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SUPPORTING INFORMATION FOR:

Excited-state deactivation in 8-oxo-deoxyguanosine: comparison between anionic and neutral forms

Deniz Tuna[1*] and Wolfgang Domcke[2]

[1] *Max-Planck-Institut für Kohlenforschung, 45470 Mülheim an der Ruhr, Germany*

[2] *Department of Chemistry, Technische Universität München, 85747 Garching, Germany.*

[*] *email: tuna@kofo.mpg.de*

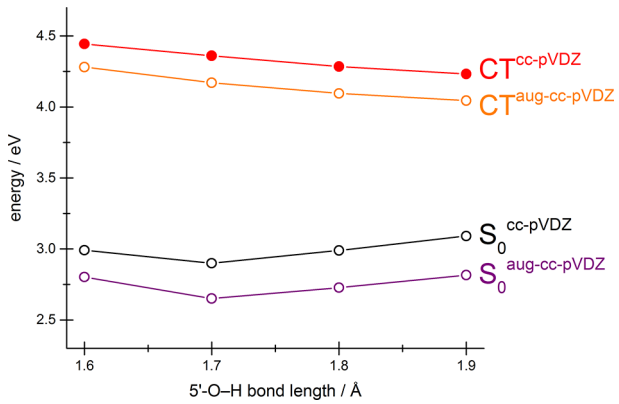

Figure S1 Energy profiles of the intramolecularly 5′-O–H···N3 hydrogen-bonded *syn* conformer of anionic 8-oxo-deoxyguanosine obtained by a relaxed scan with the cc-pVDZ basis set along the 5′-O–H internuclear distance in the charge-transfer state (full red circles). The energy profile of the charge-transfer state obtained at the same geometries with the aug-cc-pVDZ basis set is given by empty orange circles. The energy profile of the ground state obtained at the same geometries is given by empty black circles for the basis set cc-pVDZ and in empty purple circles for the basis set aug-cc-pVDZ.

Table S1 Cartesian coordinates of the MP2/aug-cc-pVDZ optimized ground-state equilibrium geometry of neutral 8-oxo-deoxyguanosine (energy: $-1036.22803\ E_h$).

```
33

O     1.8775793  -4.5789001  -2.9191495
C     0.6562333  -4.9516293  -2.2548402
C    -0.4414658  -4.8160876  -3.3165329
C     0.2853171  -5.2877992  -4.5733218
C     1.7358939  -4.8018592  -4.3462653
N     0.4996582  -4.0884730  -1.1045127
C     0.4787517  -2.7061855  -1.1014950
C     0.4140858  -2.2880345   0.2201970
N     0.4021321  -3.4256313   1.0151266
C     0.4774554  -4.5751393   0.2288270
C     0.3774402  -0.8972040   0.5494681
N     0.4192321  -0.1230901  -0.6528363
C     0.5079351  -0.6133302  -1.9302013
N     0.5439722  -1.9050785  -2.2049744
O     0.3141511  -0.3493823   1.6558561
N     0.4916104   0.3014616  -2.9700987
O     0.5050092  -5.7487831   0.5878588
O     0.1957368  -6.7238079  -4.5694561
C     2.0887492  -3.5085680  -5.0737763
O     1.1198893  -2.4824011  -4.8599148
H     1.0025609  -2.3915847  -3.8860193
H     0.7076277  -7.0624087  -5.3178892
H    -0.1417658  -4.8659100  -5.4977370
H    -0.7406400  -3.7641977  -3.4196766
H     0.7229324  -5.9746412  -1.8516815
H     2.4484609  -5.5941874  -4.6442236
H     3.0952697  -3.1875480  -4.7472530
H     2.1225607  -3.7002488  -6.1592312
H    -1.3157509  -5.4432267  -3.0937287
H     0.7211596  -0.1268000  -3.8663592
H     0.9901570   1.1710685  -2.8062252
H     0.3710863  -3.4512551   2.0277230
H     0.3380412   0.8814077  -0.5035119
```

