1 -1.005743 -1.870642 0.000004
C2 -1.463132 -0.507856 0.000004
H3 0.817609 -2.806884 -0.000012
C4 1.243279 -0.769051 -0.000006
C5 -2.616946 1.370775 0.000000
N6 0.414238 -1.876591 -0.000003
N7 -2.729342 0.043162 0.000007
N8 -1.315874 1.709055 -0.000008
N9 0.771343 0.474832 -0.000008
C10 -0.558991 0.537703 -0.000004
N11 2.561849 -0.977056 -0.000014
H12 3.213579 -0.189246 0.000021
H13 2.951386 -1.905765 0.000052
O14 -1.661193 -2.887197 0.000009
H15 -3.439110 2.067308 0.000001
C16 -0.759951 3.067974 -0.000010
H17 -0.145744 3.203642 0.889173
H18 -0.145567 3.203556 -0.889083
H19 -1.579081 3.784300 -0.000128
H20 -3.598752 -0.476867 0.000010
O21 4.730713 0.898329 0.000009
H22 5.211704 1.221538 -0.769395
H23 5.211235 1.222130 0.769460

[9MG + H]⁺_2^{...}W7

C1 -0.017064 -1.516452 -0.000047
C2 -0.439598 -0.175926 -0.000079
C3 2.168611 -0.766647 0.000004
C4 -1.386098 1.804248 -0.000052
N5 1.265168 -1.789374 -0.000020
N6 -1.647825 0.501963 -0.000113
N7 -0.057336 2.019531 0.000006

N8 1.875340 0.549506 0.000027
 C9 0.576545 0.778289 -0.000015
 N10 3.463723 -1.120283 0.000017
 H11 4.177387 -0.410070 0.000043
 H12 3.719042 -2.093952 0.000010
 O13 -0.921455 -2.497276 -0.000010
 H14 -2.130328 2.584074 -0.000059
 C15 0.628513 3.316660 0.000078
 H16 1.253005 3.393806 0.889308
 H17 1.253041 3.393888 -0.889119
 H18 -0.116859 4.109644 0.000099
 H19 -0.452987 -3.347364 0.000010
 H20 -2.589837 0.067158 -0.000213
 O21 -4.033489 -0.875509 0.000164
 H22 -3.982452 -1.838297 0.000958
 H23 -4.969393 -0.647040 -0.001029

[9MG + H]⁺_2⁺⁺⁺W6

C1 1.078816 -0.507784 0.000103
 C2 -0.296473 -0.832875 0.000068
 C3 0.447551 1.721243 0.000031
 C4 -2.341877 -1.666327 -0.000014
 N5 1.418746 0.765099 0.000103
 N6 -1.049603 -1.996831 0.000045
 N7 -2.470812 -0.330639 -0.000037
 N8 -0.887090 1.513053 -0.000018
 C9 -1.190777 0.230454 0.000009
 N10 0.871486 2.996446 0.000039
 H11 0.201241 3.747603 -0.000070
 H12 1.857129 3.197826 -0.000020
 O13 1.962090 -1.479446 0.000121
 H14 -3.161475 -2.366286 -0.000042
 C15 -3.722886 0.435429 -0.000104
 H16 -3.758072 1.063803 0.888979
 H17 -3.757949 1.063839 -0.889166
 H18 -4.561845 -0.257700 -0.000176
 H19 2.900078 -1.140799 -0.000074
 H20 -0.689047 -2.942270 0.000059
 O21 4.514470 -0.772587 -0.000440
 H22 4.871838 0.121289 0.000806
 H23 5.260400 -1.381781 0.000776

[9MG + H]⁺_2⁺⁺⁺W2a

C1 -0.278975 1.516214 0.000000
 C2 0.998862 0.925437 0.000003
 C3 -1.196702 -0.609456 -0.000009
 C4 3.112300 0.283643 0.000007
 N5 -1.339919 0.752058 -0.000007
 N6 2.317978 1.355260 0.000009
 N7 2.372373 -0.835190 0.000001
 N8 -0.014691 -1.274738 -0.000007
 C9 1.022737 -0.467497 -0.000002
 N10 -2.319253 -1.329124 -0.000014
 H11 -2.247178 -2.334018 -0.000016
 H12 -3.240886 -0.893979 -0.000009
 O13 -0.381726 2.843914 0.000005

H14 4.189835 0.311945 0.000011
 C15 2.862870 -2.218756 -0.000002
 H16 2.493905 -2.728812 0.888961
 H17 2.493916 -2.728804 -0.888975
 H18 3.951073 -2.208601 0.000004
 H19 -1.321705 3.085716 0.000008
 H20 2.637716 2.315207 0.000013
 O21 -5.100343 -0.503002 0.000013
 H22 -5.671109 -0.400991 0.768947
 H23 -5.670974 -0.400324 -0.768932

[9MG + H]⁺_2⁺⁺⁺W2b

C1 0.874841 -1.778389 -0.000012
 C2 1.437600 -0.488045 -0.000002
 C3 -1.223720 -0.793965 0.000021
 C4 2.591560 1.395166 -0.000003
 N5 -0.426227 -1.909358 -0.000001
 N6 2.709325 0.066391 -0.000012
 N7 1.295473 1.740276 0.000013
 N8 -0.781493 0.486270 0.000026
 C9 0.530258 0.569125 0.000015
 N10 -2.539871 -1.009299 0.000037
 H11 -3.213531 -0.244752 0.000081
 H12 -2.872004 -1.960233 0.000007
 O13 1.680089 -2.838768 -0.000030
 H14 3.416070 2.089487 -0.000008
 C15 0.742587 3.099940 0.000016
 H16 0.127610 3.235388 -0.888777
 H17 0.127523 3.235345 0.888756
 H18 1.562396 3.815607 0.000074
 H19 1.140524 -3.645458 -0.000034
 H20 3.585740 -0.439209 -0.000023
 O21 -4.780118 0.845281 -0.000036
 H22 -5.296271 1.109931 -0.768837
 H23 -5.297024 1.108843 0.768634

[9MG + H]⁺_3⁺⁺⁺W67

C1 -0.783910 -1.177439 -0.016584
 C2 -0.551372 0.194778 -0.015649
 C3 1.639036 -1.450425 0.003663
 C4 -0.592730 2.317836 -0.019733
 N5 0.349317 -1.956720 -0.007505
 N6 -1.398000 1.289343 -0.026487
 N7 0.748066 1.975104 -0.007617
 N8 1.886621 -0.156311 0.006519
 C9 0.794136 0.612544 -0.003495
 N10 2.652525 -2.333014 0.009810
 H11 3.593215 -1.969801 0.025773
 H12 2.522539 -3.331128 0.021156
 O13 -1.899006 -1.826510 -0.026247
 H14 -0.905221 3.351931 -0.024326
 C15 1.897642 2.883464 0.018372
 H16 2.402301 2.822345 0.982880
 H17 2.593908 2.613692 -0.774724
 H18 1.540765 3.899042 -0.142528
 H19 -2.725108 -1.204868 -0.001946

H20 0.190026 -2.958674 -0.005004
 O21 -3.773253 -0.150371 0.108109
 H22 -4.611665 -0.124350 -0.365269
 H23 -3.309192 0.703502 0.006623

[9MG + H]⁺_3⁺W12

C1 -0.278975 1.516214 0.000000
 C2 0.998862 0.925437 0.000003
 C3 -1.196702 -0.609456 -0.000009
 C4 3.112300 0.283643 0.000007
 N5 -1.339919 0.752058 -0.000007
 N6 2.317978 1.355260 0.000009
 N7 2.372373 -0.835190 0.000001
 N8 -0.014691 -1.274738 -0.000007
 C9 1.022737 -0.467497 -0.000002
 N10 -2.319253 -1.329124 -0.000014
 H11 -2.247178 -2.334018 -0.000016
 H12 -3.240886 -0.893979 -0.000009
 O13 -0.381726 2.843914 0.000005
 H14 4.189835 0.311945 0.000011
 C15 2.862870 -2.218756 -0.000002
 H16 2.493905 -2.728812 0.888961
 H17 2.493916 -2.728804 -0.888975
 H18 3.951073 -2.208601 0.000004
 H19 -1.321705 3.085716 0.000008
 H20 2.637716 2.315207 0.000013
 O21 -5.100343 -0.503002 0.000013
 H22 -5.671109 -0.400991 0.768947
 H23 -5.670974 -0.400324 -0.768932

