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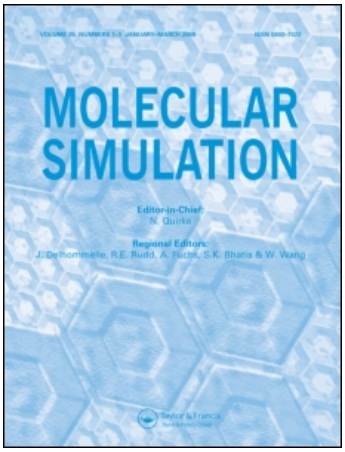

Molecular Simulation

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The role of spin in biological processes: O_2, NO, nucleobases, nucleosides, nucleotides and Watson-Crick base pairs

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To cite this Article Chen, Edward S. and Chen, Edward C. M.(2009) 'The role of spin in biological processes: O_2, NO, nucleobases, nucleosides, nucleotides and Watson-Crick base pairs', Molecular Simulation, 35: 9, 719 — 724
To link to this Article: DOI: 10.1080/08927020902865931
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Molecular Simulation
Vol. 35, No. 9, August 2009, 719–724

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The role of spin in biological processes: O_2, NO, nucleobases, nucleosides, nucleotides and Watson–Crick base pairs

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(*Received 11 January 2009; final version received 25 February 2009*)

The experimental electron affinities of adenine, guanine, cytosine, thymine and uracil have been determined from reduction potentials and negative ion photoelectron spectra. Updated values for purine, pyrimidine and other nitrogen heterocyclics, which have not been measured in the gas phase, are presented. The electron affinity of Watson–Crick guanine–cytosine is estimated empirically. The experimental values are consistent with quantum mechanical semi-empirical multiconfiguration configuration interaction calculations. The bulk hydration energies of the nucleobase anions, 2.34 eV, determined from the experimental data and sequential anion hydration energy difference of about 0.20(5) eV suggest that 10–15 water molecules complete the hydration shell. The electron affinities for the formation of doublet and quartet anions of the nucleobases, nucleosides, nucleotides and Watson–Crick base pairs are calculated. We postulate that low-lying quartet anion states and their spin distribution can and will participate in electron conduction, radiation damage, oxidation damage and repair, strand breakage and protein synthesis.

Keywords: electron affinity; DNA; RNA; semi-empirical calculations; spin distribution

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1. Introduction

A half century ago, Szent-Gyorgi [1] observed that reduction potentials (ERED), electron affinities (E_a) and quantum mechanical calculations gave different energies for biological molecules. Nucleobases and O_2 were reduced in biological systems and NO oxidised, yet the E_a of NO was greater than that of O_2 and orbital energies gave negative E_a. These differences are partly due to the assumption that there are few excited anion states stable to autodetachment. In 1958, Mulliken assigned the photodetachment $E_a(O_2)$, 0.15(5) eV to the ground state and concluded 'It seems rather unlikely that a bound σ^* Rydberg MO exists'. In 1962, Jortner and Sokolov reported $E_a(O_2)$, 0.74(17) and E_a(NO), 0.87(17) eV from donor acceptor complex data [2,3]. Subsequently, experimental reduction potentials, gas phase electron affinities and theoretical calculations have been reported, but the differences persist. Indeed, the lower theoretical electron affinities have been used to assign experimental gas phase measurement that conflict with reduction potentials [4–23].

The energy differences between an N electron system and one of its $N + 1$ anions are: E_a in their most stable forms; vertical E_a (VE_a) in the neutral geometry and vertical detachment energy (E_{vd}) in the anion geometry. The AE_a is always positive, exothermic by convention, since it is greater than the long range E_a (LE_a), where repulsions are balanced by dipole, polarisation or other attractions [4,5]. The Nernst equation relates gas and condensed phase energetics: $E_a = 4.44 + ERED + \Delta\Delta G$; 4.44 V_{std} is the 1 M, 298 K, normal hydrogen electrode and $\Delta\Delta G$ the solution energy difference [13–16,18–20]. Shown in Figure 1 are Herschbach ionic Morse Person electron curves (HIMPEC) for anions of guanine in the N9–H dimension, NO and O_2. The acronym emphasises the seminal work of Morse, Person, and Herschbach and the multidimensional nature of anion surfaces due to the plethora of curves in the electron molecule dimensions. The curves for guanine are improvements in those predicted in 2008 [5–16].

