Oxidative Addition of Propargyl Halides, Chloroacetonitrile, or Ethyl Chloroacetate to a Dimethylplatinum (II) Complex: Kinetic and DFT Studies

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Supporting Information

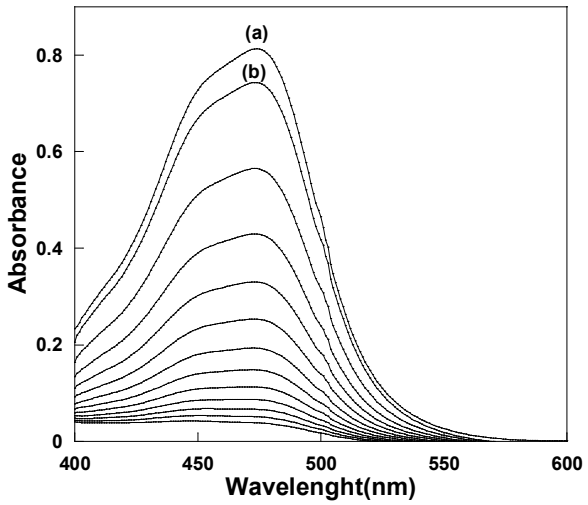

Figure S1. Changes in the UV-vis spectrum during the reaction of complex **1** (3 mL of 3×10^{-4} M solution) and $ClCH_2C{\equiv}N$ (0.1 M) in acetone, at T=25 °C: (a) initial spectrum (before adding $ClCH_2C{\equiv}N$); (b) spectrum at t = 0. Successive spectra were recorded at intervals of 40 s.

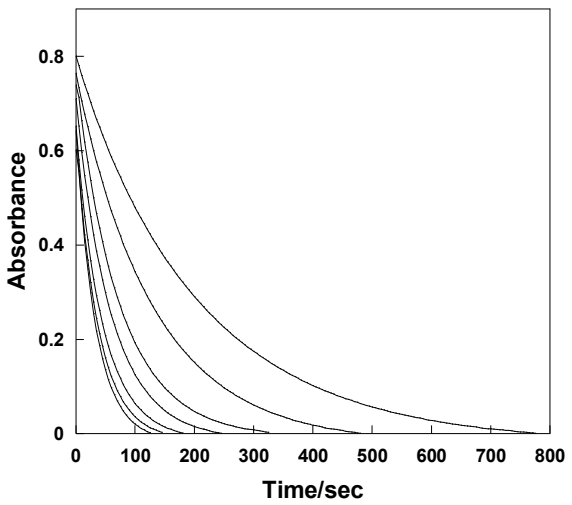

Figure S2. Absorbance-time curves for the reactions of complex **1** with $ClCH_2C{\equiv}N$ (0.125- 0.88 M, [$ClCH_2C{\equiv}N$] increase reading downwards) in acetone at 25 °C.

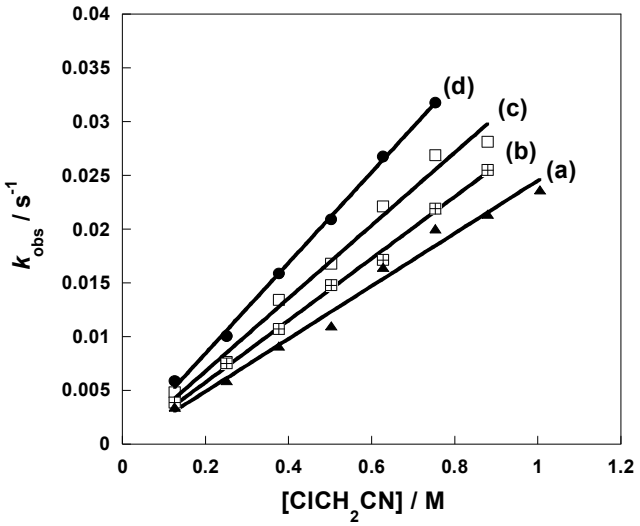

Figure S3. Plots of the observed first-order rate constants for the reaction of complex **1** with $ClCH_2C{\equiv}N$ *vs* the concentration of $ClCH_2C{\equiv}N$ in acetone: (a) T = 15 °C, (b) T = 20 °C, (c) T = 25 °C (d) T = 30 °C.

