

Kinetics and DFT Studies of the Hydrogenation of Alkenes and Alkynes Catalyzed by (Benzoimidazol-2-ylmethyl)amine palladium (II) Complexes

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Supplementary Information

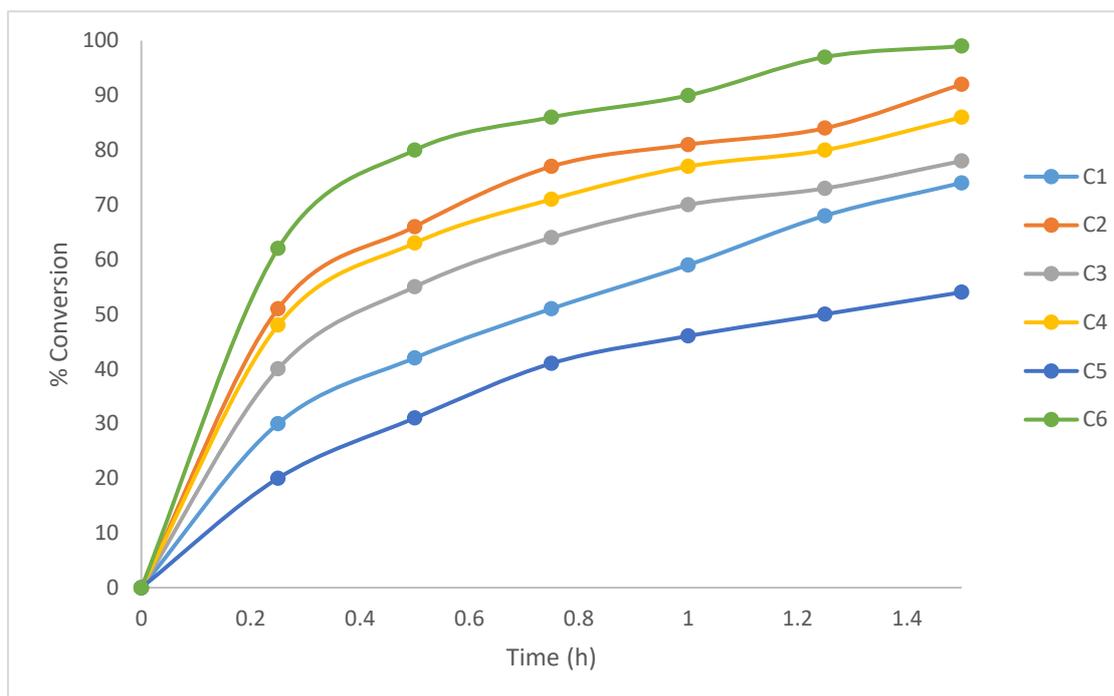


Fig. S1: Plot of % conversion vs time for styrene hydrogenation using complexes **1-6**. Reaction conditions: styrene, substrate/catalyst = 600; substrate; solvent, toluene (50 mL); pressure, 5 bar; temperature, 30 °C; time, 1.5 h.

