Supporting Information

DFT Study on the Mechanism of Bimetallic Pd−Zn-Catalyzed Cycloaddition
of Alkynyl Aryl Ethers with Internal Alkynes

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Figure S1. Free energy profiles at ωB97XD/6-311+G(d,p)-SDD-SMD//M06/6-31g(d,p)-LANL2DZ level for (a) bimetallic Pd−Zn complex 1 catalyzed coordination of substrate C6H5OC≡CSiPr3, C−H activation, acetic acid rotation and H transformation steps and (b) monometallic Pd(PMe3)2 catalyzed C−H activation step. The free energies are in kcal/mol.
Figure S2. The optimized 3D structures of transition states $\text{TS}_{23X}$ and $\text{TS}_{45X}$ (X = O, CH2, CO, S, and NH). The lengths are given in angstrom.
Figure S3. Free energy profile for the reaction of $C_6H_5SC≡SiPr_3$ with $MeC≡CMe$ to generate the cycloaddition product $P_S$. The free energies are given in kcal/mol.

Figure S4. Free energy profile for the reaction of $C_6H_5N(H)C≡SiPr_3$ with $MeC≡CMe$ to generate the cycloaddition product $P_{NH}$. The free energies are given in kcal/mol.
Table S1. Calculated thermodynamic corrections, solution-phase single-point energies in toluene and solution-phase Gibbs free energies in toluene of all the intermediates and transition states at M06/6-311+G(d,p)-SDD-SMD//M06/6-31g(d,p)-LANL2DZ level (in Hartree).

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TS$_{45NH-PCy3}$ 0.889404, -2866.785416, -2865.896012
Table S2. Calculated thermodynamic corrections, solution-phase single-point energies in toluene and solution-phase Gibbs free energies in toluene of several intermediates and transition states at ωB97XD/6-311+G(d,p)-SDD-SMD//M06/6-31g(d,p)-LANL2DZ level ( in Hartree).

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