In 2002, uncertainties in experimental methods were estimated. Significantly different electron affinities were identified: (in eV) O_2, 0.05(2)–1.07(2); NO, 0.02(1)–0.91(10); Watson–Crick adenine–thymine (AT), 1.4(1); G, 1.66(2), 0.3(1); A, 1.10(2), 0.3(1), 0.02(1); C, 1.04(2), 0.77(2), 0.230(8), 0.216(1), 0.13(12), 0.098(1), 0.085(8); U, 1.00(2), 0.80(5), 0.50(5), 0.30(5), 0.15(12), 0.090(6); T, 0.99(1), 0.80(5), 0.50(5), 0.30(5), 0.12(12), 0.068(8). Twenty-seven $E_a(O_2)$ were assigned to predicted doublet and quartet states. An E_a, 0.05(5) eV was assigned to polarisation states [4,5,11–16]. In 2008, Toader and Graham [10] presented a theoretical model for experimentally observed long range anions.

The adiabatic E_a (AE_a) of the nucleobases and Watson–Crick AT have been reported to be 1.0–1.7 eV from ERED and/or gas phase studies [4,5,7,13–21]. Bowen and

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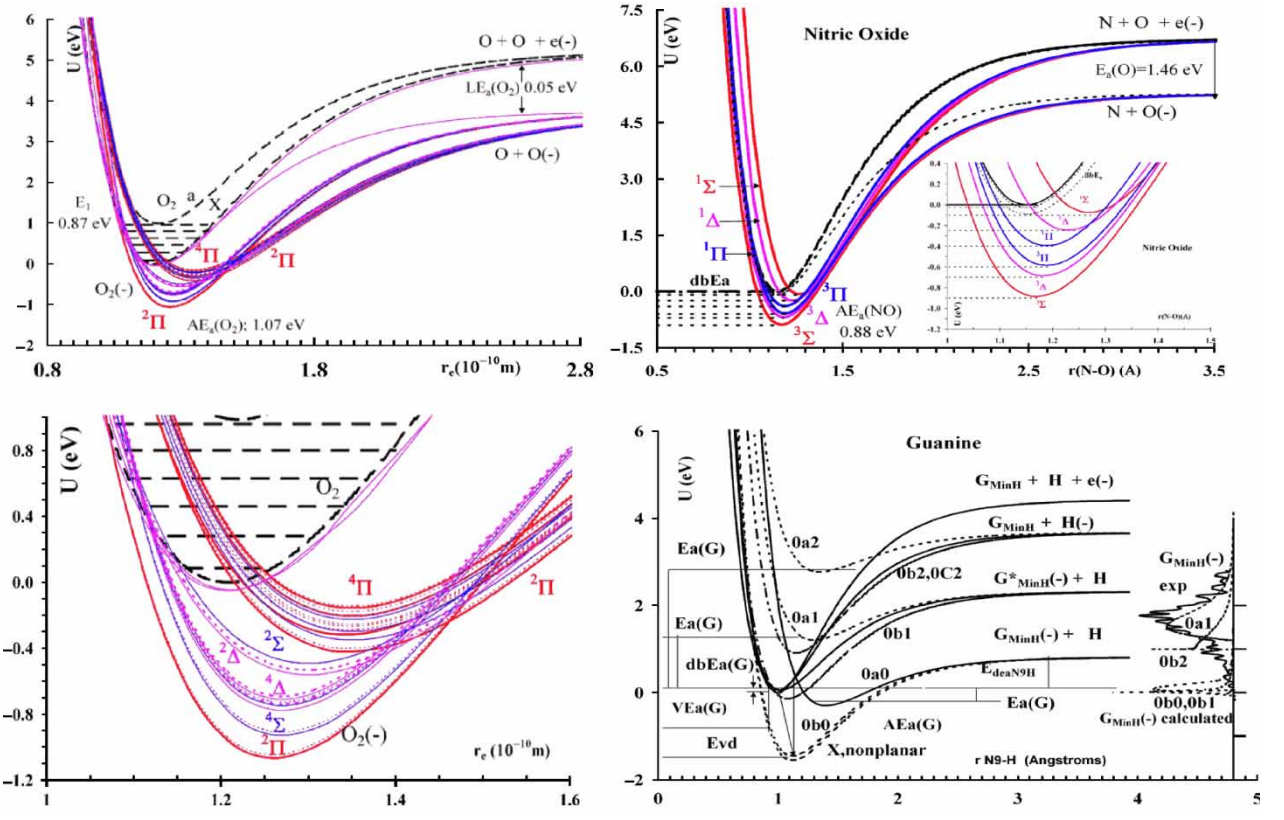

