Supporting Information

Synthesis and characterization of heterometallic molecular triangles using ambidentate linker: Self-selection of single linkage isomer

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Preparation of cis-(dppf)Pd(OTf)$_2$

The *cis*-(dppf)Pd(OTf)$_2$ was prepared using standard Schlenk technique by treating the *cis*-(dppf)PtCl$_2$ with 2. equivalents CF_3SO_3Ag at room temperature in dry CH_2Cl_2 under N_2 atmosphere for 16 hours stirring in absence of light. The precipitated AgCl was removed by filtration and the product was isolated as deep blue solid by adding diethyl ether to the concentrated filtrate. Yield: 80%. $^{31}P\{^1H\}$: δ = 46.3 ppm in $CDCl_3$.

Preparation of cis-(dppf)Pt(OTf)$_2$

The *cis*-(dppf)Pt(OTf)$_2$ was prepared using standard Schlenk technique by treating the *cis*-(dppf)PtCl$_2$ with 2.3 equivalents CF_3SO_3Ag at room temperature in dry CH_2Cl_2 under N_2 atmosphere for overnight in absence of light. The precipitated AgCl was removed by filtration and the product was isolated as orange solid by adding diethyl ether to the concentrated filtrate. Yield: 76%. $^{31}P\{^1H\}$: δ = 9.4 ppm in $CDCl_3$.

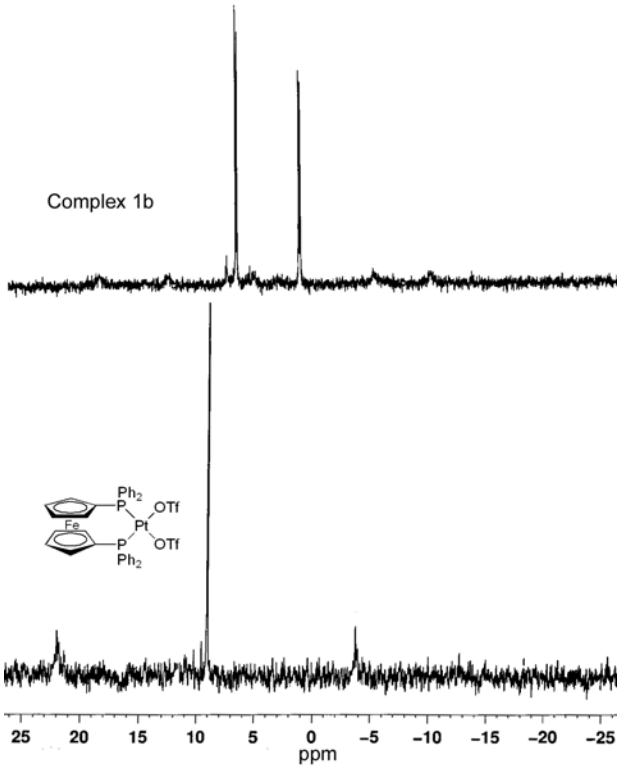

Fig. S1. ^{31}P NMR spectrum of **1b** and *cis*-(dppf)Pt(OTf)$_2$ in CD_3OD.

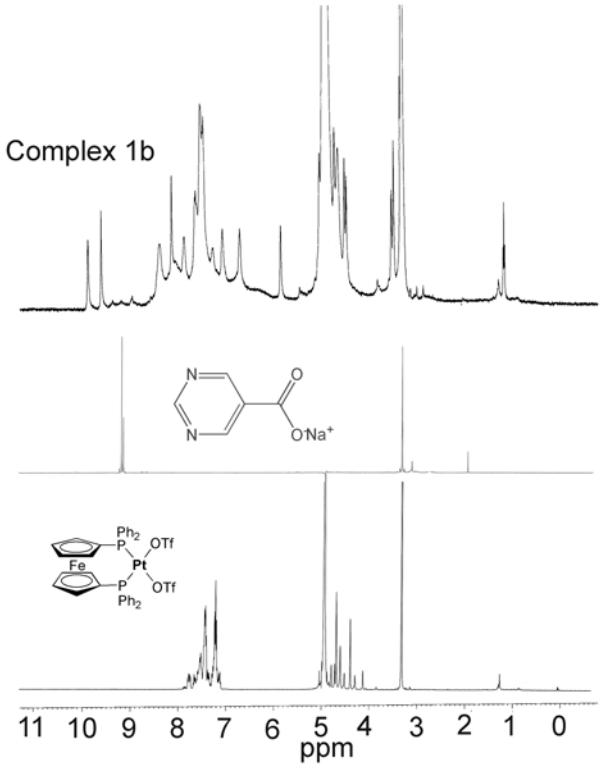

Fig. S2. ^{1}H NMR (400 MHz, CD_3OD, 293 K) spectrum of **1a**, Sodium 5-pyrimidine carboxylate and *cis*-(dppf)Pd$(OTf)_2$.