[9MG + H]⁺_3⁺W2

C1 -0.989274 -1.720252 -0.000008
 C2 -1.490452 -0.441621 0.000017
 C3 1.235988 -0.749653 -0.000032
 C4 -2.621142 1.337245 0.000071
 N5 0.370904 -1.843316 -0.000037
 N6 -2.780447 0.044311 0.000060
 N7 -1.287834 1.746663 0.000050
 N8 0.784429 0.494551 -0.000023
 C9 -0.541776 0.609181 0.000002
 N10 2.546716 -1.002979 -0.000043
 H11 3.221981 -0.232086 -0.000015
 H12 2.911818 -1.941663 -0.000028
 O13 -1.652881 -2.858263 -0.000010
 H14 -3.422949 2.062038 0.000110
 C15 -0.788271 3.124075 -0.000110
 H16 -1.134720 3.646459 0.891979
 H17 0.299188 3.087646 0.000852
 H18 -1.133157 3.645751 -0.893227
 H19 -2.609978 -2.695371 0.000010
 H20 0.741426 -2.787445 -0.000063
 O21 4.717098 0.833806 0.000072
 H22 5.172913 1.190998 -0.769784
 H23 5.172927 1.190866 0.769979

**Cartesian coordinates for mono-hydrated
deprotonated 9-methylguanine tautomers
in Fig. S5, optimized at B3LYP/6-311++G****

[9MG – H]⁻_1^{...}W67

C1 -0.761939 -1.296982 0.004202
C2 -0.533450 0.117535 0.002410
H3 0.379764 -2.999374 0.003433
C4 1.769481 -1.480288 -0.002102
C5 -0.655735 2.252350 -0.007195
N6 0.447881 -1.991440 0.002829
N7 -1.413443 1.188664 -0.001350
N8 0.698791 1.949257 -0.014659
N9 1.936595 -0.119327 -0.001568
C10 0.798029 0.565467 -0.002385
N11 2.716754 -2.371006 -0.005523
H12 3.604967 -1.873963 -0.007846
O13 -1.837234 -1.914514 0.006688
H14 -1.005148 3.275078 -0.014349
C15 1.816492 2.866436 0.015077
H16 2.705176 2.317767 -0.298085
H17 1.643396 3.700920 -0.670113
H18 1.990229 3.262617 1.022158
O19 -4.117184 -0.100928 -0.000863
H20 -3.436725 0.592412 -0.002391
H21 -3.549615 -0.892073 0.002443

[9MG – H]⁻_1^{...}W2

C1 0.323000 1.625487 0.037336
C2 -0.964949 0.989609 -0.005990
H3 2.286012 1.022651 0.136861
C4 1.228473 -0.745088 0.093463
C5 -3.035976 0.481392 -0.068876
N6 1.344576 0.656494 0.084208
N7 -2.243743 1.518747 -0.055829
N8 -2.351199 -0.727615 -0.025492
N9 -0.011274 -1.303954 0.055588
C10 -1.003605 -0.412442 0.011759
N11 2.353548 -1.417213 0.135824
H12 2.135314 -2.409345 0.144471
O13 0.604874 2.823066 0.038051
H14 -4.116348 0.512351 -0.103517
C15 -2.898564 -2.065993 -0.050264
H16 -2.083579 -2.758156 0.162949
H17 -3.678092 -2.181338 0.709038
H18 -3.319850 -2.311956 -1.031603
O19 4.929131 -0.456207 -0.098447
H20 4.011088 -0.827880 0.047302
H21 4.959795 -0.304208 -1.046984

[9MG – H]⁻_1^{...}W3

C1 2.128070 -0.281496 -0.105225
C2 1.164232 0.785326 -0.062698
H3 2.094756 -2.331850 0.026528
C4 0.118631 -1.812095 0.199915
C5 0.115800 2.640183 -0.045285

N6 1.488950 -1.523526 0.033820
N7 1.323378 2.158034 -0.148860
N8 -0.856568 1.656215 0.097116
N9 -0.761484 -0.757275 0.223491
C10 -0.187547 0.447630 0.095560
N11 -0.189412 -3.071088 0.313002
H12 -1.194937 -3.143504 0.452462
O13 3.350825 -0.223139 -0.237123
H14 -0.153756 3.686983 -0.073939
C15 -2.276474 1.852590 0.315010
H16 -2.856527 1.158882 -0.295120
H17 -2.542387 1.687222 1.364535
H18 -2.535174 2.877893 0.042158
O19 -3.408105 -1.276647 -0.520502
H20 -2.482934 -1.111243 -0.191771
H21 -3.281124 -1.855437 -1.277502

[9MG – H]⁻_1^{...}W6

C1 1.133190 -0.492905 0.117315
C2 -0.245490 -0.864236 0.059690
H3 2.229378 1.245032 0.136779
C4 0.278904 1.892446 0.029762
C5 -2.139620 -1.842162 -0.004921
N6 1.282588 0.892579 0.097074
N7 -0.863527 -2.104627 0.057118
N8 -2.417365 -0.479089 -0.039186
N9 -1.030123 1.490705 -0.024524
C10 -1.194596 0.172335 -0.003541
N11 0.707551 3.119814 0.024675
H12 -0.107178 3.727867 -0.025963
O13 2.128718 -1.236472 0.178248
H14 -2.934209 -2.575559 -0.022666
C15 -3.706370 0.167334 -0.138948
H16 -3.561476 1.226283 0.077025
H17 -4.132027 0.071636 -1.144685
H18 -4.408770 -0.257126 0.584767
O19 4.826588 -0.775778 -0.149385
H20 3.875697 -0.910989 0.066466
H21 4.886153 -1.061682 -1.064864

[9MG – H]⁻_2^{...}W67

C1 -0.672065 -1.362116 -0.010446
C2 -0.544080 0.086144 -0.015545
C3 1.689253 -1.362281 -0.013996
C4 -0.795918 2.215771 -0.011894
N5 0.542154 -2.031189 -0.007798
N6 -1.487639 1.105611 -0.016192
N7 0.571663 1.998723 -0.013993
N8 1.909277 -0.030911 -0.005612
C9 0.739528 0.626031 -0.010397
N10 2.849982 -2.149741 -0.064298
H11 3.657648 -1.693230 0.334686
H12 2.689251 -3.087160 0.274926
O13 -1.753566 -1.978629 -0.001570
H14 -1.204673 3.216741 -0.015969
C15 1.630015 2.982466 0.027403

H16 2.058445 3.070777 1.031719
 H17 2.427981 2.689981 -0.657769
 H18 1.231991 3.953325 -0.275345
 O19 -4.107183 -0.372491 0.031177
 H20 -3.506837 0.389173 0.013376
 H21 -3.446269 -1.094192 0.022029

[9MG – H]₂^{W16}

C1 1.033527 -0.898620 -0.004954
 C2 -0.416664 -0.944765 -0.008308
 C3 0.753658 1.458087 -0.022383
 C4 -2.494903 -1.446529 -0.001440
 N5 1.553910 0.395187 -0.014806
 N6 -1.312973 -2.003827 -0.002871
 N7 -2.444981 -0.059753 -0.012151
 N8 -0.590960 1.509808 -0.010773
 C9 -1.103096 0.267696 -0.009826
 N10 1.392894 2.704727 -0.079346
 H11 0.830628 3.454422 0.296685
 H12 2.338511 2.677789 0.273288
 O13 1.777490 -1.894308 0.011536
 H14 -3.442027 -1.969272 -0.003079
 C15 -3.547375 0.873837 0.031366
 H16 -3.711698 1.259488 1.043846
 H17 -3.333421 1.720297 -0.623826
 H18 -4.457412 0.375074 -0.309564
 O19 4.330737 -0.596344 0.019095
 H20 3.731022 -1.364571 0.034785
 H21 3.642457 0.090753 -0.024282

[9MG – H]₂^{W3}

C1 -1.958315 -0.899051 -0.065630
 C2 -1.357933 0.430171 -0.047080
 C3 0.270702 -1.681736 0.108127
 C4 -0.905929 2.520572 -0.036497
 N5 -1.022753 -1.934736 0.030443
 N6 -1.919306 1.697856 -0.101665
 N7 0.318819 1.874161 0.049073
 N8 0.912707 -0.488913 0.130100
 C9 0.026598 0.525610 0.050980
 N10 1.120141 -2.801490 0.137955
 H11 1.984883 -2.643215 0.637434
 H12 0.625712 -3.633207 0.427468
 O13 -3.168642 -1.127011 -0.147416
 H14 -0.962384 3.600676 -0.056471
 C15 1.625254 2.476155 0.220855
 H16 1.939007 2.460950 1.270478
 H17 2.370667 1.932740 -0.361454
 H18 1.587323 3.512775 -0.121123
 O19 3.665321 -0.436576 -0.311412
 H20 3.722956 -0.956861 -1.118062
 H21 2.688889 -0.423639 -0.113528

