Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

One-electron oxidation of ds(5'-GGG-3') and ds(5'-G(8OG)G-3') and the nature of hole distribution: A density functional theory (DFT) study†

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Figure S7- Spin density plots of one-electron oxidized ds(5'-GGG-3') calculated using the HF-PCM/6-31++G**//ωb97xd-PCM/6-31G** method. (a) in NEPCM, (b) in EQPCM and (c) finally the fully optimized cation radical (adiabatic).

Figure S8- Spin density plots of one-electron oxidized ds(5'-G8OGG-3') calculated using the HF-PCM/6-31++G**//ωb97xd-PCM/6-31G** method. (a) in NEPCM, (b) in EQPCM and (c) fully optimized cation radical (adiabatic).

Figure S9- Time evolution of the total spin density after vertical electron removal from ds(5'-GGG-3'), depicted at times: (a) 0 fs, (b) 10 fs, (c) 20 fs, (d) 30 fs, (e) 40 fs and (f) 50 fs. Molecular dynamics simulations were carried out using the atom centered density matrix propagation (ADMP) *ab initio* molecular dynamics method implemented in Gaussian 16. The ωB97XD-PCM/6-31G** method was used in the ADMP simulations. Simulations were run for 50 fs with a time step of 0.1 fs using default values set in the Gaussian 16 program.

Figure S10- ωB97XD-PCM/6-31G** calculated singlet and triplet states of double oxidized ds(5'-GGG-3') [ds(5'-GGG-3')$^{2+}$]. Single point calculations were carried out using the ωB97XD-PCM/6-31G** optimized geometry of one-electron oxidized ds(5'-GGG-3'). (a) HOMO of ds(5'-GGG-3')$^{2+}$ in the singlet state and (b) Spin density distribution of ds(5'-GGG-3')$^{2+}$ in the triplet state. The triplet state is more stable (19.95 kcal/mol) than the singlet.

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Figure S12- ωB97XD-PCM/6-31++G** calculated singlet and triplet states of double oxidized ds(5'-GGG-3') [ds(5'-GGG-3')$^{2+}$]. Single point calculations were carried out using the ωB97XD-PCM/6-31G** optimized geometry of one-electron oxidized ds(5'-GGG-3'). (a) HOMO of ds(5'-GGG-3')$^{2+}$ in the singlet state and (b) Spin density distribution of ds(5'-GGG-3')$^{2+}$ in the triplet state. The triplet state is more stable (18.81 kcal/mol) than the singlet.

Figure S13- ωB97XD-PCM/6-31++G** calculated singlet and triplet states of double oxidized ds(5'-G8OGG-3') [ds(5'-G8OGG-3')$^{2+}$]. Single point calculations were carried out using the ωB97XD-PCM/6-31G** optimized geometry of one-electron oxidized ds(5'-G8OGG-3'). (a) HOMO of ds(5'-G8OGG-3')$^{2+}$ in the singlet state and (b) Spin density distribution of ds(5'-G8OGG-3')$^{2+}$ in the triplet state. The triplet state is more stable (9.95 kcal/mol) than the singlet.

Optimized X, Y, Z coordinates.

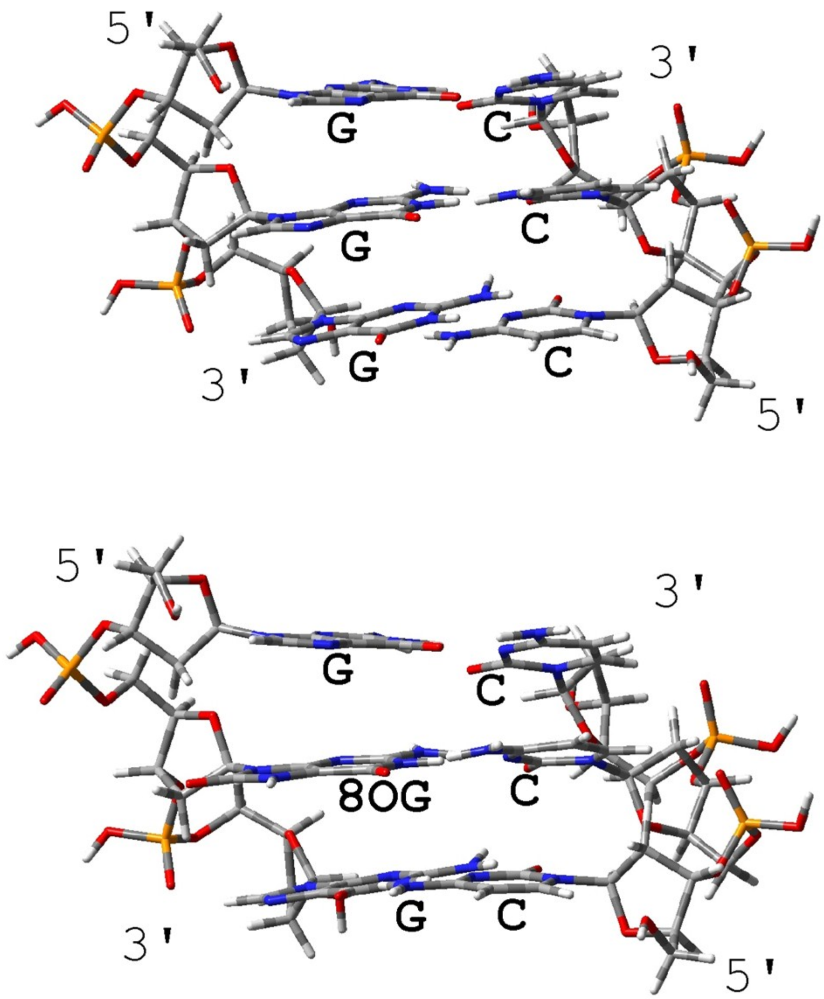


Figure S1- Structures of ds(5'-GGG-3') and ds(5'-G8OGG-3').

The calculated $IP^{vert}_{(NEPCM)}$, $IP^{vert}_{(EQPCM)}$ and IP^{adia} by ωB97XD-PCM/6-31G** method are 6.4, 5.7 and 5.3 eV, respectively. The calculated E^o of -GGG- is 5.3 – 4.44(SHE) = 0.9 V is quite low in comparison to the experimental estimate of 1.3 V of -GGG- stack.

The ωB97XD-PCM/6-31G** calculated $IP^{vert}_{(NEPCM)}$, $IP^{vert}_{(EQPCM)}$ and IP^{adia} of ds(5'-G8OGG-3') in B-DNA conformation are 6.19, 5.49 and 5.05 eV, respectively, see Table S1. (see main text for details). The Calculated E^o of -G8OGG- is 5.05 -4.44 = 0.61 V.

The ωB97XD-PCM/6-31G** calculated solvent relaxation energy (λ_1) of ds(5'-GGG-3') and ds(5'-G8OGG-3') are the same and these are 0.72 and 0.7 eV, respectively, see Table S1. The solute relaxation energy (λ_2) calculated by ωB97XD-PCM/6-31G** for ds(5'-GGG-3') and ds(5'-G8OGG-3') are 0.37 and 0.44 eV, respectively, see Table S1.

Table S1- ωB97XD-PCM/6-31G** and ωB97XD-PCM/6-31++G** calculated vertical and adiabatic ionization potentials and relaxation energies (λ_1, λ_2, and λ_{total}) of ds(5'-GGG-3') and ds(5'-G8OGG-3') oligos in eV. The estimated oxidation potential E^o is given in volt.

System	ωB97XD-PCM/6-31G**[a]							Exp
	$IP^{vert}_{(NEPCM)}$	$IP^{vert}_{(EQPCM)}$	IP^{adia}	λ_1	λ_2	λ_{total}	$E^{o\,b}$	E^o
ds(5'-GGG-3')	6.39	5.67	5.30	0.72	0.37	1.09	0.86	
ds(5'-G8OGG-3')	6.19	5.49	5.05	0.7	0.44	1.14	0.61	
	ωB97XD-PCM/6-31++G**//ωB97XD-PCM/6-31G**[a]							
ds(5'-GGG-3')	6.64	5.96	5.59	0.68	0.37	1.06	1.2	"1.3"[d]
ds(5'-G8OGG-3')	6.43	5.74	5.34	0.69	0.4	1.09	0.9	1.18[e]
	HF-PCM/6-31++G//ωB97XD-PCM/6-31G****[a]							
ds(5'-GGG-3')	5.70	4.95	4.74	0.75	0.21	0.96		
ds(5'-G8OGG-3')	5.61	4.88	4.61	0.73	0.27	1.00		

[a]All values in eV except E^o in volt.
[b]$E^o = IP^{vert}_{(NEPCM)} - \lambda_{total}$ – SHE; SHE = 4.44 volt.
[c]Calculated using SHE = 4.28 volt.
[c]Estimated from DPV measurements showed lowering of 0.1 V oxidation potential in per GG step in single- and double-stranded DNA.[1]
[d]8-oxoG (monomer).[2]

References

1 A. Capobianco, T. Caruso, A. M. D'Ursi, S. Fusco, A. Masi, M. Scrima, C. Chatgilialoglu and A. Peluso, Delocalized Hole Domains in Guanine-Rich DNA Oligonucleotides, *J. Phys. Chem. B*, 2015, **119**, 5462–5466. (Ref. 46 in main text)

2 S. Steenken, S. V. Jovanovic, M. Bietti and K. Bernhard, The trap depth (in DNA) of 8-oxo-7, 8-dihydro-2'deoxyguanosine as derived from electron-transfer equilibria in aqueous solution, *Journal of the American Chemical Society*, 2000, **122**, 2373–2374. (Ref. 9 in main text)

Table S2- ωB97XD and MP2 calculated $IP^{Vert}_{(NEPCM)}$, $IP^{Vert}_{(PCM)}$, IP^{adia}, λ_1 and λ_2 of guanine monomer in PCM using different basis sets.

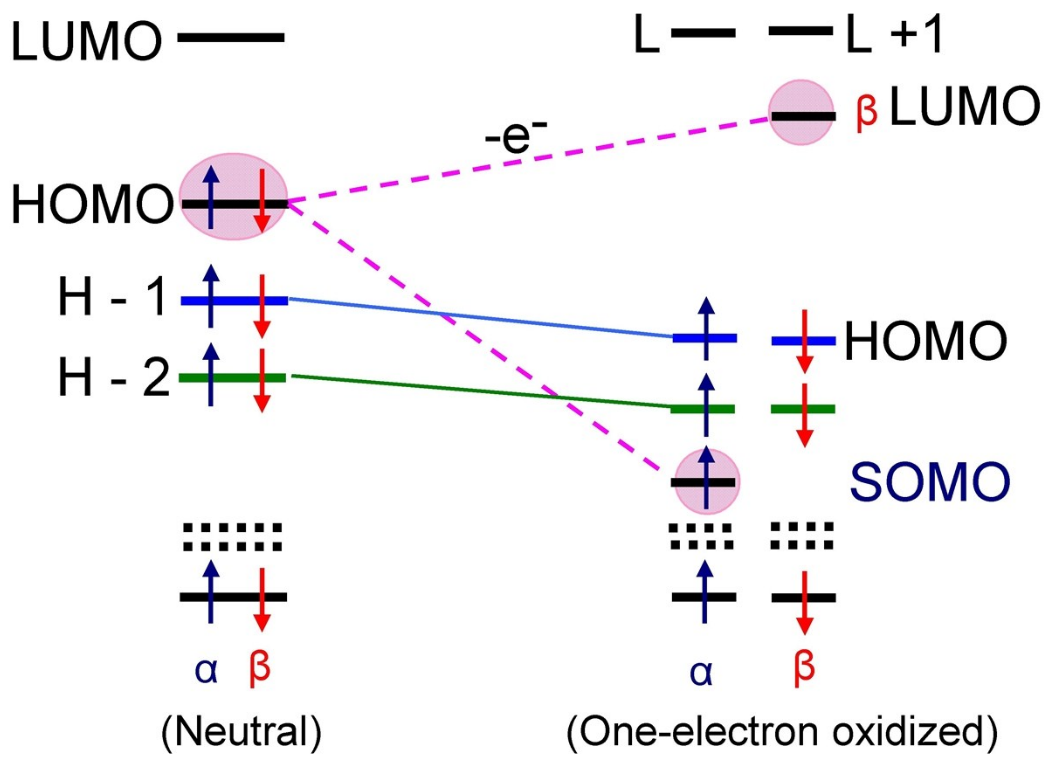
Method	Guanine (values in eV)					
	$IP^{Vert}_{(NEPCM)}$	$IP^{Vert}_{(PCM)}$	IP^{adia}	λ_1	λ_2	λ_{total}
ωb97xd-PCM/6-31G**	7.03	5.92	5.59	1.11	0.33	1.44
ωb97xd-PCM/6-31++G**// ωb97xd-PCM/6-31G**	**7.28**	**6.18**	**5.85**	**1.10**	**0.33**	**1.43**
MP2-PCM/6-31G**	7.56	6.47	5.88	1.09	0.59	1.68
MP2-PCM/6-31++G**// MP2-PCM/6-31G**	7.85	6.76	6.22	1.09	0.55	1.64
PMP2-PCM/aug-cc-pVDZ	7.36	6.28	6.04	1.08	0.24	1.32
PMP2/aug-cc-pVDZ[a]	**7.34Guanine**	**-**	**-**	**-**	**-**	**-**
	7.4Guanosine	**-**	**-**	**1.1**	**0.44**	**1.54**
	7.3 GMP	**-**	**-**	**1.1**	**0.45**	**1.55**

[a](i)Schroeder et al. *J. Am. Chem. Soc.*, 2015, **137**, 201–209 (ref. 69 in text). (ii) Pluhařová et al. *J. Phys. Chem. B*, 2011, **115**, 1294–1305 (Ref 26 in text)

Table S3- ωB97XD and MP2 calculated $IP^{Vert}_{(NEPCM)}$, $IP^{Vert}_{(PCM)}$, IP^{adia}, λ_1 and λ_2 of 8oxoguanine monomer in PCM using different basis sets.

