Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electric-field induced mutation on DNA: a theoretical investigation of the GC base pair (Supporting Information)

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Table S-1: Computed H-bond distances (Å) and dipole moments (D) of the GC base pair under the influence of several external electric fields (au/10^{-4}).

E_{ext}	O_6–N_4	N_1–N_3	N_2–O_2	dipole moment
0	2.80	2.94	2.92	7.04
10	2.83	2.94	2.90	8.01
20	2.85	2.93	2.88	8.98
40	2.89	2.93	2.84	10.94
60	2.93	2.92	2.79	12.93
80	2.97	2.92	2.75	14.97
100	3.01	2.92	2.71	17.11

Table S-2: Mulliken atomic charges ($|e|$) computed for the canonical GC base pair at E_{ext}=0 and E_{ext}=100 au.

atom	E_{ext}=0	E_{ext}=100 au
Guanine		
O6	-0.442	-0.394
N1	-0.248	-0.208
H1	0.602	0.621
N2	-0.472	-0.439
H2	0.382	0.400
Cytosine		
H4	0.417	0.384
N4	-0.434	-0.452
N3	-0.351	-0.417
O2	-0.473	-0.491

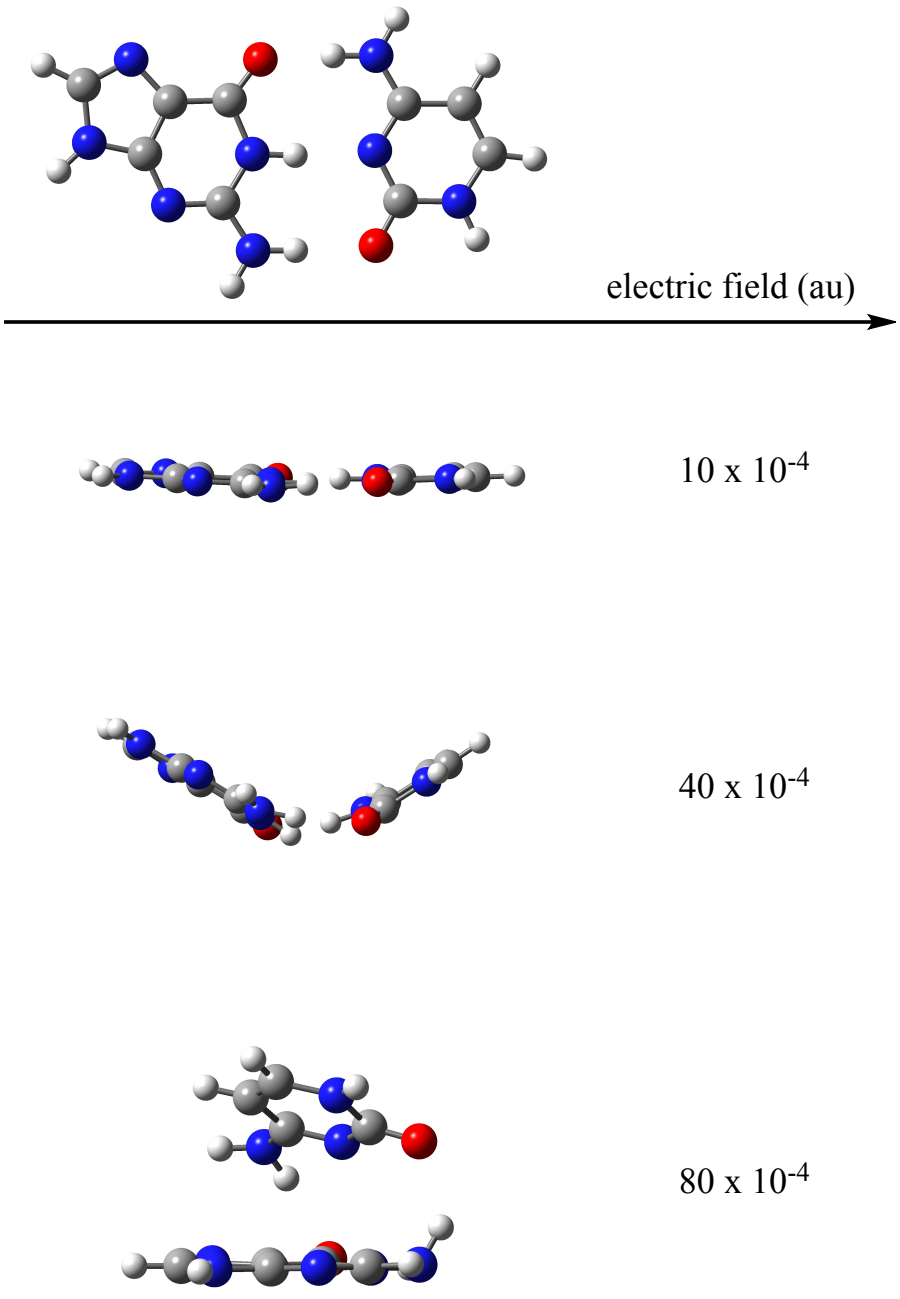

Figure S-1: Evolution of the GC canonical structure under positive electric fields [$E_{ext}(N_1 \Rightarrow H_1)$]. As noted in the text, positive fields result in the folding of cytosine on the guanine base.

Table S-3: Relative total electronic energies (before applying thermal corrections) of transition states and rare tautomeric forms (in kcal/mol). The canonical GC base pair is taken as reference for computing energies.[a]

	M06-2X				MP2			
E_{ext}	GC1ts	GC1	GC21ts	GC21	GC1ts	GC1	GC21ts	GC21