Figure 1. Morse potential energy curves for O_2, NO, and guanine and their anions. The data are from [4,5,11–16]. The letters for guanine refer to bonding (b) and antibonding (a) curves. The superscripts are for the multiplicity, quartet or doublet while the other numbers are for the order of the dissociation limits (0–2). One dipole bound curve of the multitude of such curves in the electron–molecule dimension is drawn to the lowest dissociation limit. The curves in the N9–H dimension can be drawn in other single bond dimensions when sufficient data are available.

co-workers assigned the first valence state photoelectron spectra E_a to rare tautomers of the nucleobases based on theoretical electron affinities from 0.05 to −0.5 eV. In contrast, they noted theoretical AE_a: (in eV) dA, −0.038, −0.035, 0.06 eV and dG, 0.09 and reported ground state electron affinities of the nucleosides: (in eV) dA, and rG, 0.7(2) and rA, 0.9(2) [22,23]. Here, we (a) report the first set of electron affinities and reduction potentials of DNA and RNA nucleobases and nucleosides that are consistent with theory (b) update electron affinities of purine, pyrimidine and other nitrogen heterocyclics not measured in the gas phase (c) estimate the electron affinity of Watson–Crick guanine-cytosine (GC) (d) determine the bulk hydration energy of the nucleobases (e) calculate electron affinities for doublet and quartet anions of the nucleobases, nucleosides, nucleotides and Watson–Crick GC and AT (f) postulate that spin is an important property in biological processes.

2. Experiments and calculations

The 1991 ERED were collected using standard techniques. The solvent was dimethyl sulphoxide carefully purified over CaH_2 to remove water and purged with nitrogen to remove O_2. The samples were freshly prepared at the 1–2 mM concentration. The runs were carried out at 295(2) K at 50 mV/s, where the reactions were reversible. The instrument was a Bioanalytical BAS-CV-27 system with commercially available electrodes [13].

The anion photoelectron spectra NPES-98-CUT; NPES-05-[AT]; NPES-07-nucleosides and NPES-07-AGCUT were obtained by electronically digitising spectra in the literature. The original article should be consulted for the details, but significantly different conditions are presented. The NPES-98-CUT were obtained with a microplasma ion source, mass selected with a quadrupole selector and photodetached with a 1.15 eV laser. They were energy analysed by time of flight. The NPES-05-[AT] used a similar setup with a higher energy photodetachment laser. The NPES-07-AGCUT and nucleosides were obtained using a new ion source based on laser ablation of a nucleobase or nucleoside coated Cu or Ag rod with a low-power 532 nm (2.34 eV) laser. The ions were mass selected by time of flight and photodetached with a 3.493 eV laser. They were energy analysed with a magnetic bottle [17,21–23].