Method	8-Oxoguanine (values in eV)					
	$IP^{Vert}_{(NEPCM)}$	$IP^{Vert}_{(PCM)}$	IP^{adia}	λ_1	λ_2	λ_{total}
ωb97xd-PCM/6-31G**	6.69	5.60	5.27	1.09	0.33	1.42
ωb97xd-PCM/6-31++G**// ωb97xd-PCM/6-31G**	**6.97**	**5.90**	**5.57**	**1.07**	**0.33**	**1.40**
MP2-PCM/6-31G**	6.94	5.88	5.36	1.06	0.52	1.58
MP2-PCM/6-31++G**// MP2-PCM/6-31G**	7.28	6.23	5.74	1.05	0.48	1.53
PMP2-PCM/aug-cc-pVDZ	7.09	6.05	5.66	1.04	0.39	1.43
PMP2/aug-cc-pVDZ[a]	**6.94**	**-**	**-**	**-**	**-**	**-**

[a]Palivec et al. *J. Phys. Chem. B*, 2014, **118**, 13833–13837 (ref 74 in text)



Scheme S1- Diagram showing the electronic configuration (α- and β-MOs) of a neutral parent molecule and its one-electron oxidized radical. In the neutral molecule, each MO is doubly occupied; however, on one-electron oxidation (removal of an electron), α- and β-MOs rearranged independently. Removal of an electron from HOMO of neutral molecule splits HOMO of neutral molecule into β-LUMO and α-SOMO, with the SOMO buried in the filled MOs. As expected, the SOMO and the β-LUMO have near identical wave functions. HOMO = highest occupied molecular orbital; LUMO = lowest unoccupied molecular orbital; and SOMO = singly occupied molecular orbital. Blue and red arrows represent α and β spin of an electron, respectively.

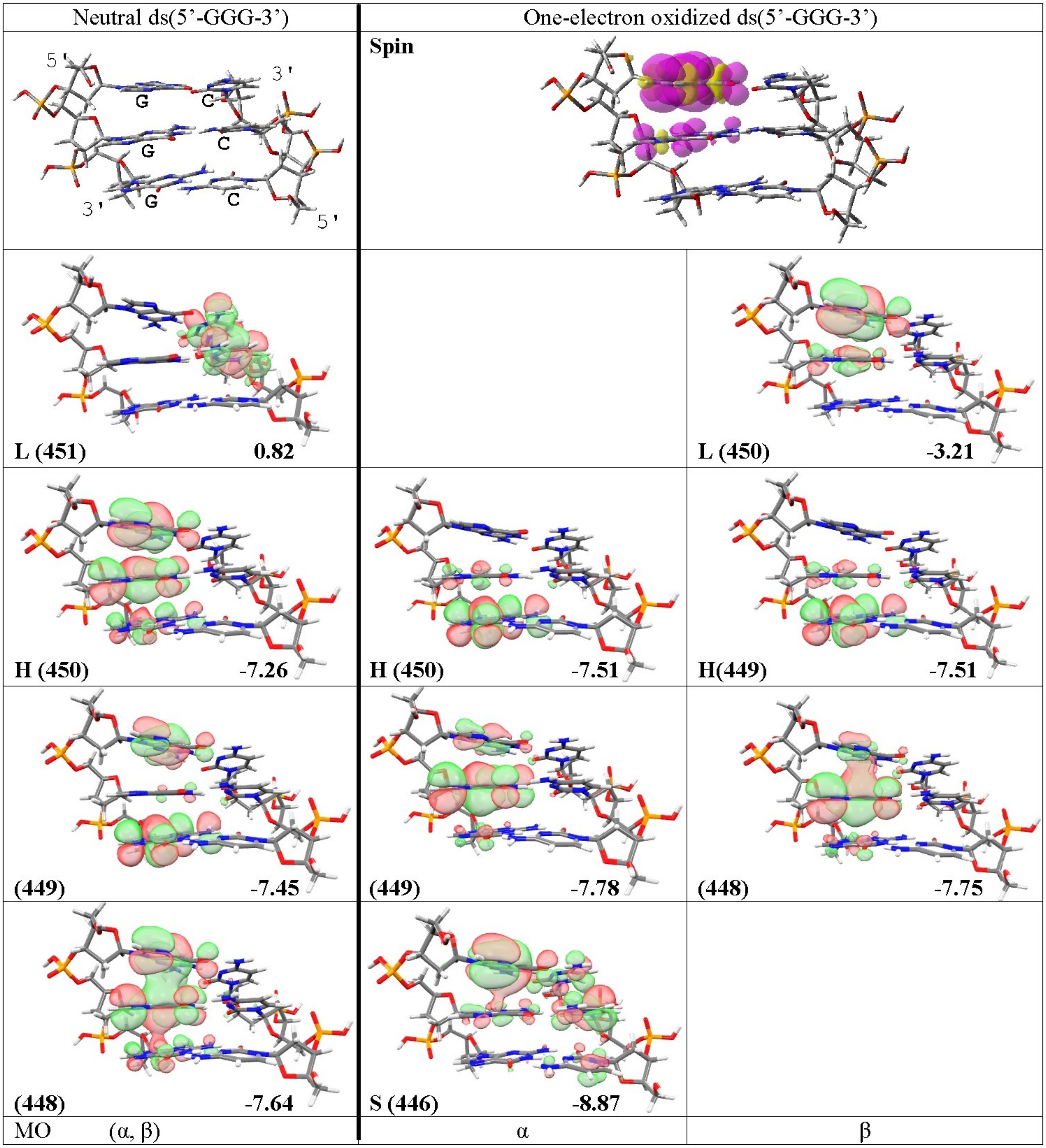


Figure S2- ωb97xd-PCM/6-31G** calculated molecular orbital of neutral ds(5’-GGG-3’) and spin density and α- and β-MOs of one-electron oxidized ds(5’-GGG-3’) are shown. In the figure H, L and S designate the highest occupied molecular orbital, the lowest unoccupied molecular orbital and singly occupied molecular orbital, respectively.

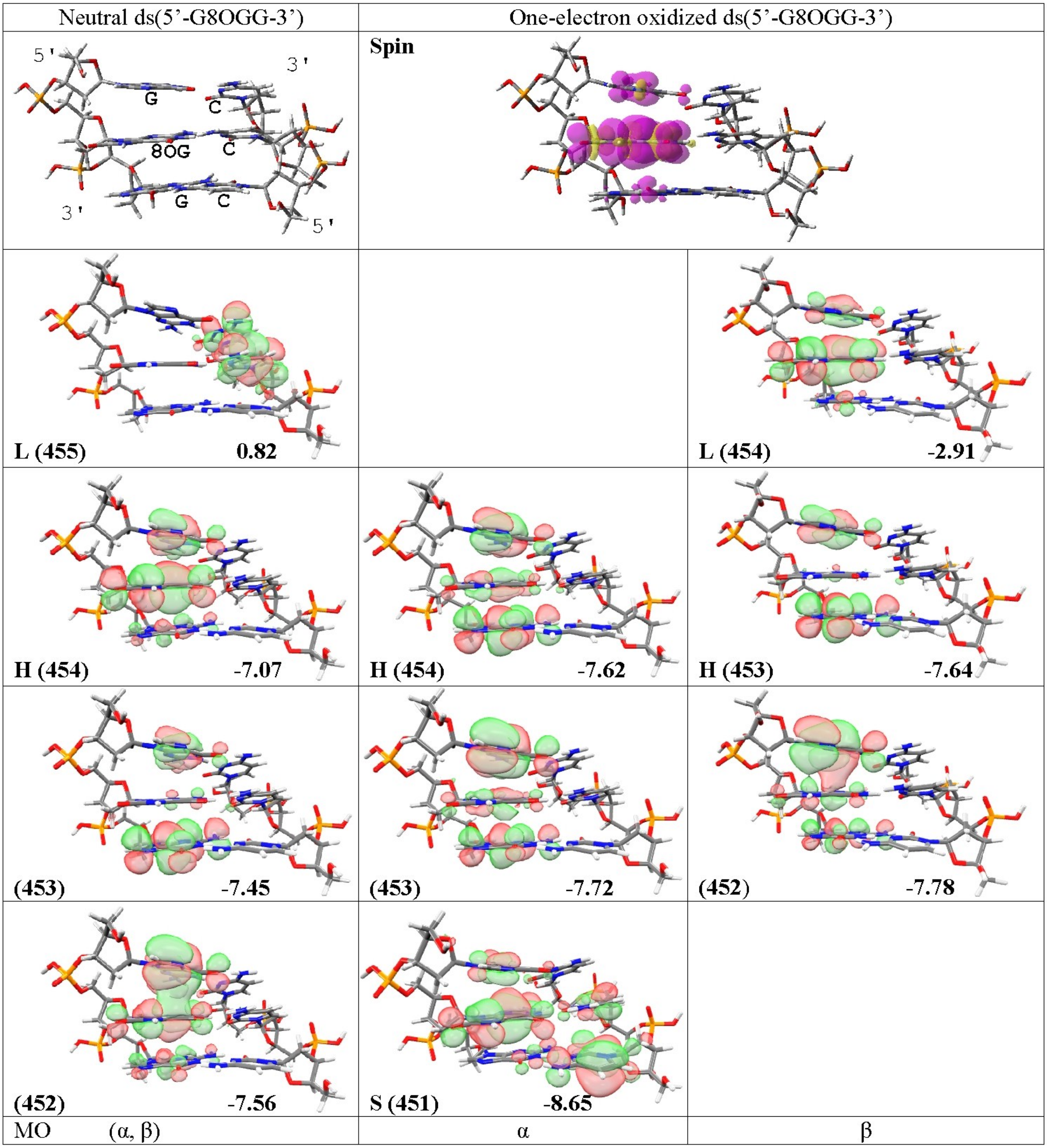


Figure S3- ωb97xd-PCM/6-31G** calculated molecular orbital of neutral ds(5'-G8OGG-3') and spin density and α- and β-MOs of one-electron oxidized ds(5'-G8OGG-3') are shown. In the figure H, L and S designate the highest occupied molecular orbital, the lowest unoccupied molecular orbital and singly occupied molecular orbital, respectively.

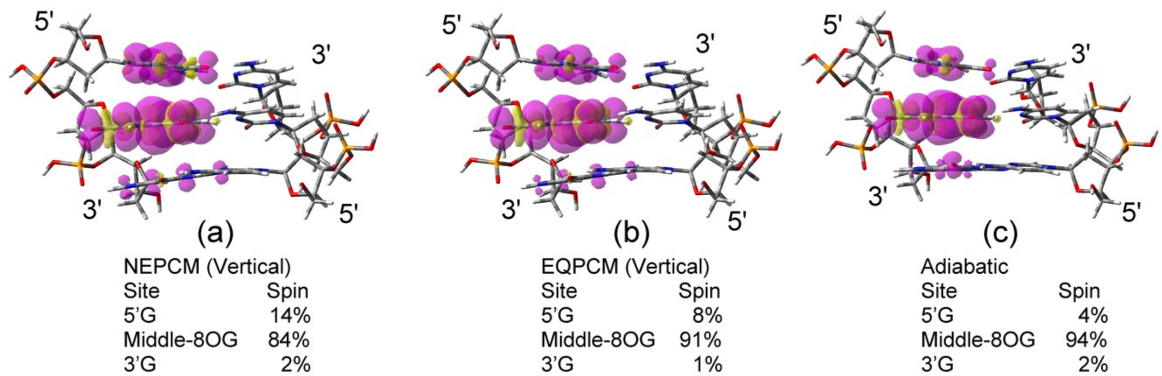


Figure S4. Spin density plots of one-electron oxidized ds(5'-G8OGG-3') calculated using the ωb97xd-PCM/6-31G** method. (a) in NEPCM, (b) in EQPCM and (c) fully optimized cation radical (adiabatic).

