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ADDITION/CORRECTION

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Density Functional Theory Study of the Mechanism and Origins of Stereoselectivity in the Asymmetric Simmons−Smith Cyclopropanation with Charette Chiral Dioxaborolane Ligand [*Journal of the American Chemical Society* **2011**, *133*, 9343–9353. DOI: 10.1021/ja111330z]. Tao Wang, Yong Liang, and Zhi-Xiang Yu*

Pages 9345−9347. Our drawings in Figures 1−3 using 1/4 mol of **2-T** as the reference point are not correct mathematically. The corrected Figures 1−3, using 1 mol of **2-T** as the reference point, are presented here. To reduce the overestimation of the entropy contribution in solution for the bimolecular processes (the dimerizations of **2-M** to **2-D** and **2-D** to **2-T**), the entropy values in solution from **2-M** to **2-D** and **2-D** to **2-T** are estimated to be 50% of their originally computed gas-phase values (for details, see the Supporting Information). Therefore, aggregates **2-D** (2 mol) and **2-T** (1 mol) in dichloromethane are more stable than **2-M** (4 mol) by 37.2 and 40.2 kcal in terms of free energy, respectively. The background cyclopropanation requires an overall activation free energy of 16.5 kcal/mol (from **2-T** to **TS-2-T**). In the absence of ligand **1**, tetramer **2-T** is the most stable and reactive cyclopropanation precursor. However, in the presence of a stoichiometric amount of ligand **1** (4 mol), tetramer **2-T** (1 mol) can be completely transformed to the chiral complex **2-L-O** (4 mol) because this process is exergonic by 15.7 kcal in CH_2Cl_2, and the overall activation free energy for the generation of the racemic cyclopropane product via **TS-2-T** is 32.2 kcal/mol (**2-L-O** → **2-T** → **TS-2-T**).

These corrections do not affect the conclusions in the original paper. We thank Prof. Daniel A. Singleton (Texas A&M University) for calling these to our attention.

■ ASSOCIATED CONTENT

Supporting Information. Computational details, full citation of ref 11, and Cartesian coordinates of computed stationary points [corrected]. This material is available free of charge via the Internet at http://pubs.acs.org.

DOI: 10.1021/ja205871t
Published on Web 08/04/2011

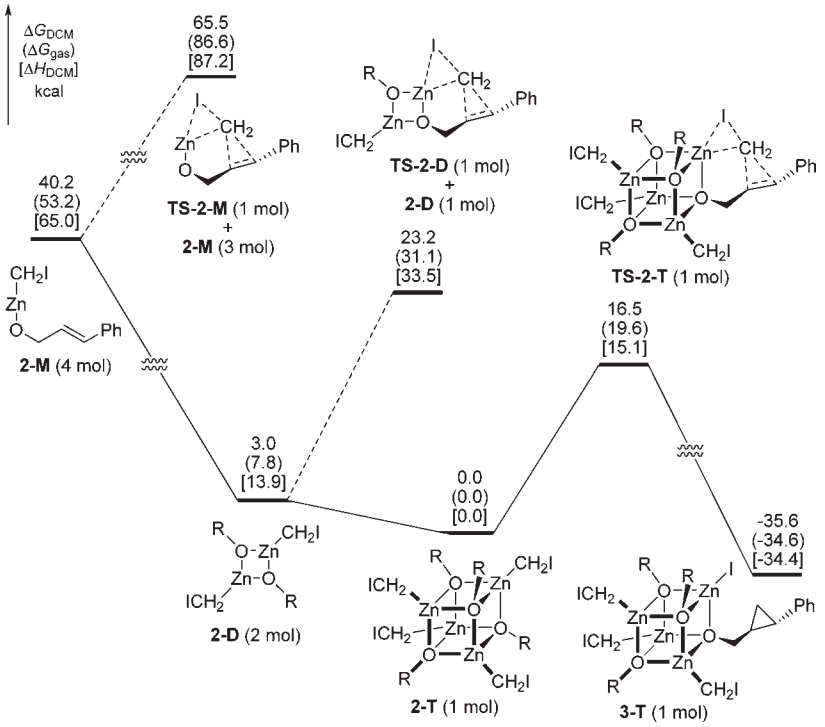

Figure 1. DFT-computed free energy surfaces for the cyclopropanation reactions of monomer **2-M**, dimer **2-D**, and tetramer **2-T** (R = (*E*)-PhCH=CHCH$_2$).