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The theoretical calculations were carried out using the HYPERCHEM-7 suite of programs. The electron affinities for the nucleobases are the differences between the energies of the anion and the neutral in the global minimum geometries. This process has been used to support the majority of electron affinities of organic molecules in the literature within the quoted uncertainties. The three-dimensional spin distributions and the charges are automatically calculated in the program [5,14–16]. The procedures for the calculation of the HIMPEC in Figure 1 have been previously described in detail. The curves for the diatomic molecules are presented for comparison with HIMPEC for guanine from this work [5,6,11,12,14,16].

3. Results and discussion

In 1991, Wiley et al. [13] measured reversible reduction potentials, ERED and reported the first experimental gas phase E_a for the nucleobases and several nitrogen heterocyclic compounds. This used the Nernst equation: $E_a = 4.44 + \mathrm{ERED} + \Delta\Delta G$ (solution energy differences). The $\Delta\Delta G$, is now -2.00 eV from E_a and ERED for A, C, U, T and many other similar compounds. The updated E_a not in the National Institute of Standards and Technology web site are: (in eV) *s*-tetrazine, 1.85(10); G, 1.66(5); purine, 1.22(5); 1,2,4 triazine, 1.10(5); 1,3,5-triazine, 0.70(10); 1,4-diazine, 0.56(5); 1,2-diazine, 0.50(5) and pyrimidine, 0.37(5) [4,5,13]. Faraggi et al. measured aqueous ERED(AGCUT) comparable to literature values. The average ERED for A, U, and T that give $\Delta\Delta G$, $-2.35(3)$ and the ERED for C and G give $AE_a(C)$, 1.02(5) and $E_a(G)$, 1.28(5) [18]. In 1996, Seidel et al. [19] reported aprotic reduction potentials relative to $AE_a(U)$, 1.00(2) eV gives E_a: (in eV) ribopurine 1.20(9); dT, 0.90(9);dC, 0.81(6) and dA, 0.40(6). The E_a of ribopurine and dT overlap the AE_a of the parents and E_a of dA and dC overlap excited state E_a within the uncertainties [19].

Scheidt et al. reported dipole bound E_a: (in eV) C, 0.085(8), 0.230(8); U, 0.090(6) and T, 0.065(6) from the negative ion photoelectron spectra NPES-98-CUT in Figure 2. They obtained valence state E_a(C,U,T), 0.13(12)