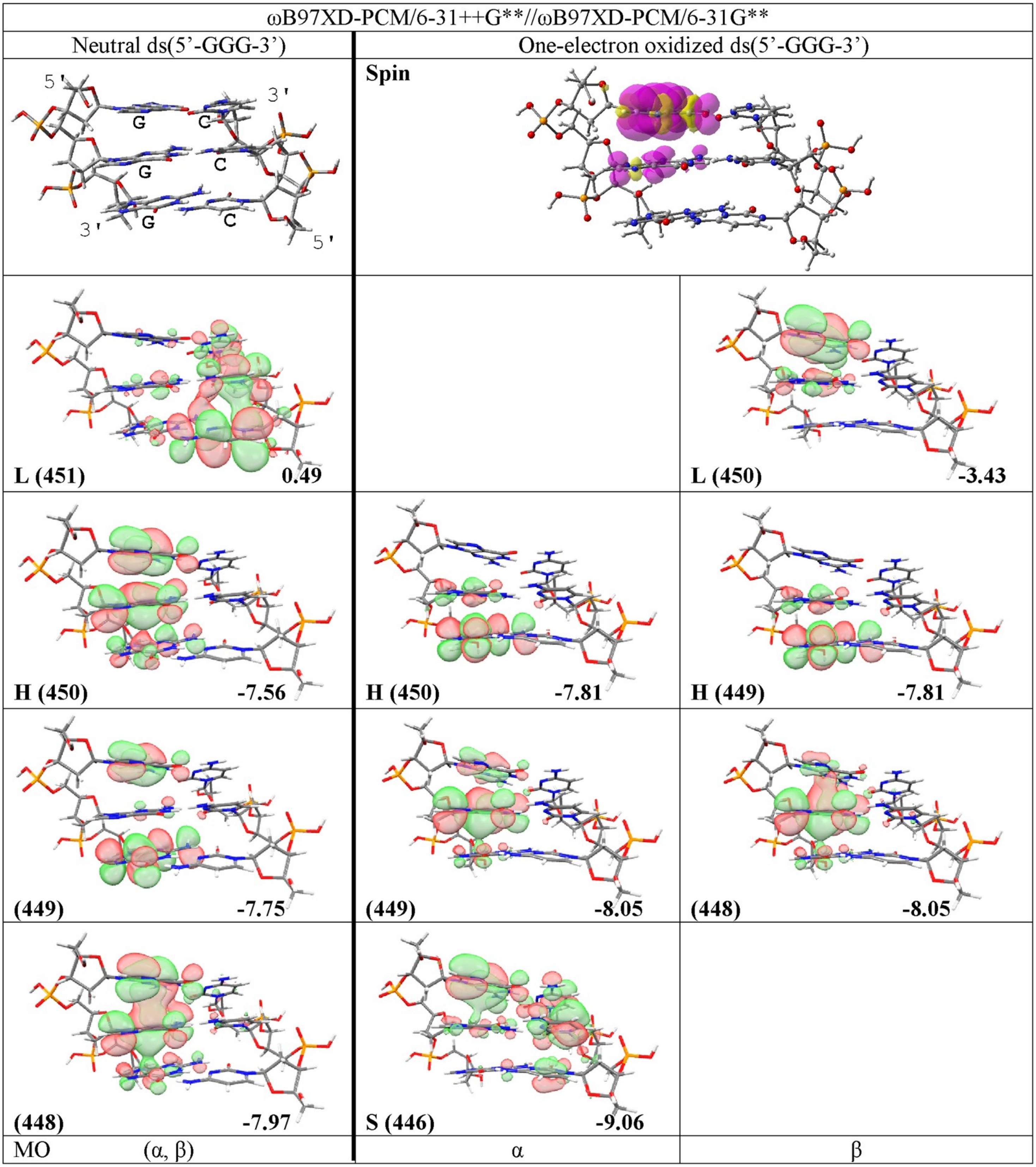


Figure S5- ωb97xd-PCM/6-31++G**//ωb97xd-PCM/6-31G** calculated molecular orbital of neutral ds(5'-GGG-3') and spin density and α- and β-MOs of one-electron oxidized ds(5'-GGG-3') are shown. In the figure H, L and S designate the highest occupied molecular orbital, the lowest unoccupied molecular orbital and singly occupied molecular orbital, respectively.

<table>
<tr><td colspan="3">ωB97XD-PCM/6-31++G**//ωB97XD-PCM/6-31G**</td></tr>
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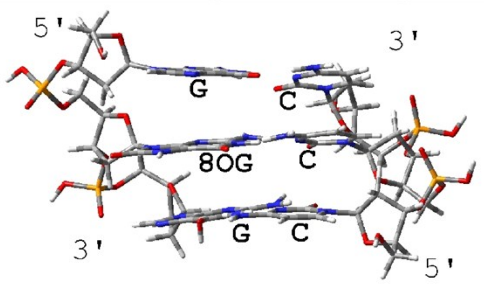
<tr><td>
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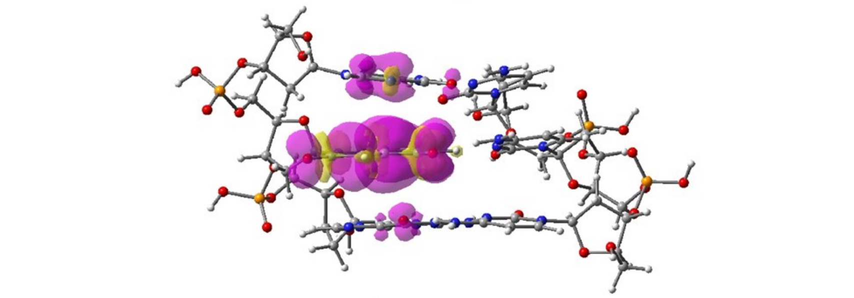
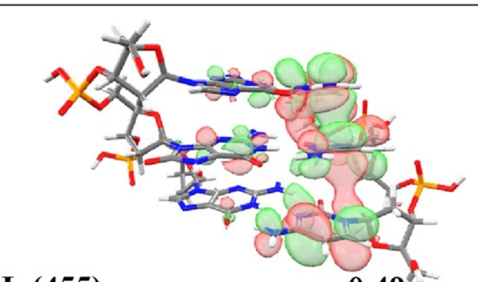
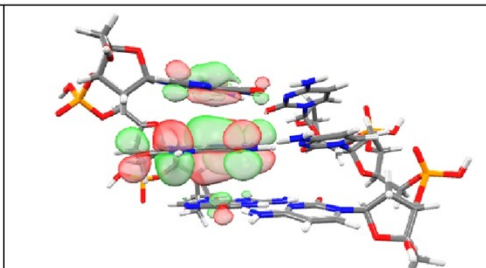
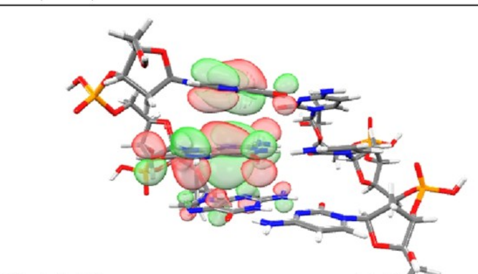
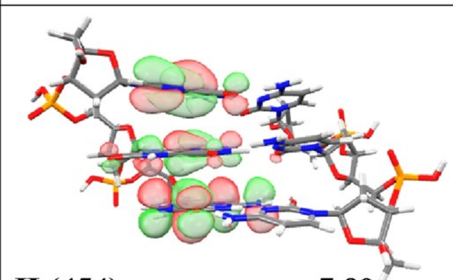
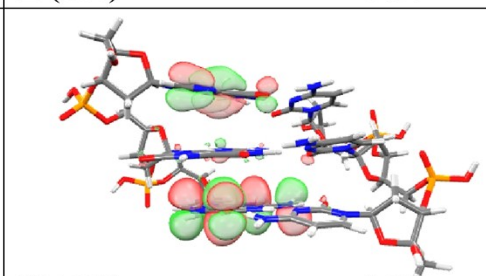
</td></tr>
<tr><td>
L (455) 0.49</td><td></td><td>
L (454) -3.10</td></tr>
<tr><td>
H (454) -7.40</td><td>
H (454) -7.89</td><td>
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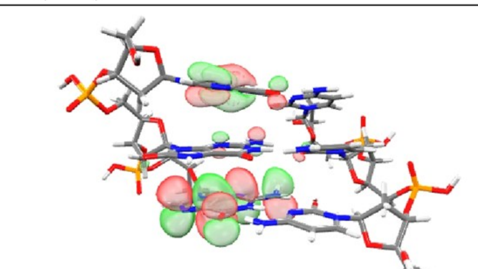
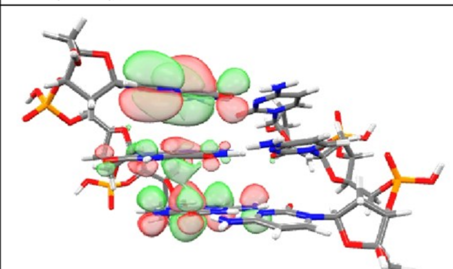
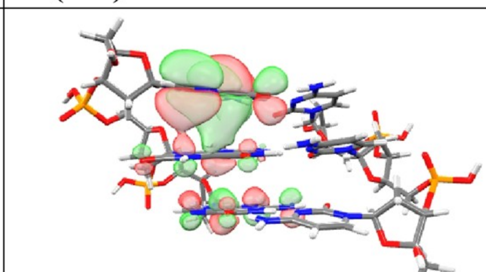
<tr><td>
(453) -7.75</td><td>
(453) -8.00</td><td>
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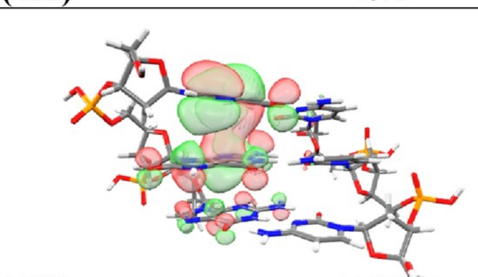
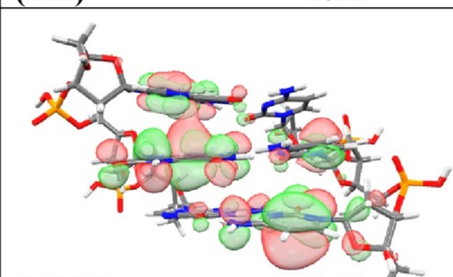
<tr><td>
(452) -7.89</td><td>
S (451) -8.84</td><td></td></tr>
<tr><td>MO (α, β)</td><td>α</td><td>β</td></tr>
</table>

Figure S6- ωb97xd-PCM/6-31++G**//ωb97xd-PCM/6-31G** calculated molecular orbital of neutral ds(5’-G8OGG-3’) and spin density and α- and β-MOs of one-electron oxidized ds(5’-G8OGG-3’) are shown. In the figure H, L and S designate the highest occupied molecular orbital, the lowest unoccupied molecular orbital and singly occupied molecular orbital, respectively.

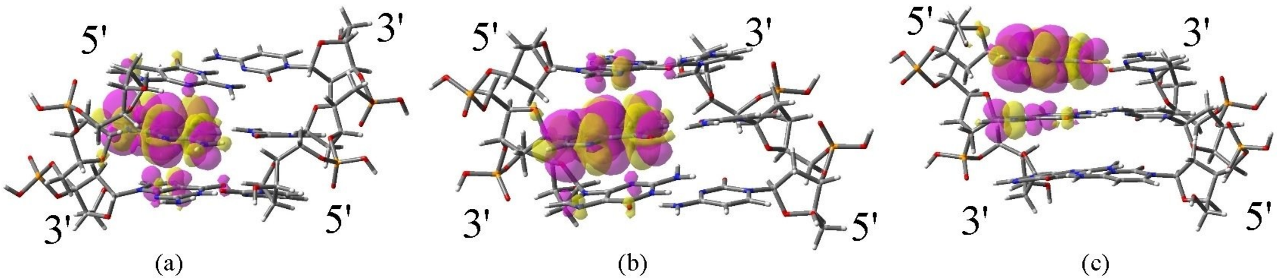


Figure S7- Spin density plots of one-electron oxidized ds(5'-GGG-3') calculated using the HF-PCM/6-31++G**//ωb97xd-PCM/6-31G** method. (a) in NEPCM, (b) in EQPCM and (c) finally the fully optimized cation radical (adiabatic).

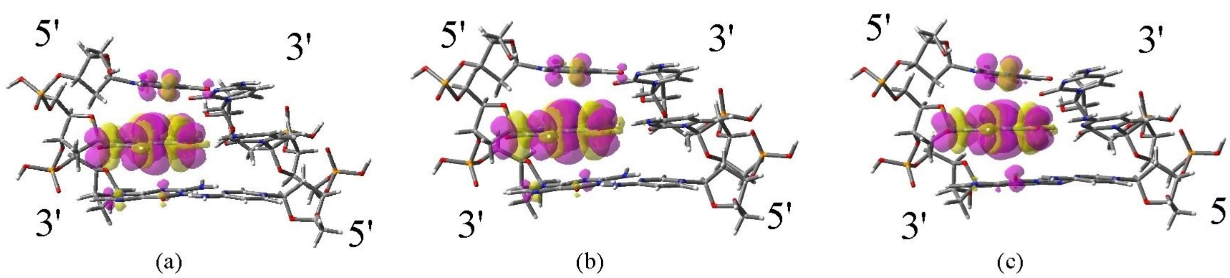


Figure S8- Spin density plots of one-electron oxidized ds(5'-G8OGG-3') calculated using the HF-PCM/6-31++G**//ωb97xd-PCM/6-31G** method. (a) in NEPCM, (b) in EQPCM and (c) fully optimized cation radical (adiabatic).

