

**Correction to “Theoretical Determination of One-Electron Redox Potentials for DNA Bases, Base Pairs, and Stacks”**

[*The Journal of Physical Chemistry A* **2011**, *115*, 4804–4810. DOI: 10.1021/jp201281t]. Y. Paukku, and G. Hill\*

**ELECTRON AFFINITIES**

In Tables 1, 5, and S1 (Supporting Information) calculated values of electron affinities have the wrong sign. The corrected data are given in the tables below.

	EA, eV	EA <sup>zpe</sup> , eV
Ade	−0.72	−0.59
Gua	−0.34	−0.28
Cyt	−0.24	−0.13
Thy	−0.09	0.03
1-MeC	−0.25	−0.14
3-MeC	−0.23	−0.10
5-MeC	−0.25	−0.14
1-MeG	−0.42	−0.37
7-MeG	−0.46	−0.39
1-MeA	0.08	0.18
3-MeA	0.02	0.13
7-MeA	−0.37	−0.24
G·C	0.35	0.48
A·T	0.03	0.18
G·5-MeC	0.31	0.45
GG	0.11	0.17

**Supporting Information**

	adenine EA, eV	cytosine EA, eV
mPWB1K/6-31++G(d,p)	−0.55	−0.34
M05	−0.45	−0.18
M052X	−0.74	−0.23
M06	−0.52	−0.19
M062X	−0.72	−0.24
MP2	−0.57	
experimental	0.012	0.23

As a result of this change, the order of AEAs for DNA bases obtained in this study is  $T > C > G > A$ . The discussion section corresponding to the electron affinities should be as follows: The ZPE-corrected electron affinity for thymine is slightly positive. Because obtained values of AEAs for adenine, guanine, and cytosine are negative, there is no evidence of the existence of stable anion-radical species of these bases. The conclusion section is also affected by this change. AEAs for all base pairs and GG stack are positive. Positive values are in excellent agreement with previous work of Li et al. (ref 11), where AEAs for A·T and G·C were determined to be 0.30 and 0.49 eV, respectively.

Reported experimental values of electron affinity (Table 1) for adenine, guanine, and cytosine are for the dipole-bound states of

these bases. However, obtained theoretical results have mixed dipole-bound and valence character. Therefore, these values differ from experimental data and are not appropriate for dipole-bound energies or the valence energy.

DOI: 10.1021/jp204493j

Published on Web 05/23/2011