[9MG – H]₃^{W23}

C1 -1.192034 -1.740867 -0.021949
 C2 -1.437855 -0.330303 -0.014541

H3 0.425553 -2.977322 0.013754
 C4 1.279649 -1.076114 0.052627
 C5 -2.241268 1.643930 -0.016769
 N6 0.198861 -1.992870 0.012486
 N7 -2.618190 0.395537 -0.038987
 N8 -0.860180 1.798413 0.025614
 N9 0.980773 0.254165 0.054784
 C10 -0.323372 0.524669 0.023802
 N11 2.520473 -1.490865 0.086281
 H12 2.570313 -2.506293 0.061862
 O13 -1.981551 -2.685488 -0.052088
 H14 -2.897535 2.503423 -0.024352
 C15 -0.099074 3.028324 0.040769
 H16 -0.782899 3.867958 0.180096
 H17 0.624813 3.013593 0.858705
 H18 0.450094 3.164795 -0.895736
 O19 3.906696 1.006727 -0.124194
 H20 2.976568 1.276844 -0.090141
 H21 3.763494 0.038597 -0.058817

[9MG – H]₃^{W67}

C1 0.744274 -1.293747 0.000019
 C2 0.537807 0.118333 0.000012
 H3 -0.388472 -2.977041 0.000035
 C4 -1.812118 -1.440610 -0.000011
 C5 0.682861 2.250991 -0.000014
 N6 -0.483364 -1.971333 0.000010
 N7 1.430480 1.180141 0.000000
 N8 -0.674142 1.964430 -0.000038
 N9 -1.938176 -0.080416 -0.000006
 C10 -0.791082 0.580189 -0.000005
 N11 -2.850575 -2.225677 -0.000027
 H12 -2.552427 -3.200474 -0.000027
 O13 1.803779 -1.939569 0.000033
 H14 1.044712 3.269519 -0.000039
 C15 -1.785006 2.891391 0.000039
 H16 -2.698711 2.296137 -0.000726
 H17 -1.772179 3.526708 0.891803
 H18 -1.771312 3.527778 -0.890940
 O19 4.110651 -0.155711 -0.000020
 H20 3.441297 0.548602 -0.000002
 H21 3.531674 -0.938300 -0.000014

[9MG – H]₃^{W16}

C1 1.054655 -0.749962 -0.080063
 C2 -0.357000 -0.918191 -0.037650
 H3 2.403825 0.774407 -0.099717
 C4 0.553335 1.753428 -0.032006
 C5 -2.376147 -1.600528 0.018753
 N6 1.405630 0.604285 -0.076262
 N7 -1.153801 -2.053440 -0.025361
 N8 -2.448721 -0.212125 0.037291
 N9 -0.794256 1.528898 0.007723
 C10 -1.141329 0.252182 0.001711
 N11 1.048309 2.956862 -0.029510
 H12 2.065984 2.916021 -0.066181

O13	1.944928	-1.624649	-0.116173
H14	-3.270961	-2.207790	0.039618
C15	-3.626253	0.625427	0.085388
H16	-3.283997	1.660944	0.074034
H17	-4.273044	0.452577	-0.781468
H18	-4.203511	0.450120	0.999740
O19	4.460986	-0.635621	0.084678
H20	3.587261	-1.084212	-0.048201
H21	4.683438	-0.825404	1.000167

**Cartesian coordinates for the structures in Fig. 1,
optimized at B3LYP/6-31+G***

Fig. 1a

[9MG + H_{N7}]⁺

C1 1.157636 1.402851 -0.000001
C2 -0.214588 0.968754 -0.000004
H3 2.995888 0.484355 0.000003
C4 1.592661 -1.058927 0.000013
C5 -2.414343 0.793099 -0.000015
N6 2.004303 0.258586 0.000009
N7 -1.406254 1.668030 -0.000014
N8 -1.921147 -0.459926 -0.000007
N9 0.312687 -1.418746 0.000011
C10 -0.529914 -0.378916 0.000000
N11 2.537684 -2.014621 0.000011
H12 2.240963 -2.981834 0.000041
H13 3.528673 -1.818999 0.000065
O14 1.595249 2.536931 -0.000006
H15 -3.464266 1.047256 -0.000022
C16 -2.693968 -1.710054 -0.000005
H17 -2.442270 -2.286751 -0.892086
H18 -2.442288 -2.286738 0.892091
H19 -3.756874 -1.466608 -0.000017
H20 -1.497623 2.679768 -0.000020

PC⁺

C1 1.231769 -1.426390 -0.349751
C2 -0.060466 -0.790474 -0.489389
H3 3.139533 -0.816630 0.106297
C4 1.975378 0.914095 0.092906
C5 -2.170736 -0.266520 -0.812981
N6 2.202787 -0.441938 -0.023633
N7 -1.287306 -1.279295 -0.841253
N8 -1.523260 0.890824 -0.579358
N9 0.775690 1.473122 -0.075093
C10 -0.187648 0.598350 -0.347582
N11 3.015834 1.705361 0.385347
H12 2.848221 2.698739 0.486797
H13 3.953479 1.361128 0.540985
O14 1.506945 -2.599901 -0.482207
H15 -3.226199 -0.355923 -1.023421
H16 -1.523054 -2.262040 -0.951306
O17 -0.942283 -0.564274 1.838593
O18 -2.132977 -0.855354 1.633680
C19 -2.136117 2.218134 -0.423280
H20 -2.172653 2.471999 0.638708
H21 -1.528785 2.947687 -0.960398
H22 -3.143306 2.191581 -0.839805

TS1⁺

C1 1.251084 -1.431135 -0.251978
C2 -0.068662 -0.827092 -0.386768
H3 3.155384 -0.778605 0.154537
C4 1.965138 0.933096 0.048431

C5 -2.186822 -0.353261 -0.554456
N6 2.211320 -0.425132 0.017513
N7 -1.251730 -1.341288 -0.784807
N8 -1.536257 0.855576 -0.560023
N9 0.756210 1.475308 -0.133810
C10 -0.213843 0.597604 -0.330837
N11 2.995040 1.751713 0.273703
H12 2.814093 2.747930 0.314526
H13 3.941417 1.431811 0.433021
O14 1.535260 -2.602972 -0.350425
H15 -3.233987 -0.461320 -0.798874
H16 -1.476487 -2.333111 -0.755338
O17 -0.888661 -0.469008 1.621795
O18 -2.112407 -0.760427 1.328859
C19 -2.191436 2.153504 -0.347389
H20 -2.455771 2.258490 0.708863
H21 -1.489667 2.935986 -0.635601
H22 -3.083348 2.208533 -0.973026

5,8-OO-[9MG + H_{N7}]⁺

C1 1.187439 -1.412785 -0.200656
C2 -0.197529 -0.811011 -0.084002
H3 3.141801 -0.821328 -0.050338
C4 1.995407 0.918416 0.061258
C5 -2.201585 -0.310705 -0.303102
N6 2.195956 -0.445134 -0.035986
N7 -1.248499 -1.165782 -0.996204
N8 -1.507703 0.997721 -0.349692
N9 0.797861 1.515433 -0.021061
C10 -0.226812 0.703713 -0.180866
N11 3.062630 1.692072 0.233777
H12 2.920917 2.694579 0.295983
O13 1.424082 -2.575359 -0.393065
H14 -3.232209 -0.301543 -0.651396
C15 -2.158793 2.302091 -0.236311
H16 -2.703664 2.363318 0.711202
H17 -1.388032 3.072885 -0.265278
H18 -2.848245 2.437567 -1.073362
O19 -2.173719 -0.749296 1.067492
O20 -0.736442 -1.066090 1.260679
H21 4.006353 1.337208 0.327123
H22 -1.498770 -2.155210 -0.928540

8-OO[9MG + H_{N7}]⁺

C1 1.348906 -1.517220 -0.164184
C2 0.081826 -0.803785 -0.303610
C3 2.264164 0.763303 0.142815
C4 -2.123311 -0.137620 -0.604579
N5 2.408059 -0.605395 0.045041
N6 -1.141978 -1.260149 -0.342639
N7 -1.224352 1.035129 -0.369105
N8 1.096671 1.408188 0.018699
C9 0.034657 0.647427 -0.204962
N10 3.355465 1.493119 0.367373
H11 3.250814 2.498924 0.443805
H12 4.281455 1.100174 0.481216

O13 1.509565 -2.716463 -0.212793
 H14 -2.499866 -0.101039 -1.636156
 H15 -1.412174 -2.241523 -0.421815
 O16 -3.122385 -0.343967 0.269128
 O17 -2.358425 -0.800264 1.405601
 H18 3.322206 -1.039070 0.153636
 C19 -1.763526 2.385307 -0.227311
 H20 -2.284710 2.471303 0.731248
 H21 -0.936025 3.093956 -0.269218
 H22 -2.465088 2.582108 -1.042790