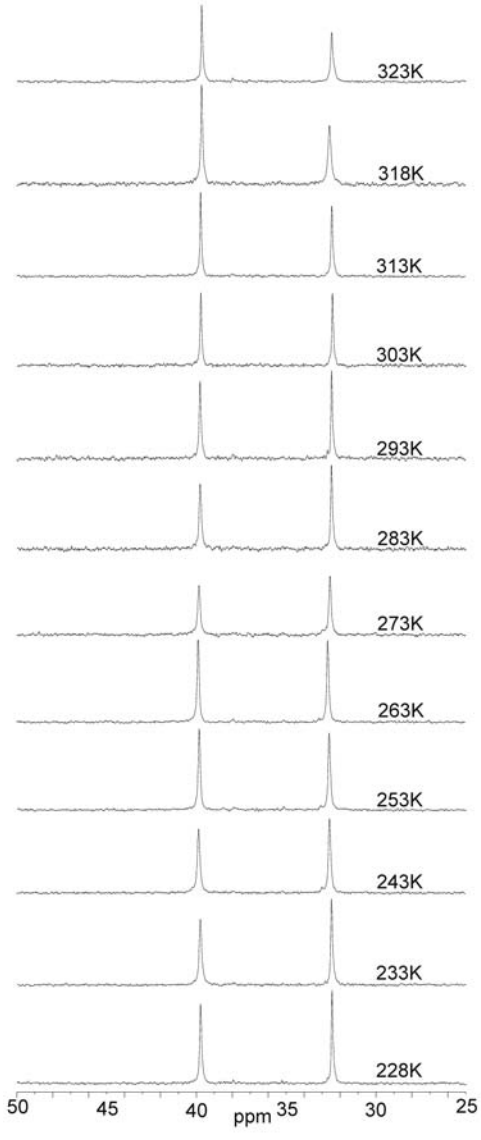

Fig. S3. Variable temperature ^{31}P NMR spectra of **1a** in CD_3OD

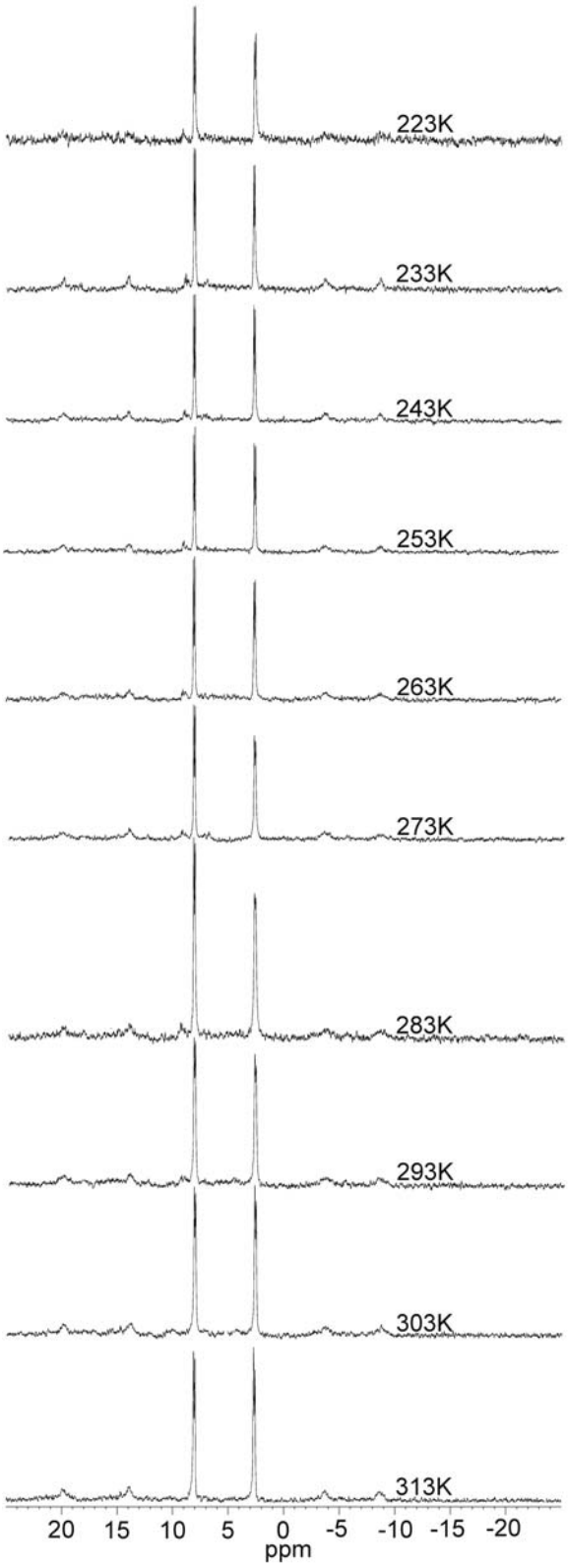

Fig. S4. Variable temperature ^{31}P NMR spectra of **1b** in CD_3OD.