Table S2 Cartesian coordinates of the MP2/aug-cc-pVDZ optimized ground-state equilibrium geometry of anionic 8-oxo-deoxyguanosine (energy: $-1035.70739\ E_h$).

```
32

N     1.9443289  -4.6943281  -2.9114169
C     0.7833279  -4.9706357  -2.2675138
C    -0.4681944  -4.9967097  -2.8542853
C    -0.6391336  -4.7088517  -4.2553526
N     0.5634585  -4.4329670  -4.9110015
C     1.7172363  -4.4487374  -4.2316566
N    -1.3890960  -5.2937633  -1.8429262
C    -0.7577225  -5.4456771  -0.6223164
N     0.6133180  -5.2666411  -0.9061184
C     1.6225881  -5.2544872   0.1125937
O     2.1858417  -3.9214862   0.1958108
C     3.6126542  -3.9941579   0.3918095
C     3.9574554  -5.4863752   0.5657199
C     2.8143016  -6.1850367  -0.1598724
O     3.8872042  -5.8992932   1.9506470
C     4.3402995  -3.3312534  -0.7810016
O     4.3990540  -4.1379649  -1.9460728
O    -1.2598278  -5.7010280   0.4856369
O    -1.7592181  -4.6999577  -4.8286479
N     2.8867111  -4.2252353  -4.9906839
H     3.4580092  -4.3208229  -2.2543008
H     4.4702571  -5.3163054   2.4568324
H     4.9459502  -5.7242099   0.1399081
H     3.0161177  -6.2254929  -1.2388146
H     1.1053155  -5.4991197   1.0536611
H     3.8541896  -3.4346967   1.3190601
H     3.8458182  -2.3591202  -0.9746289
H     5.3836707  -3.1298119  -0.4741735
H     2.6396519  -7.1962264   0.2348911
H     3.6440712  -3.8288700  -4.4371665
H     2.6776413  -3.6847326  -5.8254765
H    -2.3906900  -5.3686503  -1.9660817
```

Table S3 Cartesian coordinates of the [ADC(2)-s/MP2]/cc-pVDZ optimized proton-transfer conical intersection of neutral 8-oxo-deoxyguanosine (energy: −1035.87383 E_h).

```
33

C   -1.2744809470  -0.2628770193  -2.0312003596
C   -0.0853186637  -1.0474003605  -1.4655495137
O    1.0748841300  -0.2831379435  -1.8355795435
C    0.7706987753   0.5260518053  -2.9621524235
C   -0.6940132276   0.2265393623  -3.3513266752
N   -0.0739141085  -1.2032075455  -0.0419018823
C   -0.0611647179  -0.1990591720   0.9096966658
C    0.0759125181  -0.7908872199   2.1519290453
N    0.1614748591  -2.1634344457   1.9441010309
C    0.1160974040  -2.4666587533   0.5935996211
C    0.0778616481  -0.0254657465   3.3793402156
N   -0.0910434225   1.3400782101   3.0907503038
C    0.0050120128   1.9786700441   1.8347241377
N   -0.2009363723   1.1394130107   0.7192975678
O    0.1804252055  -0.4650995554   4.5258390150
N   -0.5162926340   3.2967641380   1.8125586476
O    0.1995776960  -3.5490729258   0.0316346261
C    1.0294500267   1.9988295897  -2.6095996312
O    0.1069745251   2.4748877849  -1.6833458918
O   -0.7730291893  -0.8735211590  -4.2470712739
H   -0.0138161486   1.5672966789  -0.2257617205
H   -0.3039989940  -0.6183651321  -5.0543183807
H   -1.2090117613   1.1244974225  -3.7463353060
H   -1.5290548357   0.5901625844  -1.3840016002
H   -0.0295035089  -2.0652464986  -1.8863577507
H    1.4466643485   0.2585458179  -3.8000584916
H    2.0442813975   2.0403531931  -2.1600537941
H    1.0261567358   2.6116576267  -3.5351365618
H   -2.1587589831  -0.8974499283  -2.1871996195
H   -1.5320394129   3.2839622607   1.6465416857
H   -0.1051438475   3.8146584515   1.0333029473
H    0.3200666251  -2.8576403279   2.6656051229
H   -0.0237471525   1.9670558707   3.8928598095
```

