Electronic Supplementary Information (ESI) for

Mechanistic Insights into the Photogeneration and Quenching of Guanine Radical Cation in One-electron Oxidation of G-Quadruplex DNA

Yumei Yang,[†] Wenjing Yang,[‡] Hongmei Su,[†] Weihai Fang[†] and Xuebo Chen[†]*

[†]Key Laboratory of Theoretical and Computational Photochemistry of Ministry of Education, Department of Chemistry, Beijing Normal University, Xin-wai-da-jie No. 19, Beijing, 100875, People's Republic of China

[‡]College of Material Science & Engineering, Taiyuan University of Technology, Shanxi 030024, People's Republic of China

Corresponding email: xuebochen@bnu.edu.cn

Contents

2.QM/MM Partition

Scheme S1. *The chosen QM/MM partitioning: QM1 includes G-G (G-quartet) and $Na_2S_2O_8$ molecule as well as three crystal water molecules. QM2 includes G-T (loop) and $Na_2S_2O_8$ molecule as well as three crystal water molecules. The red wavy lines indicate the bonds between the QM and MM regions. See text for details.*

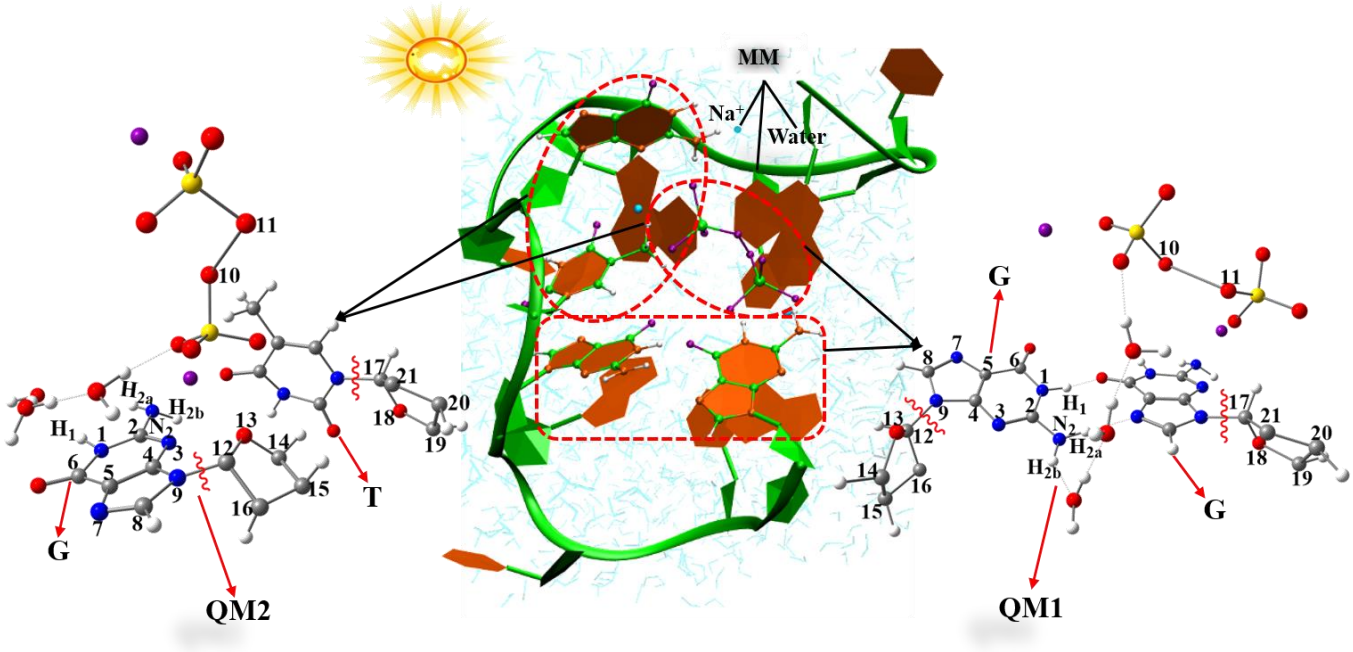


Table S1. *Re-parameterized point charges (a.u.) for the MM atoms near the QM/MM boundary.*

QM1		***QM2***	
C12	0.0000	C12	0.0000
O13	0.3491	O13	0.3291
C14	0.1729	C14	0.1829
C15	0.0741	C15	0.0763
C16	0.0824	C16	0.0824
C17	0.0000	C17	0.0000
O18	0.3491	O18	0.3291
C19	0.1729	C19	0.1829
C20	0.0741	C20	0.0763
C21	0.0824	C21	0.0824

2.Molecular Orbitals in Active Space

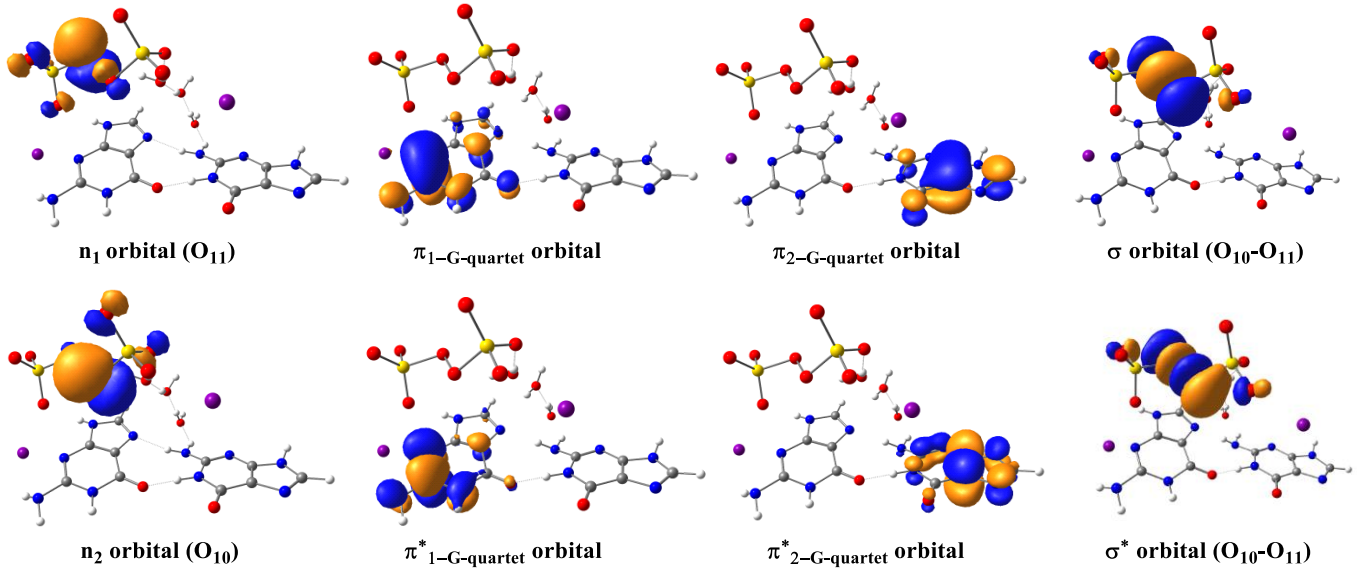


Figure S2.1 *Molecular orbitals for the QM1 subsystem including the G-G (G-quartet) and $Na_2S_2O_8$ molecule as well as three crystal water molecules used in defining the active space calculated at the CASPT2//CASSCF(10e,8o)/AMBER QM/MM level of theory.*

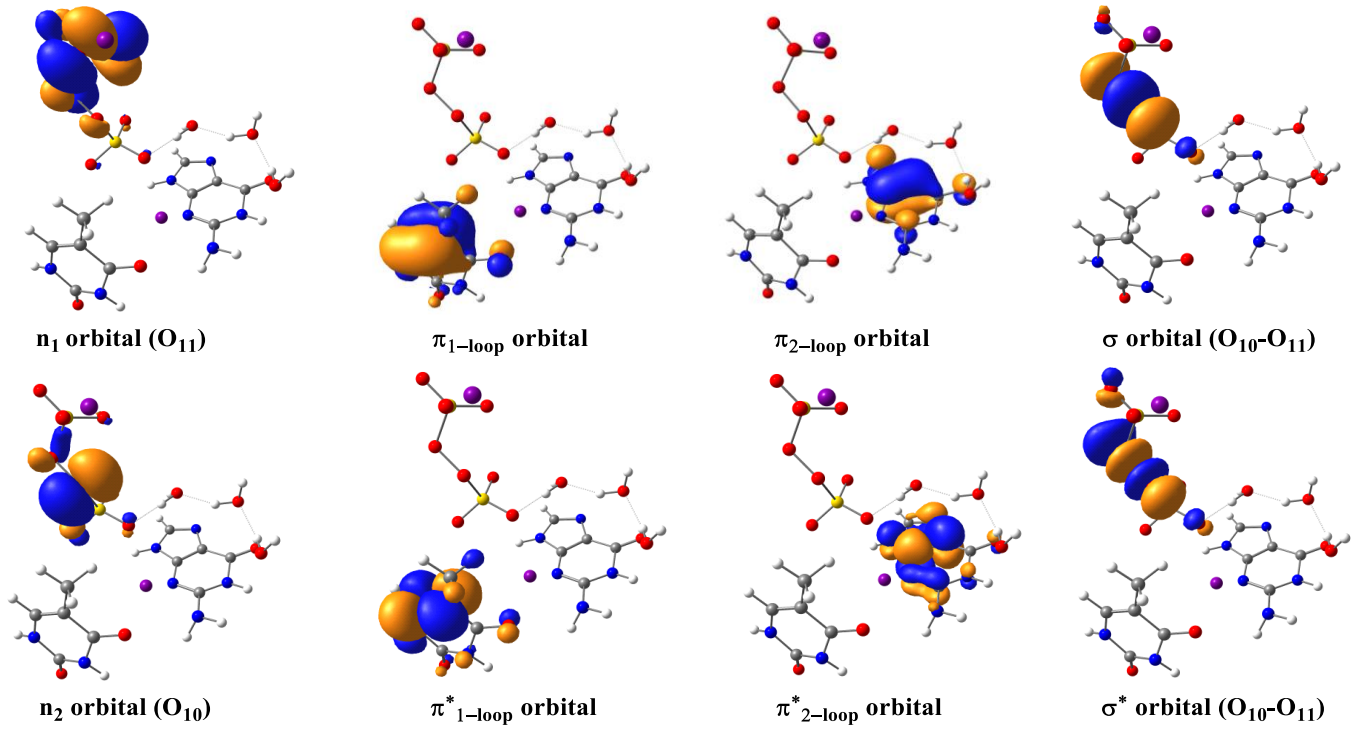


Figure S2.2 *Molecular orbitals for the QM2 subsystem including the G-T (loop) and $Na_2S_2O_8$ molecule as well as three crystal water molecules used in defining the active space calculated at the CASPT2//CASSCF(10e,8o)/AMBER QM/MM level of theory.*

2.1.Molecular Orbitals in Active Space CAS(14e,12o)

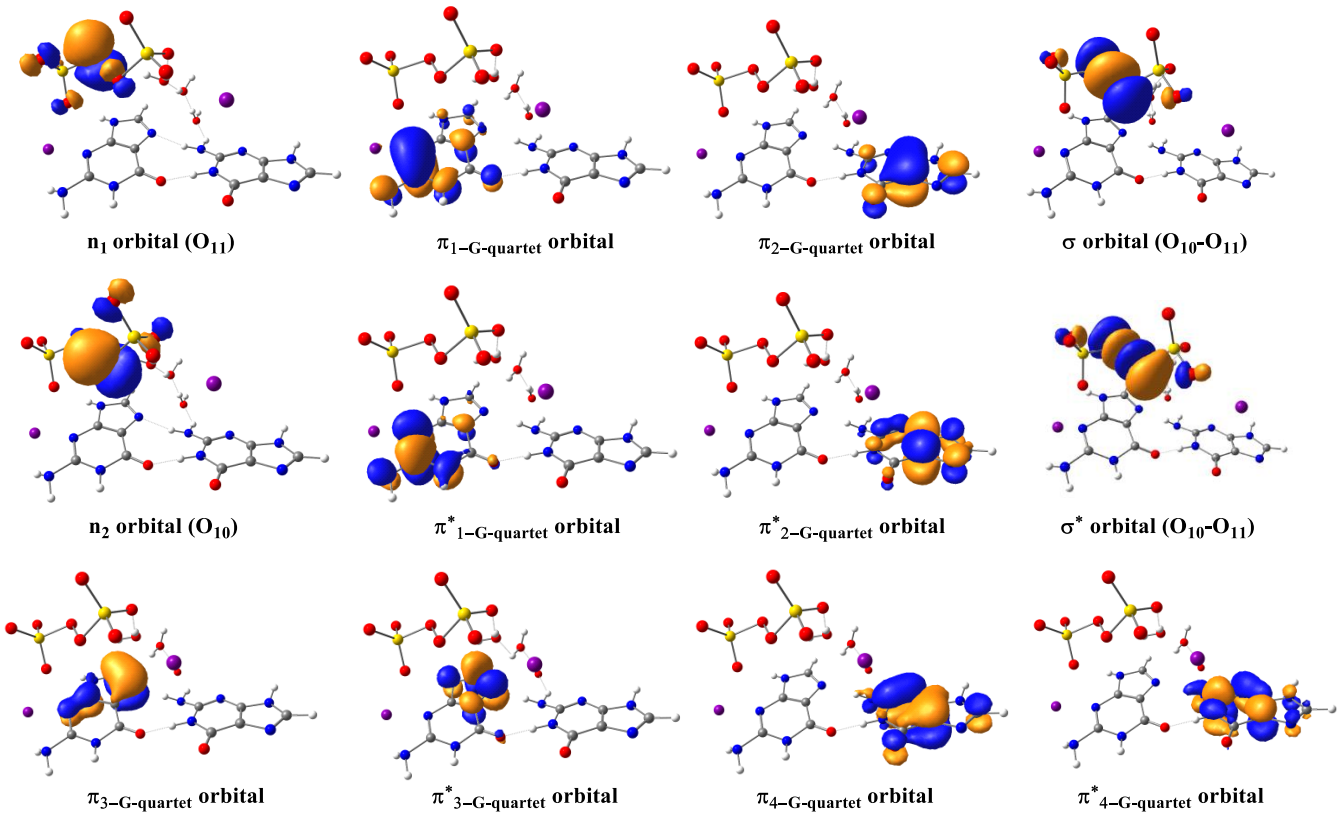


Figure S2.3 *Molecular orbitals for the QM1 subsystem including the G-G (G-quartet) and $Na_2S_2O_8$ molecule as well as three crystal water molecules used in defining the active space calculated at the CASPT2//CASSCF(14e,12o)/AMBER QM/MM level of theory.*

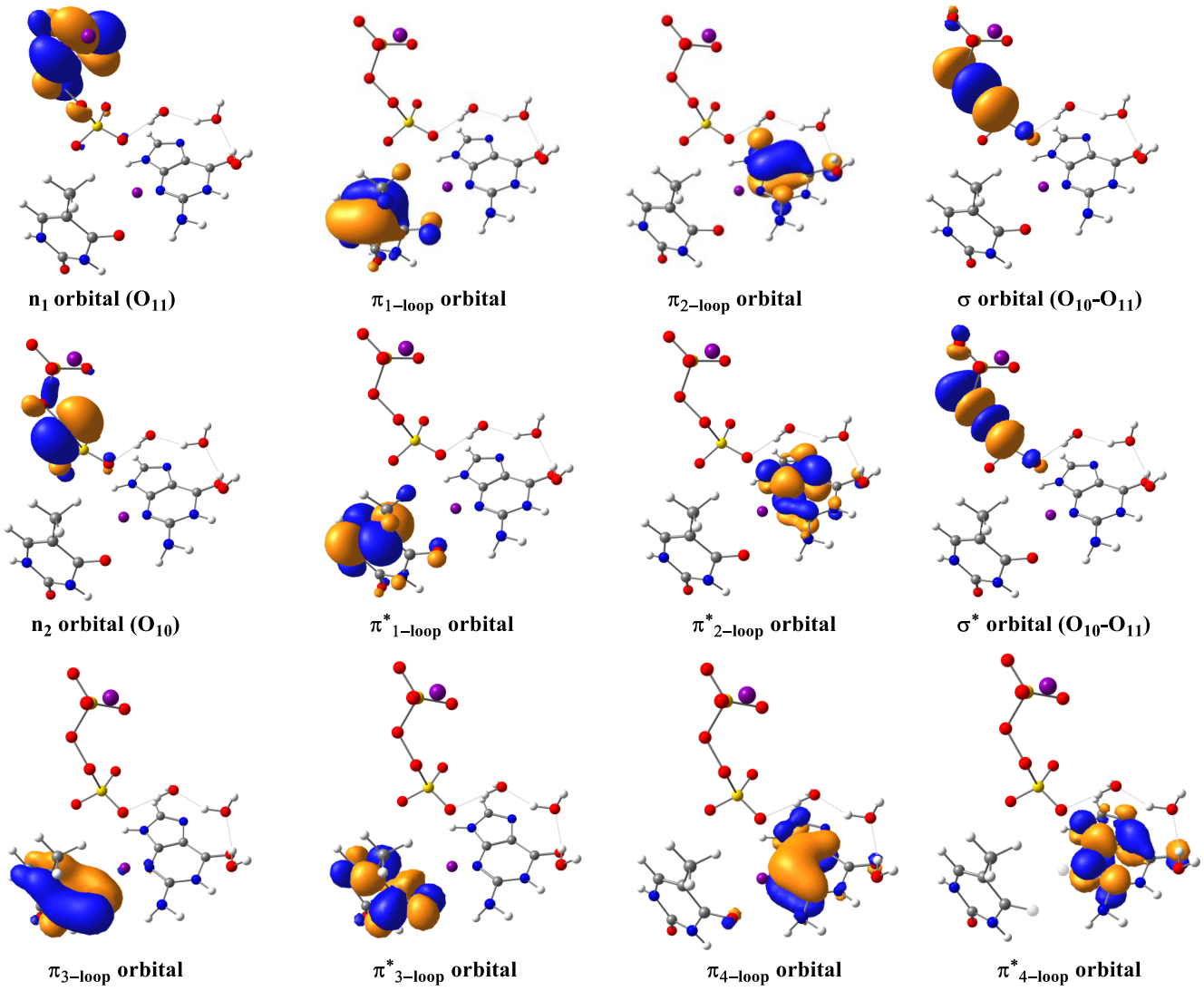


Figure S2.4 *Molecular orbitals for the QM2 subsystem including the G-T (loop) and $Na_2S_2O_8$ molecule as well as three crystal water molecules used in defining the active space calculated at the CASPT2//CASSCF(14e,12o)/AMBER QM/MM level of theory.*

