JACS
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
pubs.acs.org/JACS
Addition/Correction

Correction to "Excited-State Turn-On of Aurophilicity and Tunability of Relativistic Effects in a Series of Digold Triazolates Synthesized via iClick"

Charles J. Zeman IV, Yu-Hsuan Shen, Jessica K. Heller, Khalil A. Abboud, Kirk S. Schanze,* and Adam S. Veige*

J. Am. Chem. Soc. **2020**, *142* (18), 8331−8341. DOI: 10.1021/jacs.0c01624

Cite This: *J. Am. Chem. Soc.* 2020, 142, 14391−14391

Read Online

ACCESS | Metrics & More | Article Recommendations | Supporting Information

Page 8339 and Supporting Information. There was an error in the structure assigned as **4,5-Au$_1$-Th**. As shown in Supporting Information (SI) Figure S30, the X-ray crystallography structure indicates the proton is attached to N_1 rather than N_3. The incorrect tautomer structure appears in Figure 8b and in the SI on p S25. Excited-state optimized geometry computational analysis using CAM-B3LYP of the correct tautomer reveals bond lengths and angles similar to those reported in the original paper. The corrected Figure 8b is shown here, and a new SI file with the corrected structure on p S25 is provided. These corrections do not alter any conclusions.

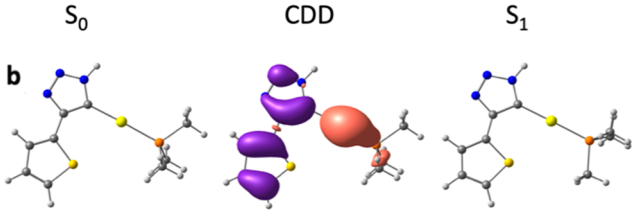

Figure 8b. Excited-state optimized structure of **4,5-Au$_1$-Th** using CAM-B3LYP.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/jacs.0c07691.

Syntheses, NMR, X-ray crystallography data; fluorescence of **Au$_2$-Th** and **4,5-Au$_1$-Th**; computational results; references (PDF)

Published: August 4, 2020