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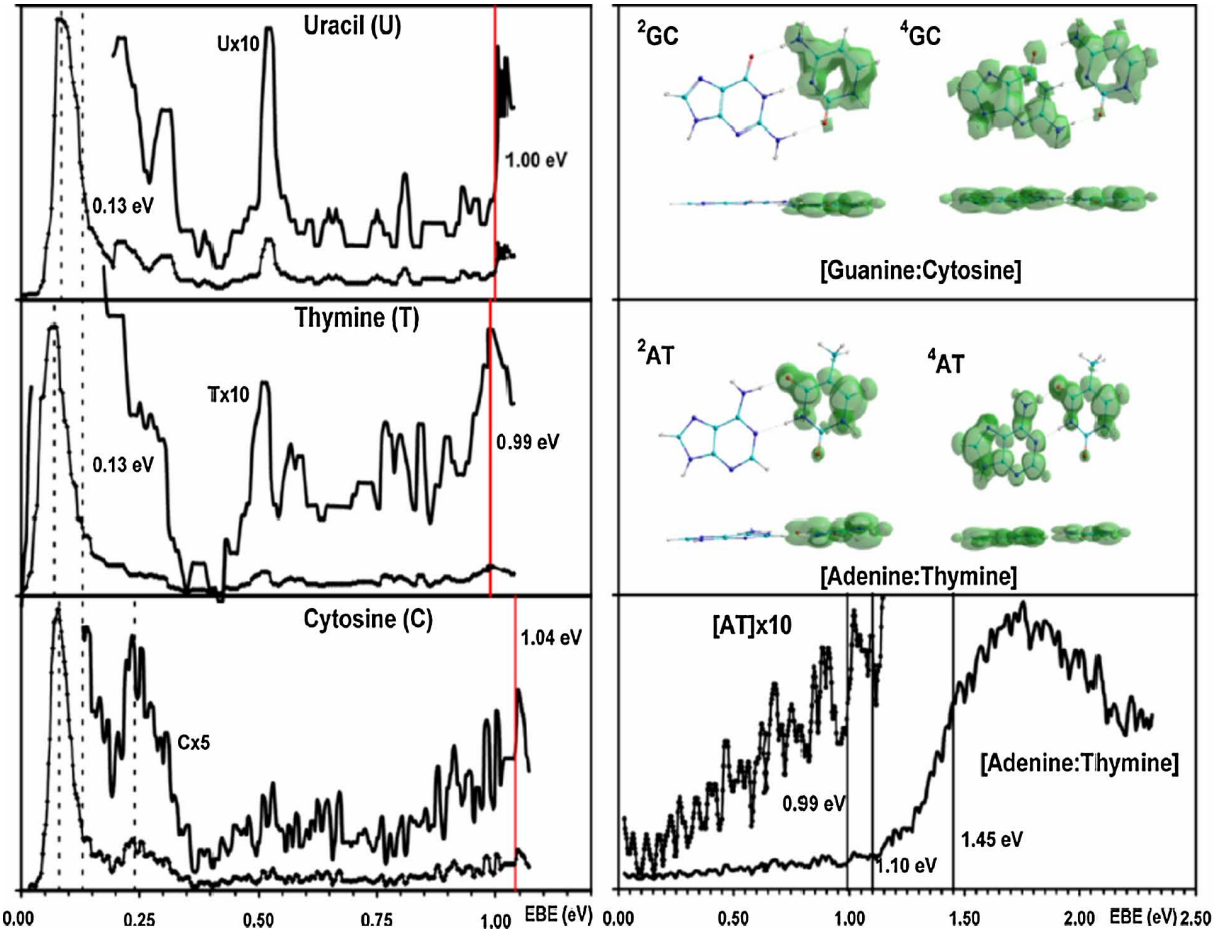

Figure 2. Negative ion photoelectron spectra from [17,21]. Vertical lines at the highest energy are for the adiabatic electron affinities identified from reduction potential data discussed in the text. The spin distributions for Watson–Crick AT and GC are from this work.

eV from onsets of photoelectron spectra of anion hydrates [7,17]. We reported AE_a(C,U,T) from the onsets identified using reduction potentials. These are shown in Figure 2 [5,7–19]. Water molecules (10–15) will complete the inner hydration shell for C, U, and T anions based on the experimental sequential hydration energy, 0.20(5) eV and the bulk hydration energy of 2.34 eV. Radisic et al. [21] assigned the NPES-05-AT in Figure 2 to non-Watson–Crick structures. We determined an onset at the E_a of Watson–Crick AT, 1.45(2) eV calculated using semi-empirical PM3 calculations. We also identified onsets at the AE_a(T), 0.99(2) eV and AE_a,(A), 1.10(2) eV. The latter was the first determination of the AE_a for adenine in the gas phase.

The doublet anion of Watson–Crick AT is designated [^{2}AT(−)]. Thus, it is ^{2}T(−) with two hydrogen bonds to adenine [5,14,15]. The ^{2}GC(−) is ^{2}C(−) with three hydrogen bonds to guanine and E_a of Watson–Crick GC is $AE_a(C) + 3(0.2) = 1.04 + 0.6 = 1.64$ eV in agreement with our theoretical value, but this is much larger than other theoretical values [7]. In 2003, Kawai et al. [20] 'experimentally demonstrated that the reduction potential of cytosine is lowered by base pairing with guanine thus making cytosine the base with the most (selected-ion chromatogram, largest) E_a in duplex DNA'. These data support the postulate that the E_a (G and A) in DNA are for excited states. The activation energy for electron conduction in B-DNA is thus $1.65 - 1.45 = 0.2$ eV [5,14,15].