3. Optimized Structures

Figure S3.1 *Schematically critical points with the key bond lengths/distances (Å) for G-G (G-quartet) leading to the G(N_2-H_{2b})$^{\cdot}$ radical obtained at the CASSCF/AMBER QM/MM level of theory. The corresponding energy profiles are plotted in Figure 1 of the main article.*

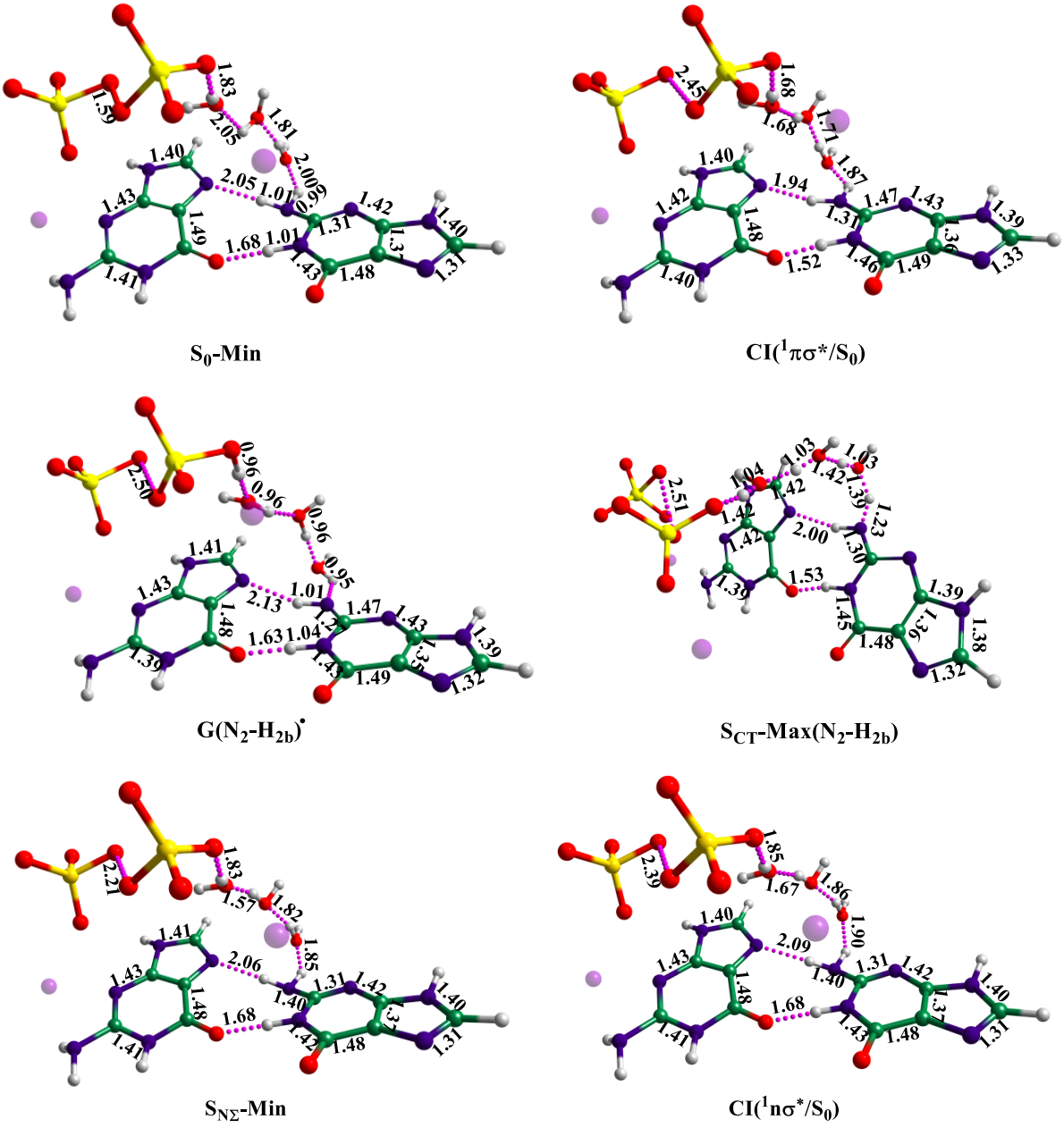
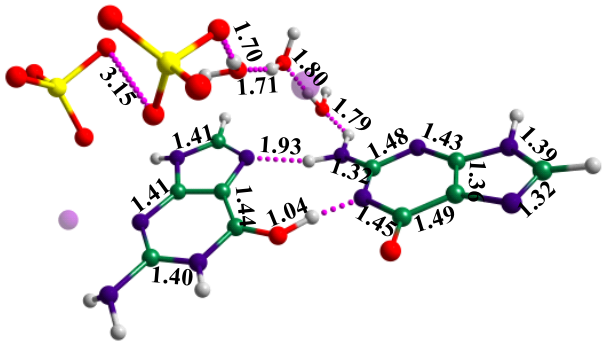
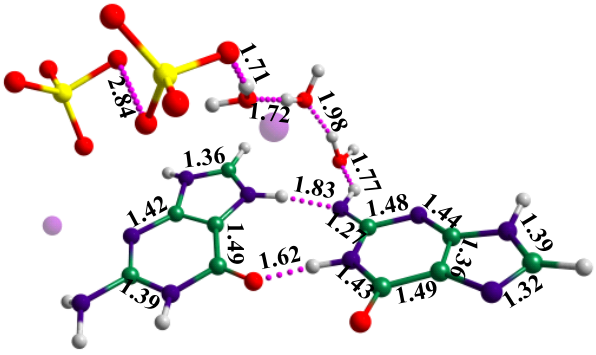


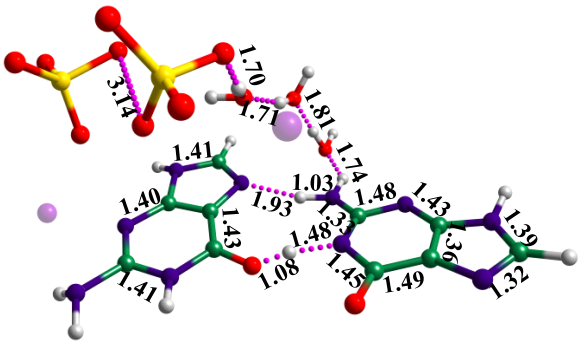
Figure S3.2 *Schematically critical points with the key bond lengths/distances (Å) for G-G (G-quartet) leading the G(N_1-H_1)$^{\cdot}$ and G(N_2-H_{2a})$^{\cdot}$ radicals obtained at the CASSCF/AMBER QM/MM level of theory. The corresponding energy profiles are plotted in Figure 2 of the main article.*



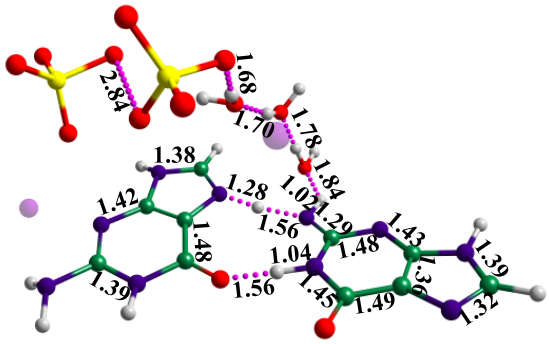
$G(N_1\text{-}H_1)^{\bullet}$



$G(N_2\text{-}H_{2a})^{\bullet}$

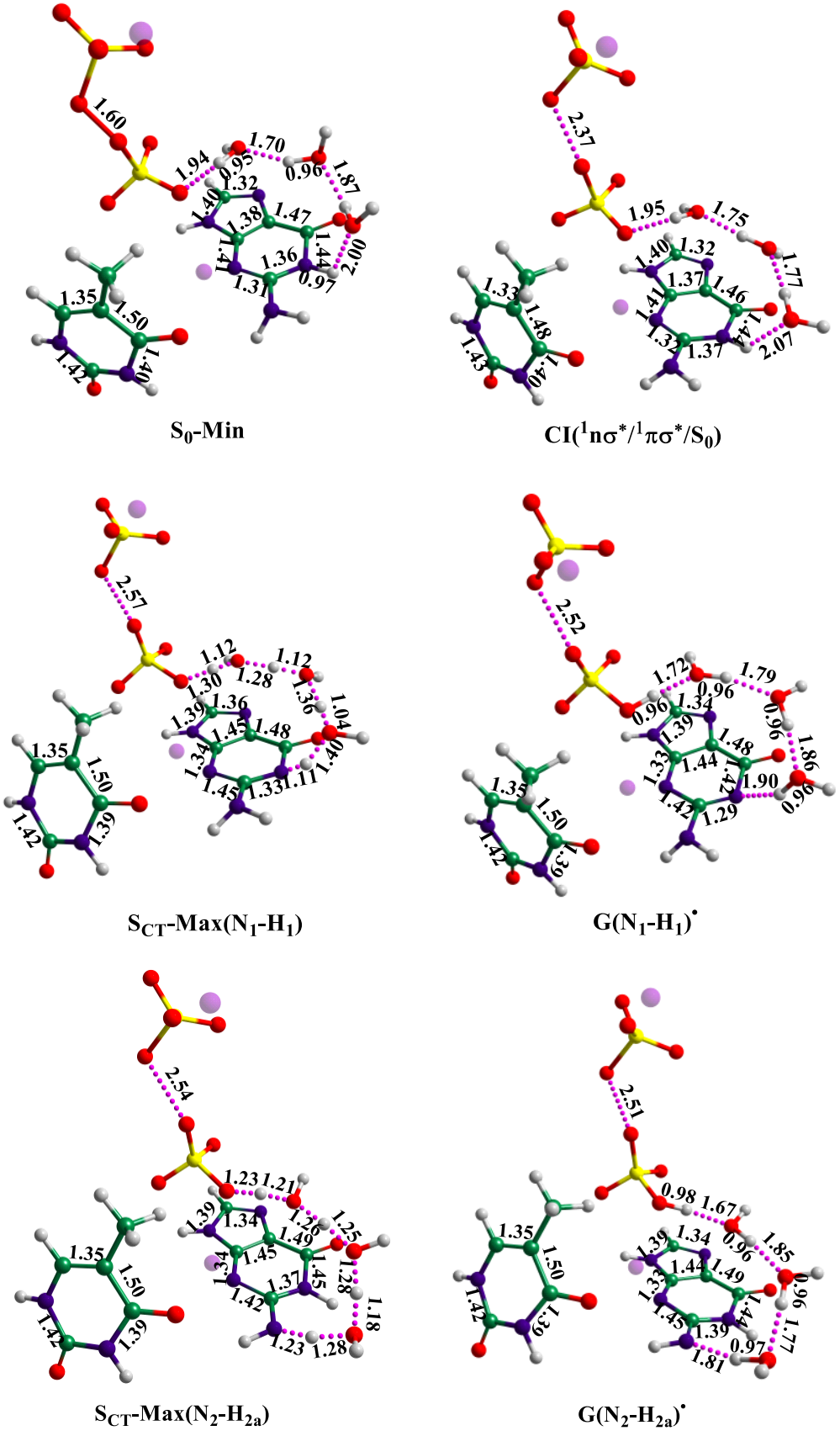


S_{CT}-Max(N_1-H_1)



S_{CT}-Max(N_2-H_{2a})

Figure S3.3 *Schematically critical points with the key bond lengths/distances (Å) for G-T (loop) leading to the G(N_1-H_1)$^{\cdot}$ and G(N_2-H_{2a})$^{\cdot}$ radicals obtained at the CASPT2//CASSCF/AMBER QM/MM level of theory. The corresponding energy profiles are plotted in Figure 3 of the main article.*



4. MEPs of the photogeneration and quenching of guanine radical cation obtained at the CASPT2//CASSCF(14e,12o) QM/MM level of theory.

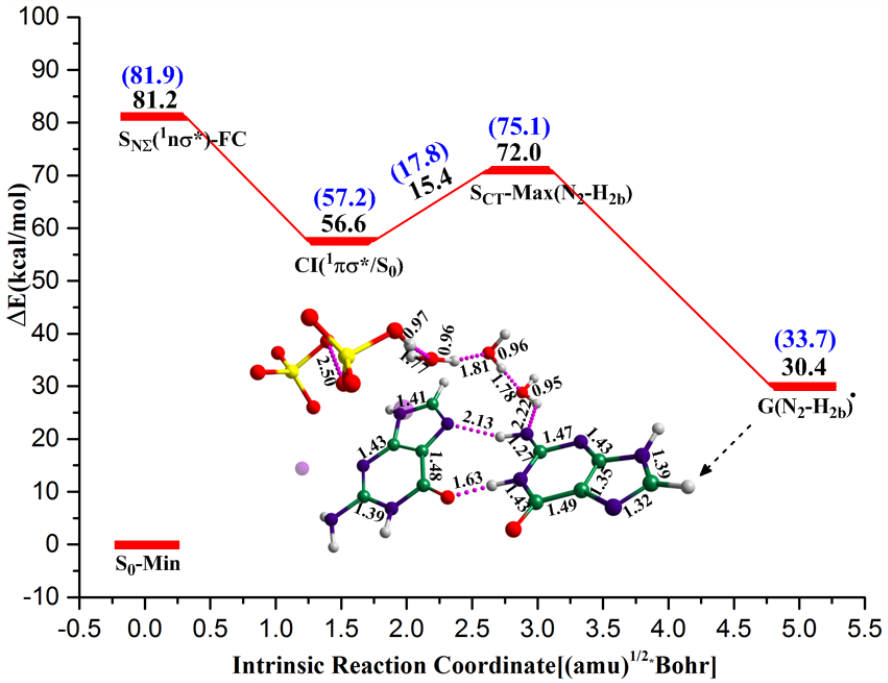
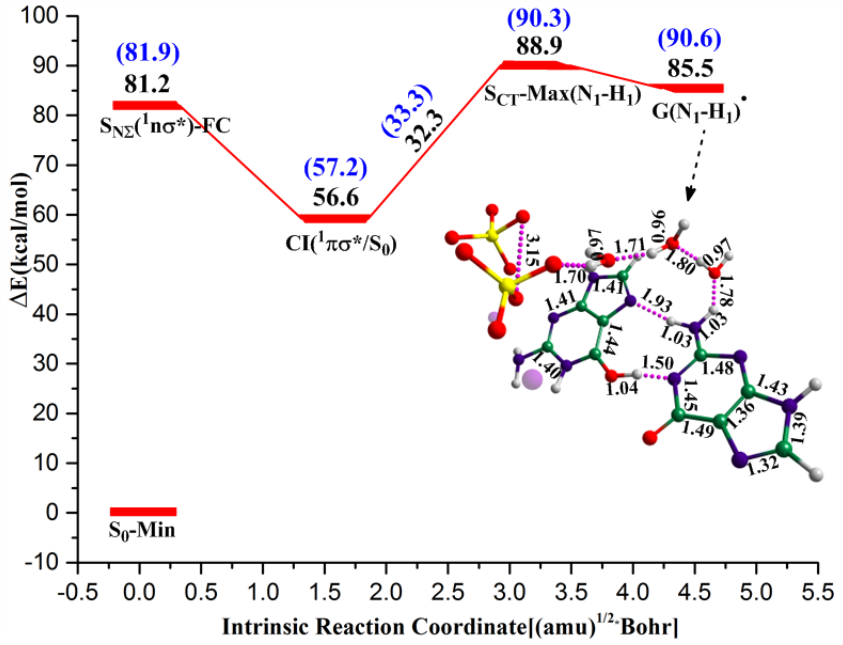
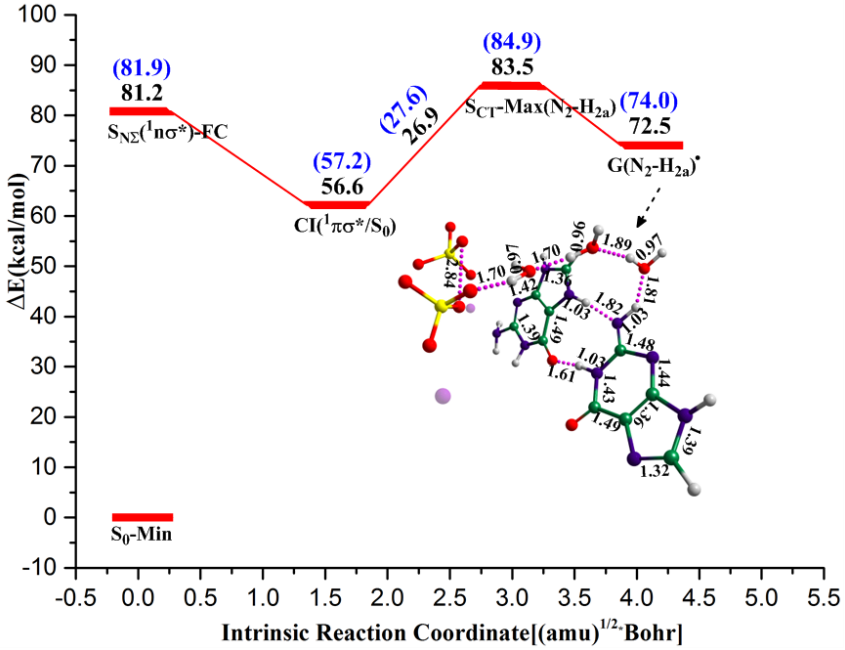


Figure 4.1 *MEPs of the relaxation process for the photo-excited peroxydisulfate followed by the free amino proton (N_2−H_{2b}) transfer for the G-G (G-quartet) moiety of TBA calculated at the CASPT2//IRC/CASSCF(14e,12o)/Amber level of theory. The relative energies (in blue) are also provided at the CASPT2//IRC/CASSCF(10e,8o)/Amber level of theory. Selected stationary structures are provide with their key bond lengths in Å.*

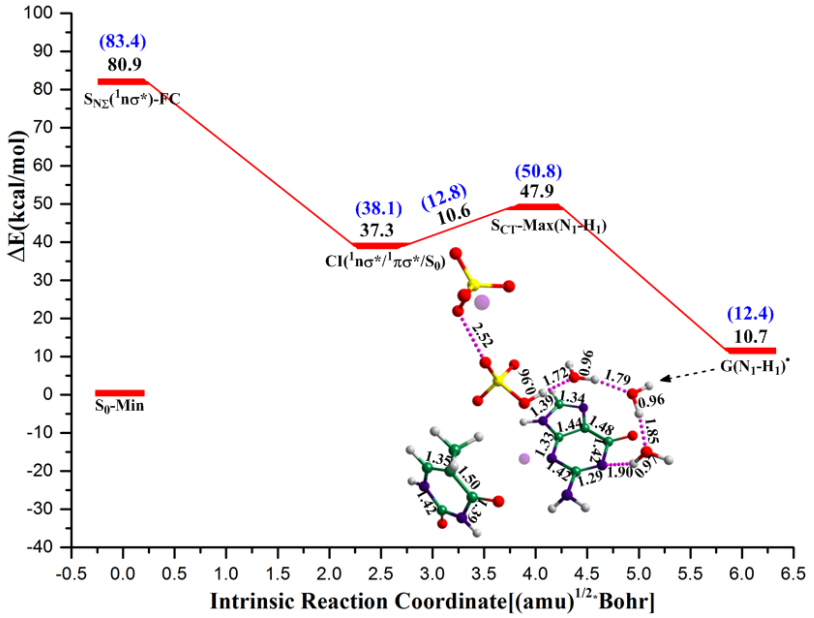


(a)