Molecular Dynamics (MD) Calculations-

We note that our optimization calculations converge to a single minimum structure for a ds(5'-GGG-3') stack which show spin localization on a single guanine at 5'-site in ds(5'-GGG-3') as observed in ESR experiment. Our calculations do not take into account the effect of thermal fluctuations which may produce some isoenergic structures having localized/delocalized spin densities on the other guanines in ds(5'-GGG-3'). To check the effect of thermal fluctuations on ds(5'-GGG-3'), we employed *ab initio* Atom Centered Density Matrix Propagation (ADMP) molecular dynamics (MD) implemented in the Gaussian 16 programs.[68] We started MD simulations using the vertical cation geometry (electron removed from the optimized neutral geometry of ds(5'-GGG-3')) using the ωb97xd-PCM/6-31G** method. The total MD simulations were run for 50 fs at the step size of 0.1 fs. From the MD steps, we took geometries at 0, 1, 10, 20, 30, 40 and 50 fs and then calculated the spin density distributions, shown in Figure S9, using the ωb97xd-PCM/6-31G** method. The spin density plot at 0 fs shows delocalized spin density distribution on middle and 5’-guanines but within 1 fs the spin is becomes more localized to the 5’-G. From 10 to 20 fs the hole appears to oscillate somewhat to the central G but after 30 fs and up to 50 fs it remains on 5’G. This suggests some energy barrier to hole transfer from the 5’-G site to other Gs but our MD simulations are too short to provide a meaningful description of thermal fluctuations on hole distribution on the other Gs.

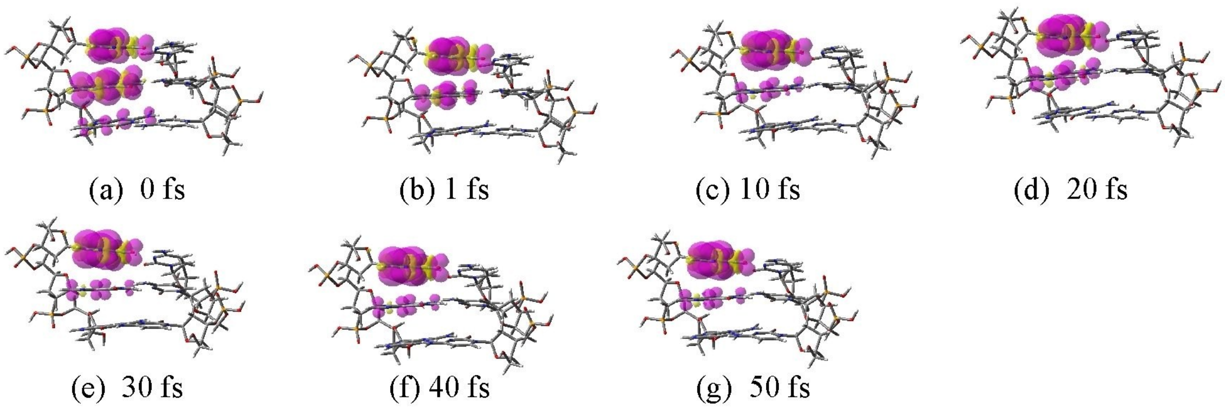
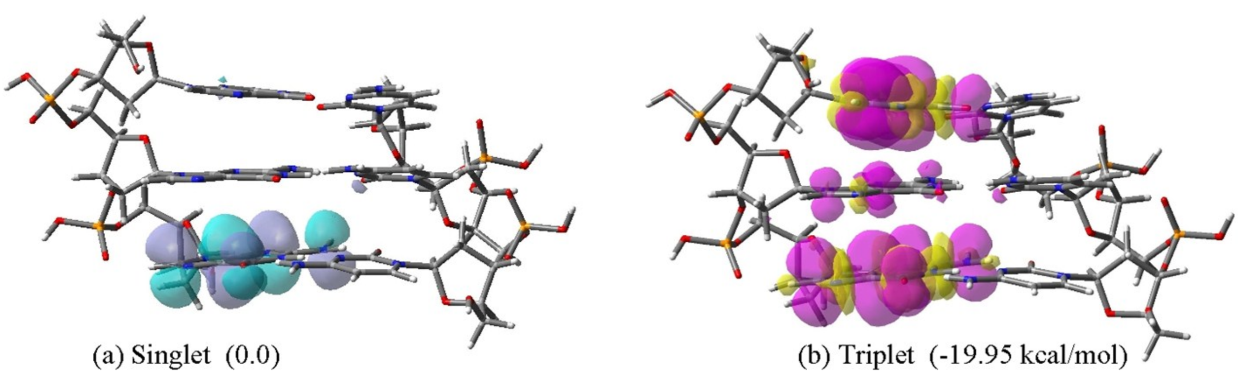


Figure S9- Time evolution of the total spin density after vertical electron removal from ds(5’-GGG-3’), depicted at times: (a) 0 fs, (b) 1 fs, (c) 10 fs, (d) 20 fs, (e) 30 fs, (f) 40 fs and (g) 50 fs. Molecular dynamics simulations were carried out using the atom centered density matrix propagation (ADMP) *ab initio* molecular dynamics method implemented in Gaussian 16. The ωB97XD-PCM/6-31G** method was used in the ADMP simulations. Simulations were run for 50 fs with a time step of 0.1 fs using default values set in the Gaussian 16 program.



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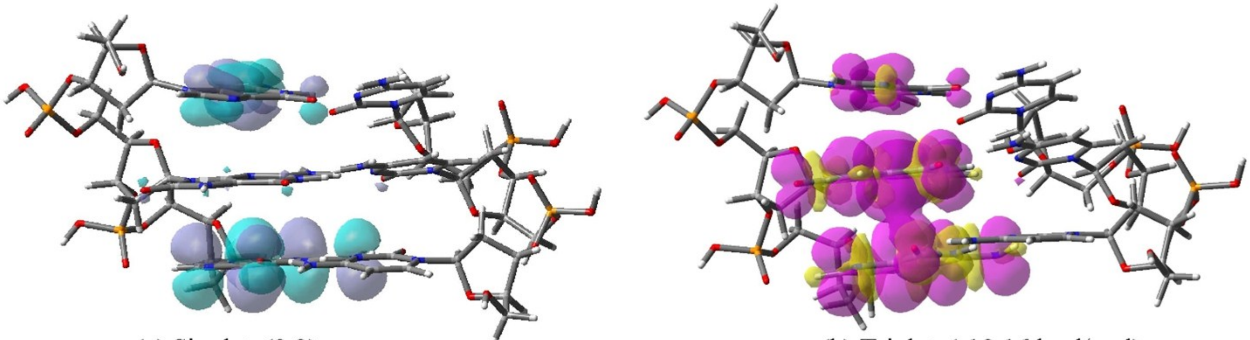
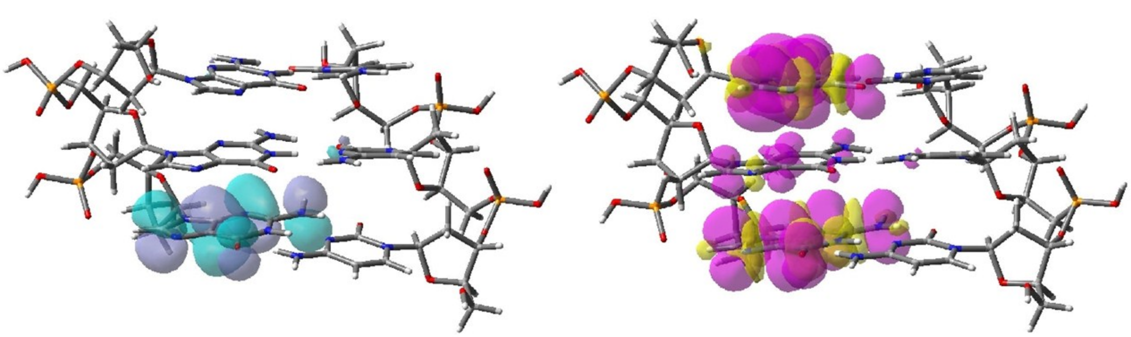


(a) Singlet (0.0) (b) Triplet (-10.16 kcal/mol)

Figure S11- ωB97XD-PCM/6-31G** calculated singlet and triplet states of double oxidized ds(5'-G8OGG-3') [ds(5'-G8OGG-3')$^{2+}$]. Single point calculations were carried out using the ωB97XD-PCM/6-31G** optimized geometry of one-electron oxidized ds(5'-GGG-3'). (a) HOMO of ds(5'-GGG-3')$^{2+}$ in the singlet state and (b) Spin density distribution of ds(5'-GGG-3')$^{2+}$ in the triplet state. The triplet state is more stable (10.16 kcal/mol) than the singlet.



(a) Singlet (0.0) (b) Triplet (-18.81 kcal/mol)

Figure S12- ωB97XD-PCM/6-31++G** calculated singlet and triplet states of double oxidized ds(5'-GGG-3') [ds(5'-GGG-3')$^{2+}$]. Single point calculations were carried out using the ωB97XD-PCM/6-31G** optimized geometry of one-electron oxidized ds(5'-GGG-3'). (a) HOMO of ds(5'-GGG-3')$^{2+}$ in the singlet state and (b) Spin density distribution of ds(5'-GGG-3')$^{2+}$ in the triplet state. The triplet state is more stable (18.81 kcal/mol) than the singlet.

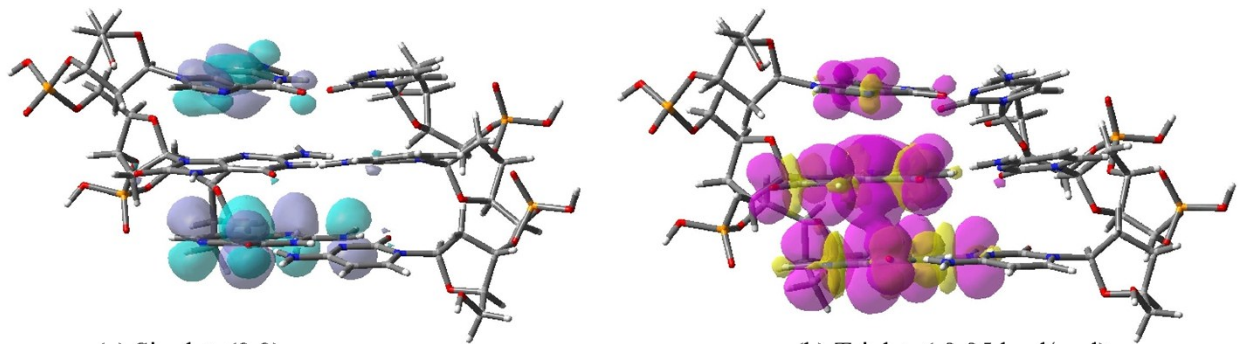


Figure S13- ωB97XD-PCM/6-31++G** calculated singlet and triplet states of double oxidized ds(5'-G8OGG-3') [ds(5'-G8OGG-3')$^{2+}$]. Single point calculations were carried out using the ωB97XD-PCM/6-31G** optimized geometry of one-electron oxidized ds(5'-G8OGG-3'). (a) HOMO of ds(5'-G8OGG-3')$^{2+}$ in the singlet state and (b) Spin density distribution of ds(5'-G8OGG-3')$^{2+}$ in the triplet state. The triplet state is more stable (9.95 kcal/mol) than the singlet.