TS2⁺

C1 1.274915 -1.415911 -0.232932
 C2 -0.101728 -0.841516 0.165908
 H3 3.227497 -0.796383 -0.233558
 C4 2.055883 0.908655 0.071577
 C5 -2.257139 -0.300206 -0.316769
 N6 2.280009 -0.448267 -0.098538
 N7 -1.276586 -1.316010 -0.618487
 N8 -1.432189 0.963408 -0.338955
 N9 0.851231 1.487042 0.015739
 C10 -0.176175 0.664073 -0.100418
 N11 3.116460 1.688192 0.255383
 H12 2.964720 2.686200 0.356535
 H13 4.062830 1.338712 0.343344
 O14 1.484585 -2.550352 -0.562133
 H15 -2.928778 -0.328044 -1.230138
 H16 -1.598190 -2.260124 -0.386978
 O17 -0.479527 -1.128633 1.407126
 O18 -3.044468 -0.431746 0.703853
 C19 -2.056224 2.285579 -0.362257
 H20 -2.810258 2.332949 0.428477
 H21 -1.284030 3.035680 -0.190049
 H22 -2.528173 2.452261 -1.335058

TS3⁺

C1 1.268758 -1.384188 -0.339604
 C2 -0.000548 -0.850657 0.322621
 H3 3.225335 -0.751472 -0.522089
 C4 2.076934 0.912009 0.017363
 C5 -2.300659 -0.284257 -0.278949
 N6 2.295735 -0.421611 -0.268185
 N7 -1.310436 -1.369086 0.017753
 N8 -1.436396 0.929951 -0.147145
 N9 0.856661 1.471092 0.074471
 C10 -0.164612 0.638780 0.055259
 N11 3.131598 1.704015 0.168415
 H12 2.971029 2.691471 0.338436
 H13 4.087738 1.369487 0.167298
 O14 1.426843 -2.491820 -0.780355
 H15 -2.102228 -0.756218 -1.375885
 H16 -1.552967 -2.363589 0.049954
 O17 -0.180464 -1.239435 1.602834
 O18 -3.497286 -0.258037 -0.003010
 C19 -2.025249 2.264105 -0.299015
 H20 -1.376370 2.986461 0.196661

H21 -2.121207 2.514523 -1.360015
 H22 -3.011963 2.248389 0.166676

TS4⁺

C1 1.204180 -1.379772 -0.371620
 C2 -0.001602 -0.845918 0.390895
 H3 3.169994 -0.758289 -0.617491
 C4 2.047863 0.905278 -0.057058
 C5 -2.272471 -0.245301 -0.168498
 N6 2.247667 -0.415613 -0.353598
 N7 -1.383375 -1.388821 0.097519
 N8 -1.483556 0.921142 -0.067072
 N9 0.813690 1.472188 0.028688
 C10 -0.176945 0.628971 0.085895
 N11 3.090689 1.710366 0.072321
 H12 2.919985 2.695893 0.245712
 H13 4.051244 1.387281 0.056738
 O14 1.346508 -2.480185 -0.834568
 H15 -1.514786 -2.194357 -0.526200
 H16 -1.228759 -1.623222 1.281023
 O17 0.059825 -1.121616 1.716601
 O18 -3.438787 -0.318962 -0.402275
 C19 -2.057584 2.269832 -0.210999
 H20 -1.570400 2.782838 -1.042562
 H21 -3.123417 2.156949 -0.408013
 H22 -1.900680 2.825635 0.716030

5-OH-8-oxo9MG⁺

C1 1.187537 -1.357346 -0.385964
 C2 -0.062962 -0.862004 0.349832
 H3 3.105816 -0.694684 -0.749577
 C4 1.995894 0.943671 -0.080779
 C5 -2.264281 -0.339568 -0.164621
 N6 2.197767 -0.376227 -0.417241
 N7 -1.323773 -1.347612 -0.107908
 N8 -1.511239 0.906292 -0.019494
 N9 0.777295 1.483100 0.095059
 C10 -0.225510 0.638149 0.131576
 N11 3.048631 1.748280 -0.002053
 H12 2.888845 2.730162 0.198361
 H13 4.005176 1.430462 -0.101497
 O14 1.358333 -2.480096 -0.787243
 H15 -1.607483 -2.320724 -0.084427
 H16 0.290831 -1.965674 1.955510
 O17 0.194190 -1.019705 1.738102
 O18 -3.446674 -0.393467 -0.347438
 C19 -2.129875 2.221700 -0.205877
 H20 -1.824604 2.644165 -1.167029
 H21 -3.210288 2.076044 -0.188828
 H22 -1.820669 2.881929 0.606569

TS5⁺

C1 1.236729 -1.330025 -0.415495
 C2 -0.104371 -0.840388 0.125110
 H3 3.144300 -0.630202 -0.696130
 C4 2.009878 0.990133 -0.017003

C5 -2.241351 -0.332493 -0.260447
 N6 2.222226 -0.324474 -0.390198
 N7 -1.331327 -1.374672 -0.244460
 N8 -1.489646 0.952435 -0.014366
 N9 0.799120 1.513334 0.198377
 C10 -0.217340 0.671389 0.138092
 N11 3.067115 1.789986 0.082051
 H12 2.909457 2.765564 0.312792
 H13 4.021029 1.483076 -0.064543
 O14 1.479626 -2.458734 -0.753950
 H15 -1.107988 -1.913785 1.085525
 H16 0.515252 -2.109205 1.864322
 O17 -0.173218 -1.444081 1.633922
 O18 -3.425229 -0.324673 -0.428679
 C19 -2.114564 2.270143 -0.098733
 H20 -1.758523 2.794584 -0.990284
 H21 -3.191586 2.110894 -0.164514
 H22 -1.867681 2.850166 0.793512

TS6⁺

C1 0.392405 -0.982093 -0.776836
 C2 0.044860 0.378420 -0.481595
 C3 -2.160120 0.544716 -0.121061
 C4 -0.708478 -0.897336 1.065953
 C5 2.274681 0.103201 -0.072861
 N6 -1.980438 -0.438079 0.865841
 N7 -1.124514 1.000780 -0.766710
 O8 -0.240693 -1.568716 1.929533
 N9 1.206267 1.014430 -0.114758
 N10 -3.398596 1.012727 -0.314314
 H11 -4.218833 0.577253 0.084639
 H12 -3.538065 1.717529 -1.028852
 O13 3.405728 0.292464 0.282740
 N14 1.715535 -1.126927 -0.526091
 O15 -0.379007 -1.794531 -1.489713
 H16 2.250082 -1.988677 -0.480533
 H17 -2.688211 -0.613985 1.577803
 H18 -0.037435 -2.706011 -1.536213
 C19 1.316583 2.384152 0.395514
 H20 1.094127 2.417414 1.466571
 H21 2.341367 2.717624 0.229503
 H22 0.621378 3.018231 -0.155858

8-oxo[9MG – H]⁺

C1 -1.288248 1.491393 -0.000005
 C2 0.100664 0.948917 -0.000009
 H3 -3.211863 0.753314 0.000012
 C4 -1.956768 -0.905148 0.000019
 C5 2.232989 0.546834 -0.000017
 N6 -2.244256 0.434615 0.000009
 N7 1.208967 1.583942 -0.000020
 N8 1.581517 -0.747547 -0.000002
 N9 -0.701030 -1.417914 0.000016
 C10 0.267286 -0.535815 0.000003
 N11 -2.954417 -1.777913 0.000032
 H12 -2.725718 -2.767272 0.000039

H13 -3.933578 -1.515299 0.000036
 O14 -1.622145 2.644380 -0.000013
 O15 3.411641 0.718881 -0.000025
 C16 2.294145 -2.029557 0.000004
 H17 2.028655 -2.596861 0.895050
 H18 2.028692 -2.596850 -0.895061
 H19 3.361972 -1.809143 0.000027

[9MSp + H]⁺

C1 -0.700236 1.377687 -0.259614
 C2 0.051096 0.063987 -0.112973
 C3 2.197828 -0.231434 -0.501081
 C4 0.817771 0.042098 1.280438
 C5 -2.272833 -0.303704 -0.249901
 N6 2.127250 -0.145344 0.897202
 N7 1.054677 -0.119947 -1.122644
 O8 0.345298 0.153777 2.381361
 N9 -1.056575 -0.884941 -0.145168
 N10 3.376498 -0.418635 -1.105545
 H11 4.248699 -0.500000 -0.602834
 H12 3.398366 -0.475728 -2.116160
 O13 -3.391269 -0.730878 -0.297683
 N14 -1.980391 1.161009 -0.318772
 O15 -0.044003 2.494362 -0.302412
 H16 -2.741105 1.832132 -0.414032
 H17 2.889549 -0.248840 1.558355
 H18 -0.592014 3.298723 -0.396473
 C19 -0.866598 -2.334259 -0.077020
 H20 -1.832688 -2.806761 -0.258922
 H21 -0.157387 -2.642296 -0.848978
 H22 -0.506012 -2.626560 0.914316

Fig. 1b

[9MG + H_{N7}]⁺(H₂O)