0			17.10	9.59			16.63	8.29
10			13.08	9.62			12.21	8.45
20			10.15	9.66			8.79	8.81
40			6.09	9.66			4.39	9.37
60	3.84	1.75	1.85	9.56	2.07	0.45	3.30	9.53
80	1.95	-2.72	4.47	9.13	0.27	-4.03	6.46	9.40
100	0.55	-7.23			-0.97	-8.50		

[a] Thermal corrections at M06-2X/ 6-311++G(d,p) level.

Cartesian coordinates for the optimized geometries of rare tautomers

GC21 at $E_{ext} = 0$ au

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.83975800
N	1.37198000	0.00000000	-1.97787400
C	-1.05892600	-0.21814600	-2.10141700
C	-1.12917000	-0.13579300	-0.69973800
O	-2.28858900	-0.19262000	-0.09618500
N	-2.00942200	-0.35986300	-3.09649400
H	2.26987800	0.08799900	1.10447100
N	2.29582100	0.25126900	0.10519800
C	-1.32143800	-0.36898100	-4.19561400
H	0.76938800	-0.21740500	-4.68607100
N	0.04111800	-0.24001900	-3.99056300
H	3.17806900	0.15385100	-0.36816000
C	0.22443100	-0.14073600	-2.63837500
H	-1.73245300	-0.46599300	-5.18950000
H	-2.22762600	-0.05506700	0.89614300
O	2.18417900	-0.12485500	3.08426600
C	-1.35900500	0.15139400	3.40257600
N	-0.07898300	0.02834400	2.88140200
C	-1.43226700	0.23998000	4.85430900
C	1.08538600	-0.02119500	3.59158000
N	0.92660700	0.05577200	4.96739400
C	-0.29907600	0.18827500	5.57044800
H	-3.23221600	0.26796800	3.04075600
H	-2.39396700	0.34364600	5.33400700

H	1.78052800	0.02204800	5.50307800
H	-0.28642400	0.24600000	6.65108200
N	-2.33632900	0.17337300	2.57393500
C	1.18850400	0.06767100	-0.66049000