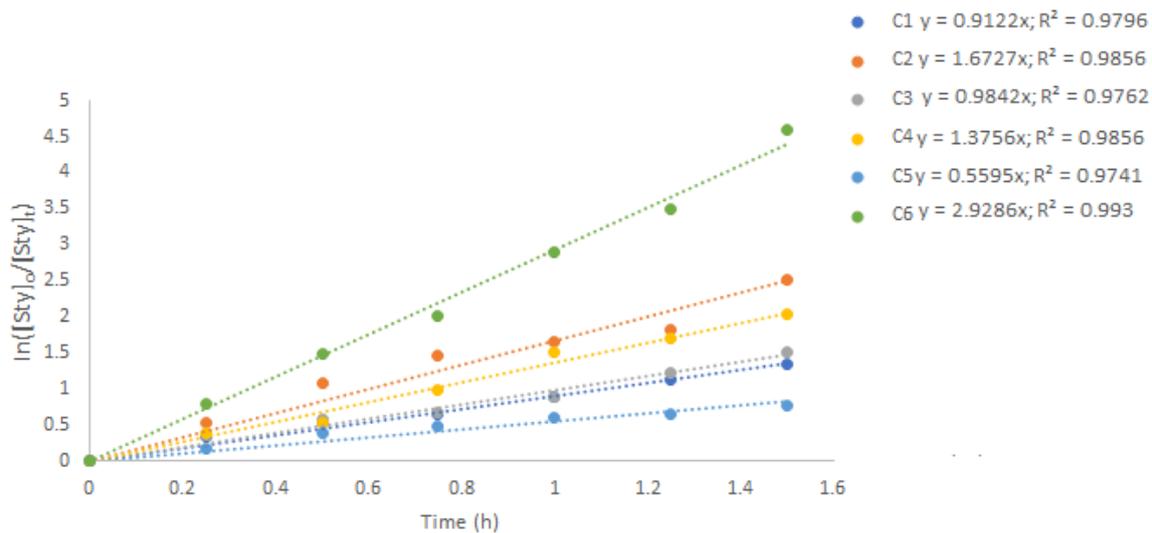


Fig. S2: Plot of $\ln[Sty]_0/[Sty]_t$ vs time for styrene hydrogenation using complexes **1-6**. Reaction conditions: styrene, substrate/catalyst = 600; solvent, toluene (50 mL); pressure, 5 bar; temperature, 30 °C; time, 1.5 h.

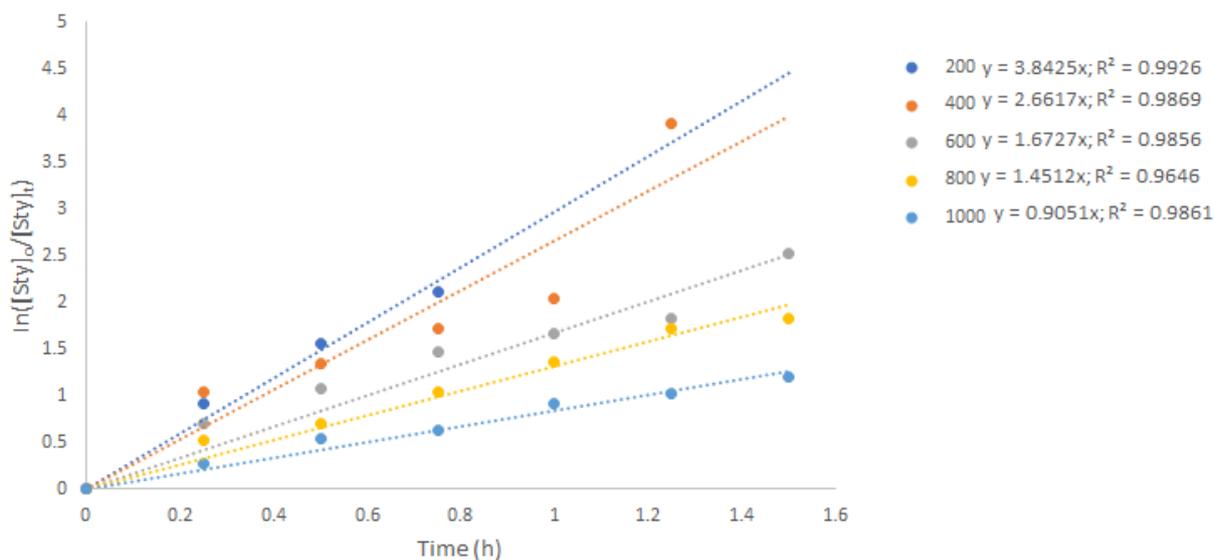


Fig. S3: Plot of $\ln[Sty]_0/[Sty]_t$ vs time for effect of catalyst concentration using complex **2**. Reaction conditions: solvent, toluene (50 mL); pressure, 5 bar; temperature, 30 °C.