C1 0.482869 -1.459901 0.000009
 C2 0.545811 -0.025888 0.000004
 H3 -0.992178 -2.883382 0.000005
 C4 -1.975534 -1.042090 -0.000008
 C5 1.127274 2.090336 0.000000
 N6 -0.871479 -1.873712 0.000002
 N7 1.610984 0.853643 0.000007
 N8 -0.224513 2.058201 -0.000008
 N9 -1.883288 0.281577 -0.000012
 C10 -0.619058 0.725784 -0.000006
 N11 -3.192576 -1.615234 -0.000013
 H12 -4.004797 -1.012174 -0.000020
 H13 -3.339244 -2.614481 -0.000010
 O14 1.396971 -2.275179 0.000017
 H15 1.720078 2.993507 0.000000
 C16 -1.133428 3.211550 -0.000018
 H17 -1.761980 3.175866 -0.892009
 H18 -1.761994 3.175871 0.891963
 H19 -0.539594 4.126207 -0.000016
 H20 2.604805 0.540104 0.000015
 O21 3.779167 -0.719471 0.000022

H22 4.730234 -0.905195 0.000020
H23 3.294059 -1.569193 0.000023

PC⁺(H₂O)

C1 0.079329 -1.696642 -0.115808
C2 -0.350138 -0.337478 -0.339274
H3 1.858115 -2.659130 0.219327
C4 2.333616 -0.641775 -0.033993
C5 -1.438628 1.522660 -0.699608
N6 1.483529 -1.729783 0.044966
N7 -1.582138 0.198824 -0.585330
N8 -0.129028 1.855423 -0.639936
N9 1.912735 0.599883 -0.261466
C10 0.590632 0.700227 -0.392106
N11 3.647092 -0.860767 0.124559
H12 4.272133 -0.065498 0.083155
H13 4.044311 -1.770942 0.311854
O14 -0.599780 -2.709941 -0.063627
H15 -2.241590 2.221843 -0.880883
H16 -2.462480 -0.371622 -0.567313
O17 -3.327693 -1.828385 -0.530186
H18 -2.677619 -2.521579 -0.301333
H19 -4.170662 -2.065237 -0.113329
O20 -0.489113 0.656339 1.982364
O21 -1.521881 1.331912 1.852473
C22 0.429397 3.213925 -0.661384
H23 0.678690 3.517253 0.358276
H24 1.328085 3.212760 -1.279393
H25 -0.311824 3.892199 -1.085059

TS1⁺(H₂O)

C1 0.087434 -1.710600 -0.088488
C2 -0.356870 -0.339414 -0.295303
H3 1.866590 -2.674479 0.243189
C4 2.336712 -0.656986 -0.034356
C5 -1.435641 1.531044 -0.433030
N6 1.489040 -1.746703 0.066620
N7 -1.560418 0.166448 -0.605328
N8 -0.100441 1.861592 -0.595393
N9 1.922676 0.591219 -0.256484
C10 0.607286 0.723572 -0.356983
N11 3.647370 -0.876176 0.101414
H12 4.271993 -0.080164 0.048006
H13 4.049352 -1.787216 0.278179
O14 -0.597005 -2.714724 -0.048122
H15 -2.232423 2.222610 -0.668988
H16 -2.441235 -0.392084 -0.508560
O17 -3.405172 -1.797282 -0.404211
H18 -2.819806 -2.544160 -0.181361
H19 -4.249114 -1.945355 0.050462
O20 -1.527150 1.346288 1.404546
O21 -0.462982 0.658561 1.695732
C22 0.430030 3.224406 -0.472020
H23 0.372728 3.546657 0.572079
H24 1.469243 3.212583 -0.800484
H25 -0.150152 3.892089 -1.110806

5,8-OO-[9MG + H_{N7}]⁺(H₂O)

C1 0.056133 -1.667917 -0.037441
C2 -0.394221 -0.224653 0.028273
H3 1.794679 -2.744229 0.012573
C4 2.355371 -0.733571 -0.029056
C5 -1.357815 1.591710 -0.202062
N6 1.455087 -1.784829 0.003336
N7 -1.427701 0.283851 -0.816695
N8 0.079388 1.932298 -0.382453
N9 2.012341 0.553541 -0.143917
C10 0.714091 0.784766 -0.209276
N11 3.650578 -1.029844 0.046445
H12 4.316650 -0.265697 0.015920
H13 4.008233 -1.970536 0.154593
O14 -0.669793 -2.628063 -0.095683
H15 -2.058348 2.356568 -0.529571
H16 -2.329476 -0.202431 -0.675722
O17 -3.576693 -1.554581 -0.434070
H18 -4.539760 -1.665666 -0.416778
H19 -3.190001 -2.423293 -0.237603
O20 -1.540419 1.363978 1.211530
O21 -0.809980 0.092350 1.413099
C22 0.635522 3.283101 -0.370924
H23 1.718046 3.210356 -0.480783
H24 0.217417 3.855063 -1.203156
H25 0.395309 3.774658 0.577416

Cartesian coordinates for the structures in Fig. 3.

Fig. 3a (optimized at B3LYP/6-31+G*)

[9MG – H_{N10}][−]

C1 -1.252372 1.299121 0.001445
 C2 0.155288 1.004565 -0.000302
 H3 -3.006854 0.226547 0.002073
 C4 -1.552061 -1.230333 -0.000838
 C5 2.291033 1.020346 -0.002348
 N6 -2.000431 0.111120 0.000920
 N7 1.267107 1.835022 -0.000432
 N8 1.923421 -0.322458 -0.007153
 N9 -0.199191 -1.464822 -0.001552
 C10 0.537950 -0.350989 -0.002640
 N11 -2.488999 -2.142513 -0.001116
 H12 -2.023806 -3.052270 -0.002158
 O13 -1.827261 2.398849 0.003365
 H14 3.334684 1.313902 -0.004771
 C15 2.782852 -1.482447 0.007321
 H16 2.677820 -2.039980 0.946669
 H17 2.524305 -2.158025 -0.815772
 H18 3.822463 -1.156981 -0.103466

PC[−]

C1 -1.667944 1.421159 -0.023295
 C2 -0.353097 0.889542 -0.345156
 H3 -3.498414 0.659886 0.512576
 C4 -2.315733 -1.010539 0.290334
 C5 1.693485 0.541034 -0.823192
 N6 -2.553901 0.382924 0.270699
 N7 0.790870 1.517931 -0.683808
 N8 1.128036 -0.723368 -0.692113
 N9 -1.059504 -1.477114 -0.025458
 C10 -0.183252 -0.532514 -0.324449
 N11 -3.333940 -1.753787 0.609967
 H12 -3.022706 -2.726607 0.586948
 O13 -2.033295 2.598563 0.002910
 H14 2.666385 0.678648 -1.269334
 C15 1.853196 -1.977078 -0.614392
 H16 2.496408 -1.987362 0.271753
 H17 1.120697 -2.785011 -0.556348
 H18 2.473115 -2.109659 -1.508386
 O19 2.842007 0.588184 1.091451
 O20 4.041745 0.145050 0.986724

TS1[−]

C1 -1.669454 1.407418 -0.026394
 C2 -0.330741 0.893352 -0.312617
 H3 -3.504110 0.619691 0.444005
 C4 -2.291061 -1.033799 0.247972
 C5 1.749736 0.576553 -0.691677
 N6 -2.548118 0.359210 0.229574
 N7 0.794437 1.539221 -0.607632
 N8 1.174478 -0.706174 -0.621187
 N9 -1.020742 -1.485753 -0.031317

C10 -0.141518 -0.538101 -0.298966
 N11 -3.310288 -1.786299 0.530685
 H12 -2.991235 -2.756659 0.512346
 O13 -2.041413 2.580816 -0.005882
 H14 2.657732 0.729836 -1.256631
 C15 1.913455 -1.955064 -0.558825
 H16 2.733736 -1.850726 0.159024
 H17 1.220946 -2.738567 -0.243490
 H18 2.320981 -2.210933 -1.545287
 O19 2.736027 0.703221 0.984873
 O20 3.874271 0.048935 0.930036

***syn*-8-OO[9MG – H_{N10}][−]**

C1 1.456725 -1.363778 -0.143357
 C2 0.067298 -0.897569 -0.358382
 H3 3.275759 -0.516651 0.266355
 C4 1.998996 1.091506 0.086532
 C5 -2.053522 -0.619440 -0.474345
 N6 2.305167 -0.293019 0.076612
 N7 -0.986616 -1.578351 -0.680287
 N8 -1.471295 0.702720 -0.739744
 N9 0.710371 1.511774 -0.177915
 C10 -0.170462 0.560139 -0.345318
 N11 2.996842 1.876202 0.330843
 H12 2.644599 2.835124 0.310330
 O13 1.859837 -2.522252 -0.161221
 H14 -2.958400 -0.822462 -1.048924
 C15 -2.221235 1.900364 -0.403317
 H16 -2.423457 1.932084 0.674705
 H17 -1.629158 2.773508 -0.690241
 H18 -3.163635 1.905144 -0.962095
 O19 -2.420028 -0.711822 0.917366
 O20 -1.326533 -0.224596 1.695409

