THE JOURNAL OF PHYSICAL CHEMISTRY A

Addition/Correction

pubs.acs.org/JPCA

Correction to "Catalytic Activity of Phosphine–Copper Complexes for Hydroboration of Styrene with Pinacolborane: Experiment and Theory"

Jiyeon Won, Dongwan Noh, Jaesook Yun,* and Jin Yong Lee*

J. Phys. Chem. A **2010**, *114* (45), 12112–12115. DOI: 10.1021/jp1081966

Page 12114. Figure 2 and Table 1 should be replaced by

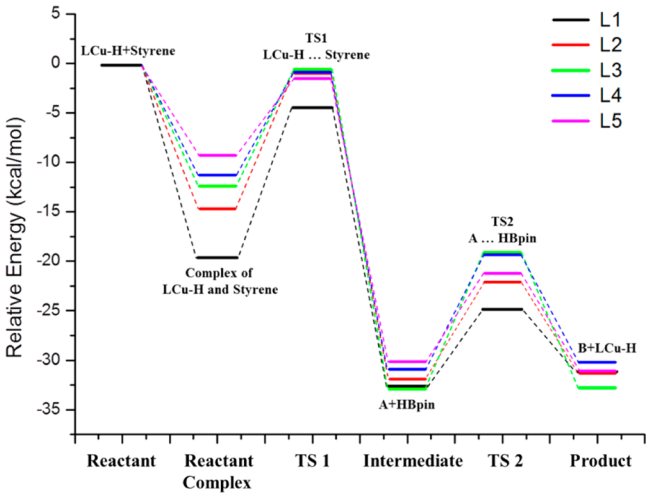

Figure 2. Energy profiles for step I and step II with **L1**–**L5**.

Table 1. Calculated Activation Barriers ($\Delta E^{\ddagger}$) and Enthalpy Changes (ΔH) in Steps I and II

	step I			step II		
ligand	$\Delta E_1^{\ddagger}$	$\Delta E_{-1}^{\ddagger}$	ΔH_1	$\Delta E_2^{\ddagger}$	ΔH_2	conversion[a]
L1	15.19	28.12	−12.93	7.77	1.46	
L2	13.69	30.89	−17.20	9.82	0.58	29
L3	11.85	32.33	−20.48	13.79	0.09	18
L4	10.43	330.03	−19.63	11.61	0.75	71
L5	7.73	28.62	−20.89	8.95	−0.96	100

[a]Reactions were run using 5 mol % CuCl, 6 mol % NaO-*t*-Bu, and 5 mol % ligand at room temperature. Conversions were measured by GC analysis with an internal standard after 24 h. Energies are in kcal/mol. $\Delta E_1^{\ddagger}$, $\Delta E_{-1}^{\ddagger}$, and $\Delta E_2^{\ddagger}$ denote the activation barriers for the forward and backward reactions in step I and the forward reaction in step II, respectively. ΔH_1 and ΔH_2 denote the enthalpy changes in steps I and II, respectively.

Published: December 11, 2013