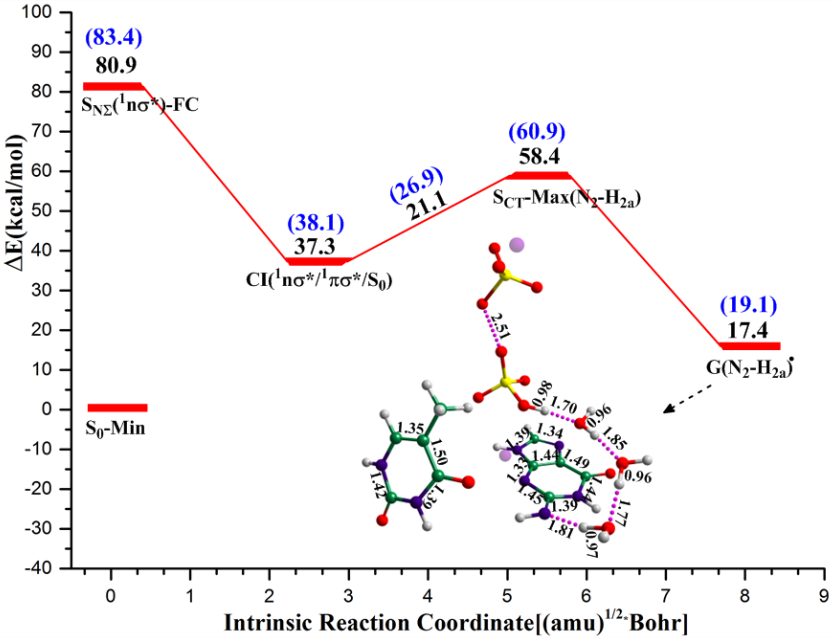


(b)

Figure 4.2 *MEPs of the relaxation process for the photo-excited peroxydisulfate along the inter-base hydrogen bonded imino N_1-H_1 (a) and the amino N_2-H_{2a} protons (b) transfer of G-quartet calculated at the CASPT2//IRC/CASSCF(14e,12o)/Amber level of theory. The relative energies (in blue) are also provided at the CASPT2//IRC/CASSCF(10e,8o)/Amber level of theory. Selected stationary structures are provide with their key bond lengths in Å.*



(a)



(b)

Figure 4.3 *MEPs of the relaxation process for the photo-excited peroxydisulfate followed by the free imino N_1–H_1 (a) and the free amino N_2-H_{2a} protons (b) transfer of the G-T (loop) of TBA calculated at the CASPT2//IRC/CASSCF(14e,12o)/Amber level of theory. The relative energies (in blue) are also provided at the CASPT2//IRC/CASSCF(10e,8o)/Amber level of theory. Selected stationary structures are provide with their key bond lengths in Å.*

5. Tables

Table S5.1 *Vertical excitation energies (⊿E, kcal/mol), oscillator strength (f), dipole moment (D.M., Debye), and the character of singly occupied orbital involved in the $S_0 \rightarrow S_{N\Sigma}(^1n\sigma^*)$ and $S_0 \rightarrow S_{\Sigma\Sigma}(^1\sigma\sigma^*)$ electronic transitions for the optimized structures of $Na_2O_2S_8$ in the isolated form of ground state computed with the 11-root state-averaged CASPT2 method. The absolute energies (A.E.) in Hartree and relative energies (R.E.) in kcal/mol.*

$Na_2O_2S_8$	CASSCF	CASPT2	
	A.E.	A.E.	R.E.
S_0	-1717.5621		
Root1		-1719.2790	0
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]		-1719.1509	80.3949
Root3		-1719.1338	91.1079
Root4		-1719.1265	95.7027
Root5		-1719.1119	104.8179
Root6		-1719.0863	120.8995
Root7		-1719.0516	142.7044
Root8[**$S_{\Sigma\Sigma}(^1\sigma\sigma^*)$**]		-1719.0247	159.6074
Root9		-1719.0007	174.6304
Root10		-1718.9469	208.3552
Root11		-1718.9368	214.7130

Species	*Transition*	*D.M.*	*f*	*⊿E*	*Singly occupied orbitals*	
$Na_2O_2S_8$	S_0	11.5		0		
	$S_0 \rightarrow S_{N\Sigma}(^1n\sigma^*)$	11.2	1.7×10^{-4}	80.4	n_{10}	σ^*
	$S_0 \rightarrow S_{N\Sigma}(^1n\sigma^*)$	11.7	0.0017	91.1	n_{12}	σ^*
	$S_0 \rightarrow S_{N\Sigma}(^1n\sigma^*)$	9.78	0.0042	95.7	n_{11}	σ^*
	$S_0 \rightarrow S_{N\Sigma}(^1n\sigma^*)$	12.0	5.5×10^{-4}	104.8	n_{12}	σ^*
	$S_0 \rightarrow S_{N\Sigma}(^1n\sigma^*)$	13.2	0.0032	120.9	n_{12}	σ^*
	$S_0 \rightarrow S_{N\Sigma}(^1n\sigma^*)$	4.39	0.0018	142.7	n_{10}	σ^*
	$S_0 \rightarrow S_{\Sigma\Sigma}(^1\sigma\sigma^*)$	3.09	0.1094	159.6	σ	σ^*

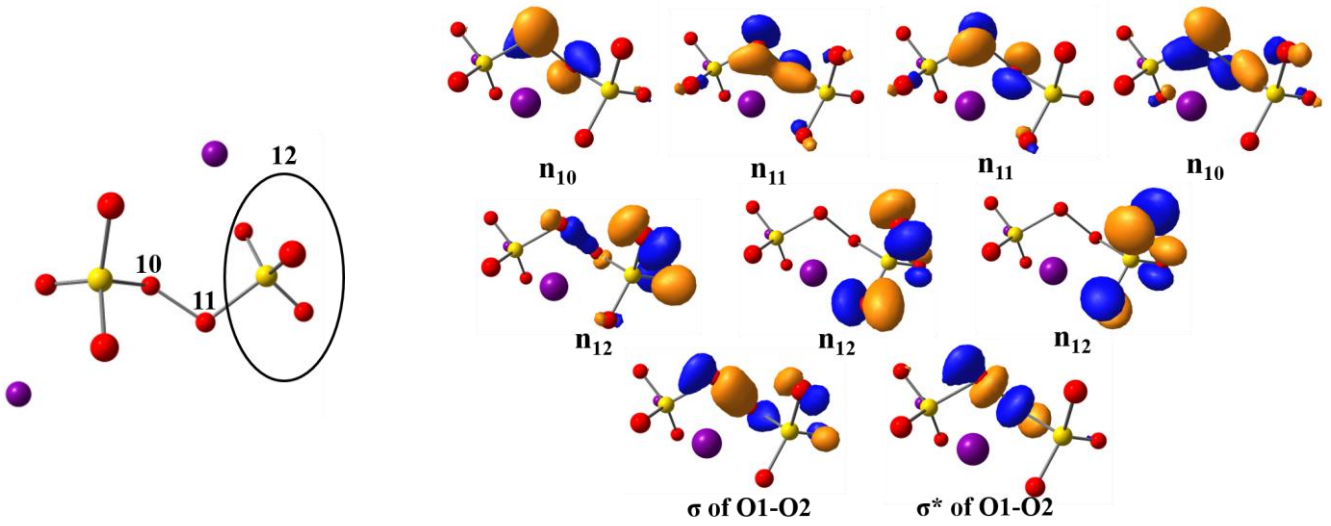


Table S5.2 *The absolute energies (A.E.) in Hartree and the relative energies (R.E.) in kcal/mol for the optimized ground state structure of G-G (G-quartet) together with $Na_2S_2O_8$ molecule and three crystal water molecules obtained at the CASPT2//CASSCF(10e,8o)/AMBER QM/MM and CASPT2//CASSCF(14e,12o)/AMBER QM/MM level of theory, respectively.*

G-G (G-quartet)	**CASSCF**	**MM**	**CASPT2**	
	A.E.	**A.E.**	**A.E.**	**R.E.**
S_0				
Root1	-3053.2420	-41.4755	-3014.9477	0
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]			-3014.8172	81.8818
Root3			-3014.7708	
Root4			-3014.6639	
Root5[**$S_{\Sigma\Sigma}(^1\sigma\sigma^*)$**]			-3014.6899	161.7084
G-G (G-quartet) CAS(14e,12o)	**CASSCF**	**MM**	**CASPT2**	
	A.E.	**A.E.**	**A.E.**	**R.E.**
S_0				
Root1	-3053.2420	-41.4755	-3014.9494	0
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]			-3014.8199	81.2346
Root3			-3014.7809	
Root4			-3014.6839	
Root5[**$S_{\Sigma\Sigma}(^1\sigma\sigma^*)$**]			-3014.6657	178.0170

Table S5.3 *The absolute energies (A.E.) in Hartree and relative energies (R.E.) in kcal/mol for the optimized ground state structure of G-T (loop) together with $Na_2S_2O_8$ molecule and three crystal water molecules obtained at the CASPT2//CASSCF(10e,8o)/AMBER QM/MM and CASPT2//CASSCF(14e,12o)/AMBER QM/MM level of theory, respectively.*

G-T (loop)	**CASSCF**	**MM**	**CASPT2**	
	A.E.	**A.E.**	**A.E.**	**R.E.**
S_0				
Root1		-41.5467	-2928.1359	0
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]	-2966.4778		-2928.0030	83.4091
Root3			-2927.9670	
Root4[**$S_{\Sigma\Sigma}(^1\sigma\sigma^*)$**]			-2928.1359	163.2060
Root5			-2928.0030	
G-T (loop) CAS(14e,12o)	**CASSCF**	**MM**	**CASPT2**	
	A.E.	**A.E.**	**A.E.**	**R.E.**
S_0				
Root1		-41.5467	-2928.1395	0
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]	-2966.4778		-2928.0106	80.8792

Root3			-2927.9718	
Root4[$\mathbf{S_{\Sigma\Sigma}(^1\sigma\sigma^*)}$]			-2927.8513	180.8444
Root5			-2927.9985	

Table S5.4 *The absolute energies (A.E.) in Hartree and relative energies (R.E.) in kcal/mol for the optimized structures of G-G (G-quartet) together with $Na_2S_2O_8$ molecule and three crystal water molecules along the reaction pathway leading to the G(N_2-H_{2b})˙ radical obtained at the CASPT2//CASSCF/AMBER QM/MM level of theory. The corresponding energy profiles are plotted in Figure 1 of the main article.*

G-G	**CASSCF**	**MM**	**CASPT2**	
	A.E.	**A.E.**	**A.E.**	**R.E.**
$S_{N\Sigma}(^1n\sigma^*)$-FC G-G(G-quartet)				
Root1	-3053.2420	-41.4755	-3014.9477	0
Root2[$\mathbf{S_{N\Sigma}(^1n\sigma^*)}$]			-3014.8172	81.8818
Root3			-3014.7708	
Root4			-3014.6639	
Root5[$\mathbf{S_{\Sigma\Sigma}(^1\sigma\sigma^*)}$]			-3014.6899	161.7084
Path-$S_{N\Sigma}(^1n\sigma^*)$-3				
Root1		-41.4725	-3014.8863	40.4101
Root2[$\mathbf{S_{N\Sigma}(^1n\sigma^*)}$]	-3053.1357		-3014.8372	71.2292
Root3			-3014.8156	
Root4			-3014.7788	
Root5			-3014.6763	
$S_{N\Sigma}$-Min				
Root1		-41.4648	-3014.8821	47.8525
Root2[$\mathbf{S_{N\Sigma}(^1n\sigma^*)}$]	-3053.1643		-3014.8685	56.3741
Root3			-3014.8485	
Root4			-3014.8418	
Root5			-3014.6898	
CI($^1n\sigma^*/S_0$)				
Root1($\mathbf{S_0}$)		-41.4685	-3014.8663	55.5098
Root2[$\mathbf{S_{N\Sigma}(^1n\sigma^*)}$]	-3053.1873		-3014.8647	56.5090
Root3			-3014.8471	
Root4			-3014.8459	
Root5			-3014.6816	
CI($^1\pi\sigma^*/S_0$)				
Root1($\mathbf{S_0}$)		-41.4328	-3014.8992	57.2401
Root2[$\mathbf{S_{N\Sigma}(^1n\sigma^*)}$]	-3053.2377		-3014.8646	57.4304
Root3[$\mathbf{S_{CT}(^1\pi\sigma^*)}$]			-3014.8546	58.1138
Root4			-3014.8722	
Root5			-3014.8415	

S_{CT}-Min				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]		-41.4329	-3014.9041	54.0559
Root2	-3053.2344		-3014.8217	
Root3			-3014.8096	
Root4			-3014.8066	
Root5			-3014.7941	
Path-$S_{CT}(^1\pi\sigma^*)$-9				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-3053.2297	-41.4331	-3014.9013	55.7660
Root2			-3014.8185	
Root3			-3014.8071	
Root4			-3014.8034	
Root5			-3014.7915	
Path-$S_{CT}(^1\pi\sigma^*)$-11				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-3053.2124	-41.4334	-3014.8891	63.2299
Root2			-3014.8004	
Root3			-3014.7903	
Root4			-3014.7843	
Root5			-3014.7745	
S_{CT}-Max				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-3053.1887	-41.4352	-3014.8683	75.1344
Root2			-3014.8435	
Root3			-3014.8057	
Root4			-3014.8051	
Root5			-3014.7828	
Path-$S_{CT}(^1\pi\sigma^*)$-14				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-3053.1785	-41.4479	-3014.8837	57.5059
Root2			-3014.8604	
Root3			-3014.8067	
Root4			-3014.7907	
Root5			-3014.7694	
Path-$S_{CT}(^1\pi\sigma^*)$-15				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-3053.1947	-41.4496	-3014.8942	49.8041
Root2			-3014.8708	
Root3			-3014.8391	
Root4			-3014.7969	
Root5			-3014.7761	
Path-$S_{CT}(^1\pi\sigma^*)$-16				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-3053.2206	-41.4549	-3014.9046	39.9398
Root2			-3014.8820	
Root3			-3014.7969	
Root4			-3014.7964	
Root5			-3014.7763	

Path-$S_{CT}(^1\pi\sigma^*)$-18				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]		-41.4540	-3014.9098	37.2313
Root2	-3053.2330		-3014.8882	
Root3			-3014.7973	
Root4			-3014.7988	
Root5			-3014.7992	
Path-$S_{CT}(^1\pi\sigma^*)$-20				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]		-41.4517	-3014.9142	35.9177
Root2	-3053.2413		-3014.8929	
Root3			-3014.8001	
Root4			-3014.8009	
Root5			-3014. 8021	
G(N_2-H_{2b})$^{\cdot}$				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-3053.2389	-41.4517	-3014.9178	33.6665
Root2			-3014.8974	
Root3			-3014.7995	
Root4			-3014.8009	
Root5			-3014.7992	

Table S5.5 *The absolute energies (A. E.) in Hartree and relative energies (R.E.) in kcal/mol for the optimized structures of G-G (G-quartet) together with $Na_2S_2O_8$ molecule and three crystal water molecules along the reaction pathway leading to the G(N_1-H_1)$^{\cdot}$ radical obtained at the CASPT2//CASSCF/AMBER QM/MM level of theory. The corresponding energy profiles are plotted in Figure 2(a) of the main article.*

G-G	**CASSCF**	**MM**	**CASPT2**	
	A.E.	**A.E.**	**A.E.**	**R.E.**
$S_{N\Sigma}(^1n\sigma^*)$-FC G-G(G-quartet)				
Root1	-3053.2420	-41.4755	-3014.9477	0
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]			-3014.8172	81.8818
Root3			-3014.7708	
Root4			-3014.6639	
Root5[**$S_{\Sigma\Sigma}(^1\sigma\sigma^*)$**]			-3014.6899	161.7084
Path-$S_{N\Sigma}(^1n\sigma^*)$-3				
Root1		-41.4725	-3014.8863	40.4101
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]	-3053.1357		-3014.8372	71.2292
Root3			-3014.8156	
Root4			-3014.7788	
Root5			-3014.6763	
$S_{N\Sigma}$-Min				
Root1		-41.4648	-3014.8821	47.8525
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]	-3053.1643		-3014.8685	56.3741

Root3			-3014.8485	
Root4			-3014.8418	
Root5			-3014.6898	
CI(^{1}nσ*/S_0)				
Root1(**S_0**)		-41.4685	-3014.8663	55.5098
Root2[**$S_{N\Sigma}$(^{1}nσ*)**]	-3053.1873		-3014.8647	56.5090
Root3			-3014.8471	
Root4			-3014.8459	
Root5			-3014.6816	
CI(^{1}πσ*/S_0)				
Root1(**S_0**)		-41.4328	-3014.8992	57.2401
Root2[**$S_{N\Sigma}$(^{1}nσ*)**]	-3053.2377		-3014.8646	57.4304
Root3[**S_{CT}(^{1}πσ*)**]			-3014.8546	58.1138
Root4			-3014.8722	
Root5			-3014.8415	
Path-S_{CT}(^{1}πσ*)-9				
Root1[**S_{CT}(^{1}πσ*)**]	-3053.2701	-41.3947	-3014.9568	61.3886
Root2			-3014.9050	
Root3			-3014.9030	
Root4			-3014.8569	
Root5			-3014.8392	
Path-S_{CT}(^{1}πσ*)-11				
Root1[**S_{CT}(^{1}πσ*)**]	-3053.2572	-41.3944	-3014.9456	68.6209
Root2			-3014.8914	
Root3			-3014.8914	
Root4			-3014.8443	
Root5			-3014.8275	
Path-S_{CT}(^{1}πσ*)-12				
Root1[**S_{CT}(^{1}πσ*)**]	-3053.2490	-41.3943	-3014.9382	73.3328
Root2			-3014.9122	
Root3			-3014.8825	
Root4			-3014.8299	
Root5			-3014.8205	
Path-S_{CT}(^{1}πσ*)-14				
Root1[**S_{CT}(^{1}πσ*)**]	-3053.2344	-41.3940	-3014.9126	89.6009
Root2			-3014.8660	
Root3			-3014.8664	
Root4			-3014.8055	
Root5			-3014.8032	
S_{CT}-Max(N_1-H_1)				
Root1[**S_{CT}(^{1}πσ*)**]	-3053.2304	-41.3965	-3014.9090	90.2682
Root2			-3014.8665	
Root3			-3014.8664	

