ADDITIONS AND CORRECTIONS

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Leon D. Betowski,* Mark Enlow, Lee Riddick, and Donald H. Aue*: Calculation of Electron Affinities of Polycyclic Aromatic Hydrocarbons and Solvation Energies of Their Radical Anions

Page 12927. References were missed in computer literature searches of electron affinities (EAs) of aromatic hydrocarbons. We present here a summary of relevant results from those papers. Chen et al. have reviewed the electron capture detector (ECD) data for electron affinities in 2004.[1] This review contains updated experimental ECD data since the 1995 summary paper we referenced.[2] New experimental data are based upon a multistate model of the temperature dependence of the ECD response.[3] The lowest energy states of the anions give new EAs (followed by a prior ECD value and our assigned value of the electron attachment energy at 0 K, all in eV) for seven aromatic hydrocarbons: cyclooctatetraene (0.80, 0.58, 0.65), azulene (0.90, 0.70, 0.79), naphthalene (0.16, 0.15, −0.2), acenaphthalene (0.80, 0.41, 0.8), anthracene (0.69, 0.66, 0.53), pyrene (0.61, 0.56, 0.54), tetracene (naphthacene) (1.10, 0.88, 1.00). These papers also present estimated EAs from solution reduction potentials and empirically estimated solvation energies and from semiempirical quantum calculations that generally support their experimental data.[1,3,4] Newly proposed EAs (in eV) based upon such estimates are benzene (0.1), biphenylene (0.45), and coronene (0.8). All of these estimated values differ substantially from our assigned values. In all cases above where there are significant differences, we believe that our assignments are based upon more reliable experimental data, theoretical estimates, and/or values from reduction potentials and calculated solvation energies. We also note that a recent theoretical paper using density functional methods gives EA values for eight PAHs virtually identical with our theoretical results.[5]

References and Notes

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(4) Chen, E. S.; Chen, E. C. M.; Sane, N.; Talley, L.; Kozanecki, N.; Schulze, S. *J. Chem. Phys.* **1999**, *110*, 9319.
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