Supporting Information

Does 8-Nitroguanine Form 8-Oxoguanine? An Insight from Its Reaction with ·OH Radical

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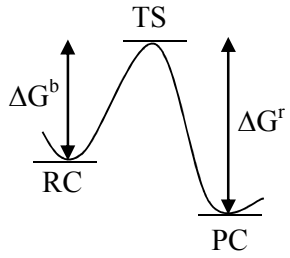
Table S1: Gibbs free reaction energies and their corresponding enthalpy changes (kcal/mol) involved in addition reactions of OH radical at the different sites of 8-nitroG as obtained at the different levels of theory in gas phase and aqueous media.

	Reaction sites			
Level of theory	**C2**	**C4**	**C5**	**C8**
Gas phase				
M06-2X/6-31G(d,p)	-13.59(-23.72)	-9.78(-19.45)	-6.24(-16.10)	-33.53(-43.18)
M06-2X/ aug-cc-pVDZ// M06-2X/6-31G(d,p)	-11.29(-21.42)	-8.72(-18.38)	-5.18(-15.05)	-31.83(-41.47)
M06-2X/aug-cc-pVDZ	-11.47(-21.53)	-9.02(-18.57)	-5.28(-15.15)	-32.19(-41.60)
DLPNO-CCSD(T)/cc-pVDZ// M06-2X/6-31G(d,p)	-12.06(-22.19)	-4.69(-14.35)	-0.41(-10.27)	-26.02(-35.66)
Aqueous media				
CPCM-DLPNO-CCSD(T)/cc-pVDZ// M06-2X/6-31G(d,p)	-5.96(-16.09)	9.99(0.32)	5.22(-4.64)	-24.59(-34.23)

The corresponding enthalpy changes are given in parentheses.

Definitions:

The Gibbs free energy barrier (ΔG^b) and released energy (ΔG^r) for a one step chemical reaction in the present contribution are defined as below:



Relative Boltzmann Populations:

Boltzmann populations of adducts formed by addition of ·OH radical at the C2, C4 and C5 sites of 8-nitroG relative to that of the C8-site adduct at 298.15 K were calculated using the following formula:

$$\frac{N_j}{N_i} = e^{-\frac{(G_j - G_i)}{K_b T}}$$

where G_j = Gibbs free energies of adducts (j= C2, C4, C5)

G_i = Gibbs free energy of C8-site adduct.

K_b= Boltzmann constant