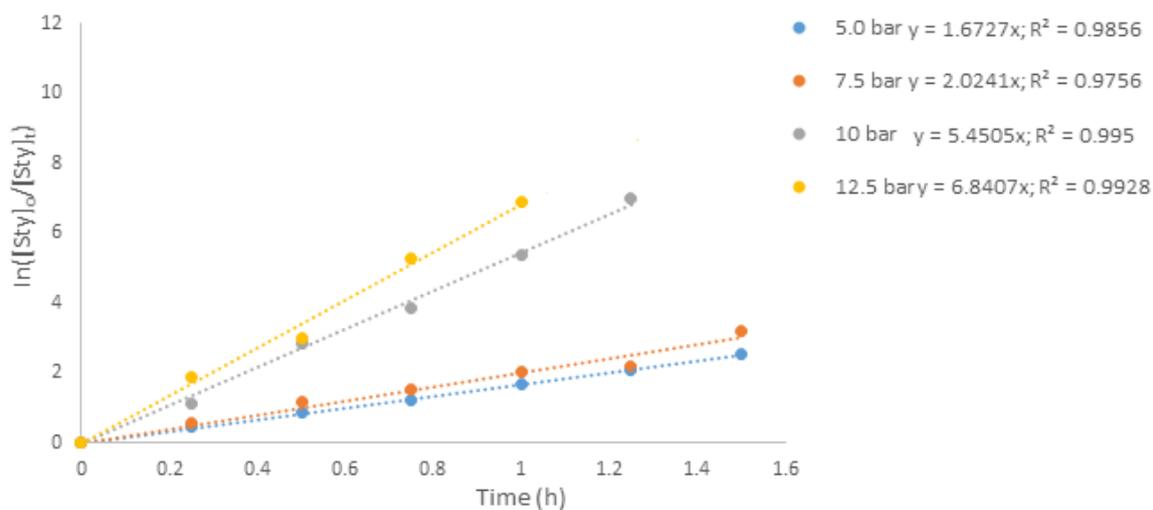


Fig. S4: Plot of $\ln([\text{Sty}]_0/[\text{Sty}]_t)$ vs time for styrene hydrogenation pressures. Reaction conditions: styrene, substrate/catalyst = 600; solvent, toluene (50 mL); temperature, 30 °C; time, 1.5 h.

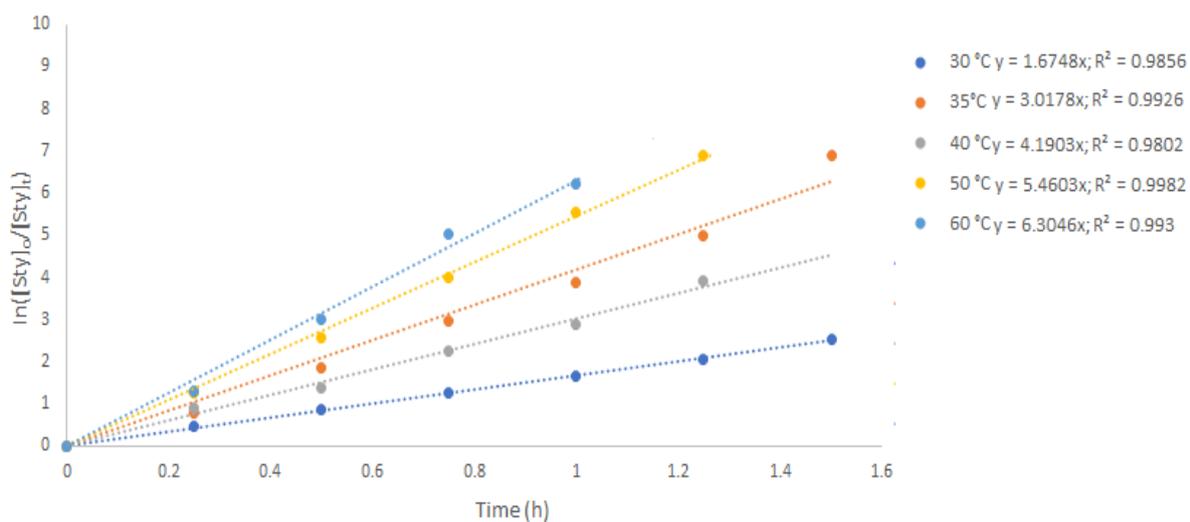


Fig. S5: Plot of $\ln([\text{Sty}]_0/[\text{Sty}]_t)$ vs time for effect of temperature using complex **2**. Reaction conditions: solvent, toluene (50 mL); pressure, 5 bar.