Root4			-3014.8055	
Root5			-3014.8032	
G(N_1-H_1)·				
Root1[**S_{CT}($^1\pi\sigma^*$)**]	-3053.2271	-41.3974	-3014.9021	90.5057
Root2			-3014.7812	
Root3			-3014.9695	
Root4			-3014.8055	
Root5			-3014.8032	

Table S5.6 *The absolute energies (A. E.) in Hartree and relative energies (R.E.) in kcal/mol for the optimized structures of G-G (G-quartet) together with $Na_2S_2O_8$ molecule and three crystal water molecules along the reaction pathway leading to the G(N_2-H_{2a})· radical obtained at the CASPT2//CASSCF/AMBER QM/MM level of theory. The corresponding energy profiles are plotted in Figure 2(b) of the main article.*

G-G	CASSCF	MM	CASPT2	
	A.E.	A.E.	A.E.	R.E.
$S_{N\Sigma}$(^{1}nσ^*)-FC G-G(G-quartet)				
Root1	-3053.2420	-41.4755	-3014.9477	0
Root2[**$S_{N\Sigma}$(^{1}nσ^*)**]			-3014.8172	81.8818
Root3			-3014.7708	
Root4			-3014.6639	
Root5[**$S_{\Sigma\Sigma}$($^1\sigma\sigma^*$)**]			-3014.6899	161.7084
Path-$S_{N\Sigma}$(^{1}nσ^*)-3				
Root1		-41.4725	-3014.8863	40.4101
Root2[**$S_{N\Sigma}$(^{1}nσ^*)**]	-3053.1357		-3014.8372	71.2292
Root3			-3014.8156	
Root4			-3014.7788	
Root5			-3014.6763	
$S_{N\Sigma}$-Min				
Root1		-41.4648	-3014.8821	47.8525
Root2[**$S_{N\Sigma}$(^{1}nσ^*)**]	-3053.1643		-3014.8685	56.3741
Root3			-3014.8485	
Root4			-3014.8418	
Root5			-3014.6898	
CI(^{1}nσ^*/S_0)				
Root1(**S_0**)		-41.4685	-3014.8663	55.5098
Root2[**$S_{N\Sigma}$(^{1}nσ^*)**]	-3053.1873		-3014.8647	56.5090
Root3			-3014.8471	
Root4			-3014.8459	
Root5			-3014.6816	

CI($^1\pi\sigma^*/S_0$)				
Root1(**S_0**)		-41.4328	-3014.8992	57.2401
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]	-3053.2377		-3014.8646	57.4304
Root3[**$S_{CT}(^1\pi\sigma^*)$**]			-3014.8546	58.1138
Root4			-3014.8722	
Root5			-3014.8415	
Path-$S_{CT}(^1\pi\sigma^*)$-9				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-3052.9387	-41.3945	-3014.5548	60.2258
Root2			-3014.8646	
Root3			-3014.8546	
Root4			-3014.8722	
Root5			-3014.8415	
Path-$S_{CT}(^1\pi\sigma^*)$-11				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-3052.9049	-41.4047	-3014.5548	72.6250
Root2			-3014.8646	
Root3			-3014.8546	
Root4			-3014.8722	
Root5			-3014.8415	
S_{CT}-Max(N_2-H_{2a})				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-3052.8988	-41.4058	-3014.5341	84.9019
Root2			-3014.5151	
Root3			-3014.4469	
Root4			-3014.4284	
Root5			-3014.4045	
Path-$S_{CT}(^1\pi\sigma^*)$-14				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-3052.9155	-41.4033	-3014.5489	77.1820
Root2			-3014.5298	
Root3			-3014.4624	
Root4			-3014.4436	
Root5			-3014.4182	
Path-$S_{CT}(^1\pi\sigma^*)$-15				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-3052.9233	-41.4019	-3014.5520	74.1406
Root2			-3014.5329	
Root3			-3014.4663	
Root4			-3014.4475	
Root5			-3014.4214	
G(N_2-H_{2a})·				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-3052.9282	-41.4019	-3014.5553	74.0348
Root2			-3014.5364	
Root3			-3014.4690	
Root4			-3014.4504	
Root5			-3014.4241	

Table S5.7 *The absolute energies (A. E.) in Hartree and relative energies (R.E.) in kcal/mol for the optimized structures of G-T (loop) together with $Na_2S_2O_8$ molecule and three crystal water molecules along the reaction pathway leading to the G(N_1-H_1)$^{\cdot}$ radical obtained at the CASPT2//CASSCF/AMBER QM/MM level of theory. The corresponding energy profiles are plotted in Figure 3(a) of the main article.*

G-T	**CASSCF**	**MM**	**CASPT2**	
	A.E.	**A.E.**	**A.E.**	**R.E.**
$S_{N\Sigma}(^1n\sigma^*)$-FC G-T (loop)				
Root1		-41.5467	-2928.1359	0
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]	-2966.4778		-2928.0030	83.4091
Root3			-2927.9670	
Root4[**$S_{\Sigma\Sigma}(^1\sigma\sigma^*)$**]			-2928.1359	163.2060
Root5			-2928.0030	
Path-$S_{N\Sigma}(^1n\sigma^*)$-3				
Root1		-41.5448	-2928.1163	13.4663
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]	-2966.5566		-2928.0326	66.0367
Root3			-2927.9534	
Root4			-2927.8855	
Root5			-2927.8648	
Path-$S_{N\Sigma}(^1n\sigma^*)$-5				
Root1		-41.5433	-2928.1052	21.4170
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]	-2966.5828		-2928.0499	56.0580
Root3			-2927.9661	
Root4			-2927.8982	
Root5			-2927.8847	
Path-$S_{N\Sigma}(^1n\sigma^*)$-7				
Root1		-41.5425	-2928.1011	25.9670
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]	-2966.5992		-2928.0561	49.5609
Root3			-2927.9712	
Root4			-2927.9026	
Root5			-2927.9212	
Path-$S_{N\Sigma}(^1n\sigma^*)$-9				
Root1		-41.5422	-2928.0915	30.6826
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]	-2966.6110		-2928.0665	46.3616
Root3			-2927.9121	
Root4			-2927.9001	
Root5			-2927.8582	
CI($^1n\sigma^*/^1\pi\sigma^*/S_0$)				
Root1(**S_0**)		-41.5422	-2928.0818	36.7148
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]	-2966.5967		-2928.0797	38.0864

Root3[$S_{CT}(^1\pi\sigma^*)$]			-2927.9144	33.9694
Root4			-2927.9034	
Root5			-2927.8707	
Path-$S_{CT}(^1\pi\sigma^*)$-13				
Root1[$S_{CT}(^1\pi\sigma^*)$]	-2966.5794	-41.5197	-2928.0919	44.5401
Root2			-2928.0806	
Root3			-2928.0775	
Root4			-2927.9983	
Root5			-2927.9173	
Path-$S_{CT}(^1\pi\sigma^*)$-14				
Root1[$S_{CT}(^1\pi\sigma^*)$]	-2966.5716	-41.5219	-2928.0826	49.0297
Root2			-2928.0734	
Root3			-2928.0682	
Root4			-2927.9936	
Root5			-2927.9133	
S_{CT}-Max(N_1-H_1)				
Root1[$S_{CT}(^1\pi\sigma^*)$]	-2966.5875	-41.5186	-2928.0829	50.8815
Root2			-2928.0894	
Root3			-2928.0818	
Root4			-2928.0058	
Root5			-2927.9230	
Path-$S_{CT}(^1\pi\sigma^*)$-18				
Root1[$S_{CT}(^1\pi\sigma^*)$]	-2966.5310	-41.5323	-2928.0783	48.5297
Root2			-2928.0318	
Root3			-2928.0132	
Root4			-2928.2975	
Root5			-2927.9173	
Path-$S_{CT}(^1\pi\sigma^*)$-20				
Root1[$S_{CT}(^1\pi\sigma^*)$]	-2966.5350	-41.5353	-2928.0829	40.4040
Root2			-2928.0294	
Root3			-2928.0194	
Root4			-2927.9996	
Root5			-2927.9098	
Path-$S_{CT}(^1\pi\sigma^*)$-22				
Root1[$S_{CT}(^1\pi\sigma^*)$]	-2966.5372	-41.5546	-2928.1002	27.5346
Root2			-2928.0389	
Root3			-2928.0757	
Root4			-2928.1399	
Root5			-2928.1259	
Path-$S_{CT}(^1\pi\sigma^*)$-24				
Root1[$S_{CT}(^1\pi\sigma^*)$]		-41.5425	-2928.1164	14.8713
Root2	-2966.5755		-2928.0305	
Root3			-2928.0202	

Root4			-2927.9527	
Root5			-2928.0517	
G(N_1-H_1)·				
Root1[**S_{CT}(^{1}πσ*)**]	-2966.5848	-41.5422	-2928.1206	12.4039
Root2			-2928.0360	
Root3			-2928.0249	
Root4			-2927.9569	
Root5			-2928.0611	

Table S5.8 *The absolute energies (A. E.) in Hartree and relative energies (R.E.) in kcal/mol for the optimized structures of G-T (loop) together with $Na_2S_2O_8$ molecule and three crystal water molecules along the reaction pathway leading to the G(N_2-H_{2a})· radical obtained at the CASPT2//CASSCF/AMBER QM/MM level of theory. The corresponding energy profiles are plotted in Figure 3(b) of the main article.*

G-T (loop)	**CASSCF**	**MM**	**CASPT2**	
	A.E.	**A.E.**	**A.E.**	**R.E.**
$S_{N\Sigma}$(^{1}nσ*)-FC G-T (loop)				
Root1		-41.5467	-2928.1359	0
Root2[**$S_{N\Sigma}$(^{1}nσ*)**]	-2966.4778		-2928.0030	83.4091
Root3			-2927.9670	
Root4[**$S_{\Sigma\Sigma}$(^{1}σσ*)**]			-2928.1359	163.2060
Root5			-2928.0030	
Path-$S_{N\Sigma}$(^{1}nσ*)-3				
Root1		-41.5448	-2928.1163	13.4663
Root2[**$S_{N\Sigma}$(^{1}nσ*)**]	-2966.5566		-2928.0326	66.0367
Root3			-2927.9534	
Root4			-2927.8855	
Root5			-2927.8648	
Path-$S_{N\Sigma}$(^{1}nσ*)-5				
Root1		-41.5433	-2928.1052	21.4170
Root2[**$S_{N\Sigma}$(^{1}nσ*)**]	-2966.5828		-2928.0499	56.0580
Root3			-2927.9661	
Root4			-2927.8982	
Root5			-2927.8847	
Path-$S_{N\Sigma}$(^{1}nσ*)-7				
Root1		-41.5425	-2928.1011	25.9670
Root2[**$S_{N\Sigma}$(^{1}nσ*)**]	-2966.5992		-2928.0561	49.5609
Root3			-2927.9712	
Root4			-2927.9026	
Root5			-2927.9212	

Path-$S_{N\Sigma}(^1n\sigma^*)$-9				
Root1		-41.5422	-2928.0915	30.6826
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]	-2966.6110		-2928.0665	46.3616
Root3			-2927.9121	
Root4			-2927.9001	
Root5			-2927.8582	
CI($^1n\sigma^*/^1\pi\sigma^*/S_0$)				
Root1(**S_0**)		-41.5422	-2928.0818	36.7148
Root2[**$S_{N\Sigma}(^1n\sigma^*)$**]	-2966.5967		-2928.0797	38.0864
Root3[**$S_{CT}(^1\pi\sigma^*)$**]			-2927.9144	33.9694
Root4			-2927.9034	
Root5			-2927.8707	
Path-$S_{CT}(^1\pi\sigma^*)$-13				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-2966.6309	-41.4856	-2928.0770	46.6868
Root2			-2928.0749	
Root3			-2928.0543	
Root4			-2928.0529	
Root5			-2927.9889	
Path-$S_{CT}(^1\pi\sigma^*)$-15				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-2966.6286	-41.4765	-2928.0736	54.6151
Root2			-2928.0597	
Root3			-2928.0507	
Root4			-2928.0423	
Root5			-2928.0164	
Path-$S_{CT}(^1\pi\sigma^*)$-17				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-2966.6250	-41.4769	-2928.0718	55.4441
Root2			-2928.0563	
Root3			-2928.0485	
Root4			-2928.0361	
Root5			-2927.9987	
Path-$S_{CT}(^1\pi\sigma^*)$-19				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-2966.6174	-41.4794	-2928.0688	55.7503
Root2			-2928.0502	
Root3			-2928.0450	
Root4			-2928.0289	
Root5			-2927.9980	
Path-$S_{CT}(^1\pi\sigma^*)$-21				
Root1[**$S_{CT}(^1\pi\sigma^*)$**]	-2966.6026	-41.4839	-2928.0635	56.2852
Root2			-2928.0408	
Root3			-2928.0396	
Root4			-2928.0183	
Root5			-2927.9847	

S_{CT}-Max(N_2-H_{2a})				
Root1[**S_{CT}($^1\pi\sigma^*$)**]	-2966.5410	-41.4920	-2928.0480	60.9136
Root2			-2928.0246	
Root3			-2927.9908	
Root4			-2927.9852	
Root5			-2927.9660	
Path-S_{CT}($^1\pi\sigma^*$)-26				
Root1[**S_{CT}($^1\pi\sigma^*$)**]	-2966.5561	-41.4936	-2928.0599	52.3980
Root2			-2928.0373	
Root3			-2927.9736	
Root4			-2927.9511	
Root5			-2927.8948	
Path-S_{CT}($^1\pi\sigma^*$)-28				
Root1[**S_{CT}($^1\pi\sigma^*$)**]	-2966.5621	-41.4948	-2928.0599	44.1240
Root2			-2928.0373	
Root3			-2927.9736	
Root4			-2927.9511	
Root5			-2927.8948	
Path-S_{CT}($^1\pi\sigma^*$)-30				
Root1[**S_{CT}($^1\pi\sigma^*$)**]	-2966.5818	-41.4992	-2928.0840	33.8018
Root2			-2928.0624	
Root3			-2927.9922	
Root4			-2927.9706	
Root5			-2927.9192	
Path-S_{CT}($^1\pi\sigma^*$)-32				
Root1[**S_{CT}($^1\pi\sigma^*$)**]	-2966.5935	-41.5039	-2928.0599	25.1931
Root2			-2928.0373	
Root3			-2927.9736	
Root4			-2927.9511	
Root5			-2927.8948	
G(N_2-H_{2a})·				
Root1[**S_{CT}($^1\pi\sigma^*$)**]	-2966.5977	-41.5057	-2928.1009	19.0649
Root2			-2928.0788	
Root3			-2928.0075	
Root4			-2927.9854	
Root5			-2927.9364	

6. Cartesian Coordinates

6.1 Cartesian coordinates for critical points of G-G (G-quartet) along the reaction pathway leading to the G(N_2-H_{2b})· radical. The corresponding energy profiles are plotted in Figure 1 of the main article.

S_0-Min(N_2-H_{2b})

N 2.745695525 -5.474150836 3.138661714

C	3.065746375	-5.262087483	1.791208641
H	3.812274512	-5.872104986	1.291133670
N	2.449947198	-4.246865587	1.241998070
C	1.609981356	-3.769542618	2.290061689
C	0.626589800	-2.663078658	2.238437930
O	0.355340290	-1.944331492	1.282274427
N	-0.032491695	-2.532599757	3.495420172
H	-0.746033302	-1.787938310	3.582976728
C	0.219569886	-3.354951537	4.588853274
N	-0.454718306	-3.021438576	5.768932039
H	-1.438457203	-2.768182256	5.693484169
H	-0.307100550	-3.728975498	6.455054952
N	1.043984838	-4.370286269	4.648776650
C	1.750933543	-4.518009554	3.429026874
N	-5.342699291	-1.272491755	6.597657213
C	-4.369268481	-2.265971276	6.730891715
H	-4.445303743	-3.064642125	7.463257576
N	-3.379353620	-2.137319275	5.863655931
C	-3.686341508	-0.943672104	5.160480302
C	-2.941306720	-0.264165897	4.065526614
O	-1.943513161	-0.615498171	3.454178574
N	-3.537522313	1.019505088	3.772704261
H	-3.282567307	1.403394977	2.857484991
C	-4.776305768	1.435180918	4.292702656
N	-5.380466460	2.639204091	3.772251074
H	-5.752142991	3.206685041	4.550301696
H	-4.742123590	3.204079680	3.192360727
N	-5.504623243	0.783254614	5.190381388
C	-4.849152478	-0.414880752	5.621142464
O	-7.495542785	-4.937280493	0.384347574
S	-6.239426865	-4.398594431	0.801569592
O	-5.496544665	-5.221675513	1.728873667
O	-5.408246784	-3.852868233	-0.244337027
O	-6.584117473	-3.001266435	1.660314431
O	-7.438587967	-3.348572226	2.955851618

S	-8.366295482	-2.001252866	3.292569726
O	-9.209414278	-1.858436562	2.122987213
O	-9.062416670	-2.391649280	4.477227540
O	-7.418390277	-0.936755562	3.465869798
Na	-7.053637290	1.212985133	3.285571791
Na	-3.321446209	-4.148434602	-1.258246256
H	2.797429110	-6.372932146	3.659606933
H	-6.005112418	-0.952636356	7.336456070
O	-4.708284769	-4.593934857	4.290910946
H	-4.887419481	-4.663454264	3.359153390
H	-5.366156608	-3.998454673	4.622529336
O	-3.185491572	-5.088358184	6.460453195
H	-3.387721240	-4.387355622	5.847220638
H	-3.525956123	-5.886215709	6.078523960
O	-1.093458466	-4.467050012	8.139396713
H	-1.781148008	-4.777685672	7.554038038
H	-1.286862812	-4.890990009	8.975293827

$S_{N\Sigma}$-Min(N_2-H_{2b})

N	2.558901930	-5.539256412	3.102329727
C	2.809160620	-5.376689351	1.732502897
H	3.506216123	-6.024689647	1.208629502
N	2.194792232	-4.358597627	1.190051263
C	1.430792891	-3.826009857	2.270148040
C	0.480877443	-2.693458153	2.242466530
O	0.177118650	-1.996064113	1.278847846
N	-0.105702589	-2.514434113	3.528686635
H	-0.798587615	-1.756896984	3.631494180
C	0.177016026	-3.305941474	4.639085102
N	-0.447110879	-2.933416063	5.838730994
H	-1.452662659	-2.675702996	5.764559923
H	-0.264762046	-3.663262987	6.524699652
N	0.982170882	-4.343711353	4.678724542
C	1.612558084	-4.544092621	3.422416191
N	-5.415760995	-1.212311967	6.575650795
C	-4.428819660	-2.206901003	6.718475153