The largest theoretical E_a for ^{4}AT(−) is −0.1 eV. Over 95% of the charge is on thymine in both the ^{2}AT(−) and ^{4}AT(−). The three-dimensional spin distributions in Figure 2 show that the majority of the spin is on the thymine in the ^{2}AT(−). The spin is distributed to adenine in ^{4}AT(−), but the majority of the charge remains on thymine. The largest theoretical E_a for ^{4}GC(−) is 0.3(1) eV. The charge on guanine is about $-0.15q$ in both the doublet and quartet GC anions. The distributions in Figure 2 show that the majority of the spin is on cytosine in the ^{2}GC(−) while the spin in the ^{4}GC(−) is distributed to guanine. However, the charge remains on the cytosine [5].

Bowen and co-workers recently published the valence state NPES-07-AGCUT and NPES-07-nucleosides shown

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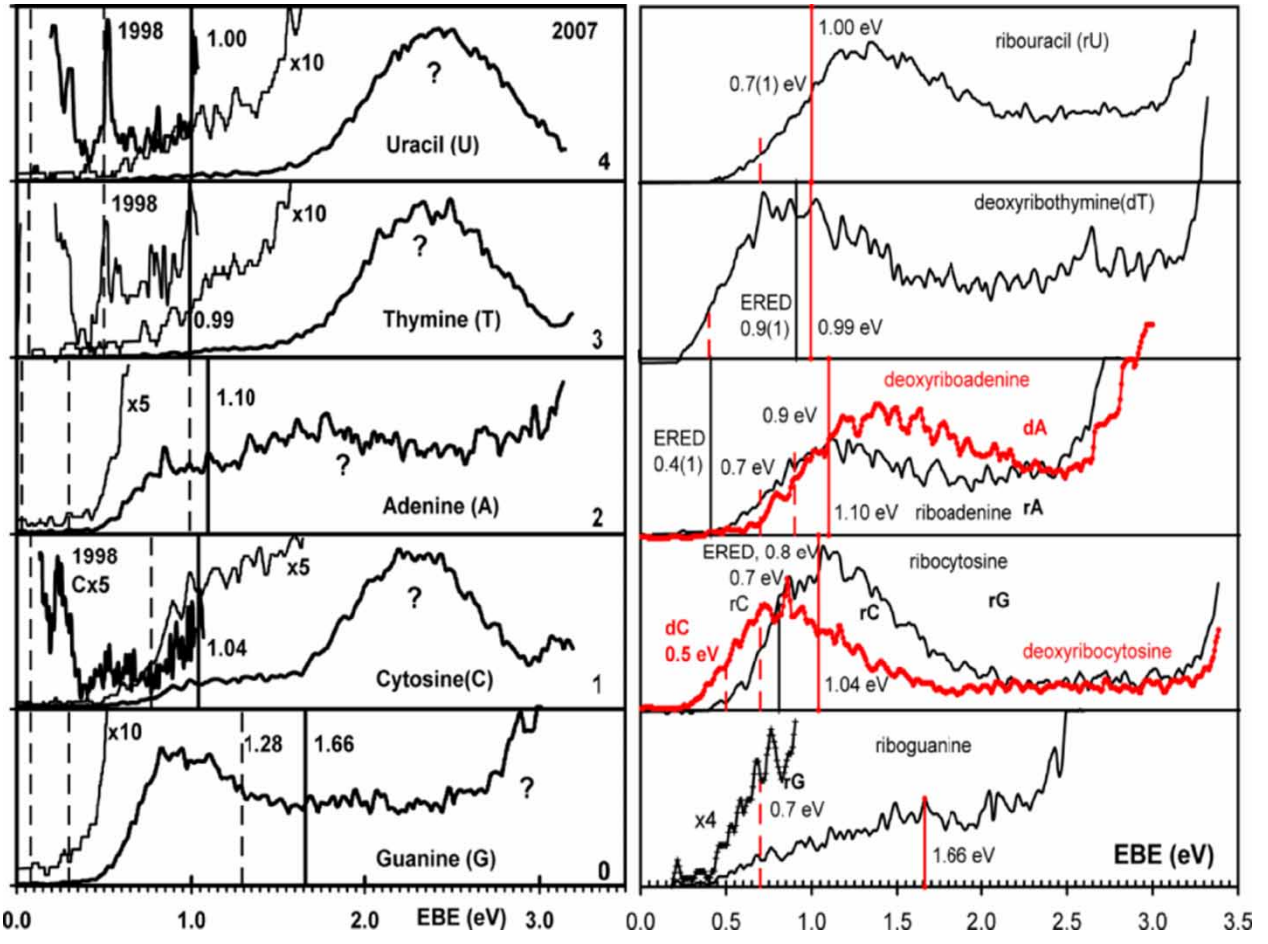