Table S4 Cartesian coordinates of the [ADC(2)-s/MP2]/cc-pVDZ optimized C2-puckered conical intersection of neutral 8-oxo-deoxyguanosine (energy: −1035.88160 E_h).

```
33

C   -0.1930360714  -0.3169306759   0.1828714313
C   -0.0860379949   0.1412344620   1.5488067681
C    2.2952633752  -0.0104528236   1.0581393530
C    0.9384426782  -0.9343790448  -0.4918135225
C   -0.9870039807  -1.3830852576  -1.6774799532
O   -1.7502916359  -1.8135355351  -2.5172267969
O   -1.0075934279   0.5630188284   2.2460398063
N    1.2568072873  -0.0195136843   2.0260818481
N    2.1422109337  -0.9834751121  -0.0110962945
N    0.4175337672  -1.5379223240  -1.6224820423
N   -1.3120203421  -0.6069279835  -0.5501162458
N    2.7987474528   1.2307435660   0.6062312136
H   -2.2701417489  -0.3778356206  -0.2955940396
H    3.6410460438   1.0764643717   0.0442726669
H    3.0303472175   1.8503807808   1.3892961918
H    1.4224939300   0.5144389129   2.8815900848
H    1.8186859674  -0.9677288814  -4.2337274054
H    2.7465608642  -0.8265082963  -2.6782859620
C    2.2260826125  -1.5084066619  -3.3646487697
H    4.1867095126  -2.2884881886  -4.0013000843
C    3.1586390294  -2.6366347511  -3.7895109356
O    2.5467251184  -3.2309044856  -4.9330007968
O    4.4190266872  -1.9755706332  -1.2518978564
C    1.1547401182  -2.3044187348  -2.6133037100
H    3.0526955107  -4.0303898317  -5.1356779870
H    3.6113436588  -1.7079108647  -0.7535966766
H    0.3917732027  -2.7045320509  -3.3032757242
C    3.1165632387  -3.5756972937  -2.5701323972
C    4.2408314408  -3.3381010782  -1.5668473260
H    5.1835703112  -3.7000040209  -2.0175484635
O    1.8397082928  -3.3474502017  -1.9363205711
H    3.1463280802  -4.6318843646  -2.9038106563
H    4.0369987570  -3.9556822940  -0.6679449661
```

Table S5 Cartesian coordinates of the [ADC(2)-s/MP2]/cc-pVDZ optimized C6-puckered conical intersection of neutral 8-oxo-deoxyguanosine (energy: −1035.87623 E_h).

```
33

C   -0.0796583007  -0.1122483551   0.0454045820
C   -0.0193486395   0.1110161187   1.4951290341
C    2.2445118920   0.0670590204   0.8466627544
C    0.9649381934  -0.9492715567  -0.5862735891
C   -1.0098337078  -1.2239821836  -1.7359763547
O   -1.8215289786  -1.6014636402  -2.5514149297
O   -1.0060097081   0.2015385502   2.2225713711
N    1.3133390733   0.1224019862   1.9245603110
N    2.1711538627  -1.0213773971  -0.1333942557
N    0.3461791046  -1.6124700752  -1.6250653075
N   -1.2153976514  -0.2901747120  -0.6994465936
N    3.5507292187   0.4211719817   1.1879637691
H   -2.1458155073   0.0399840073  -0.4536107308
H    4.1774326329   0.3505277909   0.3842755888
H    3.5982737771   1.3485538433   1.6149391489
H    1.4936982192  -0.3596480701   2.8134203160
H    1.8430602542  -1.7899481122  -4.2574867859
H    2.7564499943  -1.5020389042  -2.7180112418
C    2.1382261136  -2.2106919581  -3.2845054301
H    3.9537813329  -3.3945099045  -3.6472795709
C    2.8762394994  -3.5340177497  -3.4476954974
O    2.2170927048  -4.2251074287  -4.5073873030
O    4.2370430303  -2.6661363893  -1.0474212542
C    0.9355542851  -2.6557674211  -2.4501713801
H    2.6227723262  -5.1021485121  -4.5602010558
H    3.5108333421  -2.1341925261  -0.6458800674
H    0.1131157694  -3.0267399842  -3.0854592218
C    2.6423003834  -4.2163471577  -2.0862210450
C    3.7733939186  -3.9966461726  -1.0840967142
H    4.6234067151  -4.6378975344  -1.3839885379
O    1.4089790333  -3.6662304827  -1.5729837618
H    2.4907361490  -5.3052107895  -2.2268209806
H    3.4262019065  -4.3500762800  -0.0926250662
```

