

Correction to π -Extended and Six-Coordinate Iron(II) Complexes: Structures, Magnetic Properties, and the Electrochemical Synthesis of a Conducting Iron(II) Metallocopolymer

Brandon Djukic, Takele Seda, Serge I. Gorelsky, Alan J. Lough, and Martin T. Lemaire*

Inorganic Chemistry 2011, 50, 7334–7343 DOI: 10.1021/ic2010503

Page 7336. The Computational Details section is incorrect and should read as follows: All DFT calculations were performed using the Gaussian 09 package¹⁶ using the B3LYP hybrid functional¹⁷ and the DZVP basis set for all atoms.¹⁸ Closed- and open-shell species were optimized using the spin-restricted and spin-unrestricted MO formalism, respectively. Tight SCF convergence criteria were used for all calculations. The converged wave functions were tested to confirm that they correspond to the ground-state surface.

Page 7343. References 16, 17b, 18, and 19 from the original manuscript should be removed. Reference 17a in the original manuscript becomes ref 18, as noted in the corrected text above. Reference 17 noted in the above corrected text is as follows: Becke, A. D. *J. Chem. Phys.* 1993, 98, 5648. Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev.* 1988, B37, 785. Reference 16 noted in the above corrected text is as follows: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, revision A.02; Gaussian, Inc.: Wallingford, CT, 2009. References 20 and 21 in the original manuscript, along with their corresponding citations in the text, become refs 19 and 20.

Published: September 19, 2011