Figure 3. Negative ion photoelectron spectra from [17,22,23]. The vertical lines at the highest energy are for the adiabatic electron affinities identified from reduction potential data discussed in the text. The question marks indicate unassigned structure, some of which was assigned to rare tautomers of the nucleobases in [23].

in Figure 3. It was noted that for AGCUT 'calculations on the AE_a of their canonical tautomers find all of them to lie in the narrow range between about 0.05 and −0.5 eV'. The parts of the spectra marked by question marks in Figure 3 were assigned to mixtures of rare tautomers based on theoretical E_{vd} [22]. The AE_a of canonical nucleosides were reported: (in eV) rA, 0.9(2); dA, rU, rC, rU, 0.7(2); dT, 0.4(2) and dC, 0.5(2) although they cited theoretical AE_a: (in eV) dA, −0.038, −0.035, 0.06 eV and dG, 0.09 [21–23]. They concluded that 'the E_a of the nucleosides are greater than those of their corresponding nucleobases' [23]. We note that the AE_a (rA, dA, rU and rC) overlap the AE_a (in eV) A, 1.10(2); U, 1.00(2) and C, 1.04(2) within twice the mutual errors. The values for rC, dC, dA and dT overlap excited state E_a: (in eV) dC, 0.81(5); C, 0.77(5); dA, 0.40(5) and T, 0.30(10).

We identify onsets at the AE_a(AGCUT) in the NPES-07-AGCUT and NPES-07-nucleosides in Figure 3. Thus, the AE_a of the nucleosides are about the same as the AE_a for the corresponding nucleobases. This is predicted by empirical substitution rules and semi-empirical quantum mechanical calculations. The latter give AE_a(dG), 1.66(5) eV. Onsets at excited valence and dipole bound electron affinities are also shown in Figure 3. The theoretical E_a for the quartet states of G(−), rG(−) and dG(−) are about 0.1 eV. The E_a for the the other nucleosides are −0.45 to −0.55 eV in agreement with the relative E_a of the nucleobases. To our knowledge, these