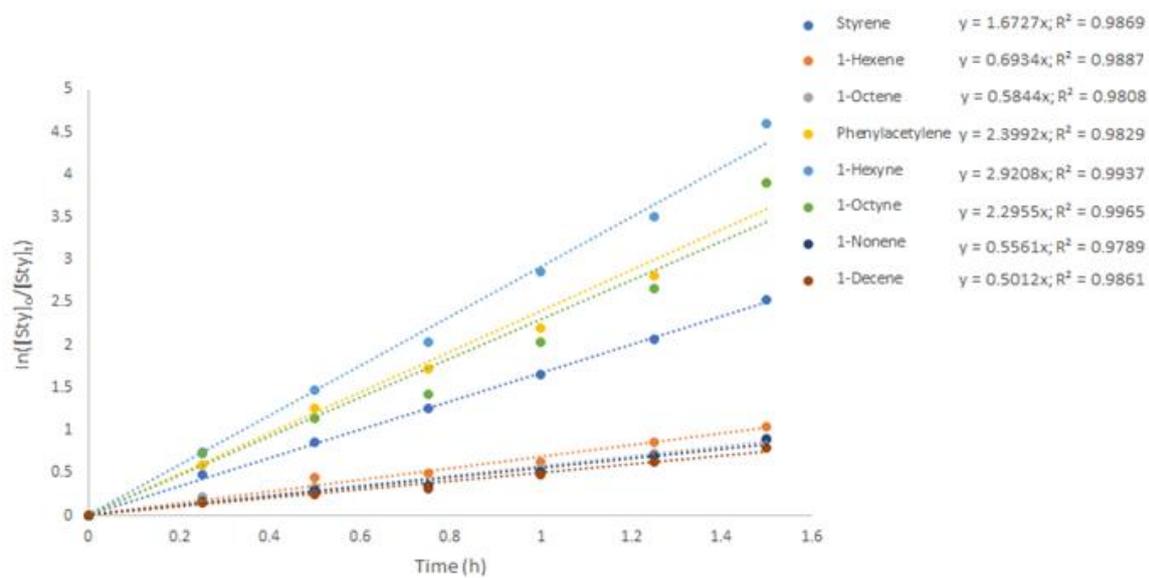


Fig. S6: Plot of $\ln[\text{Sty}]_0/[\text{Sty}]_t$ vs time for effect of substrate using complex **2**. Reaction conditions: solvent, toluene (50 mL); pressure, 5 bar; temperature, 30 °C.

