## ADDITIONS AND CORRECTIONS

## 1999, Volume 103

**Daniel E. Wheeler, Jorge H. Rodriguez, and James K. McCusker\*:** Density Functional Theory Analysis of Electronic Structure Variations across the Orthoquinone/Semiquinone/ Catechol Redox Series

The following typographical errors were found: Page 4102 Geometry Optimizations. Last sentence of first paragraph should read: The final optimization was performed at both BLYP/6-31G\* and B3LYP/6-31G\* levels using either RDFT (for singlet ground state molecules) or unrestricted density functional theory UDFT (for doublet ground state molecules). Page 4103 TABLE 2: The labels for 3,6-DTBSQ and 3,5-DBTSQ should be U-BLYP and U-B3LYP. Page 4104 TABLE 3: The values of 2S+1 for 3,6-DTBQ and 3,6-DTBCat should be 1. Page 4105: Last paragraph should read: Clearly the reduction of 3,6-DTBQ to 3,6-DTBSQ causes some important changes in the molecular properties, e.g., the diamagnetism of 3,6-DTBQ versus the paramagnetism of 3,6-DTBSQ. Page 4106: MO 61a should be MO 61α. Page 4108: First line of last paragraph should read Natural Population Analysis (NPA) Charge Densities.

None of the data or conclusions in the paper are affected by the previous corrections.

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