Inorganic Chemistry

Correction to Prediction of Reliable Metal–PH₃ Bond Energies for Ni, Pd, and Pt in the 0 and +2 Oxidation States [Inorganic Chemistry 2010, 49, 5546–5553 DOI: 10.1021/ic1004853]. Raluca Craciun, Andrew J. Vincent, Kevin H. Shaughnessy, and David A. Dixon* Department of Chemistry, The University of Alabama, Shelby Hall, Box 870336, Tuscaloosa, Alabama 35487-0336, United States

Page 5553. The values for the density functional theory (DFT) bond dissociation energies in Table S7 for $PdCl_2-PH_3$ in the Supporting Information have been changed. The previous DFT values were for ¹PdCl₂ rather than for the ground state ³PdCl₂. The DFT bond dissociation energies to the ground state ³PdCl₂ are now provided.

ASSOCIATED CONTENT

Supporting Information. Figure of general catalytic cycle, T_1 diagnostics, $M-PH_3$ binding energies as a function of basis set, singlet-triplet energy splittings, metal-phosphine bond dissociation energies calculated with various exchange-correlation functionals, and the aD-PP basis sets and deviations from the CCSD(T)/CBS calculated BDEs and optimized MPH_3, M(PH_3)_2, MPH_3Cl_2, M(PH_3)_2Cl_2, and MCl_2 XYZ coordinates at the B3LYP/ aD-PP level. This material is available free of charge via the Internet at http://pubs.acs.org.

DOI: 10.1021/ic200849s Published on Web 05/05/2011