Table S6 Cartesian coordinates of the [ADC(2)-s/MP2]/cc-pVDZ optimized folded conical intersection of anionic 8-oxo-deoxyguanosine (energy: −1035.30111 E_h).

```
32

C   -0.0930316378  -0.4307420529   0.0734013038
C   -0.0023808573   0.0311640376   1.4280855144
C    2.2717790120   0.0964829383   1.2068659671
C    1.3520696508  -0.5939351109  -0.7602908740
C   -0.2695121783   0.4149689552  -2.1142283268
N    1.2808945561  -0.0950178179   2.0541500722
N    2.2326508938   0.2633870749  -0.1971236291
N    0.8813854912  -0.3853384362  -2.1258429867
N   -0.8465327207   0.3271244687  -0.8485086914
N    3.5696181716   0.1631351612   1.7061542865
O   -0.6804034146   1.1077092659  -3.0434332469
O   -0.9705875831   0.5230521260   2.0491763197
H   -1.4239792376   1.1084175363  -0.5353867333
H    4.2060244904   0.6547226977   1.0805109039
H    3.5915650665   0.4938098709   2.6679988792
H    1.7208714925   1.8502812801  -4.0703582981
H    2.4662996334   1.7364417595  -2.4314644771
C    2.3612206294   1.2482040584  -3.4098538433
H    4.4506373842   1.7925217915  -3.8506227213
C    3.7265761067   0.9738286250  -4.0234243164
O    3.5137585857   0.7508881342  -5.4246000065
O    4.5547882714   1.0037566089  -1.2597051799
C    1.8078174157  -0.1765808347  -3.2285310036
H    4.3149953936   0.3137835132  -5.7455686556
H    3.6426888776   0.7323146608  -0.9092573173
H    1.3004523107  -0.4952673805  -4.1584035006
C    4.1508589900  -0.3168738300  -3.3050345311
C    4.9999881530  -0.0689004976  -2.0536911734
H    6.0265145731   0.1752853179  -2.3949763168
O    2.9402920399  -1.0143036490  -2.9885638406
H    4.7400767943  -0.9640781032  -3.9917630989
H    5.0520337386  -1.0250921130  -1.4909305351
```

Table S7 Cartesian coordinates of the [ADC(2)-s/MP2]/cc-pVDZ optimized twisted conical intersection of anionic 8-oxo-deoxyguanosine (energy: −1035.31362 E_h).

```
32

C    0.0032191839   0.1793678597   0.0943002585
C   -0.0772861075  -0.0792808250   1.5746242775
C    2.2294427005  -0.0925251727   1.3381265612
C    1.1841870613   0.7872792320  -0.4551332932
C   -0.5881630685   1.1738261457  -1.8902807594
N    1.1211563668  -0.0410931236   2.1904585546
N    2.3190039875   0.8657348877   0.1781958485
N    0.7864586209   1.3687391558  -1.6747820581
N   -1.0234421807   0.4568032362  -0.7757959202
N    2.6217163684  -1.4067963472   0.8558234542
O   -1.2547832692   1.5479280416  -2.8486822417
O   -1.2292733042  -0.1566749365   2.0678926331
H   -2.0017696802   0.2636774441  -0.5798157401
H    3.6255923436  -1.3807872961   0.6386063443
H    2.5060551253  -2.0376671173   1.6571768902
H    1.4900488784   4.2670309171  -2.1549982531
H    2.3783736262   3.2836414050  -0.9222859047
C    2.1724396145   3.4185515835  -1.9930768973
H    4.2191770683   4.1897383138  -2.2033458904
C    3.4762893583   3.5864704511  -2.7569524608
O    3.1486096894   4.1804681250  -4.0196591048
O    4.5559590545   2.1928231648  -0.5298418157
C    1.6126623534   2.1194110475  -2.5882764850
H    3.9107189668   4.0155382590  -4.5925056816
H    3.7431942028   1.6887315625  -0.2214645758
H    0.9795328043   2.3157011430  -3.4707708571
C    3.9387544588   2.1289527853  -2.9149619100
C    4.8780102442   1.6741165791  -1.7922025788
H    5.8965069154   2.0289622997  -2.0504259740
O    2.7447711552   1.3318008630  -2.9621328027
H    4.4622794080   1.9955797871  -3.8865127674
H    4.8937079442   0.5641804988  -1.8115107766
```