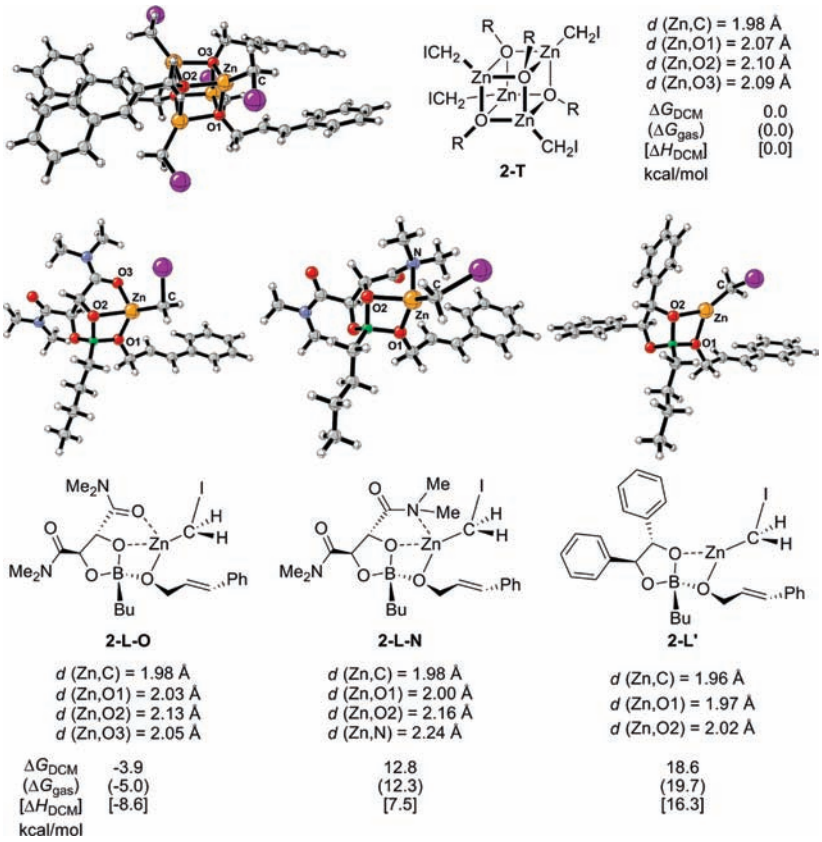

Figure 2. DFT-optimized structures of iodomethylzinc allyloxide complexes **2-T**, **2-L-O**, **2-L-N**, and **2-L′** (carbon, gray; hydrogen, white; oxygen, red; nitrogen, blue; boron, green; zinc, orange; iodine, purple; energies are given in kcal/mol; R = (*E*)-PhCH═CHCH$_2$).

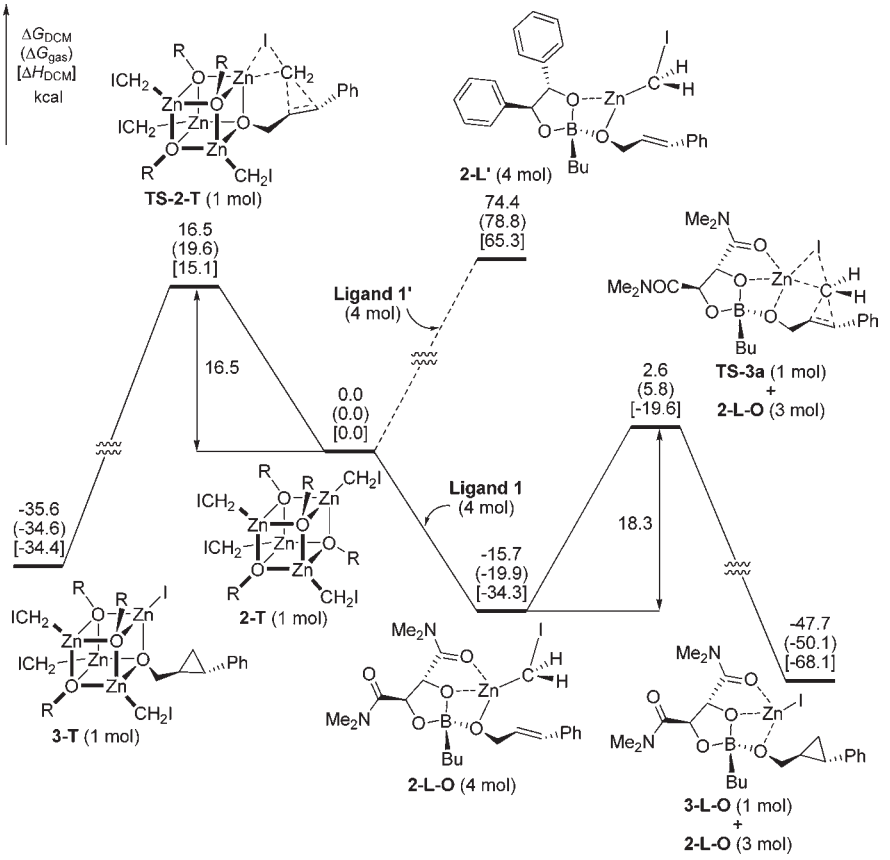

Figure 3. DFT-computed free energy surfaces for the cyclopropanation reactions of tetramer **2-T** and the chiral zinc complex **2-L-O** (R = (*E*)-PhCH═CHCH$_2$).

dx.doi.org/10.1021/ja205871t |*J. Am. Chem. Soc.* 2011, 133, 13762–13763