Optimized geometries by ωb97xd/6-31G in PCM.**

1. Optimized X, Y, Z coordinates of neutral ds(5'-GGG-3') in Angstroms.

Charge = 0 Multiplicity = 1

H	6.58237	-6.04873	-3.62811
O	6.70923	-5.12604	-3.38989
C	5.87717	-1.84388	-3.08035
C	6.70993	-2.46050	-1.95372
C	8.03894	-2.77773	-2.62271
C	7.64951	-3.02860	-4.07993
C	7.47294	-4.50226	-4.40670
O	6.44794	-2.29004	-4.29809
H	5.88958	-0.75094	-3.04143
H	6.25633	-3.38966	-1.60628
H	6.80401	-1.77079	-1.11557
H	8.55333	-3.62688	-2.17094
H	8.41876	-2.62458	-4.74503
H	8.46978	-4.95725	-4.48195
H	6.98421	-4.58162	-5.38553
O	8.92809	-1.63662	-2.61655
N	1.09366	-0.19700	-3.28003
C	2.25233	0.52515	-3.15547
N	2.11787	1.86699	-3.12977
N	3.45292	-0.02287	-3.09747

C	3.40643	-1.36855	-3.12735
C	2.29658	-2.19458	-3.23598
C	1.01240	-1.58802	-3.34313
O	-0.08251	-2.14953	-3.48227
N	2.66798	-3.52744	-3.23914
C	3.96682	-3.49853	-3.12808
N	4.47924	-2.21699	-3.04618
H	0.19005	0.31627	-3.29704
H	1.20683	2.28516	-2.92137
H	2.93983	2.37531	-2.84578
H	4.63369	-4.35099	-3.12893
O	-6.42315	5.63017	-1.07305
C	-2.80821	4.43580	-2.29899
C	-3.41414	5.57308	-3.11283
C	-3.78085	6.56495	-2.00253
C	-3.98054	5.64684	-0.76933
C	-5.34631	5.69718	-0.12261
O	-3.69314	4.31849	-1.19108
H	-1.80125	4.69276	-1.96262
H	-4.31926	5.23303	-3.62364
H	-2.72146	5.99728	-3.84137
H	-4.69420	7.11940	-2.24177
H	-3.25004	5.95909	-0.01001
H	-5.47027	6.65838	0.37764
H	-5.44994	4.89474	0.61016
O	-2.72184	7.44860	-1.68241
H	-2.63498	8.07790	-2.40526
N	-2.69866	3.14227	-2.93916
C	-1.45878	2.47871	-2.95182
O	-0.44544	3.08738	-2.58340
N	-1.42212	1.19436	-3.37832
C	-2.53238	0.56840	-3.77705
N	-2.44685	-0.72412	-4.09035
C	-3.78333	1.25826	-3.86911
C	-3.81947	2.52834	-3.41399
H	-1.58580	-1.24669	-3.88543
H	-3.28127	-1.23431	-4.32918
H	-4.67357	0.76888	-4.24023
H	-4.73587	3.11079	-3.38192
O	8.76320	-0.30190	-0.44682
C	5.31205	0.33592	0.76656
C	6.47273	0.19305	1.74000
C	7.34053	1.36047	1.29776
C	7.10158	1.40701	-0.22684
C	8.27396	0.91043	-1.04153
O	5.95910	0.59418	-0.47969
H	4.67355	1.18338	1.04347
H	7.02139	-0.73268	1.55116
H	6.18534	0.24318	2.78680
H	8.39446	1.25549	1.56162
H	6.89637	2.44283	-0.52082
H	9.07219	1.65738	-1.03939
H	7.95453	0.72608	-2.07118
O	6.84040	2.60646	1.81462
N	0.59295	-1.11384	-0.16639
C	1.12671	0.15050	-0.11572
N	0.27802	1.15548	-0.35734

N	2.40443	0.39460	0.13158
C	3.11208	-0.73293	0.32484
C	2.68234	-2.04944	0.27953
C	1.30576	-2.29959	0.00130
O	0.73743	-3.39395	-0.09600
N	3.72269	-2.92106	0.54804
C	4.74726	-2.14485	0.75549
N	4.44874	-0.79942	0.63462
H	-0.41815	-1.20291	-0.38592
H	-0.73175	1.01650	-0.43780
H	0.64453	2.09136	-0.36265
P	9.71714	-1.28759	-1.27474
O	10.14129	-2.42131	-0.43381
O	10.84531	-0.37061	-1.93319
O	-9.04985	-0.14301	0.33591
C	-5.29965	0.68400	-0.55909
C	-6.41997	1.04155	-1.52989
C	-7.28866	1.90247	-0.62428
C	-7.08040	1.26258	0.76808
C	-8.30890	0.57936	1.33412
O	-6.01837	0.32636	0.62293
H	-4.65871	1.55000	-0.37721
H	-6.98624	0.15184	-1.81702
H	-6.09582	1.57466	-2.41809
H	-8.33838	1.93590	-0.92082
H	-6.78571	2.05165	1.47138
H	-9.00019	1.33495	1.70947
H	-8.02603	-0.08755	2.15046
O	-6.77845	3.25022	-0.53669
N	-4.40970	-0.39938	-0.90385
C	-3.02687	-0.24922	-0.66654
O	-2.58576	0.87187	-0.37980
N	-2.22934	-1.33591	-0.77088
C	-2.73648	-2.53156	-1.08101
N	-1.92750	-3.58654	-1.06169
C	-4.12215	-2.69088	-1.41212
C	-4.91653	-1.60890	-1.27814
H	-0.94971	-3.49638	-0.76412
H	-2.29000	-4.49985	-1.27859
H	-4.52735	-3.64925	-1.70749
H	-5.98888	-1.65497	-1.43822
P	-7.03899	4.31102	-1.69832
O	-6.58759	3.94681	-3.06231
O	-8.60963	4.60110	-1.62475
O	6.38257	4.49297	3.31418
C	2.88273	2.76949	3.61597
C	3.37780	3.51911	4.84481
C	3.62738	4.90428	4.24615
C	3.99132	4.57897	2.77588
C	5.39862	4.95093	2.36995
O	3.78612	3.17822	2.59588
H	1.86178	3.07602	3.36072
H	4.31854	3.07874	5.18708
H	2.65541	3.53448	5.66246
H	4.44139	5.43133	4.75491
H	3.30250	5.14045	2.13061
H	5.49381	6.03755	2.36150

H	5.62875	4.56142	1.37718
O	2.45473	5.69828	4.20762
H	2.23564	5.94296	5.11226
N	-0.00865	-1.29276	3.01713
C	-0.30276	0.03233	2.80558
N	-1.55049	0.31398	2.40408
N	0.56806	1.00923	2.99556
C	1.76708	0.55740	3.40138
C	2.17583	-0.74663	3.63699
C	1.22969	-1.79436	3.42206
O	1.39745	-3.01388	3.55109
N	3.49133	-0.77924	4.07046
C	3.85472	0.47398	4.10372
N	2.85277	1.33856	3.70230
H	-0.73982	-1.99594	2.80226
H	-2.22090	-0.42634	2.17631
H	-1.69798	1.21822	1.98644
H	4.82218	0.85750	4.40279
P	7.03167	3.04609	3.33362
O	6.55545	2.11477	4.38211
O	8.59366	3.36935	3.45929
H	-7.34095	-7.08311	3.02892
O	-7.27200	-6.20166	2.65173
C	-5.76225	-3.20521	2.03354
C	-6.59910	-3.85609	0.93560
C	-7.99905	-3.67164	1.49009
C	-7.79374	-3.88107	2.99246
C	-8.01408	-5.30873	3.46279
O	-6.45375	-3.46060	3.25004
H	-5.66316	-2.13106	1.86873
H	-6.39606	-4.92463	0.85331
H	-6.46604	-3.38643	-0.03399
H	-8.75191	-4.33413	1.05890
H	-8.47715	-3.23293	3.55038
H	-9.08912	-5.52841	3.41159
H	-7.70236	-5.36897	4.51264
O	-8.42417	-2.29435	1.34527
N	-4.40355	-3.71068	2.16518
C	-3.33954	-2.79588	2.22224
O	-3.57176	-1.59536	2.03721
N	-2.09532	-3.26351	2.48407
C	-1.88316	-4.56580	2.69325
N	-0.63871	-4.95817	2.96213
C	-2.95691	-5.51679	2.65581
C	-4.19582	-5.03632	2.41824
H	0.10665	-4.26625	3.09224
H	-0.44967	-5.92511	3.16762
H	-2.79034	-6.56649	2.85498
H	-5.08740	-5.65629	2.44437
P	-8.87668	-1.67304	-0.04729
O	-8.03674	-1.97521	-1.23042
O	-10.39330	-2.14047	-0.22951
H	-10.55198	-2.49911	-1.11118
H	-9.02422	4.54457	-2.49415
H	11.50733	-0.07442	-1.29591
H	8.98732	2.93109	4.22328
H	5.74062	-2.48345	1.01012

2. Optimized X, Y, Z coordinates of cation radical ds(5'-GGG-3') in Angstroms (**Spin localized on 5'-G most stable (Figure 4(a)**)

Charge = 1 Multiplicity = 2

H	6.59129	-5.88924	-3.69986
O	6.69147	-4.96017	-3.47268
C	5.95030	-1.72108	-3.00569
C	6.82716	-2.38869	-1.94559
C	8.12549	-2.65420	-2.69534
C	7.65882	-2.86573	-4.13505
C	7.43841	-4.32412	-4.49638
O	6.45426	-2.09985	-4.26230
H	5.94016	-0.63253	-2.90681
H	6.40357	-3.34243	-1.62897
H	6.95250	-1.74276	-1.07848
H	8.68107	-3.50495	-2.29859
H	8.38974	-2.44773	-4.83217
H	8.42120	-4.79790	-4.61371
H	6.91721	-4.36663	-5.46025
O	8.98038	-1.49112	-2.70319
N	1.04908	-0.20227	-3.18298
C	2.17957	0.54540	-3.01911
N	2.05121	1.84552	-2.91883
N	3.43730	0.01910	-2.95499
C	3.45380	-1.28653	-2.98870
C	2.34043	-2.17219	-3.10938
C	1.01546	-1.58824	-3.24878
O	-0.02168	-2.20999	-3.41572
N	2.73099	-3.45169	-3.14176
C	4.05904	-3.38855	-3.03808
N	4.54428	-2.11991	-2.93042
H	0.11659	0.29327	-3.24602
H	1.11719	2.30058	-2.84977
H	2.89343	2.38287	-2.77250
H	4.73591	-4.23509	-3.07949
O	-6.34030	5.65796	-1.13065
C	-2.74641	4.37853	-2.34216
C	-3.32500	5.51585	-3.17483
C	-3.67932	6.52793	-2.07802
C	-3.89696	5.62970	-0.83315
C	-5.25956	5.71733	-0.18438
O	-3.63791	4.28953	-1.23944
H	-1.73620	4.61951	-2.00420
H	-4.23314	5.18633	-3.68700
H	-2.61957	5.91784	-3.90360
H	-4.58345	7.09251	-2.32788
H	-3.15779	5.93458	-0.07947
H	-5.36186	6.68857	0.30106
H	-5.37769	4.92886	0.56124
O	-2.60803	7.39887	-1.76609
H	-2.51436	8.02289	-2.49263
N	-2.66158	3.07246	-2.96701
C	-1.43883	2.39241	-2.98238
O	-0.41100	2.99328	-2.63366
N	-1.42014	1.10062	-3.38812
C	-2.54059	0.49132	-3.79088

N	-2.47981	-0.80260	-4.10183
C	-3.77677	1.20184	-3.88670
C	-3.79255	2.47479	-3.43724
H	-1.63575	-1.33674	-3.90320
H	-3.31778	-1.30064	-4.35346
H	-4.67443	0.72495	-4.25555
H	-4.69907	3.07322	-3.40704
O	8.79788	-0.22956	-0.49468
C	5.28037	0.21328	0.75770
C	6.43807	0.05145	1.73142
C	7.28869	1.24925	1.33390
C	7.03767	1.36367	-0.18635
C	8.23070	0.97706	-1.02960
O	5.93421	0.50702	-0.47596
H	4.63668	1.05036	1.05444
H	6.99979	-0.86019	1.51259
H	6.14702	0.05890	2.77834
H	8.34568	1.14166	1.58292
H	6.77410	2.40103	-0.42163
H	8.98133	1.77085	-0.99248
H	7.91977	0.82577	-2.06729
O	6.78197	2.46412	1.91142
N	0.54651	-1.19401	-0.18647
C	1.08359	0.06532	-0.08232
N	0.24873	1.08749	-0.29246
N	2.36999	0.29452	0.15193
C	3.07688	-0.83823	0.29520
C	2.64569	-2.15241	0.18372
C	1.25936	-2.39005	-0.07470
O	0.69191	-3.47581	-0.21778
N	3.68738	-3.03458	0.39802
C	4.71436	-2.26813	0.63778
N	4.41675	-0.91906	0.58467
H	-0.47253	-1.27381	-0.38798
H	-0.76854	0.96015	-0.34270
H	0.61227	2.01248	-0.13443
P	9.79302	-1.12405	-1.37740
O	10.31797	-2.24937	-0.58473
O	10.82936	-0.11574	-2.04914
O	-9.06851	-0.03372	0.36695
C	-5.29677	0.69383	-0.56590
C	-6.41265	1.06554	-1.53682
C	-7.26200	1.95091	-0.63640
C	-7.05686	1.32325	0.76219
C	-8.29568	0.67731	1.34884
O	-6.01870	0.35958	0.61950
H	-4.63837	1.54833	-0.39201
H	-6.99701	0.18484	-1.81447
H	-6.08262	1.58476	-2.43091
H	-8.31250	1.99780	-0.92813
H	-6.73573	2.11366	1.45218
H	-8.96201	1.45396	1.72610
H	-8.02001	0.01018	2.16750
O	-6.73007	3.29088	-0.56680
N	-4.42982	-0.41019	-0.90862
C	-3.04376	-0.28775	-0.68150
O	-2.57971	0.82225	-0.38902