H	-4.511478205	-3.006150910	7.444647153
N	-3.421398292	-2.064983079	5.874455221
C	-3.742241184	-0.880348738	5.171165396
C	-2.985524443	-0.213075470	4.083845318
O	-1.987076011	-0.572528767	3.480075069
N	-3.578730912	1.064604431	3.766796008
H	-3.316343061	1.434379633	2.848201206
C	-4.822925242	1.480064394	4.271676274
N	-5.423140530	2.672083339	3.720507541
H	-5.805020022	3.260287633	4.479366533
H	-4.777480214	3.221387146	3.137677661
N	-5.560776146	0.842099309	5.171074690
C	-4.913512867	-0.354074051	5.612854913
O	-7.216703576	-4.834543122	0.133384647
S	-5.966865550	-4.324412973	0.594930501
O	-5.263021787	-5.094300977	1.602968302
O	-5.062761002	-3.841076502	-0.412201464
O	-6.427944249	-3.003834537	1.438835126
O	-7.725881312	-3.370086594	3.191388766
S	-8.492629988	-1.986297211	3.397879549
O	-9.276969892	-1.814282208	2.179026200
O	-9.243275801	-2.322448332	4.567320248
O	-7.503025352	-0.941298623	3.553993563
Na	-7.104091377	1.218907325	3.275101680
Na	-2.932594034	-4.251348819	-1.203953623
H	2.610033211	-6.422209290	3.647970019
H	-6.091761012	-0.900888124	7.304599229
O	-4.592336499	-4.575153277	4.237583480
H	-4.727917235	-4.614825214	3.288530262
H	-5.239210198	-3.968915359	4.586549438
O	-3.079753311	-4.969114013	6.261253997
H	-3.695731583	-4.959061391	5.465121696
H	-3.073698412	-5.891554367	6.536883270
O	-0.960313025	-4.580991494	7.966799097
H	-1.648230886	-4.891480964	7.382879785

H	-1.059931192	-5.085332714	8.777080487

CI(^{1}nσ*/S_0)(N_2-H_{2b})

N	2.732942385	-5.458296844	3.249627913
C	3.060681742	-5.256017269	1.902228742
H	3.807685809	-5.871380225	1.409301860
N	2.454801552	-4.238904174	1.344568094
C	1.612942611	-3.748801822	2.385549988
C	0.640245479	-2.632307393	2.326846065
O	0.381332618	-1.916954845	1.364479330
N	-0.018991374	-2.490454499	3.583563464
H	-0.732477353	-1.744073273	3.663536064
C	0.222534882	-3.307208155	4.684773239
N	-0.445384361	-2.973633365	5.871194219
H	-1.432033531	-2.694977976	5.780479427
H	-0.300761682	-3.721217718	6.523595947
N	1.033131862	-4.335297863	4.744248645
C	1.740562748	-4.494335359	3.527594101
N	-5.385622498	-1.153350032	6.559171158
C	-4.416395853	-2.156975035	6.705430510
H	-4.503250170	-2.948821858	7.444401720
N	-3.415119609	-2.031979320	5.853939707
C	-3.716948749	-0.853306051	5.133533739
C	-2.949000254	-0.213886591	4.035562095
O	-1.936764125	-0.585224242	3.460274738
N	-3.547209321	1.055139476	3.679055139
H	-3.284130502	1.400381799	2.751022641
C	-4.790421296	1.487338343	4.173398952
N	-5.396050571	2.657916095	3.582621190
H	-5.761248703	3.278952328	4.322345303
H	-4.755066250	3.179738362	2.967700441
N	-5.524684141	0.878803361	5.098025962
C	-4.884724810	-0.313852548	5.569899056
O	-7.529839662	-4.837793492	0.188170556
S	-6.239900372	-4.327685310	0.536638876
O	-5.502068587	-5.090823695	1.527425207

O	-5.430271564	-3.879280348	-0.564338341
O	-6.614835207	-3.011484265	1.394654927
O	-7.836760509	-3.358836635	3.429896863
S	-8.591735256	-1.956591084	3.597673293
O	-9.414506075	-1.836482268	2.402126233
O	-9.305946315	-2.197680762	4.813953798
O	-7.559312824	-0.951682943	3.654371598
Na	-7.103944266	1.198838468	3.239938783
Na	-3.415320993	-4.326448919	-1.527907399
H	2.780570703	-6.351270910	3.779358157
H	-6.045264165	-0.821446839	7.295177176
O	-4.666395040	-4.578439865	4.132266253
H	-4.847512161	-4.629298688	3.196547476
H	-5.214511310	-3.891803804	4.488490867
O	-3.090937715	-5.109585537	6.161090216
H	-3.695508779	-5.048600775	5.405599204
H	-3.109819490	-6.043083478	6.368149389
O	-0.962982994	-4.807131179	7.937657412
H	-1.635868374	-5.087233878	7.324575723
H	-1.061968265	-5.365407663	8.704280514

CI($^1\pi\sigma^*/S_0$)(N_2-H_{2b})

N	2.742272695	-5.414700524	2.993830663
C	3.066906501	-5.111873429	1.680264138
H	3.821933049	-5.671936019	1.133945642
N	2.416886039	-4.059004446	1.202822946
C	1.583080901	-3.684609235	2.259281671
C	0.584284238	-2.579898112	2.263982845
O	0.315602337	-1.814669355	1.357833472
N	-0.129999460	-2.507373708	3.537398067
H	-0.890262440	-1.762045678	3.598656901
C	0.073555705	-3.343622260	4.565005219
N	-0.616199543	-3.272576070	5.677268167
H	-1.486052257	-2.712841529	5.755629052
H	-0.457261702	-3.910194846	6.442691625
N	1.059208431	-4.433120093	4.588322187

C	1.747181703	-4.495428110	3.339998390
N	-5.288819173	-1.243841660	6.689940063
C	-4.299182077	-2.229290090	6.816264780
H	-4.366029647	-3.015962729	7.562107198
N	-3.321251180	-2.120899868	5.940669900
C	-3.650988462	-0.938591061	5.215689121
C	-2.934673537	-0.298632143	4.090120815
O	-1.927249317	-0.652002315	3.482486043
N	-3.553059126	0.953786200	3.753419058
H	-3.260488403	1.358673483	2.857456553
C	-4.750468959	1.407147457	4.308479530
N	-5.358308750	2.582704228	3.755064254
H	-5.809593013	3.124209719	4.512656942
H	-4.724953244	3.174101609	3.198021934
N	-5.455619154	0.799380232	5.241697913
C	-4.816601722	-0.391797738	5.683270466
O	-7.384446732	-4.839239189	0.630825425
S	-6.086547399	-4.263556383	1.009172198
O	-5.328408278	-5.260762634	1.836339687
O	-5.308466815	-4.005067653	-0.218022691
O	-6.271695882	-3.052421571	1.805790649
O	-7.756510779	-3.436078214	3.722990535
S	-8.519019634	-2.028235995	3.538429894
O	-9.091299323	-1.989633964	2.217222235
O	-9.505987645	-2.154827903	4.591926069
O	-7.534972735	-1.010307643	3.786846656
Na	-6.964675291	1.037860701	3.239503667
Na	-3.464783132	-4.501134604	-1.227147890
H	2.835069387	-6.324293825	3.505676072
H	-5.909469715	-0.896406283	7.451889049
O	-4.598342391	-4.536439993	4.272141040
H	-4.788485391	-4.706437745	3.331405700
H	-5.403499217	-4.145860113	4.588742687
O	-3.276669055	-5.156526469	6.449263583
H	-3.621150115	-4.845433071	5.599610401

H	-3.275389261	-6.116050565	6.423238381
O	-1.330270396	-4.294606159	8.058348825
H	-2.072929808	-4.607195283	7.529488130
H	-1.282565046	-4.881841561	8.810313136

S_{CT}-Min(N_2-H_{2b})

N	2.789240515	-5.349108263	2.911743471
C	3.112576144	-4.969685863	1.617996116
H	3.859304743	-5.506856318	1.039754034
N	2.479048814	-3.878853376	1.211936214
C	1.652049619	-3.563030890	2.294488162
C	0.671177312	-2.446161331	2.374380131
O	0.422128734	-1.619515506	1.517007978
N	-0.057655883	-2.451942725	3.634899066
H	-0.841345666	-1.708205353	3.705771579
C	0.119770666	-3.364803002	4.598309312
N	-0.635287733	-3.385376186	5.666038179
H	-1.535699052	-2.854389326	5.747421883
H	-0.515653479	-4.090228333	6.372626705
N	1.139338123	-4.432674325	4.587813875
C	1.805298419	-4.444386033	3.318478831
N	-5.283348708	-1.271205304	6.596705753
C	-4.317592391	-2.282887258	6.708656587
H	-4.423378347	-3.093626243	7.422937603
N	-3.304114156	-2.155118406	5.874546610
C	-3.598034885	-0.942673213	5.182532377
C	-2.834549174	-0.268007035	4.114243476
O	-1.799316446	-0.609630262	3.540703933
N	-3.426549849	1.002056579	3.793811570
H	-3.121288338	1.407738961	2.901954719
C	-4.652025364	1.440650817	4.306321128
N	-5.248501439	2.617684648	3.745159226
H	-5.687927543	3.179861401	4.494367078
H	-4.614113809	3.188325713	3.167738279
N	-5.382924012	0.817332311	5.208558452
C	-4.768999275	-0.392754232	5.636722183

O	-7.411527377	-5.156011850	1.008574000
S	-6.119785763	-4.498752561	1.254227208
O	-5.306956490	-5.453808416	2.066797797
O	-5.426841120	-4.284347587	-0.036585521
O	-6.274253237	-3.235560572	1.964018155
O	-7.938327245	-3.367504812	3.863193444
S	-8.576710009	-1.924764189	3.539245425
O	-9.031456573	-1.911800871	2.171415996
O	-9.647316071	-1.930900179	4.508876055
O	-7.542844775	-0.957908121	3.821808597
Na	-6.861689990	1.050064667	3.260481275
Na	-3.742717046	-4.657879006	-1.265393250
H	2.889630604	-6.280935846	3.379799589
H	-5.912720398	-0.934428367	7.355166031
O	-4.657286053	-4.575763710	4.337243362
H	-4.856215666	-4.904221864	3.440160552
H	-5.430010839	-4.088089653	4.589208278
O	-3.304367870	-5.212960805	6.326692691
H	-3.746500193	-4.927351164	5.512746061
H	-3.001109512	-6.111384756	6.219994682
O	-1.612915448	-4.147811888	7.908459264
H	-2.309862719	-4.482909131	7.339069465
H	-1.563251174	-4.752524241	8.645149984

S_{CT}-Max(N_2-H_{2b})

N	2.776297242	-5.340397741	2.903084073
C	3.107405621	-4.965311832	1.612327897
H	3.854892024	-5.507062062	1.040620064
N	2.481005891	-3.873340878	1.208356616
C	1.656561924	-3.554123032	2.290300798
C	0.677717673	-2.443951593	2.375805988
O	0.427629151	-1.618867152	1.515402009
N	-0.033216869	-2.464841680	3.634031845
H	-0.788262065	-1.723202480	3.721018615
C	0.130834048	-3.382729453	4.626358415
N	-0.609303315	-3.418412574	5.691782123

H	-1.421307161	-2.779549793	5.697320228
H	-0.777542146	-3.977811606	6.774426757
N	1.140149902	-4.449272720	4.579105618
C	1.804343503	-4.433262061	3.312266491
N	-5.283731949	-1.270701739	6.598481830
C	-4.324818148	-2.289488135	6.700961661
H	-4.429136240	-3.103264434	7.410149400
N	-3.319412533	-2.163639096	5.861188959
C	-3.603691657	-0.944516163	5.180025167
C	-2.839470565	-0.266417704	4.112644948
O	-1.809068278	-0.599965776	3.537830892
N	-3.440156779	1.000154367	3.789498072
H	-3.125624326	1.417296130	2.907054268
C	-4.653262364	1.440975457	4.314501885
N	-5.249410195	2.614954247	3.747756401
H	-5.696154345	3.171759941	4.496517046
H	-4.606239170	3.192383169	3.186698435
N	-5.383288509	0.820442381	5.219978520
C	-4.769652656	-0.393224226	5.638843126
O	-7.397506350	-5.170055283	1.005814738
S	-6.141829117	-4.488112367	1.256787124
O	-5.286330336	-5.432012134	2.130996258
O	-5.427153334	-4.293223382	-0.019868050
O	-6.278643979	-3.233515926	1.967698826
O	-7.927556583	-3.365244347	3.857385687
S	-8.574544298	-1.925272358	3.542362830
O	-9.034931733	-1.915772727	2.173856964
O	-9.643895205	-1.940143170	4.512715204
O	-7.542704543	-0.959009428	3.825849458
Na	-6.862957793	1.055647285	3.254857322
Na	-3.732567961	-4.662591033	-1.279935152
H	2.862545042	-6.271836802	3.369727235
H	-5.904601338	-0.931704205	7.361849963
O	-4.634243066	-4.612197712	4.350542661
H	-4.847227014	-4.898002518	3.376143980

H	-5.428973016	-4.217805432	4.686441280
O	-3.292913956	-5.160746293	6.308591442
H	-3.773076294	-4.867625209	5.444202102
H	-3.046731762	-6.082473633	6.239901590
O	-1.661625934	-4.165506765	7.832650707
H	-2.369209630	-4.553625177	7.197267954
H	-1.508184127	-4.814821929	8.521482478

G(N_2-H_{2b})· [N_2-H_{2b}(G-quartet)]

N	2.883798923	-5.420804477	3.006479375
C	3.207769056	-5.120107332	1.688258102
H	3.965514834	-5.677847458	1.146307165
N	2.551256325	-4.077426271	1.211743927
C	1.710381193	-3.703326256	2.273429215
C	0.688928447	-2.613030286	2.291158203
O	0.420666730	-1.860972628	1.365696903
N	-0.012509646	-2.559135472	3.536254129
H	-0.748937110	-1.825926325	3.615680962
C	0.174878058	-3.412449423	4.620014162
N	-0.505341513	-3.441120898	5.685873383
H	-1.326481487	-2.829483238	5.721991794
H	-0.696749893	-4.167081973	7.783154801
N	1.224034587	-4.450918991	4.617212476
C	1.888180203	-4.505501058	3.349834642
N	-5.326117787	-1.320792245	6.634287921
C	-4.343795709	-2.322344962	6.751144916
H	-4.426798801	-3.134844917	7.466287697
N	-3.347419260	-2.196206109	5.900929906
C	-3.653226860	-0.993004574	5.200543084
C	-2.903928899	-0.328541993	4.107024837
O	-1.896608684	-0.672803321	3.504109501
N	-3.514271953	0.944900235	3.793864430
H	-3.209320656	1.370672471	2.912747384
C	-4.723970853	1.381816393	4.326809532
N	-5.332479714	2.557817117	3.770009268
H	-5.787297876	3.098034781	4.526342651

H	-4.692305982	3.151270468	3.222706682
N	-5.451076750	0.755684162	5.231548965
C	-4.822304781	-0.448859248	5.660038262
O	-7.562623516	-4.750940922	0.789430457
S	-6.286462943	-4.168143036	1.132534697
O	-5.550853808	-5.330907264	1.953173578
O	-5.456562889	-3.951767497	-0.042062040
O	-6.347752570	-3.046233589	2.025146171
O	-8.057530294	-3.424523999	3.809685819
S	-8.654904943	-1.963366352	3.454457768
O	-9.039666334	-1.947687851	2.062767371
O	-9.780072990	-1.955836752	4.358035413
O	-7.604107361	-1.037731852	3.785996490
Na	-6.917918195	0.986174573	3.253165621
Na	-3.648463720	-4.435001371	-1.160864312
H	2.974690878	-6.325139926	3.518316200
H	-5.938726444	-0.974677266	7.400810003
O	-4.695382227	-4.495526336	4.407896769
H	-5.163480493	-4.973332053	2.765818622
H	-5.460729155	-4.113662132	4.817679666
O	-3.263988206	-5.242034745	6.629298838
H	-4.062877172	-4.672171327	5.110659470
H	-3.028806808	-6.169521598	6.588637493
O	-1.448994757	-4.145423235	8.366955048
H	-2.607334090	-4.847755545	7.215518643
H	-1.299318814	-4.776936807	9.071784589

6.2 Cartesian coordinates for critical points of G-G (G-quartet) along the reaction pathway leading to the G(N_1-H_1)· radical. The corresponding energy profiles are plotted in Figure 2(a) of the main article.