***anti*-8-OO[9MG – H_{N10}][−]**

C1 1.705933 1.418683 0.023051
 C2 0.312183 0.895898 0.117958
 H3 3.588210 0.637731 -0.146817
 C4 2.357695 -1.019721 -0.093180
 C5 -1.875318 0.590598 0.311226
 N6 2.608705 0.382688 -0.075493
 N7 -0.780112 1.562091 0.168212
 N8 -1.188319 -0.754324 0.225090
 N9 1.068540 -1.488327 0.013395
 C10 0.125189 -0.574870 0.122780
 N11 3.414835 -1.753585 -0.206636
 H12 3.117197 -2.730987 -0.205181
 O13 2.042387 2.596334 0.034108
 H14 -2.308320 0.681871 1.323644
 C15 -1.893728 -2.022160 0.157614
 H16 -1.326931 -2.710161 -0.477985
 H17 -1.990996 -2.464478 1.158652
 H18 -2.892493 -1.798052 -0.235226
 O19 -2.836101 0.782796 -0.631832
 O20 -4.011776 -0.002417 -0.167996

TS2a⁻

C1 -1.648544 1.427165 0.015686
 C2 -0.301767 0.886242 0.004925
 H3 -3.552611 0.670717 0.156605
 C4 -2.352758 -1.005553 0.107096
 C5 1.847187 0.505101 -0.307115
 N6 -2.578841 0.393460 0.105011
 N7 0.888621 1.529426 -0.071643
 N8 1.209588 -0.730265 -0.268818
 N9 -1.056866 -1.470853 -0.027705
 C10 -0.139318 -0.529692 -0.072101
 N11 -3.407419 -1.747939 0.218982
 H12 -3.105128 -2.723286 0.195826
 O13 -1.996792 2.608256 -0.035323
 H14 1.446291 1.345358 -1.283144
 C15 1.896597 -2.009445 -0.357712
 H16 2.863410 -1.877865 0.138456
 H17 1.281414 -2.754059 0.152160
 H18 2.023508 -2.306693 -1.405701
 O19 3.147210 0.657075 -0.259888
 O20 3.580726 0.007934 1.046504

8-OO[9MG – H_{N10}]⁻1

C1 1.692835 1.411281 -0.000013
 C2 0.378790 0.878766 -0.000584
 H3 3.602388 0.640566 -0.037839
 C4 2.384830 -1.026754 -0.036801
 C5 -1.839140 0.517027 0.056894
 N6 2.626238 0.369805 -0.027937
 N7 -0.889540 1.480447 0.043395
 N8 -1.220755 -0.701443 0.026749
 N9 1.075739 -1.467100 -0.016853
 C10 0.176502 -0.495411 -0.006248
 N11 3.441115 -1.786403 -0.060969
 H12 3.123086 -2.756799 -0.064874
 O13 2.036458 2.608798 0.017004
 H14 -1.092912 2.464325 -0.048584
 C15 -1.825938 -2.024677 0.168808
 H16 -1.415512 -2.677978 -0.605774
 H17 -1.562307 -2.438814 1.148340
 H18 -2.903175 -1.893415 0.062996
 O19 -3.090542 0.836293 0.124620
 O20 -4.044470 -0.215893 -0.303785

TS3⁻

C1 -1.510209 1.462332 -0.013069
 C2 -0.241520 0.838834 -0.057725
 H3 -3.471462 0.840887 0.130036
 C4 -2.389357 -0.913394 0.069322
 C5 1.944032 0.313287 -0.170336
 N6 -2.522317 0.492723 0.070073
 N7 1.065137 1.359299 -0.259166
 N8 1.213352 -0.856936 -0.237367
 N9 -1.120398 -1.450104 -0.025079
 C10 -0.151132 -0.547588 -0.083451
 N11 -3.496225 -1.596925 0.158325

H12 -3.245956 -2.587048 0.144907
 O13 -1.777410 2.681275 -0.027018
 H14 1.348821 2.273955 0.063970
 C15 1.785787 -2.181686 -0.121326
 H16 1.113714 -2.888283 -0.613123
 H17 2.765734 -2.187841 -0.603765
 H18 1.903213 -2.468765 0.930841
 O19 3.234737 0.400998 -0.484673
 O20 3.165609 0.361477 1.044085

dioxyrane

C1 -1.499899 1.461455 -0.005482
 C2 -0.232182 0.842083 -0.014235
 H3 -3.468290 0.842018 0.073309
 C4 -2.386440 -0.911209 0.021719
 C5 1.978088 0.313656 -0.057778
 N6 -2.519434 0.490822 0.033611
 N7 1.085049 1.389024 -0.178849
 N8 1.223264 -0.862905 -0.171081
 N9 -1.113502 -1.444498 -0.041273
 C10 -0.142833 -0.541651 -0.055364
 N11 -3.492898 -1.602177 0.071899
 H12 -3.235336 -2.590453 0.053258
 O13 -1.774937 2.680740 -0.003559
 H14 1.335748 2.215971 0.351223
 C15 1.776164 -2.188589 0.002907
 H16 1.048457 -2.903345 -0.387359
 H17 2.714200 -2.268794 -0.553632
 H18 1.967213 -2.420814 1.060286
 O19 3.257495 0.380323 -0.627264
 O20 3.067850 0.373823 0.887342

TS4⁻

C1 1.492019 -1.459646 -0.006141
 C2 0.221952 -0.840226 -0.035924
 H3 3.460648 -0.842652 0.063709
 C4 2.376623 0.909460 0.010828
 C5 -2.014084 -0.316960 -0.029648
 N6 2.511363 -0.492138 0.025767
 N7 -1.079295 -1.386798 -0.153995
 N8 -1.228310 0.869880 -0.119933
 N9 1.105427 1.446272 -0.031881
 C10 0.127112 0.551341 -0.051497
 N11 3.484089 1.599087 0.043400
 H12 3.227068 2.587633 0.028827
 O13 1.759629 -2.679751 0.014762
 H14 -1.315121 -2.233630 0.351783
 C15 -1.779013 2.198901 0.028373
 H16 -1.172980 2.895908 -0.556465
 H17 -2.805558 2.196440 -0.346505
 H18 -1.777921 2.532391 1.075619
 O19 -3.197736 -0.379808 -0.741485
 O20 -3.026482 -0.396369 0.919669

pyr

C1 1.643466 -0.494159 -0.000578

C2 0.292898 -1.201422 0.000523
 H3 2.446851 1.379970 -0.001142
 C4 0.379794 1.637340 0.000337
 N5 1.578816 0.854515 -0.000713
 N6 0.274787 -2.480775 0.001780
 N7 -2.086680 -0.953484 -0.000563
 N8 -0.818016 1.029887 0.000605
 C9 -0.942776 -0.332635 0.000125
 N10 0.621205 2.920935 0.000793
 H11 -0.284465 3.394992 0.001466
 O12 2.709083 -1.123635 -0.001178
 H13 1.256890 -2.793135 0.001632
 C14 -3.261267 -0.104832 -0.000894
 H15 -3.297418 0.560817 -0.880460
 H16 -4.159495 -0.736837 -0.001728
 H17 -3.298496 0.559977 0.879265

TS2b⁻

C1 1.594905 1.481685 0.004368
 C2 0.262648 0.864474 -0.077551
 H3 3.537653 0.838568 0.106194
 C4 2.441293 -0.906565 0.052394
 C5 -1.853516 0.399361 -0.002217
 N6 2.581148 0.506702 0.047797
 N7 -0.920458 1.431527 -0.121681
 N8 -1.129250 -0.861805 -0.143265
 N9 1.181071 -1.460234 -0.005223
 C10 0.190249 -0.590198 -0.079575
 N11 3.552440 -1.570307 0.111036
 H12 3.318814 -2.564851 0.112129
 O13 1.865091 2.680626 0.030289
 H14 -2.531318 0.435589 1.087022
 C15 -1.742981 -2.168830 -0.065812
 H16 -1.234307 -2.847917 -0.756947
 H17 -1.669480 -2.583729 0.948461
 H18 -2.794558 -2.061543 -0.338310
 O19 -3.075168 0.468950 -0.615887
 O20 -3.894555 0.348318 0.664493

8-OOH[9MG – 2H]⁻

C1 1.318319 1.577943 0.000020
 C2 0.141145 0.765327 0.000021
 H3 3.352350 1.264409 -0.000001
 C4 2.569256 -0.639549 -0.000023
 C5 -1.823352 -0.048645 0.000027
 N6 2.468696 0.769212 0.000000
 N7 -1.225489 1.099970 0.000040
 N8 -1.004059 -1.148586 -0.000024
 N9 1.403657 -1.371556 -0.000015
 C10 0.303292 -0.626079 0.000000
 N11 3.779691 -1.129910 -0.000046
 H12 3.695809 -2.148014 -0.000056
 O13 1.420550 2.815759 0.000035
 H14 -2.994096 1.678533 -0.000060
 C15 -1.367850 -2.549633 0.000045
 H16 -0.433548 -3.115910 -0.000787