N	-2.26427	-1.38664	-0.81016
C	-2.79670	-2.57091	-1.12479
N	-2.00036	-3.63594	-1.15074
C	-4.19141	-2.70587	-1.42430
C	-4.96398	-1.60988	-1.27555
H	-1.02122	-3.56674	-0.85806
H	-2.38344	-4.54352	-1.35657
H	-4.61898	-3.65625	-1.71333
H	-6.03948	-1.63577	-1.41902
P	-6.97081	4.33982	-1.74348
O	-6.51523	3.95106	-3.09960
O	-8.53688	4.65282	-1.68350
O	6.42535	4.31532	3.48691
C	2.88778	2.71094	3.73479
C	3.42252	3.39441	4.98533
C	3.69626	4.79747	4.44188
C	4.04226	4.52541	2.95709
C	5.46370	4.85631	2.56366
O	3.78003	3.14338	2.71472
H	1.86793	3.04672	3.51474
H	4.35784	2.91766	5.29248
H	2.71510	3.39145	5.81606
H	4.52422	5.28717	4.96521
H	3.37644	5.14309	2.33992
H	5.60525	5.93721	2.60213
H	5.67694	4.50036	1.55476
O	2.53888	5.61447	4.44552
H	2.32888	5.82319	5.36131
N	-0.04595	-1.29557	2.94625
C	-0.34075	0.04136	2.83263
N	-1.59366	0.35136	2.47576
N	0.53865	1.00261	3.06518
C	1.74190	0.52252	3.42370
C	2.15023	-0.79561	3.56351
C	1.19914	-1.82448	3.29306
O	1.37048	-3.04946	3.32935
N	3.47325	-0.86151	3.96831
C	3.84170	0.38566	4.07921
N	2.83615	1.27793	3.75564
H	-0.78458	-1.98400	2.70732
H	-2.27867	-0.36418	2.21351
H	-1.76367	1.30257	2.19525
H	4.81598	0.74464	4.38696
P	7.04357	2.85710	3.43357
O	6.58346	1.90595	4.47137
O	8.61721	3.13592	3.50457
H	-7.42252	-6.97730	3.09277
O	-7.34997	-6.10067	2.70523
C	-5.81830	-3.12851	2.02458
C	-6.68539	-3.78061	0.95099
C	-8.07084	-3.57292	1.53227
C	-7.83635	-3.77063	3.03222
C	-8.06580	-5.19064	3.52086
O	-6.48513	-3.36745	3.25772
H	-5.71225	-2.05653	1.84980
H	-6.49834	-4.85252	0.87648
H	-6.56725	-3.32448	-0.02676

H	-8.84079	-4.22991	1.12356
H	-8.49878	-3.10767	3.59800
H	-9.14425	-5.39727	3.49186
H	-7.73529	-5.24450	4.56529
O	-8.48217	-2.19219	1.38195
N	-4.46260	-3.64783	2.12616
C	-3.38684	-2.74592	2.15963
O	-3.61200	-1.53875	2.00898
N	-2.13893	-3.23285	2.35919
C	-1.93501	-4.54133	2.53940
N	-0.68479	-4.95459	2.73807
C	-3.02226	-5.47714	2.54203
C	-4.26296	-4.97835	2.35949
H	0.07344	-4.27340	2.84788
H	-0.50118	-5.92608	2.92667
H	-2.86128	-6.53060	2.72483
H	-5.16091	-5.58688	2.41593
P	-8.92834	-1.56842	-0.01151
O	-8.09924	-1.89189	-1.19692
O	-10.45492	-2.00396	-0.18588
H	-10.62473	-2.36399	-1.06492
H	-8.94819	4.58952	-2.55403
H	11.50629	0.19454	-1.43454
H	9.03165	2.65992	4.23431
H	5.70837	-2.61952	0.87161

3. Optimized X, Y, Z coordinates of cation radical ds(5’-GGG-3’) in Angstroms (**Spin localized on Middle-G (Figure 4(b)**)

Charge = 1 Multiplicity = 2

8	0.698782	-3.709696	0.304637
6	1.201691	-2.600390	0.338403
7	0.453711	-1.444840	0.136584
6	0.959329	-0.178457	0.099113
7	2.284643	0.115703	0.253042
6	3.022126	-0.938559	0.480809
6	2.611935	-2.297470	0.559064
7	3.649512	-3.100884	0.839797
6	4.685774	-2.274624	0.947667
7	4.374673	-0.965012	0.731784
1	-0.571928	-1.561183	-0.076545
7	0.132994	0.817392	-0.089279
1	-0.898158	0.688958	-0.191178
1	0.521837	1.743167	-0.203039
1	5.686578	-2.593039	1.199667
1	6.859964	-6.514406	-2.773665
8	6.961219	-5.566942	-2.646430
6	6.091678	-2.303273	-2.654595
6	6.946195	-2.802179	-1.488556
6	8.278196	-3.123269	-2.147335
6	7.869714	-3.545149	-3.559992
6	7.726057	-5.049096	-3.720203
8	6.637183	-2.873677	-3.827755
1	6.097920	-1.212089	-2.726112
1	6.533154	-3.723489	-1.075170

1	7.025249	-2.047590	-0.707209
1	8.844294	-3.893330	-1.621751
1	8.611599	-3.193738	-4.283193
1	8.731611	-5.490326	-3.735698
1	7.248585	-5.247009	-4.687656
8	9.101990	-1.942485	-2.280282
8	-6.170426	5.433690	-1.789304
6	-2.524319	4.034579	-2.508482
6	-3.006406	5.113173	-3.469731
6	-3.411387	6.213460	-2.482469
6	-3.782966	5.414489	-1.207040
6	-5.208507	5.569609	-0.729058
8	-3.509130	4.043658	-1.482531
1	-1.542669	4.288833	-2.103050
1	-3.883630	4.766067	-4.022711
1	-2.237346	5.440505	-4.171009
1	-4.260279	6.797824	-2.852314
1	-3.127530	5.765801	-0.398444
1	-5.349037	6.580748	-0.345024
1	-5.426271	4.850685	0.062636
8	-2.330099	7.056852	-2.130189
1	-2.128949	7.611105	-2.890738
7	-2.407538	2.685074	-3.021757
6	-1.206639	1.982931	-2.844536
8	-0.212456	2.578599	-2.401603
7	-1.174898	0.669928	-3.166937
6	-2.258333	0.046845	-3.640403
7	-2.186536	-1.268274	-3.837796
6	-3.463007	0.766135	-3.918226
6	-3.495092	2.070167	-3.568812
1	-1.366438	-1.790456	-3.510993
1	-2.998763	-1.774600	-4.149971
1	-4.327958	0.277188	-4.345507
1	-4.386580	2.680930	-3.681469
8	8.776190	-0.364065	-0.299267
6	5.220690	0.206406	0.734291
6	6.332001	0.261008	1.771841
6	7.158795	1.401104	1.188456
6	6.978333	1.216446	-0.334853
6	8.213831	0.722353	-1.049533
8	5.914411	0.276530	-0.497415
1	4.539130	1.058207	0.849489
1	6.931088	-0.652677	1.741093
1	5.994904	0.442196	2.789094
1	8.205333	1.388253	1.496831
1	6.689844	2.177753	-0.773978
1	8.946495	1.530756	-1.116919
1	7.949730	0.393643	-2.058702
8	6.575553	2.678131	1.505914
15	9.830039	-1.363795	-0.982588
8	10.321415	-2.343014	0.002457
8	10.892151	-0.445400	-1.738229
8	-9.102610	-0.039050	0.074325
6	-5.256872	0.507459	-0.722392
6	-6.294537	0.814511	-1.797601
6	-7.178994	1.794332	-1.038205
6	-7.071690	1.302783	0.424539

6	-8.360661	0.762664	1.008050
8	-6.064865	0.296861	0.433739
1	-4.588726	1.360343	-0.579555
1	-6.884495	-0.074368	-2.034691
1	-5.890800	1.243640	-2.709522
1	-8.208419	1.827396	-1.399004
1	-6.754828	2.148471	1.047943
1	-9.019763	1.596320	1.253125
1	-8.152524	0.189554	1.913493
8	-6.627038	3.126207	-1.058342
7	-4.397995	-0.643254	-0.905065
6	-3.039395	-0.541902	-0.560239
8	-2.563548	0.576831	-0.315484
7	-2.286693	-1.665686	-0.527673
6	-2.820029	-2.857344	-0.815816
7	-2.062012	-3.941172	-0.679185
6	-4.180361	-2.975200	-1.245476
6	-4.928853	-1.852088	-1.246831
1	-1.094659	-3.871887	-0.368698
1	-2.433504	-4.850400	-0.898575
1	-4.608956	-3.931308	-1.512649
1	-5.986409	-1.863377	-1.488806
15	-6.773711	4.072819	-2.332358
8	-6.225536	3.571143	-3.614935
8	-8.337721	4.393505	-2.411167
8	6.183717	4.810950	2.684760
6	2.577772	3.558653	3.171849
6	3.210779	4.422192	4.253800
6	3.532075	5.684926	3.452728
6	3.842256	5.121078	2.046616
6	5.293690	5.212988	1.627540
8	3.424842	3.755324	2.046700
1	1.555371	3.886883	2.953513
1	4.133208	3.952518	4.608640
1	2.547333	4.610800	5.099140
1	4.385573	6.231294	3.867128
1	3.251641	5.686471	1.314769
1	5.545169	6.253403	1.416824
1	5.473984	4.610249	0.736365
8	2.404203	6.530334	3.311424
1	2.210209	6.910248	4.174297
7	-0.348413	-0.564061	3.052071
6	-0.714146	0.756180	2.940143
7	-2.014911	1.002958	2.737233
7	0.146115	1.761802	3.034910
6	1.398327	1.349856	3.288026
6	1.866419	0.052638	3.456740
6	0.948773	-1.018113	3.282981
8	1.208041	-2.231272	3.271714
7	3.229445	0.040232	3.691474
6	3.565768	1.301520	3.680294
7	2.503000	2.147922	3.435871
1	-1.061161	-1.307048	2.897758
1	-2.657564	0.247493	2.477063
1	-2.251289	1.945201	2.472441
1	4.557266	1.700530	3.857451
15	6.836667	3.388744	2.911106

8	6.384963	2.658041	4.117901
8	8.405813	3.691768	2.911349
1	-7.420175	-6.593103	3.617219
8	-7.360031	-5.759127	3.143206
6	-5.926824	-2.815130	2.198457
6	-6.716653	-3.623088	1.172387
6	-8.133563	-3.412542	1.667813
6	-7.959459	-3.433402	3.189197
6	-8.152674	-4.801384	3.821443
8	-6.636217	-2.949931	3.424024
1	-5.862984	-1.764669	1.909445
1	-6.486427	-4.687390	1.227670
1	-6.573670	-3.276313	0.154901
1	-8.857847	-4.143652	1.304385
1	-8.672626	-2.743074	3.651102
1	-9.218857	-5.060671	3.768979
1	-7.871103	-4.725843	4.878860
8	-8.590309	-2.076580	1.344260
7	-4.553969	-3.251268	2.402151
6	-3.530018	-2.290162	2.429623
8	-3.815707	-1.102266	2.234034
7	-2.262384	-2.701160	2.665115
6	-1.994170	-3.987366	2.913335
7	-0.727862	-4.322203	3.141329
6	-3.033948	-4.974422	2.964302
6	-4.292988	-4.552889	2.724493
1	-0.001189	-3.601323	3.132369
1	-0.479703	-5.279142	3.328024
1	-2.823646	-6.004759	3.216299
1	-5.159629	-5.202633	2.801409
15	-8.953258	-1.606358	-0.131771
8	-8.064069	-2.055913	-1.229011
8	-10.472939	-2.048484	-0.344183
1	-10.594414	-2.515491	-1.179772
1	-8.689492	4.250993	-3.298254
1	11.525551	-0.029730	-1.139558
1	8.834153	3.382184	3.718741
1	0.392577	-0.178004	-2.996208
7	1.301012	-0.683952	-2.903412
6	2.462693	0.046943	-2.893244
6	1.217827	-2.074025	-2.814923
7	2.329495	1.380184	-3.002023
7	3.665590	-0.495492	-2.799449
6	2.505493	-2.667290	-2.649826
8	0.121293	-2.642931	-2.862848
1	1.426810	1.827714	-2.819711
1	3.165945	1.917589	-2.839583
6	3.620848	-1.833405	-2.679991
7	2.878763	-3.992420	-2.530138
7	4.694827	-2.672011	-2.546556
6	4.181160	-3.954872	-2.473079
1	4.849318	-4.804213	-2.409094