S_0-Min(N_1-H_1)

N	2.745695525	-5.474150836	3.138661714
C	3.065746375	-5.262087483	1.791208641
H	3.812274512	-5.872104986	1.291133670
N	2.449947198	-4.246865587	1.241998070
C	1.609981356	-3.769542618	2.290061689
C	0.626589800	-2.663078658	2.238437930

O	0.355340290	-1.944331492	1.282274427
N	-0.032491695	-2.532599757	3.495420172
H	-0.746033302	-1.787938310	3.582976728
C	0.219569886	-3.354951537	4.588853274
N	-0.454718306	-3.021438576	5.768932039
H	-1.438457203	-2.768182256	5.693484169
H	-0.307100550	-3.728975498	6.455054952
N	1.043984838	-4.370286269	4.648776650
C	1.750933543	-4.518009554	3.429026874
N	-5.342699291	-1.272491755	6.597657213
C	-4.369268481	-2.265971276	6.730891715
H	-4.445303743	-3.064642125	7.463257576
N	-3.379353620	-2.137319275	5.863655931
C	-3.686341508	-0.943672104	5.160480302
C	-2.941306720	-0.264165897	4.065526614
O	-1.943513161	-0.615498171	3.454178574
N	-3.537522313	1.019505088	3.772704261
H	-3.282567307	1.403394977	2.857484991
C	-4.776305768	1.435180918	4.292702656
N	-5.380466460	2.639204091	3.772251074
H	-5.752142991	3.206685041	4.550301696
H	-4.742123590	3.204079680	3.192360727
N	-5.504623243	0.783254614	5.190381388
C	-4.849152478	-0.414880752	5.621142464
O	-7.495542785	-4.937280493	0.384347574
S	-6.239426865	-4.398594431	0.801569592
O	-5.496544665	-5.221675513	1.728873667
O	-5.408246784	-3.852868233	-0.244337027
O	-6.584117473	-3.001266435	1.660314431
O	-7.438587967	-3.348572226	2.955851618
S	-8.366295482	-2.001252866	3.292569726
O	-9.209414278	-1.858436562	2.122987213
O	-9.062416670	-2.391649280	4.477227540
O	-7.418390277	-0.936755562	3.465869798
Na	-7.053637290	1.212985133	3.285571791

Na	-3.321446209	-4.148434602	-1.258246256
H	2.797429110	-6.372932146	3.659606933
H	-6.005112418	-0.952636356	7.336456070
O	-4.708284769	-4.593934857	4.290910946
H	-4.887419481	-4.663454264	3.359153390
H	-5.366156608	-3.998454673	4.622529336
O	-3.185491572	-5.088358184	6.460453195
H	-3.387721240	-4.387355622	5.847220638
H	-3.525956123	-5.886215709	6.078523960
O	-1.093458466	-4.467050012	8.139396713
H	-1.781148008	-4.777685672	7.554038038
H	-1.286862812	-4.890990009	8.975293827

$S_{N\Sigma}$-Min(N_1-H_1)

N	2.558901930	-5.539256412	3.102329727
C	2.809160620	-5.376689351	1.732502897
H	3.506216123	-6.024689647	1.208629502
N	2.194792232	-4.358597627	1.190051263
C	1.430792891	-3.826009857	2.270148040
C	0.480877443	-2.693458153	2.242466530
O	0.177118650	-1.996064113	1.278847846
N	-0.105702589	-2.514434113	3.528686635
H	-0.798587615	-1.756896984	3.631494180
C	0.177016026	-3.305941474	4.639085102
N	-0.447110879	-2.933416063	5.838730994
H	-1.452662659	-2.675702996	5.764559923
H	-0.264762046	-3.663262987	6.524699652
N	0.982170882	-4.343711353	4.678724542
C	1.612558084	-4.544092621	3.422416191
N	-5.415760995	-1.212311967	6.575650795
C	-4.428819660	-2.206901003	6.718475153
H	-4.511478205	-3.006150910	7.444647153
N	-3.421398292	-2.064983079	5.874455221
C	-3.742241184	-0.880348738	5.171165396
C	-2.985524443	-0.213075470	4.083845318
O	-1.987076011	-0.572528767	3.480075069

N	-3.578730912	1.064604431	3.766796008
H	-3.316343061	1.434379633	2.848201206
C	-4.822925242	1.480064394	4.271676274
N	-5.423140530	2.672083339	3.720507541
H	-5.805020022	3.260287633	4.479366533
H	-4.777480214	3.221387146	3.137677661
N	-5.560776146	0.842099309	5.171074690
C	-4.913512867	-0.354074051	5.612854913
O	-7.216703576	-4.834543122	0.133384647
S	-5.966865550	-4.324412973	0.594930501
O	-5.263021787	-5.094300977	1.602968302
O	-5.062761002	-3.841076502	-0.412201464
O	-6.427944249	-3.003834537	1.438835126
O	-7.725881312	-3.370086594	3.191388766
S	-8.492629988	-1.986297211	3.397879549
O	-9.276969892	-1.814282208	2.179026200
O	-9.243275801	-2.322448332	4.567320248
O	-7.503025352	-0.941298623	3.553993563
Na	-7.104091377	1.218907325	3.275101680
Na	-2.932594034	-4.251348819	-1.203953623
H	2.610033211	-6.422209290	3.647970019
H	-6.091761012	-0.900888124	7.304599229
O	-4.592336499	-4.575153277	4.237583480
H	-4.727917235	-4.614825214	3.288530262
H	-5.239210198	-3.968915359	4.586549438
O	-3.079753311	-4.969114013	6.261253997
H	-3.695731583	-4.959061391	5.465121696
H	-3.073698412	-5.891554367	6.536883270
O	-0.960313025	-4.580991494	7.966799097
H	-1.648230886	-4.891480964	7.382879785
H	-1.059931192	-5.085332714	8.777080487

Cl(^{1}nσ*/S_0)(N_1-H_1)

N	2.732942385	-5.458296844	3.249627913
C	3.060681742	-5.256017269	1.902228742
H	3.807685809	-5.871380225	1.409301860

N	2.454801552	-4.238904174	1.344568094
C	1.612942611	-3.748801822	2.385549988
C	0.640245479	-2.632307393	2.326846065
O	0.381332618	-1.916954845	1.364479330
N	-0.018991374	-2.490454499	3.583563464
H	-0.732477353	-1.744073273	3.663536064
C	0.222534882	-3.307208155	4.684773239
N	-0.445384361	-2.973633365	5.871194219
H	-1.432033531	-2.694977976	5.780479427
H	-0.300761682	-3.721217718	6.523595947
N	1.033131862	-4.335297863	4.744248645
C	1.740562748	-4.494335359	3.527594101
N	-5.385622498	-1.153350032	6.559171158
C	-4.416395853	-2.156975035	6.705430510
H	-4.503250170	-2.948821858	7.444401720
N	-3.415119609	-2.031979320	5.853939707
C	-3.716948749	-0.853306051	5.133533739
C	-2.949000254	-0.213886591	4.035562095
O	-1.936764125	-0.585224242	3.460274738
N	-3.547209321	1.055139476	3.679055139
H	-3.284130502	1.400381799	2.751022641
C	-4.790421296	1.487338343	4.173398952
N	-5.396050571	2.657916095	3.582621190
H	-5.761248703	3.278952328	4.322345303
H	-4.755066250	3.179738362	2.967700441
N	-5.524684141	0.878803361	5.098025962
C	-4.884724810	-0.313852548	5.569899056
O	-7.529839662	-4.837793492	0.188170556
S	-6.239900372	-4.327685310	0.536638876
O	-5.502068587	-5.090823695	1.527425207
O	-5.430271564	-3.879280348	-0.564338341
O	-6.614835207	-3.011484265	1.394654927
O	-7.836760509	-3.358836635	3.429896863
S	-8.591735256	-1.956591084	3.597673293
O	-9.414506075	-1.836482268	2.402126233

O	-9.305946315	-2.197680762	4.813953798
O	-7.559312824	-0.951682943	3.654371598
Na	-7.103944266	1.198838468	3.239938783
Na	-3.415320993	-4.326448919	-1.527907399
H	2.780570703	-6.351270910	3.779358157
H	-6.045264165	-0.821446839	7.295177176
O	-4.666395040	-4.578439865	4.132266253
H	-4.847512161	-4.629298688	3.196547476
H	-5.214511310	-3.891803804	4.488490867
O	-3.090937715	-5.109585537	6.161090216
H	-3.695508779	-5.048600775	5.405599204
H	-3.109819490	-6.043083478	6.368149389
O	-0.962982994	-4.807131179	7.937657412
H	-1.635868374	-5.087233878	7.324575723
H	-1.061968265	-5.365407663	8.704280514

Cl($^1\pi\sigma^*/S_0$)(N_1-H_1)

N	2.742272695	-5.414700524	2.993830663
C	3.066906501	-5.111873429	1.680264138
H	3.821933049	-5.671936019	1.133945642
N	2.416886039	-4.059004446	1.202822946
C	1.583080901	-3.684609235	2.259281671
C	0.584284238	-2.579898112	2.263982845
O	0.315602337	-1.814669355	1.357833472
N	-0.129999460	-2.507373708	3.537398067
H	-0.890262440	-1.762045678	3.598656901
C	0.073555705	-3.343622260	4.565005219
N	-0.616199543	-3.272576070	5.677268167
H	-1.486052257	-2.712841529	5.755629052
H	-0.457261702	-3.910194846	6.442691625
N	1.059208431	-4.433120093	4.588322187
C	1.747181703	-4.495428110	3.339998390
N	-5.288819173	-1.243841660	6.689940063
C	-4.299182077	-2.229290090	6.816264780
H	-4.366029647	-3.015962729	7.562107198
N	-3.321251180	-2.120899868	5.940669900

C	-3.650988462	-0.938591061	5.215689121
C	-2.934673537	-0.298632143	4.090120815
O	-1.927249317	-0.652002315	3.482486043
N	-3.553059126	0.953786200	3.753419058
H	-3.260488403	1.358673483	2.857456553
C	-4.750468959	1.407147457	4.308479530
N	-5.358308750	2.582704228	3.755064254
H	-5.809593013	3.124209719	4.512656942
H	-4.724953244	3.174101609	3.198021934
N	-5.455619154	0.799380232	5.241697913
C	-4.816601722	-0.391797738	5.683270466
O	-7.384446732	-4.839239189	0.630825425
S	-6.086547399	-4.263556383	1.009172198
O	-5.328408278	-5.260762634	1.836339687
O	-5.308466815	-4.005067653	-0.218022691
O	-6.271695882	-3.052421571	1.805790649
O	-7.756510779	-3.436078214	3.722990535
S	-8.519019634	-2.028235995	3.538429894
O	-9.091299323	-1.989633964	2.217222235
O	-9.505987645	-2.154827903	4.591926069
O	-7.534972735	-1.010307643	3.786846656
Na	-6.964675291	1.037860701	3.239503667
Na	-3.464783132	-4.501134604	-1.227147890
H	2.835069387	-6.324293825	3.505676072
H	-5.909469715	-0.896406283	7.451889049
O	-4.598342391	-4.536439993	4.272141040
H	-4.788485391	-4.706437745	3.331405700
H	-5.403499217	-4.145860113	4.588742687
O	-3.276669055	-5.156526469	6.449263583
H	-3.621150115	-4.845433071	5.599610401
H	-3.275389261	-6.116050565	6.423238381
O	-1.330270396	-4.294606159	8.058348825
H	-2.072929808	-4.607195283	7.529488130
H	-1.282565046	-4.881841561	8.810313136

S_{CT}-Max(N_1-H_1) [N_1-H_1(G-quartet)]

N	2.832592414	-5.380643787	3.058905542
C	3.154309448	-5.047077570	1.750590705
H	3.922138207	-5.583928021	1.199879757
N	2.481953542	-4.004308850	1.290100795
C	1.633736393	-3.666547792	2.352430986
C	0.597518771	-2.600822796	2.385897684
O	0.297224340	-1.837173199	1.484017660
N	-0.129343779	-2.548872905	3.635827608
H	-1.236736762	-1.573760242	3.598646397
C	0.112080884	-3.378107000	4.640884119
N	-0.586859649	-3.331534449	5.767897444
H	-1.446758354	-2.760219911	5.830080851
H	-0.462437160	-3.988557826	6.567079077
N	1.132056363	-4.450356084	4.671647722
C	1.815938083	-4.487024522	3.417900700
N	-5.222102633	-1.178930244	6.705090567
C	-4.222151364	-2.150591797	6.885858362
H	-4.273678803	-2.880224309	7.691161940
N	-3.255777974	-2.104641051	5.992738296
C	-3.607722898	-0.992023003	5.176294923
C	-2.981154741	-0.427466805	4.019407139
O	-1.929745626	-0.774649345	3.371772780
N	-3.593043272	0.721650148	3.556607699
H	-3.306556553	1.016003019	2.605213856
C	-4.784927717	1.239171332	4.092036992
N	-5.419150799	2.340722018	3.445359951
H	-5.839892697	2.964821585	4.154301522
H	-4.831098506	2.855075134	2.773112584
N	-5.444502146	0.710707223	5.103520705
C	-4.789765032	-0.414111239	5.629854521
O	-7.426790331	-4.182036844	0.640474025
S	-6.049810485	-3.814871676	0.975138232
O	-5.395137846	-4.937887983	1.720296545
O	-5.268570851	-3.622722655	-0.269553598
O	-6.011354645	-2.622631498	1.814347483

O	-7.963460571	-3.553699314	4.099537841
S	-8.664926396	-2.118061060	3.829151853
O	-9.246111873	-2.137248582	2.520392628
O	-9.629044216	-2.118743915	4.905992861
O	-7.603664651	-1.164897479	3.987295172
Na	-7.053149441	0.771305924	3.185250262
Na	-3.547754135	-4.404801342	-1.270090079
H	2.938920999	-6.300089787	3.542754839
H	-5.848712018	-0.780090372	7.452982435
O	-4.600225770	-4.392356183	4.198365349
H	-4.789429248	-4.508172021	3.252608318
H	-5.342758030	-3.892841134	4.512758253
O	-3.330177850	-5.250509148	6.365402536
H	-3.657106042	-4.866696386	5.547102312
H	-3.415524462	-6.204552655	6.280881922
O	-1.269043245	-4.467687057	8.038113987
H	-2.062384252	-4.753610071	7.562069520
H	-1.254687581	-5.138280925	8.749672757

G(N_1-H_1)· [G-G(G-quartet)]

N	2.832554774	-5.380465825	3.059063676
C	3.154116812	-5.047164614	1.750569564
H	3.922155405	-5.582653551	1.198798177
N	2.481273067	-4.004038059	1.289877958
C	1.633850399	-3.666868907	2.352091159
C	0.598697984	-2.600350786	2.383347912
O	0.297190378	-1.836870462	1.482170641
N	-0.126240784	-2.550734556	3.635579259
H	-1.231381303	-1.543327174	3.583699235
C	0.112426183	-3.378911011	4.642042626
N	-0.584210826	-3.329830070	5.766446969
H	-1.447440733	-2.763549108	5.832506176
H	-0.439652100	-4.000564445	6.545100017
N	1.130570502	-4.450059586	4.671410587
C	1.816759425	-4.486968619	3.418791676
N	-5.221718503	-1.179721485	6.705525762

C	-4.222660681	-2.150221214	6.886524913
H	-4.274639138	-2.881850360	7.689464551
N	-3.257795959	-2.105592273	5.992927371
C	-3.609860578	-0.992087176	5.178411357
C	-2.974117059	-0.430346169	4.014474080
O	-1.933156607	-0.776803324	3.375567891
N	-3.596199852	0.725719506	3.556155200
H	-3.314199322	1.027902035	2.606657828
C	-4.785995025	1.238019742	4.092715080
N	-5.420630272	2.339258393	3.445129436
H	-5.844326726	2.961139098	4.154149706
H	-4.824384051	2.858804775	2.784439137
N	-5.445725445	0.712952131	5.103497691
C	-4.787877785	-0.414811859	5.629202204
O	-7.420015910	-4.181909239	0.641587525
S	-6.056379850	-3.814631435	0.974972912
O	-5.393715577	-4.937685028	1.721656251
O	-5.266209530	-3.623343560	-0.269494817
O	-6.010388897	-2.623774240	1.814600514
O	-7.964467013	-3.552819769	4.099592886
S	-8.663807398	-2.119594398	3.830420756
O	-9.247219229	-2.137711194	2.520392755
O	-9.628816564	-2.118617966	4.905804252
O	-7.605136240	-1.164799941	3.984639977
Na	-7.052329481	0.771883119	3.185704830
Na	-3.547487192	-4.404594619	-1.270835965
H	2.942881859	-6.296763325	3.547897897
H	-5.847311286	-0.780832168	7.453030326
O	-4.598995988	-4.393372632	4.198595520
H	-4.791284263	-4.503167873	3.252065266
H	-5.344891091	-3.904561881	4.521545923
O	-3.329591088	-5.248798111	6.366568684
H	-3.656796621	-4.873763834	5.543852370
H	-3.399134186	-6.203840065	6.283485845
O	-1.274494516	-4.469994487	8.039881545

H	-2.050535259	-4.755749587	7.537383878
H	-1.263112009	-5.133771176	8.756641439

6.3 Cartesian coordinates for critical points of G-G (G-quartet) along the reaction pathway leading to the G(N_2-H_{2a})· radical. The corresponding energy profiles are plotted in Figure 2(b) of the main article.

S_0-Min(N_2-H_{2a})

N	2.745695525	-5.474150836	3.138661714
C	3.065746375	-5.262087483	1.791208641
H	3.812274512	-5.872104986	1.291133670
N	2.449947198	-4.246865587	1.241998070
C	1.609981356	-3.769542618	2.290061689
C	0.626589800	-2.663078658	2.238437930
O	0.355340290	-1.944331492	1.282274427
N	-0.032491695	-2.532599757	3.495420172
H	-0.746033302	-1.787938310	3.582976728
C	0.219569886	-3.354951537	4.588853274
N	-0.454718306	-3.021438576	5.768932039
H	-1.438457203	-2.768182256	5.693484169
H	-0.307100550	-3.728975498	6.455054952
N	1.043984838	-4.370286269	4.648776650
C	1.750933543	-4.518009554	3.429026874
N	-5.342699291	-1.272491755	6.597657213
C	-4.369268481	-2.265971276	6.730891715
H	-4.445303743	-3.064642125	7.463257576
N	-3.379353620	-2.137319275	5.863655931
C	-3.686341508	-0.943672104	5.160480302
C	-2.941306720	-0.264165897	4.065526614
O	-1.943513161	-0.615498171	3.454178574
N	-3.537522313	1.019505088	3.772704261
H	-3.282567307	1.403394977	2.857484991
C	-4.776305768	1.435180918	4.292702656
N	-5.380466460	2.639204091	3.772251074
H	-5.752142991	3.206685041	4.550301696
H	-4.742123590	3.204079680	3.192360727
N	-5.504623243	0.783254614	5.190381388
C	-4.849152478	-0.414880752	5.621142464

O	-7.495542785	-4.937280493	0.384347574
S	-6.239426865	-4.398594431	0.801569592
O	-5.496544665	-5.221675513	1.728873667
O	-5.408246784	-3.852868233	-0.244337027
O	-6.584117473	-3.001266435	1.660314431
O	-7.438587967	-3.348572226	2.955851618
S	-8.366295482	-2.001252866	3.292569726
O	-9.209414278	-1.858436562	2.122987213
O	-9.062416670	-2.391649280	4.477227540
O	-7.418390277	-0.936755562	3.465869798
Na	-7.053637290	1.212985133	3.285571791
Na	-3.321446209	-4.148434602	-1.258246256
H	2.797429110	-6.372932146	3.659606933
H	-6.005112418	-0.952636356	7.336456070
O	-4.708284769	-4.593934857	4.290910946
H	-4.887419481	-4.663454264	3.359153390
H	-5.366156608	-3.998454673	4.622529336
O	-3.185491572	-5.088358184	6.460453195
H	-3.387721240	-4.387355622	5.847220638
H	-3.525956123	-5.886215709	6.078523960
O	-1.093458466	-4.467050012	8.139396713
H	-1.781148008	-4.777685672	7.554038038
H	-1.286862812	-4.890990009	8.975293827

$S_{N\Sigma}$-Min(N_2-H_{2a})

N	2.558901930	-5.539256412	3.102329727
C	2.809160620	-5.376689351	1.732502897
H	3.506216123	-6.024689647	1.208629502
N	2.194792232	-4.358597627	1.190051263
C	1.430792891	-3.826009857	2.270148040
C	0.480877443	-2.693458153	2.242466530
O	0.177118650	-1.996064113	1.278847846
N	-0.105702589	-2.514434113	3.528686635
H	-0.798587615	-1.756896984	3.631494180
C	0.177016026	-3.305941474	4.639085102
N	-0.447110879	-2.933416063	5.838730994