H17 -1.950803 -2.806978 0.892521
 H18 -1.952244 -2.806618 -0.891580
 O19 -3.180989 -0.220633 0.000037
 O20 -3.804535 1.095436 -0.000104

Fig. 3b (optimized at CASSCF(10,8)/6-31+G*)

[9MG – H_{N10}]⁻ (CASSCF)

C1 1.245765 1.282418 -0.000430
 C2 -0.153949 0.987242 -0.000565
 H3 2.978969 0.226177 0.000624
 C4 1.542260 -1.211402 0.000076
 C5 -2.263967 1.011124 0.000241
 N6 1.988882 0.114272 -0.000059
 N7 -1.267668 1.810052 0.000186
 N8 -1.900141 -0.320763 -0.000945
 N9 0.206515 -1.446349 -0.000595
 C10 -0.532555 -0.345837 -0.000657
 N11 2.463579 -2.109818 0.000425
 H12 2.020569 -3.009767 0.000220
 O13 1.804198 2.361539 0.000634
 H14 -3.296871 1.301983 0.000472
 C15 -2.772256 -1.464359 0.000786
 H16 -3.404713 -1.474988 -0.882235
 H17 -2.156234 -2.350979 0.002619
 H18 -3.405264 -1.471610 0.883436

TS5⁻

C1 1.405272 -1.352518 -0.172031
 C2 0.041857 -0.861997 -0.399840
 H3 3.208985 -0.544801 0.257407
 C4 1.982518 1.069760 0.090661
 C5 -2.010579 -0.570676 -0.647220
 N6 2.259575 -0.307112 0.066523
 N7 -1.039146 -1.501590 -0.738516
 N8 -1.465155 0.719592 -0.707021
 N9 0.708313 1.503870 -0.167344
 C10 -0.161840 0.564871 -0.365806
 N11 2.972631 1.826680 0.343716
 H12 2.655741 2.777862 0.336679
 O13 1.785231 -2.492264 -0.198666
 H14 -2.986798 -0.741506 -1.052478
 O15 -1.195799 -0.298120 1.713723
 O16 -2.328852 -0.745957 1.109336
 C17 -2.221450 1.902141 -0.375329
 H18 -2.438002 1.928235 0.686286
 H19 -1.643597 2.772192 -0.651190
 H20 -3.149170 1.899169 -0.935959

syn-8-OO[9MG – H_{N10}]⁻ (CASSCF)

C1 -1.552260 1.400489 -0.081512
 C2 -0.175313 0.876245 -0.288914
 H3 -3.379334 0.632029 0.305505
 C4 -2.175484 -1.005467 0.160373
 C5 1.988687 0.521422 -0.590315
 N6 -2.429526 0.379797 0.132112

N7 0.907025 1.517020 -0.451358
 N8 1.278475 -0.776704 -0.600056
 N9 -0.906716 -1.476336 -0.089288
 C10 0.009908 -0.595732 -0.296823
 N11 -3.176913 -1.737418 0.404808
 H12 -2.886414 -2.696872 0.398167
 O13 -1.881745 2.549739 -0.105076
 H14 2.444849 0.683587 -1.562678
 C15 2.006860 -2.005733 -0.388512
 H16 2.486557 -1.969705 0.580541
 H17 1.314728 -2.834020 -0.442277
 H18 2.757626 -2.117803 -1.162737
 O19 2.931682 0.595143 0.342578
 O20 2.317713 0.331483 1.640518

O19 2.173533 0.593143 1.120410
 O20 0.983863 -0.281587 1.429420

TS6⁻

C1 -1.526157 1.306303 -0.154071
 C2 -0.084951 0.950345 -0.300742
 H3 -3.252472 0.325099 0.180570
 C4 -1.862862 -1.166146 0.043545
 C5 2.021528 0.768476 -0.305122
 N6 -2.273496 0.192677 0.041718
 N7 0.908800 1.692693 -0.493193
 N8 1.540077 -0.501570 -0.790750
 N9 -0.562067 -1.485067 -0.177111
 C10 0.283518 -0.482867 -0.199044
 N11 -2.813799 -1.991691 0.224786
 H12 -2.432087 -2.918928 0.216806
 O13 -1.982994 2.413911 -0.203166
 H14 2.942518 1.103409 -0.753624
 C15 2.375457 -1.665669 -0.585979
 H16 2.583133 -1.836080 0.464008
 H17 1.865562 -2.527203 -0.994572
 H18 3.306813 -1.523720 -1.124880
 O19 2.231473 0.644290 1.075595
 O20 1.020363 -0.087515 1.550324

4,8-OO-[9MG – H_{N10}]⁻

C1 -1.547499 1.299952 -0.141771
 C2 -0.091917 0.977698 -0.226344
 H3 -3.258932 0.271954 0.083970
 C4 -1.823524 -1.188325 0.030683
 C5 2.011195 0.818066 -0.270373
 N6 -2.268192 0.172867 0.022408
 N7 0.884716 1.741014 -0.423470
 N8 1.541486 -0.420952 -0.814183
 N9 -0.523527 -1.481626 -0.054098
 C10 0.347215 -0.442131 -0.007828
 N11 -2.802097 -2.013676 0.102042
 H12 -2.424863 -2.942858 0.119678
 O13 -2.018879 2.403119 -0.212303
 H14 2.944973 1.193780 -0.654339
 C15 2.419286 -1.568986 -0.710949
 H16 2.769192 -1.750730 0.299971
 H17 1.873369 -2.436632 -1.054370
 H18 3.272890 -1.413954 -1.364519

**Cartesian coordinates for the structures in Fig. 4,
optimized at B3LYP/6-31+G***

[9MG – H_{N1}]⁺(H₂O)

C1 -0.682208 -1.356824 -0.013095
C2 -0.545855 0.091867 -0.015311
C3 1.683046 -1.373981 -0.012732
C4 -0.779713 2.225171 -0.004090
N5 0.527665 -2.036342 -0.010869
N6 -1.483996 1.119013 -0.012544
N7 0.587092 1.998362 -0.000891
N8 1.913577 -0.041693 -0.002955
C9 0.744519 0.623541 -0.006615
N10 2.839207 -2.171617 -0.064235
H11 3.647900 -1.722579 0.349866
H12 2.669415 -3.107572 0.284885
O13 -1.772632 -1.971620 -0.006921
H14 -1.181623 3.231695 -0.002042
C15 1.652123 2.975191 0.011558
H16 2.248211 2.892417 0.928317
H17 2.320390 2.825459 -0.843884
H18 1.215552 3.977377 -0.043149
O19 -4.112309 -0.355718 0.028953
H20 -3.515011 0.416095 0.014364
H21 -3.441588 -1.078034 0.017550

PC⁺(H₂O)

C1 1.719522 -0.967571 0.173018
C2 0.365849 -0.544715 -0.207916
C3 2.223264 1.333623 0.188433
C4 -1.699171 -0.328544 -0.725495
N5 2.609214 0.073383 0.363315
N6 -0.765347 -1.246671 -0.459940
N7 1.007820 1.833237 -0.174881
C8 0.132494 0.848970 -0.363906
N9 3.205093 2.300114 0.366546
H10 2.855495 3.223224 0.589190
H11 3.993607 1.985328 0.917136
O12 2.059724 -2.156299 0.316606
H13 -2.671421 -0.552704 -1.137161
O14 -2.878456 -0.169606 1.206975
O15 -3.941768 0.525235 1.105043
O16 0.107417 -4.168323 -0.335549
H17 -0.534845 -3.441289 -0.430693
H18 0.906118 -3.658332 -0.079547
N19 -1.181278 0.960731 -0.736763
C20 -1.929563 2.195402 -0.886802
H21 -2.696991 2.266259 -0.108948
H22 -1.224102 3.023823 -0.793093
H23 -2.406075 2.237096 -1.873404

TS7(H₂O)

C1 -1.691993 0.997591 0.143611
C2 -0.322431 0.542893 -0.177975
C3 -2.241405 -1.290342 0.151303
C4 1.777298 0.271338 -0.562890

N5 -2.608692 -0.019258 0.301787
N6 0.809511 1.215488 -0.376827
N7 -1.024286 -1.823957 -0.161274
C8 -0.113827 -0.871897 -0.324340
N9 -3.246211 -2.228355 0.298917
H10 -2.937608 -3.167687 0.511257
H11 -4.063257 -1.897315 0.794578
O12 -2.003501 2.194015 0.259145
H13 2.664961 0.486868 -1.141320
O14 2.742979 0.218424 1.063261
O15 3.773591 -0.598335 0.996282
O16 0.014108 4.174822 -0.332722
H17 0.653664 3.441042 -0.376005
H18 -0.802077 3.680810 -0.106567
N19 1.198416 -1.013348 -0.639506
C20 1.931645 -2.260253 -0.758543
H21 2.755456 -2.252534 -0.034506
H22 1.239547 -3.079399 -0.551473
H23 2.335010 -2.373153 -1.772369