GC21 at $E_{ext} = 10$ au

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.84673600
N	1.37713600	0.00000000	-1.97510000
C	-1.05665300	-0.18891800	-2.10481200
C	-1.12976200	-0.11737100	-0.70104200
O	-2.28933200	-0.16630300	-0.10051100
N	-2.00564400	-0.31309500	-3.10415700
H	2.26511100	0.08396300	1.11692700
N	2.29674600	0.21840800	0.11308800
C	-1.31494400	-0.32241800	-4.20140700
H	0.78005700	-0.19219100	-4.68315900
N	0.04839900	-0.21017800	-3.99150800
H	3.18240400	0.13310300	-0.35535300
C	0.22884700	-0.12257400	-2.63728800
H	-1.72434500	-0.40823600	-5.19698400
H	-2.22987300	-0.05166900	0.89871900
O	2.17979500	-0.09272400	3.09171700
C	-1.36765300	0.12455900	3.40145600
N	-0.08391600	0.02530400	2.88591400
C	-1.44791100	0.20200100	4.85247700
C	1.07917500	-0.00961500	3.59995800

N	0.91431300	0.05693000	4.97393200
C	-0.31625300	0.16457300	5.57262800
H	-3.24068700	0.21380700	3.02968200
H	-2.41243100	0.28652200	5.33020600
H	1.76571900	0.03311300	5.51466200
H	-0.30880700	0.21528600	6.65363400
N	-2.34110800	0.13693400	2.56667800
C	1.19116100	0.05900700	-0.65623700

GC21 at $E_{ext} = 20$ au

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.85247100
N	1.38118100	0.00000000	-1.97325800
C	-1.05834700	-0.09947400	-2.10958800
C	-1.13260600	-0.05947000	-0.70293600
O	-2.29260300	-0.08114400	-0.10525000
N	-2.00826100	-0.16604000	-3.11416100
H	2.26216200	0.02070700	1.12969100
N	2.30095300	0.12469600	0.12202500
C	-1.31566400	-0.17285000	-4.21007300
H	0.78501100	-0.10529500	-4.68288800
N	0.05019100	-0.11357000	-3.99482100
H	3.18885100	0.05167100	-0.34314600
C	0.22992600	-0.06558900	-2.63772100
H	-1.72509100	-0.22013200	-5.20820800
H	-2.23283400	-0.00581300	0.90218400
O	2.17352400	-0.10704800	3.09807400

C	-1.37423100	0.10522300	3.40011100
N	-0.08834700	0.01783400	2.88955400
C	-1.46059500	0.16001000	4.85082600
C	1.07247600	-0.02953200	3.60745500
N	0.90241700	0.01763800	4.97996800
C	-0.33125500	0.11354500	5.57486800
H	-3.24571900	0.19500900	3.01893100
H	-2.42665200	0.23521300	5.32697900
H	1.75062500	-0.01615500	5.52574100
H	-0.32836400	0.14750100	6.65653700
N	-2.34360300	0.12796500	2.55933800
C	1.19433700	0.03222900	-0.65207100

GC21 at $E_{ext} = 40$ au

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.85853500
N	1.39206900	0.00000000	-1.96668700
C	-1.05056600	0.02541200	-2.11435700
C	-1.13243000	0.02022000	-0.70386800
O	-2.29075200	0.03547700	-0.11056000
N	-1.99498800	0.04485000	-3.12688300
H	2.25174900	-0.05745000	1.15141100
N	2.29953800	-0.01840800	0.13820600
C	-1.29658000	0.04567400	-4.21899300
H	0.81041800	0.02713700	-4.67455600
N	0.06901600	0.02827500	-3.99426700
H	3.19380000	-0.04784800	-0.31815400

C	0.24125800	0.01566700	-2.63378700
H	-1.70122300	0.05836000	-5.22019600
H	-2.23610800	0.05633000	0.91091400
O	2.15989300	-0.09822400	3.10891300
C	-1.38968400	0.08045900	3.38876600
N	-0.09918100	0.01266100	2.89146000
C	-1.49033100	0.11010000	4.83721800
C	1.05699300	-0.03610800	3.61857900
N	0.87482000	-0.00926800	4.98704500
C	-0.36611200	0.06373600	5.57098900
H	-3.25804600	0.16070100	2.98514000
H	-2.46035400	0.16788200	5.30769400
H	1.71642400	-0.04548700	5.54397800
H	-0.37378300	0.08058100	6.65311100
N	-2.35028600	0.10971500	2.53476900
C	1.19883800	-0.00760900	-0.64328700