4. Optimized X, Y, Z coordinates of cation radical ds(5'-GGG-3') in Angstroms (**Spin localized on 3'-G (Figure 4(c)**)

Charge = 1 Multiplicity = 2

1	6.933045	-6.429138	-3.104241
8	7.033622	-5.495037	-2.900485
6	6.139612	-2.224564	-2.736458
6	6.950875	-2.782555	-1.564963
6	8.305444	-3.090434	-2.183184
6	7.961187	-3.410513	-3.639007
6	7.829402	-4.899786	-3.909641
8	6.744436	-2.717918	-3.918119
1	6.136969	-1.131008	-2.742745
1	6.508594	-3.710970	-1.200965
1	7.004382	-2.061982	-0.750159
1	8.829589	-3.906169	-1.683605
1	8.736905	-3.012670	-4.300367
1	8.837306	-5.336105	-3.923120
1	7.384844	-5.030475	-4.903868
8	9.163923	-1.926056	-2.200120
8	-6.260270	5.391037	-1.772252
6	-2.579140	4.076316	-2.441079
6	-3.070089	5.154532	-3.398984
6	-3.508507	6.239627	-2.409838
6	-3.884651	5.423705	-1.146745
6	-5.321966	5.542622	-0.693349
8	-3.575557	4.061633	-1.425778
1	-1.605821	4.342630	-2.023503
1	-3.933542	4.793977	-3.965300
1	-2.299522	5.501059	-4.089378
1	-4.361746	6.812721	-2.787397
1	-3.252355	5.784560	-0.323944
1	-5.493229	6.547467	-0.305216
1	-5.536518	4.813386	0.089696
8	-2.446980	7.098473	-2.034700
1	-2.241933	7.660129	-2.788756
7	-2.437976	2.734197	-2.965754
6	-1.218387	2.054622	-2.812359
8	-0.231519	2.671117	-2.384331
7	-1.166255	0.744380	-3.145860
6	-2.244498	0.107270	-3.611709
7	-2.154835	-1.203506	-3.829273
6	-3.467021	0.805409	-3.867469
6	-3.520482	2.104295	-3.504791
1	-1.314652	-1.720577	-3.541437
1	-2.965624	-1.716133	-4.134645
1	-4.326285	0.303573	-4.291248
1	-4.424090	2.699015	-3.604078
8	8.803506	-0.421926	-0.167649
6	5.261589	0.226477	0.797590
6	6.354030	0.302670	1.855990
6	7.201698	1.426426	1.276876
6	7.057967	1.215797	-0.246542
6	8.304374	0.693523	-0.920732
8	5.989377	0.290919	-0.423561
1	4.580805	1.083163	0.877606

1	6.945652	-0.616248	1.857124
1	5.998535	0.502940	2.864410
1	8.239110	1.423197	1.615258
1	6.801577	2.176368	-0.708409
1	9.065081	1.478336	-0.950885
1	8.066629	0.384972	-1.942684
8	6.614807	2.715646	1.548717
7	0.553272	-1.379443	0.145142
6	1.053133	-0.102186	0.158309
7	0.172604	0.888079	-0.019700
7	2.328019	0.182890	0.381391
6	3.077710	-0.922569	0.553881
6	2.681100	-2.248951	0.568096
6	1.300282	-2.545224	0.331230
8	0.754143	-3.650409	0.281263
7	3.757317	-3.079827	0.815438
6	4.769298	-2.269291	0.951755
7	4.426664	-0.938645	0.803275
1	-0.455539	-1.495471	-0.074087
1	-0.820823	0.716727	-0.210925
1	0.537908	1.806020	-0.216533
15	9.840999	-1.445820	-0.837279
8	10.226308	-2.492656	0.125698
8	10.992641	-0.552675	-1.487329
8	-9.130991	-0.119868	0.069796
6	-5.292393	0.469964	-0.726837
6	-6.334681	0.763502	-1.800618
6	-7.226613	1.734853	-1.038429
6	-7.114241	1.241485	0.423596
6	-8.399068	0.689936	1.004678
8	-6.098575	0.244702	0.430406
1	-4.642546	1.336249	-0.580835
1	-6.915142	-0.131963	-2.036118
1	-5.936985	1.198079	-2.712901
1	-8.256574	1.761874	-1.398170
1	-6.805198	2.089122	1.048368
1	-9.066936	1.517411	1.246943
1	-8.188155	0.119497	1.911126
8	-6.684295	3.071345	-1.055027
7	-4.407059	-0.658155	-0.905062
6	-3.051126	-0.514435	-0.545241
8	-2.614285	0.616567	-0.297466
7	-2.269272	-1.617209	-0.494209
6	-2.761714	-2.821914	-0.794104
7	-1.971707	-3.881391	-0.642091
6	-4.112586	-2.980929	-1.248429
6	-4.895663	-1.881162	-1.260572
1	-1.002314	-3.779930	-0.325859
1	-2.310793	-4.798978	-0.878495
1	-4.506757	-3.948992	-1.526094
1	-5.947759	-1.921303	-1.522760
15	-6.844590	4.024618	-2.322032
8	-6.287552	3.541355	-3.607756
8	-8.413894	4.320286	-2.399373
8	6.132246	4.864595	2.649836
6	2.506369	3.576555	3.039446
6	3.053319	4.493123	4.123198

6	3.417192	5.720499	3.283491
6	3.805361	5.099123	1.921061
6	5.268036	5.210395	1.553036
8	3.421909	3.720077	1.971566
1	1.494244	3.871183	2.740152
1	3.954042	4.051459	4.559936
1	2.331187	4.713682	4.910028
1	4.246919	6.284013	3.721697
1	3.227849	5.607581	1.139535
1	5.500296	6.249943	1.318230
1	5.494158	4.586359	0.687269
8	2.299338	6.554120	3.043698
1	2.070117	6.988378	3.871607
15	6.742878	3.437731	2.961813
8	6.163383	2.727013	4.127773
8	8.302023	3.735949	3.126484
1	-7.343613	-6.675147	3.539842
8	-7.294469	-5.832212	3.080587
6	-5.894963	-2.855694	2.195693
6	-6.669727	-3.652114	1.148938
6	-8.092418	-3.478536	1.642274
6	-7.925404	-3.516458	3.163850
6	-8.098593	-4.896151	3.775708
8	-6.611504	-3.012685	3.412323
1	-5.831624	-1.800891	1.923370
1	-6.421881	-4.713278	1.176148
1	-6.529555	-3.277943	0.141127
1	-8.797213	-4.222369	1.266469
1	-8.651447	-2.844112	3.631796
1	-9.161100	-5.169124	3.720442
1	-7.816131	-4.833614	4.833667
8	-8.577854	-2.150725	1.331885
7	-4.520817	-3.295212	2.404002
6	-3.500047	-2.341441	2.478270
8	-3.785516	-1.143254	2.329759
7	-2.233471	-2.758991	2.709504
6	-1.966507	-4.056677	2.904283
7	-0.704548	-4.411292	3.119928
6	-3.008384	-5.039697	2.917378
6	-4.264593	-4.607425	2.685812
1	0.029913	-3.708511	3.141769
1	-0.462322	-5.377814	3.259620
1	-2.801286	-6.078187	3.135483
1	-5.132944	-5.257029	2.739320
15	-8.951360	-1.682929	-0.143124
8	-8.054681	-2.114932	-1.241030
8	-10.463174	-2.151850	-0.355202
1	-10.575500	-2.623800	-1.189286
1	-8.762352	4.180689	-3.288221
1	11.589088	-0.171961	-0.830474
1	8.641261	3.435277	3.978501
1	5.782205	-2.570286	1.174433
8	1.212601	-2.250491	3.533340
6	0.916694	-1.073441	3.395573
7	-0.369602	-0.663897	3.072028
6	1.835360	0.045846	3.506428
6	-0.746486	0.632939	2.860834

1	-1.076205	-1.435352	2.931445
6	1.337341	1.350255	3.223806
7	3.139876	0.071281	3.809248
7	-2.000028	0.876185	2.583510
7	0.114162	1.694695	2.928734
7	2.432834	2.168773	3.369743
6	3.469356	1.361107	3.721192
1	-2.693567	0.108153	2.457900
1	-2.248120	1.825102	2.344784
1	4.458476	1.769660	3.912869
1	1.429521	1.868662	-2.678538
7	2.342492	1.444583	-2.861438
6	2.488952	0.104325	-2.847171
1	3.163706	1.972251	-2.613412
7	1.335463	-0.632794	-2.928380
7	3.694617	-0.430375	-2.787426
6	1.267588	-2.026243	-2.953721
1	0.427204	-0.128066	-2.972227
6	3.662933	-1.776811	-2.792366
6	2.560359	-2.617227	-2.866663
8	0.173730	-2.600382	-3.041832
7	4.745398	-2.612537	-2.715229
7	2.946049	-3.945694	-2.850951
6	4.246517	-3.900578	-2.762747
1	4.923519	-4.745196	-2.753859

5. Optimized X, Y, Z coordinates of neutral ds(5’-G8OXGG-3’) in Angstroms

Charge = 0 Multiplicity = 1

H	6.49926	-6.11013	-3.55346
O	6.63238	-5.18850	-3.31465
C	5.80090	-1.90564	-2.99928
C	6.65354	-2.51937	-1.88824
C	7.97205	-2.82322	-2.58130
C	7.55592	-3.08831	-4.02848
C	7.37898	-4.56452	-4.34386
O	6.34821	-2.35444	-4.22801
H	5.81175	-0.81275	-2.96363
H	6.21755	-3.45703	-1.54209
H	6.74905	-1.84882	-1.03526
H	8.50893	-3.66079	-2.13397
H	8.31061	-2.68701	-4.71184
H	8.37640	-5.01619	-4.43210
H	6.87676	-4.64981	-5.31542
O	8.84609	-1.66998	-2.60621
N	1.01271	-0.27826	-3.24987
C	2.16961	0.45060	-3.15306
N	2.03103	1.79244	-3.17131
N	3.37167	-0.09170	-3.07978
C	3.32852	-1.43775	-3.05392
C	2.22001	-2.26956	-3.12572
C	0.93465	-1.67050	-3.26091
O	-0.15852	-2.23903	-3.38356
N	2.59384	-3.60086	-3.07367

C	3.89308	-3.56480	-2.96725
N	4.40349	-2.28020	-2.93726
H	0.10763	0.23198	-3.28435
H	1.12044	2.21345	-2.96646
H	2.85339	2.31206	-2.90958
H	4.56069	-4.41614	-2.94094
O	-6.52064	5.56163	-1.17208
C	-2.90130	4.35902	-2.37062
C	-3.51092	5.47795	-3.20681
C	-3.88120	6.48992	-2.11593
C	-4.07895	5.59503	-0.86544
C	-5.44567	5.65328	-0.22159
O	-3.78663	4.25974	-1.26131
H	-1.89576	4.62683	-2.03852
H	-4.41483	5.12505	-3.71094
H	-2.81950	5.89020	-3.94342
H	-4.79606	7.03692	-2.36626
H	-3.35031	5.92434	-0.11158
H	-5.57428	6.62434	0.25800
H	-5.54711	4.86600	0.52771
O	-2.82505	7.38264	-1.81214
H	-2.73987	7.99845	-2.54668
N	-2.78614	3.05367	-2.98519
C	-1.54417	2.39395	-2.98218
O	-0.53323	3.01235	-2.62381
N	-1.50302	1.10153	-3.38311
C	-2.60996	0.46486	-3.77352
N	-2.51955	-0.83378	-4.05957
C	-3.86231	1.14940	-3.88375
C	-3.90367	2.42751	-3.45205
H	-1.65942	-1.34996	-3.83569
H	-3.35149	-1.35117	-4.29145
H	-4.75002	0.65034	-4.24804
H	-4.82214	3.00722	-3.43277
O	8.67451	-0.25812	-0.48456
C	5.21284	0.33767	0.74296
C	6.38022	0.32278	1.72138
C	7.20955	1.47254	1.17901
C	6.95299	1.40015	-0.34144
C	8.13869	0.90362	-1.13651
O	5.84971	0.52144	-0.52365
H	4.54582	1.18391	0.94779
H	6.93291	-0.60938	1.61175
H	6.08775	0.45977	2.75875
H	8.26965	1.41171	1.43282
H	6.69902	2.40380	-0.70356
H	8.90971	1.67773	-1.17932
H	7.82146	0.65469	-2.15313
O	6.69487	2.74906	1.61111
N	0.49289	-1.14369	-0.10579
C	1.03972	0.11030	-0.09289
N	0.21086	1.12331	-0.36529
N	2.32511	0.34339	0.15017
C	3.02477	-0.77439	0.38669
C	2.55615	-2.06446	0.39190
C	1.19734	-2.32559	0.12078
O	0.63447	-3.43008	0.07360