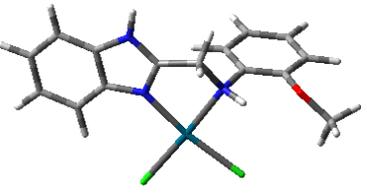
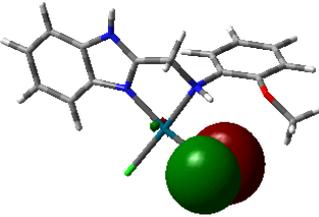
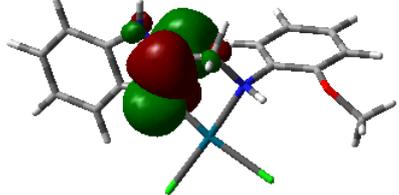
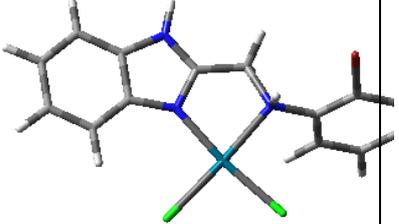
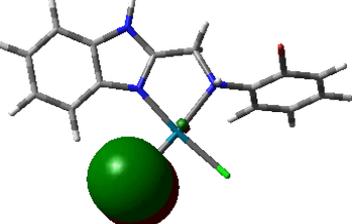
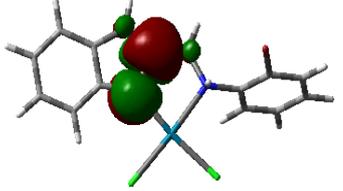
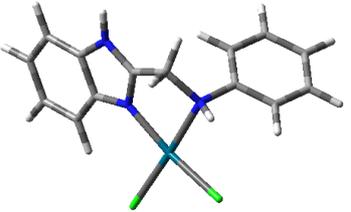
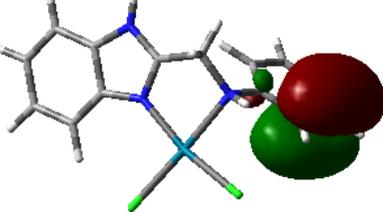
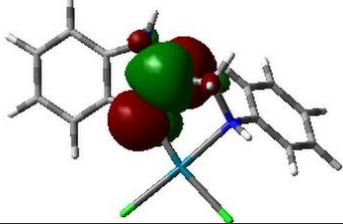
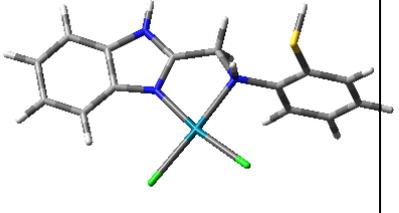
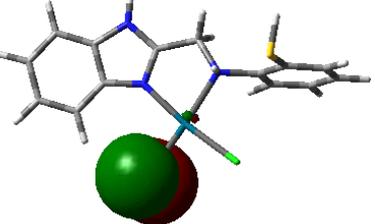
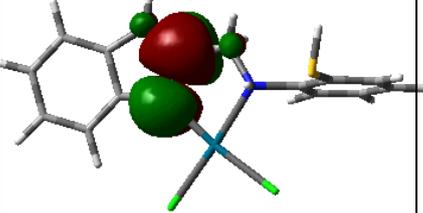
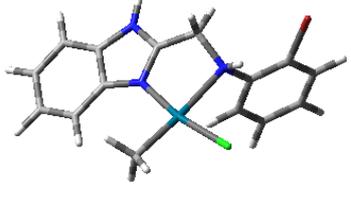
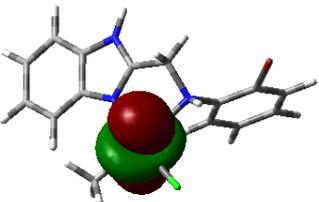
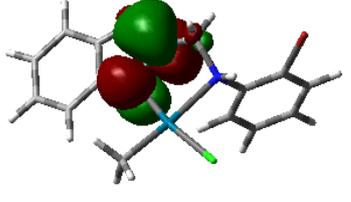
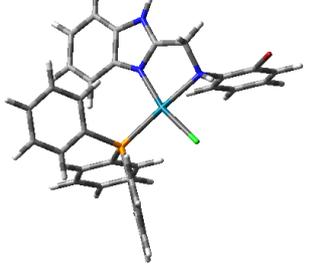
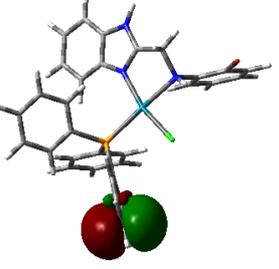
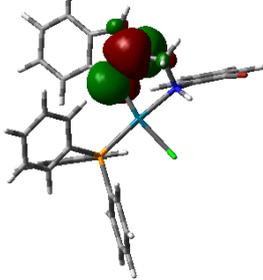
| Complex | Structure | HOMO Map | LUMO Map |
|---------|---|--|---|
| 1 |  |  |  |
| 2 |  |  |  |
| 3 |  |  |  |
| 4 |  |  |  |
| 5 |  |  |  |
| 6 |  |  |  |

Fig. S7: DFT-calculated HOMO and LUMO frontier molecular orbitals of palladium(II) complexes.

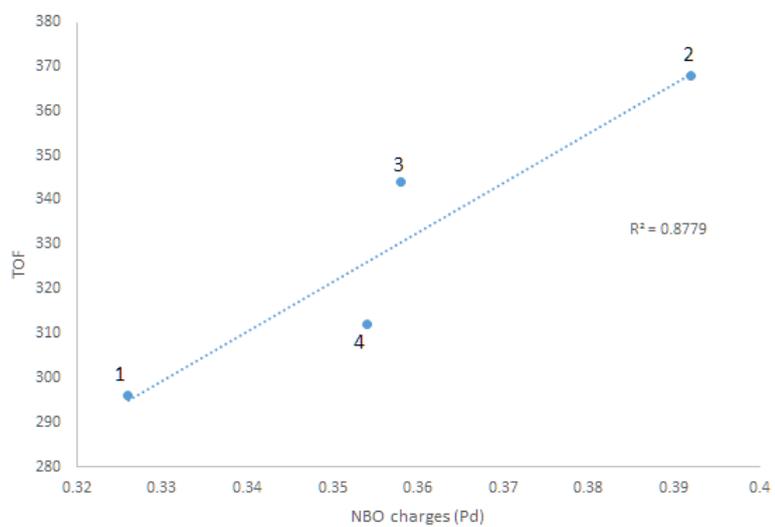


Fig. S8: Plot of TOF against NBO charges for palladium(II) depicting a correlation between catalytic activities and palladium(II) NBO charges.