GC21 at $E_{ext} = 60$ au

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.85866600
C	1.20185000	0.00000000	-0.63523100
C	-1.13300700	-0.00498800	-0.70277900
N	2.29591300	0.00986700	0.15237600
N	1.40147300	-0.00682700	-1.96018700
O	-2.28779500	-0.00368400	-0.11187700
C	-1.04285500	-0.01194600	-2.11690200
H	2.24201000	-0.00102700	1.16763700

H	3.19477000	−0.00250600	−0.29546400
C	0.25182800	−0.01254100	−2.62864400
H	−2.24039600	0.00491700	0.92617800
N	−1.98085200	−0.01918400	−3.13606900
N	0.08746600	−0.02037200	−3.99174000
C	−1.27699300	−0.02407800	−4.22472100
H	0.83506000	−0.02316500	−4.66457200
H	−1.67665400	−0.03056800	−5.22817900
N	−2.35937700	0.01890800	2.50241300
C	−1.40709000	0.01496700	3.37033800
H	−3.27372500	0.02835000	2.94179900
C	−1.52394200	0.02200300	4.81553400
N	−0.11156100	0.00245400	2.88785000
C	−0.40475600	0.01463200	5.56049400
H	−2.49906400	0.03287000	5.27876600
C	1.04034400	−0.00486900	3.62540400
N	0.84446400	0.00098900	4.98955700
H	−0.42420200	0.01883400	6.64278500
O	2.14620300	−0.01570700	3.11684200
H	1.67962500	−0.00441200	5.55853500

GC21 at $E_{ext} = 80$ au

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.85264800
C	1.20319200	0.00000000	−0.62927400
C	−1.13644700	−0.00004800	−0.69921000
N	2.29243400	0.00006500	0.16259800

N	1.40745700	-0.00005000	-1.95615500
O	-2.28430200	-0.00005300	-0.10794800
C	-1.03892200	-0.00009700	-2.11786500
H	2.23329900	0.00004300	1.17915900
H	3.19453700	0.00001500	-0.27868500
C	0.25778500	-0.00009600	-2.62405800
H	-2.24506800	-0.00002800	0.95837900
N	-1.97170400	-0.00015900	-3.14222500
N	0.09939200	-0.00015800	-3.98949400
C	-1.26424100	-0.00019400	-4.22878000
H	0.85223400	-0.00018100	-4.65588300
H	-1.66038700	-0.00024600	-5.23394600
N	-2.36764200	-0.00000700	2.46389000
C	-1.42322200	-0.00000400	3.34568700
H	-3.28800900	-0.00000700	2.89001100
C	-1.55788600	-0.00000300	4.78648100
N	-0.12519400	-0.00000400	2.87880500
C	-0.44556600	-0.00000100	5.54437500
H	-2.53735000	-0.00000400	5.24072800
C	1.02065900	0.00000000	3.62854100
N	0.81010900	0.00000000	4.98830400
H	-0.47769100	0.00000000	6.62669300
O	2.12838600	0.00000400	3.12290600
H	1.63728700	0.00000300	5.57028800

