J|A|C|S
ADDITIONS AND CORRECTIONS

Oligoacenes: Theoretical Prediction of Open-Shell Singlet Diradical Ground States [*J. Am. Chem. Soc.* **2004**, *126*, 7416−7417]. Michael Bendikov, Hieu M. Duong, Kyle Starkey, K. N. Houk, Emily A. Carter, and Fred Wudl

Page 7416 (third paragraph, line 9). The sentence "In contrast to the common view... we predict that the ground states of oligoacenes are singlets, as a result of their disjoint diradical nature." should read "In contrast to the common view... we predict that the ground states of oligoacenes are open-shell singlet diradicals."

Page 7416 (fifth paragraph, line 6). The sentence "For hexacene, the singlet−triplet gap is predicted..." should read "For hexacene, the CASSCF triplet−singlet gap is predicted..."

Page 7416 (last sentence, continued on page 7417). The sentence "The experimental band gap derived from the UV−vis spectrum for hexacene, 1.84 eV,[8] is close to the calculated HOMO−LUMO value of 1.80 eV." should be deleted.

Page 7416 (footnote *a*, Table 1). This note should read in full: "Triplet energy minus UDFT spin-contaminated open-shell singlet energy. Note that the spin-pure open-shell singlet will lie even lower in energy."

Page 7417 (second paragraph, line 3). "... two singly occupied orbitals of decacene..." should read "... two highest-energy singly occupied orbitals of decacene..."

JA045878V

10.1021/ja045878v
Published on Web 00/00/2004