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Corrigendum

Comment on Semiempirical Calculations of πElectron Affinities

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In a recent paper by one of the authors [1], a variable β-γ modification of the Pariser–Parr–Pople (PPP) approximation to the Hartree–Fock equation was used to calculate the ionization potential (*IP*) and electron affinity (*EA*) of ~100 unsaturated molecules containing C, N, O, and H atoms. Koopmans' theorem was used to relate the *EA*s and *IP*s to the energies of the unoccupied and occupied orbitals, respectively. Due to an error in the original version of the

Table 1. Calculated and experimental electron affinities for various unsaturated organic molecules

Molecule	Calculated EAs	Experimental EAs (Determined from ETS)
Adenine	−0.82, −1.43, −2.39, −4.28	
Alloxan	1.21, −1.09, −1.48, −3.22	
Aniline	−1.28, −1.49, −4.18	−1.13, −1.85, −5.07[a]
Carbazole	−0.49, −0.86, −1.48, −1.81, −3.63, −4.23	
Furan	−1.62, −3.08	−1.76, −3.14[b]
Guanine	−0.94, −1.64, −2.55, −4.39	
Imidazole	−1.63, −2.97	
Maleic anhydride	1.00, −2.24, −2.72	
Maleimide	+0.94, −2.37, −2.76	
Parabanic acid	0.54, −2.04, −2.61	
Phenol	−1.21, −1.40, −4.13	−1.01, −1.73, −4.92[a]
Phenylenediamine	−1.44, −1.86, −4.36	
Pyrrole	−1.80, −3.19	−2.38, −3.44[b]
Uracil	−0.48, −1.50, −3.35	−0.19, −1.59 −3.99
Vinylene carbonate	−2.00, −2.11	−1.54, −2.81[c]

[a] Jordan, K. D., Michejda, J. A., Burrow, P. D.: J. Am. Chem. Soc. **98**, 7189 (1976).
[b] van Veen, E. H.: Chem. Phys. Letters **41**, 535 (1976).
[c] Burrow, P. D: unpublished results.

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computer program, the *EA*s and *IP*s reported for those molecules containing N or O atoms not involved in multiple bonds are in error. The reason for this is that a charge of +1 rather than +2 was utilized for the O and N atoms in these cases for the calculation of the diagonal matrix elements of the Hamiltonian. Table 1 gives the correctly calculated *EA*s for the 15 molecules affected by this error. A favorable comparison with experiment (Electron Transmission Spectroscopy, ETS) is evident.

Reference

1. Younkin, J. M., Smith, L. J., Compton, R. N.: Theoret. Chim. Acta (Berl.) **41**, 157 (1976)

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