GC1 at $E_{ext} = 60$ au

N	0.00000000	0.00000000	0.00000000

H	0.00000000	0.00000000	1.69046300
N	1.24134300	0.00000000	-2.06722900
C	-1.20050400	-0.21018100	-2.03346300
C	-1.22173200	-0.13181300	-0.60080700
O	-2.27521600	-0.17871400	0.07790400
N	-2.20443400	-0.35215900	-2.97647700
H	2.32209300	0.10898800	0.95241100
N	2.29318100	0.25907700	-0.04898600
C	-1.58599300	-0.36863100	-4.11695600
H	0.48430900	-0.23106200	-4.71148900
N	-0.21322200	-0.24299500	-3.98731400
H	3.14198800	0.13788000	-0.57352400
C	0.04391800	-0.13992900	-2.64190900
H	-2.05482600	-0.46993800	-5.08507700
H	-2.28874600	-0.02125500	1.51034300
O	2.20940800	-0.10014100	2.88721500
C	-1.28203600	0.06150500	3.37149000
N	-0.06261600	0.00148600	2.77143900
C	-1.32857300	0.10544700	4.80643200
C	1.13786000	-0.03875800	3.44703700
N	1.03031900	-0.00305800	4.82690000
C	-0.16216600	0.06955900	5.48193200
H	-3.24269600	0.11421700	3.07049000
H	-2.27487800	0.15919500	5.32272300
H	1.90533900	-0.03231100	5.33393800
H	-0.11151900	0.09376600	6.56336000
N	-2.34437700	0.07495700	2.61215300

C	1.13457500	0.06921400	-0.73537200

GC1 at $E_{ext} = 80$ au

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.73580900
N	1.24730900	0.00000000	-2.06652300
C	-1.19073900	-0.26420700	-2.03574100
C	-1.22058300	-0.17177600	-0.59834700
O	-2.26752100	-0.24168300	0.07866400
N	-2.18577200	-0.44379300	-2.98214200
H	2.31194800	0.20759900	0.95908500
N	2.28386800	0.31391500	-0.04848400
C	-1.56304100	-0.46388100	-4.12052300
H	0.50991400	-0.29322000	-4.70417200
N	-0.19364600	-0.30418300	-3.98636300
H	3.13902400	0.21262500	-0.56615500
C	0.05468100	-0.17516100	-2.63971100
H	-2.02582900	-0.59044000	-5.08899300
H	-2.29256000	-0.13439800	1.59788200
O	2.21894800	0.04903200	2.89049200
C	-1.26626100	-0.03696600	3.42231600
N	-0.05480500	-0.00724900	2.80736000
C	-1.29972500	-0.01712300	4.85460700
C	1.15633600	0.02889600	3.46947700
N	1.06197200	0.04068200	4.84857200
C	-0.12425900	0.02074700	5.51741600
H	-3.23598000	-0.10935300	3.13819800

H	-2.24028700	-0.03685200	5.38387700
H	1.94185300	0.06876500	5.34890000
H	-0.06305400	0.03502300	6.59887700
N	-2.34011900	-0.08310200	2.67480800
C	1.13239800	0.08686100	-0.73231300

GC1 at $E_{ext} = 100$ au

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.78569600
N	1.27296000	0.00000000	-2.05340300
C	-1.16663000	-0.26580500	-2.05177800
C	-1.21632000	-0.17500000	-0.60935800
O	-2.26564300	-0.24898200	0.05558500
N	-2.14695800	-0.44808200	-3.01311100
H	2.29767300	0.23200400	0.98982800
N	2.28161900	0.31439800	-0.02101600
C	-1.50947200	-0.46947800	-4.14375200
H	0.57481700	-0.30227200	-4.69456800
N	-0.14178700	-0.30682100	-3.99012200
H	3.14509700	0.22427900	-0.52620700
C	0.08751100	-0.17640500	-2.63845400
H	-1.95939300	-0.59821500	-5.11845800
H	-2.29502800	-0.17420400	1.65411600
O	2.21480100	0.10632000	2.92063100
C	-1.26400400	-0.07760200	3.46299300
N	-0.05527400	-0.01104300	2.84738800
C	-1.29688200	-0.07000300	4.89213900

C	1.15787700	0.05375600	3.50812200
N	1.06385600	0.05358600	4.88526100
C	-0.12056000	-0.00417700	5.55469800
H	-3.23560900	-0.19871000	3.17453600
H	-2.23508900	-0.11918400	5.42416500
H	1.94206100	0.10282000	5.38871300
H	-0.05900300	0.00427700	6.63670800
N	-2.33944400	-0.14640800	2.71404300
C	1.13924200	0.08784700	-0.71677400