

2006, Volume 110A

Christopher J. Cramer*, **Marta Wloch**, **Piotr Piecuch**, **Cristina Puzzarini**, and **Laura Gagliardi**: Theoretical Models on the Cu₂O₂ Torture Track: Mechanistic Implications for Oxytyrosinase and Small-Molecule Analogues

Pages 1991–2004. The primitive basis functions used for N, O, and H in basis sets BS1 and BS2 were taken from Widmark, P. O.; Malmqvist, P. A.; Roos, B. *Theor. Chim. Acta* **1990**, *77*, 291, not reference 45 of the original paper. The contraction scheme for H was [8s4p | 2s1p], and those for N and O were [14s9p4d | 4s3p2d].

10.1021/jp073128c

Published on Web 05/16/2007

2006, Volume 110A

Christopher J. Cramer*, **Armagan Kinal**, **Marta Wloch**, **Piotr Piecuch**, and **Laura Gagliardi**: Theoretical Characterization of End-On and Side-On Peroxide Coordination in Ligated Cu₂O₂ Models

Pages 11557–11568. The primitive basis functions used for N, O, and H in basis sets BS1 and BS2 were taken from Widmark, P. O.; Malmqvist, P. A.; Roos, B. *Theor. Chim. Acta* **1990**, *77*, 291, not reference 36 of the original paper. The contraction scheme for H was [8s4p | 2s1p], and those for N and O were [14s9p4d | 4s3p2d].

In addition, while the Cartesian coordinates reported in the Supporting Information for compounds **0** and **2** provide correct geometries, they are incompatible with the use of eq 2 of the paper for the generation of intermediate geometries. A new version of the Supporting Information has been provided with geometries that are now compatible with eq 2.

Supporting Information Available: Cartesian coordinates, absolute (singlet and triplet) and relative electronic energies at all levels of theory for all structures, BS-DFT $\langle S^2 \rangle$ values, and additional technical details on software. This material is available free of charge via the Internet at <http://pubs.acs.org>.

10.1021/jp0731295

Published on Web 05/15/2007

2007, Volume 111A

Alexandru T. Balaban* and **Matevž Pompe**: QSPR for Physical Properties of *cata*-Condensed Benzenoids Using Two Simple Dualist-Based Descriptors

Pages 2448–2454. In Table 1, the code for **26** is 0102, and the code for **50** is 102102.

In Figure 1, correct numbers and codes are:

2 26 26 28

[1] [0] [0102] [1021]

In the caption of Figure 9, eq 13 should be changed to eq 12. In the caption of Figure 10, eq 15 should be changed to eq 14. In the caption of Figure 14, eq 22 should be changed to eq 21.

10.1021/jp0795199

Published on Web 05/15/2007