***syn*-8-OO[9MG – H_{N1}]⁺(H₂O)**

C1 -0.335170 -1.745821 0.053159
C2 -0.494984 -0.276508 -0.183203
C3 1.967045 -1.319747 -0.038982
C4 -1.043906 1.795775 -0.291604
N5 0.965505 -2.177653 0.148102
N6 -1.558089 0.446952 -0.364762
N7 0.334148 1.735595 -0.795742
N8 1.959665 0.014688 -0.353450
C9 0.737543 0.504612 -0.372946
N10 3.229145 -1.852836 0.052314
H11 3.982494 -1.195950 0.201383
H12 3.292278 -2.753985 0.505659
O13 -1.299769 -2.513173 0.142696
H14 -1.664031 2.552563 -0.771382
C15 1.201927 2.893117 -0.659445
H16 2.188371 2.633636 -1.052497
H17 0.790408 3.724822 -1.241427
H18 1.291578 3.180047 0.395569
O19 -3.949522 -1.399949 -0.398215
H20 -3.467996 -0.550550 -0.393803
H21 -3.214220 -2.008798 -0.184928
O22 -0.002329 1.297827 1.720760
O23 -0.986658 2.133099 1.121549

***anti*-8-OO[9MG – H_{N1}]⁺(H₂O)**

C1 1.687711 1.082069 -0.018708
C2 0.294019 0.527290 0.096691
C3 2.373541 -1.159363 -0.072123
C4 -1.883631 0.123512 0.291337
N5 2.677697 0.142408 -0.105403
N6 -0.838693 1.135657 0.114015
N7 -1.135305 -1.192934 0.259234
N8 1.169002 -1.794677 0.052507
C9 0.159243 -0.941889 0.149760
N10 3.439939 -2.011608 -0.144015

H11 3.250480 -2.984888 -0.334668
 H12 4.324453 -1.617373 -0.430360
 O13 1.907754 2.297748 -0.030531
 H14 -2.335985 0.223303 1.294197
 O15 -2.840374 0.221687 -0.676018
 O16 -3.956255 -0.632106 -0.222744
 O17 -0.279935 4.212555 0.103375
 H18 0.565982 3.722156 0.063686
 H19 -0.919676 3.480683 0.064428
 C20 -1.779040 -2.493703 0.225417
 H21 -1.114501 -3.202535 -0.277904
 H22 -1.980180 -2.847525 1.244808
 H23 -2.739637 -2.352304 -0.285454

TS8⁺(H₂O)

C1 0.856840 1.570357 0.003006
 C2 0.595166 0.098214 -0.152511
 C3 -1.482948 1.779702 -0.050119
 C4 0.481822 -2.040824 -0.200185
 N5 -0.259735 2.343448 0.068087
 N6 1.400315 -0.905036 -0.276206
 N7 -0.751765 -1.593942 -0.829274
 N8 -1.864494 0.501058 -0.218912
 C9 -0.822433 -0.352852 -0.158449
 N10 -2.517454 2.692660 -0.043350
 H11 -3.427229 2.318901 0.190772
 H12 -2.280670 3.600832 0.332236
 O13 2.010600 2.024143 0.047474
 H14 0.884961 -2.990796 -0.547915
 C15 -1.912844 -2.473570 -0.762281
 H16 -2.146865 -2.774587 0.266836
 H17 -2.767590 -1.934805 -1.180148
 H18 -1.720555 -3.362241 -1.374224
 O19 4.231120 0.191630 -0.292960
 H20 3.542500 -0.499173 -0.293598
 H21 3.670159 0.984150 -0.160967
 O22 0.153799 -2.194253 1.217554
 O23 -0.657567 -1.033490 1.501408

4,8-OO-[9MG – H_{N1}]⁺(H₂O)

C1 -0.985917 -1.501771 -0.000545
 C2 -0.611998 -0.048904 -0.115777
 C3 1.337776 -1.876230 -0.042791
 C4 -0.321003 2.073070 -0.201579
 N5 0.064777 -2.354345 0.031937
 N6 -1.335236 1.008471 -0.262250
 N7 0.854081 1.517645 -0.845632
 N8 1.822754 -0.636800 -0.098462
 C9 0.841985 0.321443 -0.020658
 N10 2.286566 -2.882728 -0.106272
 H11 3.219714 -2.609384 0.172317
 H12 1.961113 -3.782196 0.221627
 O13 -2.175578 -1.860319 0.038006
 H14 -0.655686 3.053895 -0.537215
 C15 2.074246 2.319895 -0.818465
 H16 2.329054 2.684582 0.185573

H17 2.891835 1.693712 -1.186211
 H18 1.951006 3.171736 -1.497732
 O19 -4.250700 0.120117 -0.265598
 H20 -3.521920 0.767154 -0.285764
 H21 -3.735325 -0.705629 -0.144636
 O22 0.052547 2.196196 1.209118
 O23 0.836116 0.973432 1.422935

8-OO[9MG – H_{N1}]⁺

C1 1.714081 1.434339 0.024318
 C2 0.300056 0.922139 0.122274
 C3 2.324102 -0.831930 -0.079298
 C4 -1.888198 0.588050 0.305717
 N5 2.674352 0.453744 -0.085645
 N6 -0.809072 1.568407 0.153671
 N7 -1.185539 -0.755682 0.246433
 N8 1.096179 -1.430153 0.032069
 C9 0.116148 -0.545704 0.143093
 N10 3.359433 -1.727760 -0.165921
 H11 3.122966 -2.678589 -0.411721
 H12 4.247815 -1.357802 -0.473266
 O13 1.974333 2.635465 0.044177
 H14 -2.331011 0.682745 1.313226
 O15 -2.845878 0.735646 -0.651354
 O16 -4.002679 -0.072488 -0.193347
 C17 -1.873968 -2.032230 0.181497
 H18 -1.258117 -2.738285 -0.384763
 H19 -2.039460 -2.431023 1.191205
 H20 -2.849194 -1.833923 -0.280342

TS9⁺

C1 1.603742 1.498463 0.009057
 C2 0.251973 0.883506 -0.066187
 C3 2.394954 -0.722645 0.057894
 C4 -1.864485 0.389652 -0.004805
 N5 2.643590 0.582463 0.056779
 N6 -0.943123 1.432809 -0.117968
 N7 -1.126965 -0.864695 -0.135539
 N8 1.208715 -1.402149 0.002862
 C9 0.179777 -0.564594 -0.071934
 N10 3.501877 -1.546581 0.160417
 H11 3.366697 -2.498163 -0.153781
 H12 4.379552 -1.107815 -0.083957
 O13 1.792493 2.716941 0.018002
 H14 -2.530658 0.402373 1.084780
 O15 -3.087393 0.438315 -0.616326
 O16 -3.902965 0.280283 0.663082
 C17 -1.728454 -2.178994 -0.078930
 H18 -1.195714 -2.848730 -0.760954
 H19 -1.676275 -2.596444 0.935087
 H20 -2.774391 -2.080790 -0.375665

8-oxo[9MG – H_{N1}]

C1 1.372782 1.442172 -0.000002
 C2 -0.048403 0.933381 -0.000001
 C3 2.000277 -0.816268 0.000001

C4 -2.193216 0.541164 0.000002
N5 2.336924 0.455579 0.000001
N6 -1.166254 1.565847 0.000005
N7 -1.572958 -0.739433 -0.000007
N8 0.718106 -1.417208 -0.000003
C9 -0.231042 -0.544801 -0.000004
N10 2.981292 -1.737515 0.000002
H11 2.754121 -2.721340 0.000020
H12 3.944827 -1.431660 0.000023
O13 1.617342 2.637344 -0.000004
O14 -3.381058 0.732980 0.000006
C15 -2.280641 -2.011083 -0.000002
H16 -3.349596 -1.792827 -0.000064
H17 -2.018922 -2.587552 -0.891985
H18 -2.019017 -2.587497 0.892044

8-oxo[9MG – H_{N1}]^{·-}

C1 1.308072 1.453754 -0.002143
C2 -0.060782 0.919110 -0.006438
C3 2.003272 -0.798857 -0.012141
C4 -2.205571 0.530446 0.003614
N5 2.313364 0.484007 -0.002630
N6 -1.254056 1.535673 0.000115
N7 -1.547134 -0.745580 0.001344
N8 0.771046 -1.405844 -0.009074
C9 -0.202520 -0.508873 -0.005860
N10 3.065261 -1.699106 -0.064626
H11 2.851052 -2.619655 0.297814
H12 3.944817 -1.304973 0.244749
O13 1.576539 2.663619 0.007601
O14 -3.436318 0.634320 0.008552
C15 -2.208840 -2.026892 -0.000910
H16 -3.284805 -1.835835 -0.011934
H17 -1.927367 -2.611980 -0.885385
H18 -1.946617 -2.607245 0.892909