H	-1.452662659	-2.675702996	5.764559923
H	-0.264762046	-3.663262987	6.524699652
N	0.982170882	-4.343711353	4.678724542
C	1.612558084	-4.544092621	3.422416191
N	-5.415760995	-1.212311967	6.575650795
C	-4.428819660	-2.206901003	6.718475153
H	-4.511478205	-3.006150910	7.444647153
N	-3.421398292	-2.064983079	5.874455221
C	-3.742241184	-0.880348738	5.171165396
C	-2.985524443	-0.213075470	4.083845318
O	-1.987076011	-0.572528767	3.480075069
N	-3.578730912	1.064604431	3.766796008
H	-3.316343061	1.434379633	2.848201206
C	-4.822925242	1.480064394	4.271676274
N	-5.423140530	2.672083339	3.720507541
H	-5.805020022	3.260287633	4.479366533
H	-4.777480214	3.221387146	3.137677661
N	-5.560776146	0.842099309	5.171074690
C	-4.913512867	-0.354074051	5.612854913
O	-7.216703576	-4.834543122	0.133384647
S	-5.966865550	-4.324412973	0.594930501
O	-5.263021787	-5.094300977	1.602968302
O	-5.062761002	-3.841076502	-0.412201464
O	-6.427944249	-3.003834537	1.438835126
O	-7.725881312	-3.370086594	3.191388766
S	-8.492629988	-1.986297211	3.397879549
O	-9.276969892	-1.814282208	2.179026200
O	-9.243275801	-2.322448332	4.567320248
O	-7.503025352	-0.941298623	3.553993563
Na	-7.104091377	1.218907325	3.275101680
Na	-2.932594034	-4.251348819	-1.203953623
H	2.610033211	-6.422209290	3.647970019
H	-6.091761012	-0.900888124	7.304599229
O	-4.592336499	-4.575153277	4.237583480
H	-4.727917235	-4.614825214	3.288530262

H	-5.239210198	-3.968915359	4.586549438
O	-3.079753311	-4.969114013	6.261253997
H	-3.695731583	-4.959061391	5.465121696
H	-3.073698412	-5.891554367	6.536883270
O	-0.960313025	-4.580991494	7.966799097
H	-1.648230886	-4.891480964	7.382879785
H	-1.059931192	-5.085332714	8.777080487

CI(^{1}nσ*/S_0)(N_2-H_{2a})

N	2.732942385	-5.458296844	3.249627913
C	3.060681742	-5.256017269	1.902228742
H	3.807685809	-5.871380225	1.409301860
N	2.454801552	-4.238904174	1.344568094
C	1.612942611	-3.748801822	2.385549988
C	0.640245479	-2.632307393	2.326846065
O	0.381332618	-1.916954845	1.364479330
N	-0.018991374	-2.490454499	3.583563464
H	-0.732477353	-1.744073273	3.663536064
C	0.222534882	-3.307208155	4.684773239
N	-0.445384361	-2.973633365	5.871194219
H	-1.432033531	-2.694977976	5.780479427
H	-0.300761682	-3.721217718	6.523595947
N	1.033131862	-4.335297863	4.744248645
C	1.740562748	-4.494335359	3.527594101
N	-5.385622498	-1.153350032	6.559171158
C	-4.416395853	-2.156975035	6.705430510
H	-4.503250170	-2.948821858	7.444401720
N	-3.415119609	-2.031979320	5.853939707
C	-3.716948749	-0.853306051	5.133533739
C	-2.949000254	-0.213886591	4.035562095
O	-1.936764125	-0.585224242	3.460274738
N	-3.547209321	1.055139476	3.679055139
H	-3.284130502	1.400381799	2.751022641
C	-4.790421296	1.487338343	4.173398952
N	-5.396050571	2.657916095	3.582621190
H	-5.761248703	3.278952328	4.322345303

H	-4.755066250	3.179738362	2.967700441
N	-5.524684141	0.878803361	5.098025962
C	-4.884724810	-0.313852548	5.569899056
O	-7.529839662	-4.837793492	0.188170556
S	-6.239900372	-4.327685310	0.536638876
O	-5.502068587	-5.090823695	1.527425207
O	-5.430271564	-3.879280348	-0.564338341
O	-6.614835207	-3.011484265	1.394654927
O	-7.836760509	-3.358836635	3.429896863
S	-8.591735256	-1.956591084	3.597673293
O	-9.414506075	-1.836482268	2.402126233
O	-9.305946315	-2.197680762	4.813953798
O	-7.559312824	-0.951682943	3.654371598
Na	-7.103944266	1.198838468	3.239938783
Na	-3.415320993	-4.326448919	-1.527907399
H	2.780570703	-6.351270910	3.779358157
H	-6.045264165	-0.821446839	7.295177176
O	-4.666395040	-4.578439865	4.132266253
H	-4.847512161	-4.629298688	3.196547476
H	-5.214511310	-3.891803804	4.488490867
O	-3.090937715	-5.109585537	6.161090216
H	-3.695508779	-5.048600775	5.405599204
H	-3.109819490	-6.043083478	6.368149389
O	-0.962982994	-4.807131179	7.937657412
H	-1.635868374	-5.087233878	7.324575723
H	-1.061968265	-5.365407663	8.704280514

CI($^1\pi\sigma^*/S_0$)(N_2-H_{2a})

N	2.742272695	-5.414700524	2.993830663
C	3.066906501	-5.111873429	1.680264138
H	3.821933049	-5.671936019	1.133945642
N	2.416886039	-4.059004446	1.202822946
C	1.583080901	-3.684609235	2.259281671
C	0.584284238	-2.579898112	2.263982845
O	0.315602337	-1.814669355	1.357833472
N	-0.129999460	-2.507373708	3.537398067

H	-0.890262440	-1.762045678	3.598656901
C	0.073555705	-3.343622260	4.565005219
N	-0.616199543	-3.272576070	5.677268167
H	-1.486052257	-2.712841529	5.755629052
H	-0.457261702	-3.910194846	6.442691625
N	1.059208431	-4.433120093	4.588322187
C	1.747181703	-4.495428110	3.339998390
N	-5.288819173	-1.243841660	6.689940063
C	-4.299182077	-2.229290090	6.816264780
H	-4.366029647	-3.015962729	7.562107198
N	-3.321251180	-2.120899868	5.940669900
C	-3.650988462	-0.938591061	5.215689121
C	-2.934673537	-0.298632143	4.090120815
O	-1.927249317	-0.652002315	3.482486043
N	-3.553059126	0.953786200	3.753419058
H	-3.260488403	1.358673483	2.857456553
C	-4.750468959	1.407147457	4.308479530
N	-5.358308750	2.582704228	3.755064254
H	-5.809593013	3.124209719	4.512656942
H	-4.724953244	3.174101609	3.198021934
N	-5.455619154	0.799380232	5.241697913
C	-4.816601722	-0.391797738	5.683270466
O	-7.384446732	-4.839239189	0.630825425
S	-6.086547399	-4.263556383	1.009172198
O	-5.328408278	-5.260762634	1.836339687
O	-5.308466815	-4.005067653	-0.218022691
O	-6.271695882	-3.052421571	1.805790649
O	-7.756510779	-3.436078214	3.722990535
S	-8.519019634	-2.028235995	3.538429894
O	-9.091299323	-1.989633964	2.217222235
O	-9.505987645	-2.154827903	4.591926069
O	-7.534972735	-1.010307643	3.786846656
Na	-6.964675291	1.037860701	3.239503667
Na	-3.464783132	-4.501134604	-1.227147890
H	2.835069387	-6.324293825	3.505676072

H	-5.909469715	-0.896406283	7.451889049
O	-4.598342391	-4.536439993	4.272141040
H	-4.788485391	-4.706437745	3.331405700
H	-5.403499217	-4.145860113	4.588742687
O	-3.276669055	-5.156526469	6.449263583
H	-3.621150115	-4.845433071	5.599610401
H	-3.275389261	-6.116050565	6.423238381
O	-1.330270396	-4.294606159	8.058348825
H	-2.072929808	-4.607195283	7.529488130
H	-1.282565046	-4.881841561	8.810313136

S_{CT}-Max(N_2-H_{2a}) [N_2-H_{2a}(G-quartet)]

N	2.764034766	-5.431087238	3.085850454
C	3.119837794	-5.138348448	1.776605704
H	3.878911310	-5.709582323	1.249191070
N	2.492217845	-4.083729438	1.282136370
C	1.640534124	-3.695293467	2.321546720
C	0.651806388	-2.583325260	2.295507188
O	0.414244221	-1.833279074	1.365971848
N	-0.085295498	-2.490896235	3.538778966
H	-0.794041564	-1.718629833	3.577553011
C	0.074140347	-3.314263426	4.606411296
N	-0.648597457	-3.209842393	5.674408123
H	-2.029234065	-2.487058731	5.816955509
H	-0.476466094	-3.879689661	6.426385451
N	1.059561377	-4.413757487	4.647939904
C	1.773363324	-4.497629334	3.409273550
N	-5.146276565	-1.216300820	6.744149245
C	-4.150192831	-2.161442958	6.865620930
H	-4.152927931	-2.943367940	7.624325319
N	-3.224148145	-2.039406175	5.938790474
C	-3.583605195	-0.895879091	5.192319013
C	-2.911626428	-0.277957325	4.031800836
O	-1.911315017	-0.640480380	3.429526629
N	-3.576927640	0.944164578	3.681681414
H	-3.325573447	1.324160087	2.761672005

C	-4.767666505	1.378317897	4.263012431
N	-5.424986406	2.517574664	3.700262896
H	-5.860492985	3.071700122	4.457100247
H	-4.829808044	3.102093507	3.096349362
N	-5.427399719	0.780167145	5.237760019
C	-4.741265540	-0.376644622	5.688696544
O	-7.447256261	-4.557698069	0.662393298
S	-6.050976263	-4.135990068	0.961207816
O	-5.398380803	-5.212416742	1.739585474
O	-5.337554260	-3.958367618	-0.291283691
O	-6.070392517	-2.924626032	1.751453449
O	-7.901329606	-3.516316847	3.840236640
S	-8.593043911	-2.073649462	3.663598269
O	-9.158853984	-2.003732823	2.341357782
O	-9.585297344	-2.165742914	4.714722269
O	-7.567572752	-1.097660413	3.911454584
Na	-7.021301279	0.931639476	3.298652332
Na	-3.622502723	-4.661855832	-1.328747943
H	2.838178563	-6.339499521	3.598452644
H	-5.764567173	-0.864529556	7.524693308
O	-4.626726802	-4.559931949	4.171669786
H	-4.814882816	-4.703980965	3.229352698
H	-5.403522607	-4.102826117	4.462173173
O	-3.336381332	-5.251940048	6.376884412
H	-3.678798414	-4.935208430	5.532216768
H	-3.355756019	-6.209549517	6.338731632
O	-1.317601570	-4.333305214	7.996371427
H	-2.071256285	-4.663781142	7.482317588
H	-1.286027686	-4.981555171	8.722063198

G(N_2-H_{2a})· [G-G(G-quartet)]

N	2.768454930	-5.436481830	3.081427151
C	3.123500891	-5.139606006	1.772676510
H	3.883795796	-5.710828271	1.247588282
N	2.496010913	-4.085523529	1.282108869
C	1.641450606	-3.700959590	2.324273284

C	0.651838207	-2.586657240	2.302275698
O	0.419814706	-1.838001483	1.366199156
N	-0.058792878	-2.501736383	3.540168379
H	-0.802008471	-1.782265741	3.591348921
C	0.076168334	-3.339352170	4.630862735
N	-0.687947781	-3.209409219	5.642803224
H	-2.357867615	-2.526368102	5.888204622
H	-0.513004137	-3.859406223	6.419911867
N	1.078862873	-4.425335462	4.659905940
C	1.773939545	-4.507038751	3.407609780
N	-5.141441944	-1.211582729	6.749575164
C	-4.170378308	-2.152272125	6.891504313
H	-4.145502839	-2.935560834	7.651258800
N	-3.239668675	-1.999375530	5.969162603
C	-3.571668131	-0.883199718	5.188927712
C	-2.897256048	-0.262356105	4.022751979
O	-1.909182544	-0.631893416	3.414649753
N	-3.564252977	0.964921868	3.683046146
H	-3.344851967	1.309277549	2.739401131
C	-4.764458601	1.381096691	4.256318349
N	-5.422841704	2.519959284	3.699952624
H	-5.845397675	3.088645108	4.452954773
H	-4.846062310	3.085328580	3.060562634
N	-5.429142988	0.770711198	5.224041903
C	-4.736885111	-0.379585122	5.679540454
O	-7.464818384	-4.557633261	0.676403028
S	-6.080824294	-4.137727336	0.960071297
O	-5.377596150	-5.223924325	1.712161959
O	-5.352192414	-3.950766442	-0.311667021
O	-6.073311141	-2.916768904	1.761227966
O	-7.908345967	-3.515927764	3.832094983
S	-8.595715727	-2.062765646	3.658103006
O	-9.151253994	-1.989818906	2.334907906
O	-9.586637115	-2.163048503	4.704343743
O	-7.557865578	-1.105448421	3.924823728

Na	-7.022119916	0.921950151	3.305114608
Na	-3.618861666	-4.652392999	-1.307687212
H	2.843310270	-6.348293442	3.585009393
H	-5.792798039	-0.861425154	7.510628253
O	-4.653787450	-4.531111067	4.163186508
H	-4.774461787	-4.776935135	3.231262785
H	-5.399050318	-3.962100619	4.311761609
O	-3.363075424	-5.288036276	6.358461318
H	-3.783849084	-5.019787243	5.534757612
H	-3.472884270	-6.245872349	6.390993389
O	-1.272059401	-4.297061150	8.004478634
H	-2.005295521	-4.763427965	7.571018066
H	-1.104511391	-4.921741240	8.740808032

6.4 Cartesian coordinates for critical points of G-T (loop) along the reaction pathway leading to the G(N_1-H_1)$^{\cdot}$ radical. The corresponding energy profiles are plotted in Figure 3(a) of the main article.

S_0-Min [N_1-H_1(loop)]

N	-0.482580037	-6.486360496	2.622680203
C	-1.354710104	-5.362660386	2.722970209
H	-1.713280131	-5.132390393	3.721650288
C	-1.704070129	-4.591730353	1.669330130
C	-2.560700196	-3.339640259	1.757590137
H	-2.013790154	-2.477340190	1.378670107
H	-3.472990269	-3.430740266	1.175460090
H	-2.852010219	-3.162520242	2.788170212
C	-1.149460087	-4.965870384	0.332810026
O	-1.549300120	-4.487220344	-0.754000055
N	-0.091080007	-5.873690454	0.353850027
H	0.210590016	-6.200480477	-0.573460045
C	0.113590009	-6.855590534	1.389850108
O	0.741020057	-7.872230625	1.141990089
N	-6.016780458	-7.758920599	-1.212140095
C	-7.265590558	-8.210210630	-1.640560128
H	-7.881640614	-8.856360658	-1.025620080

N	-7.594790561	-7.794120623	-2.845050220
C	-6.468530503	-7.038750528	-3.255790251
C	-6.269230498	-6.242130484	-4.470920346
O	-6.983830555	-5.989570482	-5.436020440
N	-4.955970382	-5.641400428	-4.440560341
H	-4.814110371	-4.983100384	-5.172590396
C	-4.150050318	-5.553300406	-3.340250258
N	-3.043870236	-4.656690358	-3.338220254
H	-3.006170230	-4.010770311	-4.143690317
H	-2.170780169	-5.194280398	-3.235960249
N	-4.324010332	-6.246570493	-2.245210171
C	-5.513050444	-7.008120532	-2.267370172
O	-7.336030559	-5.313350433	1.644670126
S	-6.063540465	-4.651840358	1.685480127
O	-5.012830388	-5.332820399	2.387560185
O	-5.651250427	-4.155480317	0.384340029
O	-6.274370502	-3.222260247	2.507710191
O	-7.080250566	-3.411210265	3.881940299
S	-8.285840643	-2.295610176	3.686410285
O	-9.018460667	-2.758930211	2.534880194
O	-9.023500710	-2.401180186	4.915940378
O	-7.596790586	-1.052820082	3.492630270
Na	-7.190740553	0.892000068	2.473210189
Na	-3.614200276	-4.591530355	-0.992620079
H	-5.504730402	-7.865620619	-0.327730025
H	-0.378030029	-7.175720545	3.372600260
O	-7.957990625	-4.983460384	-1.152010087
H	-8.188290627	-5.890520460	-0.957860071
H	-7.181350567	-4.776620370	-0.639890051
O	-8.227800641	-4.400910338	-3.689230286
H	-7.889700618	-4.660110356	-2.821670217
H	-8.745630689	-3.619670281	-3.468230267
O	-6.003370472	-3.405390262	-4.830640371
H	-6.737470499	-4.011130310	-4.742850363
H	-6.371760495	-2.536080193	-4.933160377

CI(^{1}nσ*/^{1}πσ*/S_0) [N_1-H_1(loop)]

N	-0.505956660	-6.481043270	2.621870440
C	-1.355713874	-5.355672865	2.702578194
H	-1.730762163	-5.127556148	3.699045307
C	-1.688511345	-4.585523802	1.667246262
C	-2.560702440	-3.346397350	1.755683469
H	-2.049427247	-2.477493207	1.344133158
H	-3.483622022	-3.463594748	1.199412462
H	-2.827455241	-3.147964470	2.789849725
C	-1.153481999	-4.959133751	0.334330630
O	-1.546132459	-4.487355982	-0.765119937
N	-0.110184631	-5.890914380	0.352553282
H	0.189183100	-6.221376205	-0.574168359
C	0.107831321	-6.857345339	1.391716442
O	0.747278557	-7.874169107	1.160653933
N	-6.010887488	-7.740634086	-1.217999003
C	-7.277632621	-8.186620597	-1.634450179
H	-7.898414950	-8.812775080	-1.004034554
N	-7.589267061	-7.778131850	-2.846904717
C	-6.465775395	-7.034017514	-3.257259056
C	-6.301074903	-6.216084486	-4.450008346
O	-7.023797461	-5.998661112	-5.423625892
N	-5.050557439	-5.495979397	-4.403366986
H	-5.039044231	-4.739545677	-5.063012848
C	-4.169919114	-5.517294181	-3.358225631
N	-3.070881490	-4.634756612	-3.344518908
H	-2.965334061	-3.998913375	-4.149588362
H	-2.211821997	-5.129491894	-3.079752681
N	-4.300943919	-6.280453183	-2.285561111
C	-5.514305917	-6.995857854	-2.270076295
O	-7.279181682	-5.266367886	1.616531020
S	-5.993262128	-4.633375385	1.629551215
O	-4.959195490	-5.274851809	2.386602030
O	-5.593976938	-4.206095549	0.302730197
O	-6.217198404	-3.289438124	2.481301749