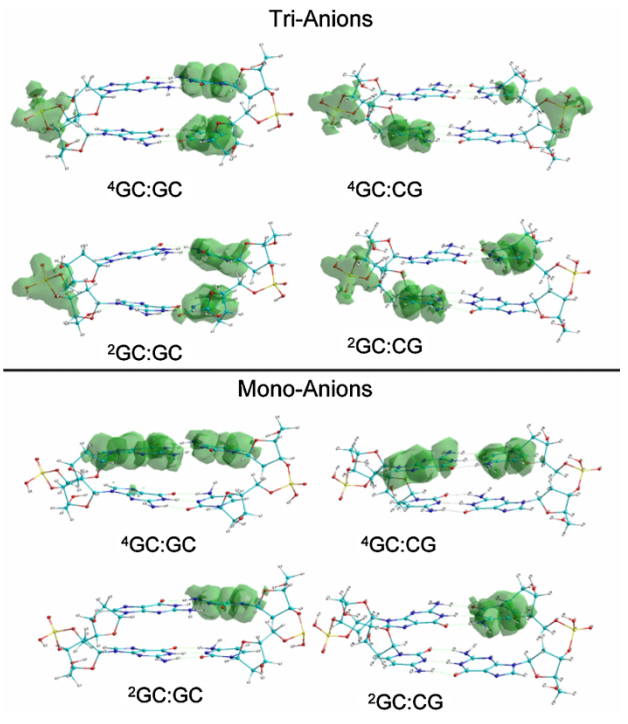

Figure 4. Three-dimensional spin distributions for doublet and quartet mono-anion and tri-anions of GC:GC and GC:CG dinucleotides.

are the first calculations for quartet anions of the nucleobases and nucleosides.

In Figure 4 are three-dimensional spin distributions of quartet and doublet mono-anions and tri-anions of B-DNA Watson–Crick dinucleotides of guanine and cytosine: ^{2}GC:GC(−n), ^{4}GC:GC(−n), ^{2}GC:CG(−n) and ^{4}GC:CG(−n), where n is 1 or 3. The charge and spin distributions for the mono-anions are similar to those of the GC base pairs shown in Figure 2. The charges (q) on the HPO_4 are about $-0.35q$, the sugars, $0.25q$, the cytosines $-0.45q$ and the guanines $-0.15q$. The spin and charge are primarily on one base pair, but some charge is distributed to the second base pair. The E_a for the doublets are about 2 eV while those for the quartet are about 0.6 eV.

In the tri-anions, the charge and spin are distributed to both base pairs and to the HPO_4 groups. In the doublet GC:GC(−3) the charge and spin are concentrated on the cytosines. In the quartet GC:GC(−3), the charge on the HPO_4 connected to the guanine dinucleotide is over $-1q$ and is accompanied by the spin. This is unlike the mono-anion, where there is no spin on the guanines. The charge on the HPO_4 connected to the cytosine dinucleotide is $-0.35q$, but is not accompanied by spin. The charges on the HPO_4 in ^{2}GC:CG(−3) and ^{4}GC:CG(−3) are over $-1q$. The spin and charge are concentrated on the cytosines and on one HPO_4 in the doublet. The spin is distributed to both HPO_4 in the quartet. The E_a for the formation of the tri-anions from the neutral are positive. This is in agreement with the recent observation of multiple charged DNA anions in mass spectrometry. The E_a for the formation of the ^{4}GC:GC(−3) is 1.25 eV while the E_a for other tri-anions are about 0.6 eV. These are lower limits based on the variational principle.

4. Conclusions

This paper moves toward the goal of a knowledge of E_a in biological media set forth by Szent-Gyorgi [1] and Chen and Chen [5]. We resolve apparent conflicts by identifying stable excited anion states. The first E_a of Watson–Crick GC and AT, the nucleobases, nucleosides and nucleotides consistent with theory are presented. These support the lower E_a of guanine and adenine in DNA. The E_a of the Watson–Crick base pairs establishes an activation energy for rapid electron conduction in B-DNA. The semi-empirical quantum mechanical values reproduce experiment. Therefore, this method can be used to predict properties of biological molecules. In contrast, the density functional E_a of Watson–Crick GC is 0.4 eV or 1.3 eV lower than experiment. The dipole bound *ab initio* E_a of Watson–Crick GC was calculated at the same time to be 0.1 eV [7]. Dipole bound anions are known to exist in the gas phase but not under biological conditions. However, ^{3}NO(−) and comparable low-lying quartet anion states such as those for guanine and superoxide can and will

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participate in electron conduction, radiation damage, oxidation damage and repair, strand breakage and protein synthesis. Thus, the knowledge of both spin and charge are required to understand biological processes. We are currently working on the predictions for spin distributions, on the 64 trinucleotides for protein synthesis.

Acknowledgement

This research was supported by the Wentworth Foundation.

Note

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