N	3.63084	-2.89884	0.69016
C	4.76082	-2.16138	0.90136
N	4.37530	-0.82253	0.69633
H	-0.52017	-1.23753	-0.32647
H	-0.80145	0.99570	-0.43551
H	0.59183	2.05318	-0.38679
P	9.63178	-1.26605	-1.27841
O	10.07069	-2.36454	-0.39876
O	10.75204	-0.36449	-1.97377
O	-9.09232	-0.20283	0.39704
C	-5.36466	0.63085	-0.58386
C	-6.50014	0.96453	-1.54541
C	-7.36031	1.83855	-0.64360
C	-7.12707	1.22856	0.75847
C	-8.34162	0.55323	1.36213
O	-6.06532	0.29240	0.61460
H	-4.72672	1.50400	-0.42657
H	-7.06748	0.06771	-1.80632
H	-6.19183	1.48203	-2.44852
H	-8.41441	1.86024	-0.92538
H	-6.82274	2.03378	1.43903
H	-9.03278	1.31385	1.72739
H	-8.04057	-0.08885	2.19180
O	-6.85743	3.19052	-0.58916
N	-4.47203	-0.45388	-0.91654
C	-3.09251	-0.30265	-0.65704
O	-2.65277	0.82186	-0.38561
N	-2.29850	-1.39480	-0.72408
C	-2.80139	-2.59411	-1.02651
N	-2.00236	-3.65361	-0.94866
C	-4.17535	-2.74939	-1.40556
C	-4.97061	-1.66485	-1.29800
H	-1.03736	-3.56202	-0.60987
H	-2.36274	-4.56915	-1.15954
H	-4.57622	-3.70896	-1.70296
H	-6.03909	-1.71269	-1.47978
P	-7.12909	4.22645	-1.77032
O	-6.67818	3.84018	-3.12845
O	-8.70174	4.50573	-1.69789
O	6.29559	4.74616	2.98680
C	2.82402	3.03286	3.54347
C	3.37779	3.84856	4.70293
C	3.58679	5.20072	4.01805
C	3.88182	4.79830	2.55153
C	5.26961	5.14080	2.05988
O	3.66763	3.39123	2.45517
H	1.78850	3.32050	3.32792
H	4.33814	3.43226	5.01977
H	2.69836	3.90632	5.55485
H	4.41938	5.75994	4.45758
H	3.16455	5.32761	1.91006
H	5.36324	6.22419	1.97337
H	5.45468	4.68416	1.08623
O	2.40620	5.98392	3.99357
H	2.22691	6.27375	4.89360
N	0.01076	-1.09570	3.04705
C	-0.31760	0.22090	2.83328

N	-1.57357	0.47157	2.43953
N	0.53163	1.21968	3.00997
C	1.74173	0.79885	3.41557
C	2.18244	-0.49314	3.65920
C	1.26559	-1.56561	3.44115
O	1.47045	-2.78100	3.55385
N	3.50342	-0.49159	4.07742
C	3.83814	0.76988	4.09481
N	2.81181	1.60768	3.69851
H	-0.70172	-1.81754	2.82936
H	-2.23555	-0.28022	2.22436
H	-1.75028	1.38062	2.04543
H	4.80170	1.17709	4.37389
P	6.94820	3.30327	3.08156
O	6.52217	2.45677	4.21995
O	8.51392	3.63576	3.11540
H	-7.15847	-7.05772	3.15148
O	-7.11881	-6.17894	2.76411
C	-5.69607	-3.15638	2.07971
C	-6.54182	-3.83987	1.00866
C	-7.93274	-3.68325	1.59270
C	-7.68862	-3.86828	3.09255
C	-7.86440	-5.29566	3.58241
O	-6.35326	-3.41523	3.31503
H	-5.62981	-2.08175	1.90211
H	-6.31611	-4.90397	0.93020
H	-6.44348	-3.37688	0.03224
H	-8.67753	-4.37099	1.18765
H	-8.37451	-3.22975	3.65857
H	-8.93479	-5.54142	3.55738
H	-7.52834	-5.33718	4.62566
O	-8.39597	-2.31941	1.43657
N	-4.32168	-3.62293	2.18428
C	-3.28645	-2.67527	2.26107
O	-3.56153	-1.47753	2.12042
N	-2.02461	-3.10862	2.49234
C	-1.76763	-4.40875	2.66170
N	-0.51166	-4.76898	2.91351
C	-2.81166	-5.39273	2.61208
C	-4.06818	-4.94687	2.40357
H	0.21992	-4.06066	3.02481
H	-0.28632	-5.73695	3.07101
H	-2.60916	-6.44094	2.78421
H	-4.93842	-5.59588	2.43070
P	-8.89845	-1.73774	0.04364
O	-8.08612	-2.04935	-1.15609
O	-10.40991	-2.23928	-0.08585
H	-10.58428	-2.62321	-0.95378
H	-9.11774	4.43282	-2.56540
H	11.39725	-0.01834	-1.34461
H	8.94030	3.25919	3.89450
O	5.87369	-2.57427	1.20317
H	3.59586	-3.89643	0.81445

6. Optimized X, Y, Z coordinates of cation radical ds(5'-G**8OG**G-3') in Angstroms

Charge = 1 Multiplicity = 2

H	6.90678	-6.33484	-3.13654
O	6.99828	-5.39723	-2.94537
C	6.06552	-2.16459	-2.71462
C	6.97023	-2.71385	-1.61339
C	8.28474	-2.94470	-2.33776
C	7.83686	-3.30004	-3.75650
C	7.72646	-4.79559	-4.00056
O	6.57721	-2.65141	-3.94083
H	6.04766	-1.07160	-2.72218
H	6.60145	-3.67458	-1.25363
H	7.04251	-2.02842	-0.77112
H	8.90146	-3.71910	-1.87973
H	8.54184	-2.88771	-4.48472
H	8.74194	-5.20924	-4.06460
H	7.23256	-4.94776	-4.96818
O	9.05948	-1.72554	-2.43409
N	1.25185	-0.63368	-2.92970
C	2.40170	0.11573	-2.92013
N	2.24762	1.44636	-3.02345
N	3.61336	-0.40780	-2.83193
C	3.58969	-1.74529	-2.70832
C	2.48810	-2.59644	-2.66769
C	1.19078	-2.02466	-2.83797
O	0.10309	-2.61035	-2.88657
N	2.88520	-3.91548	-2.54484
C	4.18790	-3.85624	-2.50112
N	4.67938	-2.56478	-2.57814
H	0.33596	-0.14200	-3.02351
H	1.33762	1.88072	-2.84380
H	3.07687	1.99673	-2.86805
H	4.86855	-4.69616	-2.45010
O	-6.27772	5.43874	-1.80329
C	-2.62769	4.04060	-2.54469
C	-3.12040	5.10632	-3.51487
C	-3.52776	6.21446	-2.53725
C	-3.88259	5.42711	-1.24970
C	-5.30262	5.58391	-0.75636
O	-3.60801	4.05436	-1.51465
H	-1.64629	4.30568	-2.14571
H	-3.99767	4.74787	-4.06039
H	-2.35612	5.43114	-4.22252
H	-4.38485	6.78653	-2.90738
H	-3.21845	5.78818	-0.45250
H	-5.43990	6.59787	-0.37870
H	-5.51010	4.87093	0.04349
O	-2.45205	7.07217	-2.20308
H	-2.26317	7.62047	-2.97105
N	-2.50276	2.68718	-3.04554
C	-1.29168	2.00070	-2.87526
O	-0.30321	2.60975	-2.43878
N	-1.24437	0.68818	-3.19863
C	-2.32198	0.05123	-3.66603

N	-2.22962	-1.26144	-3.87441
C	-3.54097	0.75262	-3.92816
C	-3.58741	2.05687	-3.58044
H	-1.40316	-1.77265	-3.54750
H	-3.03790	-1.77993	-4.17682
H	-4.40407	0.25130	-4.34476
H	-4.48712	2.65689	-3.68600
O	8.68638	-0.23864	-0.38831
C	5.12089	0.19942	0.75253
C	6.24972	0.26566	1.77328
C	7.04710	1.42588	1.19358
C	6.82973	1.27533	-0.32882
C	8.06188	0.84567	-1.09033
O	5.79341	0.30840	-0.49026
H	4.42570	1.03699	0.89117
H	6.84899	-0.64361	1.72136
H	5.92217	0.43315	2.79594
H	8.10195	1.41482	1.47269
H	6.50030	2.23999	-0.73201
H	8.76203	1.68283	-1.15500
H	7.78287	0.53516	-2.10127
O	6.46821	2.69482	1.55759
N	0.35762	-1.42469	0.09381
C	0.88962	-0.16621	0.07396
N	0.07477	0.84082	-0.11542
N	2.21341	0.10088	0.24587
C	2.94761	-0.95402	0.47171
C	2.48716	-2.29393	0.51261
C	1.09042	-2.58434	0.28392
O	0.59908	-3.70194	0.24157
N	3.54007	-3.08254	0.78131
C	4.69445	-2.30674	0.96557
N	4.29148	-0.98156	0.73683
H	-0.67037	-1.53157	-0.13036
H	-0.95287	0.71918	-0.22277
H	0.47208	1.76390	-0.21369
P	9.77259	-1.16442	-1.12095
O	10.31920	-2.15765	-0.17950
O	10.78713	-0.17103	-1.84899
O	-9.16185	-0.04109	0.12836
C	-5.33484	0.52016	-0.73250
C	-6.38960	0.82250	-1.79206
C	-7.26554	1.80113	-1.02150
C	-7.13360	1.31386	0.44087
C	-8.41106	0.77066	1.04619
O	-6.12362	0.31092	0.43720
H	-4.66581	1.37433	-0.60179
H	-6.98137	-0.06787	-2.01788
H	-6.00093	1.24976	-2.71162
H	-8.30061	1.82926	-1.36631
H	-6.81000	2.16246	1.05686
H	-9.07119	1.60222	1.29556
H	-8.18653	0.20446	1.95198
O	-6.72016	3.13528	-1.05384
N	-4.47844	-0.62953	-0.92776
C	-3.11635	-0.52914	-0.59464
O	-2.63998	0.58615	-0.34039

N	-2.36212	-1.65339	-0.58606
C	-2.89707	-2.84184	-0.88437
N	-2.13622	-3.92669	-0.77570
C	-4.26266	-2.95687	-1.29706
C	-5.01233	-1.83505	-1.27564
H	-1.16780	-3.86183	-0.46850
H	-2.51129	-4.83308	-1.00056
H	-4.69385	-3.91055	-1.56869
H	-6.07311	-1.84639	-1.50235
P	-6.87365	4.07039	-2.33569
O	-6.32473	3.56038	-3.61472
O	-8.43901	4.38377	-2.41500
O	6.14329	4.81142	2.78738
C	2.56497	3.52153	3.33969
C	3.21741	4.36388	4.42661
C	3.50770	5.64849	3.64830
C	3.78511	5.12218	2.22073
C	5.22398	5.23796	1.76616
O	3.38234	3.75278	2.19904
H	1.53588	3.84873	3.15342
H	4.15259	3.89532	4.74763
H	2.57328	4.52650	5.29211
H	4.36746	6.19189	4.05365
H	3.16929	5.69945	1.51939
H	5.46283	6.28593	1.57934
H	5.38463	4.66200	0.85365
O	2.37003	6.48777	3.55689
H	2.19538	6.84507	4.43338
N	-0.32463	-0.60618	3.04506
C	-0.69400	0.71566	2.96236
N	-1.98970	0.96266	2.72904
N	0.15834	1.71995	3.10848
C	1.40701	1.30448	3.37627
C	1.87905	0.00570	3.51221
C	0.97049	-1.06214	3.28351
O	1.23330	-2.27478	3.23213
N	3.23953	-0.00537	3.76831
C	3.56822	1.25702	3.80256
N	2.50263	2.10473	3.56944
H	-1.03416	-1.34526	2.86228
H	-2.62826	0.21370	2.44207
H	-2.22632	1.91288	2.49546
H	4.55591	1.65567	4.00076
P	6.79322	3.37929	2.96078
O	6.38935	2.63693	4.17747
O	8.36449	3.67009	2.89925
H	-7.40651	-6.58961	3.64451
O	-7.35186	-5.75615	3.16891
C	-5.92143	-2.81979	2.19448
C	-6.73633	-3.62287	1.18427
C	-8.14201	-3.40670	1.70907
C	-7.93697	-3.42720	3.22654
C	-8.12431	-4.79369	3.86361
O	-6.60694	-2.95014	3.43393
H	-5.85718	-1.76970	1.90429
H	-6.50942	-4.68823	1.23318
H	-6.61269	-3.27507	0.16446

H	-8.87615	-4.13558	1.36117
H	-8.63715	-2.73295	3.70222
H	-9.19282	-5.04696	3.83405
H	-7.81971	-4.71937	4.91470
O	-8.60051	-2.06951	1.39346
N	-4.54748	-3.26474	2.37266
C	-3.51726	-2.30995	2.38165
O	-3.79838	-1.12205	2.18018
N	-2.24928	-2.72660	2.60747
C	-1.98733	-4.01167	2.86842
N	-0.72265	-4.35150	3.09883
C	-3.03187	-4.99292	2.93133
C	-4.29067	-4.56587	2.70008
H	0.00847	-3.63517	3.08765
H	-0.48096	-5.30759	3.29808
H	-2.82537	-6.02274	3.18860
H	-5.16002	-5.21037	2.78968
P	-9.00501	-1.60806	-0.07445
O	-8.14071	-2.05397	-1.19278
O	-10.52522	-2.06679	-0.24497
H	-10.66597	-2.52948	-1.07994
H	-8.79150	4.23160	-3.30020
H	11.40391	0.25119	-1.23770
H	8.82144	3.34895	3.68606
O	5.78833	-2.71617	1.26360
H	3.52721	-4.08695	0.89711