O	-7.421126388	-3.410351611	4.523311952
S	-8.543790845	-2.329338410	4.152772967
O	-9.205110373	-2.838735770	2.980205429
O	-9.326389120	-2.381750734	5.354688384
O	-7.848693033	-1.097183381	3.915090947
Na	-7.427537847	0.856744734	2.901942257
Na	-3.666849052	-4.605222695	-0.962868903
H	-5.502447425	-7.830547174	-0.328135065
H	-0.379271971	-7.146116464	3.391727657
O	-7.942785245	-4.997006300	-1.210141859
H	-8.119114196	-5.842879056	-0.811393741
H	-7.191235969	-4.664085483	-0.720703678
O	-8.043741205	-4.153936543	-3.784516265
H	-7.970230653	-4.446272725	-2.873289018
H	-8.417924448	-4.878741011	-4.269417783
O	-6.093774055	-2.965264670	-5.262828728
H	-6.815958228	-3.428120881	-4.823998148
H	-6.434299720	-2.752575289	-6.124314832

S_{CT}-Max(N_1-H_1) [N_1-H_1(loop)]

N	-0.329020479	-6.475412506	2.562793526
C	-1.292015067	-5.434138686	2.704523550
H	-1.654296622	-5.261267353	3.713806389
C	-1.719058646	-4.663389191	1.678592886
C	-2.650778785	-3.469072368	1.822619237
H	-2.142022285	-2.561157702	1.499648635
H	-3.555466713	-3.573948208	1.230571958
H	-2.963764770	-3.363637373	2.856905727
C	-1.143825932	-4.953019912	0.327843594
O	-1.580427050	-4.472294905	-0.748097946
N	-0.015099401	-5.765047984	0.310597215
H	0.318894122	-6.034558909	-0.623976236
C	0.313266454	-6.738252306	1.323874501
O	1.062298228	-7.658160700	1.046688066
N	-5.855234868	-7.806780342	-1.087158446
C	-7.161344598	-8.152167983	-1.396337356

H	-7.781771478	-8.754983791	-0.731674258
N	-7.577825932	-7.688468163	-2.607403819
C	-6.499054982	-7.015982571	-3.088903151
C	-6.338071748	-6.205795322	-4.314781359
O	-7.126700845	-5.986365573	-5.222392659
N	-5.073351024	-5.515228484	-4.385693873
H	-5.293853427	-4.530976349	-4.832957384
C	-4.163413012	-5.607816405	-3.421271856
N	-3.051924964	-4.788437882	-3.410084403
H	-2.935853485	-4.171215471	-4.227398738
H	-2.199897295	-5.287716256	-3.108828050
N	-4.221721048	-6.415121702	-2.284296430
C	-5.399573939	-7.038590981	-2.149412155
O	-7.372479547	-5.564553149	1.181137024
S	-6.168011590	-4.723625962	1.393202695
O	-5.067870759	-5.513798595	1.922161552
O	-5.773410942	-4.296774241	-0.041766288
O	-6.445399584	-3.536415994	2.172742157
O	-7.887607828	-3.581145309	4.295241611
S	-8.715251576	-2.230889904	3.999770700
O	-9.492317674	-2.436730895	2.797535787
O	-9.500675235	-2.209760460	5.217990153
O	-7.763992446	-1.164226937	3.875595395
Na	-7.236035056	0.747465759	2.840109276
Na	-3.654661820	-4.654315008	-0.987244141
H	-5.285696784	-7.893189166	-0.226397193
H	-0.146411719	-7.173380258	3.289310147
O	-7.738121023	-4.665641740	-1.403425595
H	-8.108025234	-5.488889745	-1.104721300
H	-6.837822138	-4.454376466	-0.783877747
O	-8.002530733	-3.935052127	-3.674798697
H	-7.900741002	-4.259832753	-2.609286537
H	-8.556588361	-4.524629132	-4.171326784
O	-6.030486096	-3.333340637	-4.907185341
H	-6.907974320	-3.616526725	-4.429349906

H	-6.210121505	-3.015453587	-5.783995492

G(N_1-H_1)· [G-T(loop)]

N	-0.330381719	-6.476900976	2.561878536
C	-1.290545658	-5.433938339	2.704116116
H	-1.652560222	-5.260953487	3.713545732
C	-1.718073001	-4.663907976	1.678148091
C	-2.648826740	-3.469295030	1.822833533
H	-2.142954489	-2.560355998	1.498652544
H	-3.552408895	-3.578540953	1.229017796
H	-2.963953342	-3.363396544	2.856620014
C	-1.143192258	-4.952260130	0.326176495
O	-1.584202741	-4.472288142	-0.747549199
N	-0.014950294	-5.764574000	0.309257254
H	0.318741142	-6.034389837	-0.625498542
C	0.313086195	-6.738299614	1.322539715
O	1.062556282	-7.657919554	1.046681620
N	-5.855627147	-7.809078083	-1.087472053
C	-7.161607440	-8.151878205	-1.398888069
H	-7.776519130	-8.758600559	-0.734790990
N	-7.579988256	-7.689774755	-2.601305792
C	-6.496257222	-7.013239105	-3.090039093
C	-6.321712604	-6.201054582	-4.311879283
O	-7.130492294	-5.984735178	-5.218353004
N	-5.060721442	-5.538621082	-4.379307238
H	-5.472812176	-4.127870007	-4.992074722
C	-4.177130249	-5.615969651	-3.436119606
N	-3.052356445	-4.786944491	-3.406953537
H	-2.943242033	-4.182182490	-4.233656751
H	-2.200633211	-5.299678663	-3.133845481
N	-4.225023632	-6.418992104	-2.275804474
C	-5.395796301	-7.037206601	-2.151106528
O	-7.382504016	-5.566758812	1.178420445
S	-6.204287008	-4.731084577	1.405924164
O	-5.080136966	-5.503604101	1.911256532
O	-5.777909637	-4.297313795	-0.050313871

O	-6.452946974	-3.535673759	2.164216376
O	-7.887996879	-3.580859601	4.295462934
S	-8.716485088	-2.229835688	4.000980542
O	-9.491213228	-2.437090720	2.797412478
O	-9.500712277	-2.210332834	5.218434185
O	-7.762350726	-1.165950483	3.877886818
Na	-7.237369324	0.747730554	2.839645775
Na	-3.649116566	-4.654390739	-0.988353249
H	-5.288416977	-7.899192682	-0.228761870
H	-0.151894831	-7.179366840	3.285215374
O	-7.752857022	-4.662672453	-1.400479184
H	-8.112401847	-5.520831466	-1.206221031
H	-6.571343875	-4.377078799	-0.641833804
O	-8.015512350	-3.929053865	-3.698228893
H	-7.847260338	-4.393298018	-2.327292389
H	-8.410804951	-4.620115283	-4.219872732
O	-6.012692988	-3.321895374	-4.923604658
H	-7.202793729	-3.716949093	-4.195272001
H	-6.165997912	-3.004600537	-5.805445375

6.5 Cartesian coordinates for critical points of G-T (loop) along the reaction pathway leading to the G(N_2-H_{2a})˙ radical. The corresponding energy profiles are plotted in Figure 3(b) of the main article.

S_0-Min[N_2-H_{2a}(loop)]

N	-0.482580037	-6.486360496	2.622680203
C	-1.354710104	-5.362660386	2.722970209
H	-1.713280131	-5.132390393	3.721650288
C	-1.704070129	-4.591730353	1.669330130
C	-2.560700196	-3.339640259	1.757590137
H	-2.013790154	-2.477340190	1.378670107
H	-3.472990269	-3.430740266	1.175460090
H	-2.852010219	-3.162520242	2.788170212
C	-1.149460087	-4.965870384	0.332810026
O	-1.549300120	-4.487220344	-0.754000055
N	-0.091080007	-5.873690454	0.353850027
H	0.210590016	-6.200480477	-0.573460045
C	0.113590009	-6.855590534	1.389850108

O	0.741020057	-7.872230625	1.141990089
N	-6.016780458	-7.758920599	-1.212140095
C	-7.265590558	-8.210210630	-1.640560128
H	-7.881640614	-8.856360658	-1.025620080
N	-7.594790561	-7.794120623	-2.845050220
C	-6.468530503	-7.038750528	-3.255790251
C	-6.269230498	-6.242130484	-4.470920346
O	-6.983830555	-5.989570482	-5.436020440
N	-4.955970382	-5.641400428	-4.440560341
H	-4.814110371	-4.983100384	-5.172590396
C	-4.150050318	-5.553300406	-3.340250258
N	-3.043870236	-4.656690358	-3.338220254
H	-3.006170230	-4.010770311	-4.143690317
H	-2.170780169	-5.194280398	-3.235960249
N	-4.324010332	-6.246570493	-2.245210171
C	-5.513050444	-7.008120532	-2.267370172
O	-7.336030559	-5.313350433	1.644670126
S	-6.063540465	-4.651840358	1.685480127
O	-5.012830388	-5.332820399	2.387560185
O	-5.651250427	-4.155480317	0.384340029
O	-6.274370502	-3.222260247	2.507710191
O	-7.080250566	-3.411210265	3.881940299
S	-8.285840643	-2.295610176	3.686410285
O	-9.018460667	-2.758930211	2.534880194
O	-9.023500710	-2.401180186	4.915940378
O	-7.596790586	-1.052820082	3.492630270
Na	-7.190740553	0.892000068	2.473210189
Na	-3.614200276	-4.591530355	-0.992620079
H	-5.504730402	-7.865620619	-0.327730025
H	-0.378030029	-7.175720545	3.372600260
O	-7.957990625	-4.983460384	-1.152010087
H	-8.188290627	-5.890520460	-0.957860071
H	-7.181350567	-4.776620370	-0.639890051
O	-8.227800641	-4.400910338	-3.689230286
H	-7.889700618	-4.660110356	-2.821670217

H	-8.745630689	-3.619670281	-3.468230267
O	-6.003370472	-3.405390262	-4.830640371
H	-6.737470499	-4.011130310	-4.742850363
H	-6.371760495	-2.536080193	-4.933160377

CI(^{1}nσ*/^{1}πσ*/S_0) [N_2-H_{2a}(loop)]

N	-0.505956660	-6.481043270	2.621870440
C	-1.355713874	-5.355672865	2.702578194
H	-1.730762163	-5.127556148	3.699045307
C	-1.688511345	-4.585523802	1.667246262
C	-2.560702440	-3.346397350	1.755683469
H	-2.049427247	-2.477493207	1.344133158
H	-3.483622022	-3.463594748	1.199412462
H	-2.827455241	-3.147964470	2.789849725
C	-1.153481999	-4.959133751	0.334330630
O	-1.546132459	-4.487355982	-0.765119937
N	-0.110184631	-5.890914380	0.352553282
H	0.189183100	-6.221376205	-0.574168359
C	0.107831321	-6.857345339	1.391716442
O	0.747278557	-7.874169107	1.160653933
N	-6.010887488	-7.740634086	-1.217999003
C	-7.277632621	-8.186620597	-1.634450179
H	-7.898414950	-8.812775080	-1.004034554
N	-7.589267061	-7.778131850	-2.846904717
C	-6.465775395	-7.034017514	-3.257259056
C	-6.301074903	-6.216084486	-4.450008346
O	-7.023797461	-5.998661112	-5.423625892
N	-5.050557439	-5.495979397	-4.403366986
H	-5.039044231	-4.739545677	-5.063012848
C	-4.169919114	-5.517294181	-3.358225631
N	-3.070881490	-4.634756612	-3.344518908
H	-2.965334061	-3.998913375	-4.149588362
H	-2.211821997	-5.129491894	-3.079752681
N	-4.300943919	-6.280453183	-2.285561111
C	-5.514305917	-6.995857854	-2.270076295
O	-7.279181682	-5.266367886	1.616531020

S	-5.993262128	-4.633375385	1.629551215
O	-4.959195490	-5.274851809	2.386602030
O	-5.593976938	-4.206095549	0.302730197
O	-6.217198404	-3.289438124	2.481301749
O	-7.421126388	-3.410351611	4.523311952
S	-8.543790845	-2.329338410	4.152772967
O	-9.205110373	-2.838735770	2.980205429
O	-9.326389120	-2.381750734	5.354688384
O	-7.848693033	-1.097183381	3.915090947
Na	-7.427537847	0.856744734	2.901942257
Na	-3.666849052	-4.605222695	-0.962868903
H	-5.502447425	-7.830547174	-0.328135065
H	-0.379271971	-7.146116464	3.391727657
O	-7.942785245	-4.997006300	-1.210141859
H	-8.119114196	-5.842879056	-0.811393741
H	-7.191235969	-4.664085483	-0.720703678
O	-8.043741205	-4.153936543	-3.784516265
H	-7.970230653	-4.446272725	-2.873289018
H	-8.417924448	-4.878741011	-4.269417783
O	-6.093774055	-2.965264670	-5.262828728
H	-6.815958228	-3.428120881	-4.823998148
H	-6.434299720	-2.752575289	-6.124314832

S_{CT}-Max(N_2-H_{2a}) [N_2-H_{2a}(loop)]

N	-0.195846547	-6.364148439	2.548203829
C	-1.179123441	-5.357364963	2.753879113
H	-1.519396641	-5.228391619	3.777488648
C	-1.658958769	-4.568852094	1.767075772
C	-2.651248980	-3.437431008	1.981202440
H	-2.197282238	-2.484041659	1.713081446
H	-3.543741506	-3.568815765	1.375700316
H	-2.967988044	-3.406805669	3.019206697
C	-1.123935143	-4.796772148	0.385380327
O	-1.635136580	-4.310391506	-0.656702341
N	0.037593784	-5.556572838	0.308362595
H	0.356917502	-5.788086456	-0.641313813

C	0.439831761	-6.542853924	1.287753010
O	1.237031482	-7.407995331	0.976955258
N	-5.711067671	-7.814403194	-0.971520173
C	-7.048954494	-8.151780678	-1.163845316
H	-7.590896239	-8.751239280	-0.434795481
N	-7.566823384	-7.712764596	-2.318922546
C	-6.525744460	-7.041153363	-2.911869887
C	-6.505128031	-6.240416532	-4.168402905
O	-7.430398738	-5.975637774	-4.913397940
N	-5.173328101	-5.731194398	-4.412031871
H	-5.074418650	-5.172516333	-5.275418595
C	-4.165210331	-5.678096700	-3.493658874
N	-3.132108314	-4.900454238	-3.715921003
H	-3.301609730	-3.967472192	-4.497872512
H	-2.324789169	-5.097998010	-3.133778805
N	-4.188264266	-6.411322950	-2.279930046
C	-5.345679459	-7.046724118	-2.070534566
O	-7.450551024	-5.428595448	0.926917829
S	-6.176466943	-4.703436675	1.279183434
O	-5.172530985	-5.603628708	1.756415740
O	-5.670202540	-4.147126206	-0.056449216
O	-6.444313236	-3.598195178	2.178400956
O	-7.584564581	-3.691190052	4.442311087
S	-8.428632191	-2.327680974	4.326817295
O	-9.277046464	-2.457959560	3.165961116
O	-9.114052780	-2.392923989	5.602787052
O	-7.513401142	-1.231683315	4.233505507
Na	-6.949389742	0.808279020	3.523789846
Na	-3.636876014	-4.644607405	-0.916330876
H	-5.081227706	-7.879221691	-0.156187670
H	0.028023476	-7.084200027	3.240767575
O	-6.859535974	-4.293507783	-2.170394144
H	-7.820647538	-4.371658468	-2.133652696
H	-6.355422518	-4.260648379	-1.073460873
O	-5.969358081	-3.014841778	-4.131725889

H	-6.467843049	-3.630703949	-3.165143855
H	-6.651157933	-2.619472188	-4.663227052
O	-3.733040998	-2.938429234	-5.122718854
H	-4.802459079	-2.848469801	-4.639946179
H	-3.120809528	-2.230583378	-4.940321801

G(N_2-H_{2a})· [G-T(loop)]

N	-0.150308606	-6.379766788	2.538207930
C	-1.126071067	-5.371980415	2.760609629
H	-1.453116106	-5.243614640	3.788931207
C	-1.613955647	-4.578756318	1.783011728
C	-2.599971647	-3.447724823	2.017682592
H	-2.155298591	-2.491878520	1.743006208
H	-3.498970502	-3.586883475	1.423298482
H	-2.902881573	-3.418811515	3.060308661
C	-1.097649110	-4.795629676	0.392179805
O	-1.619616579	-4.291752359	-0.635080931
N	0.061188988	-5.559841460	0.297174306
H	0.368136801	-5.786836910	-0.657795679
C	0.465347180	-6.557385184	1.266103453
O	1.250875230	-7.429305140	0.945583466
N	-5.713451085	-7.795791077	-0.908194310
C	-7.042323797	-8.147827459	-1.114217973
H	-7.584548494	-8.753041605	-0.391256825
N	-7.553567600	-7.714368532	-2.269223700
C	-6.508570277	-7.032333301	-2.858143817
C	-6.484863136	-6.236907928	-4.119322996
O	-7.414678840	-6.015852811	-4.876506057
N	-5.170676039	-5.703509062	-4.345965119
H	-5.078041869	-5.137016593	-5.200339848
C	-4.132075421	-5.628605557	-3.428227843
N	-3.130839749	-4.857270030	-3.652127770
H	-3.333952604	-3.591288515	-4.926488928
H	-2.351089003	-5.109058397	-3.047365282
N	-4.189619933	-6.389567309	-2.200631433
C	-5.341591300	-7.024103907	-2.013415343

O	-7.462627273	-5.463049173	1.074324999
S	-6.242644368	-4.753386509	1.465218406
O	-5.185960255	-5.625440653	1.916350858
O	-5.682507816	-4.191767382	0.086882109
O	-6.474387543	-3.638264209	2.336353956
O	-7.643231499	-3.730374437	4.558420232
S	-8.485757934	-2.366087579	4.405535850
O	-9.324625690	-2.521193823	3.239011125
O	-9.179968950	-2.407146712	5.676458526
O	-7.565928704	-1.274015817	4.295426696
Na	-6.934887957	0.732379085	3.548849172
Na	-3.635407615	-4.627062793	-0.862116905
H	-5.087869145	-7.869618130	-0.093024846
H	0.081877384	-7.103630040	3.224340532
O	-7.086796118	-4.320971521	-2.144838281
H	-8.047491960	-4.417637388	-2.120766881
H	-6.283496058	-4.295525324	-0.681320264
O	-6.142548851	-2.892094983	-4.370479593
H	-6.832917935	-3.813117803	-2.919344012
H	-6.779926602	-2.499763388	-4.953406053
O	-3.648741818	-2.843927512	-5.458868250
H	-5.268125421	-2.755338579	-4.747754984
H	-2.957945926	-2.184105169	-5.329797738