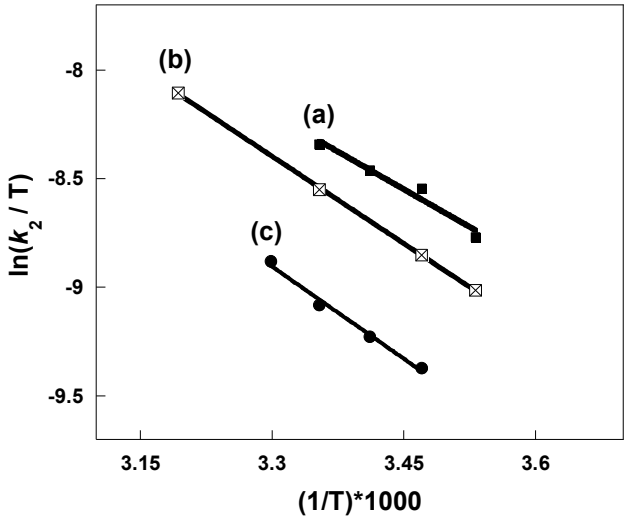

Figure S4. Eyring plots for the reaction of complex **1** with $ClCH_2C{\equiv}N$ [(a) in benzene and (c) in acetone] and $ClCH_2COOEt$ (b) in acetone.

Table S1. k_{obs} (s^{-1}) values at varying [chloroacetonitrile] and T in acetone

C_M ($mol.L^{-1}$)	k_{obs} (s^{-1}) T = 15 °C	k_{obs} (s^{-1}) T = 20 °C	k_{obs} (s^{-1}) T = 25 °C	k_{obs} (s^{-1}) T = 30 °C
0.12561	0.0034584	0.0038845	0.0048489	0.0058929
0.25121	0.0059072	0.0075263	0.0076563	0.010080
0.37682	0.0091364	0.010721	0.01362	0.015891
0.50243	0.011003	0.014797	0.016791	0.020927
0.62804	0.016452	0.01715	0.022123	0.020778
0.75364	0.020047	0.021913	0.026886	0.031764
0.87925	0.021403	0.025507	0.02814	
1.0049	0.023649			

$[Pt]_0 = 3 \times 10^{-4}$ M, Estimated errors in k_{obs} values are ±5 %.

Table S2. k_{obs} (s^{-1}) values at varying [chloroacetonitrile] and T in benzene

C_M ($mol.L^{-1}$)	k_{obs} (s^{-1}) T = 10 °C	k_{obs} (s^{-1}) T = 15 °C	k_{obs} (s^{-1}) T = 20 °C	k_{obs} (s^{-1}) T = 25 °C
0.12561	0.0032256	0.0049441	0.006897	0.008796
0.25121	0.0087754	0.012678	0.01668	0.017414
0.37682	0.017234	0.020941	0.0042546[a]	0.0047853[a]
0.50243	0.023441	0.029585	0.0044725[b]	0.0064122[b]
0.62804	0.028798	0.036387	0.01215[c]	0.014568[c]
0.75364	0.03157	0.041567		

$[Pt]_0 = 3 \times 10^{-4}$ M, Estimated errors in k_{obs} values are ±5 %, C_M ($mol.L^{-1}$) for a = 0.07536, b = 0.10049 and c = 0.20097

Table S3. k_{obs} (s^{-1}) values at varying [ethyl chloroacetate] and T in acetone

C_M ($mol.L^{-1}$)	k_{obs} (s^{-1}) T = 10 °C	k_{obs} (s^{-1}) T = 15 °C	k_{obs} (s^{-1}) T = 25 °C	k_{obs} (s^{-1}) T = 40 °C
0.15433	0.0042553	0.0067607	0.010074	0.014061
0.2345		0.0094954	0.01325	0.022582
0.31267	0.0091165	0.01233	0.019584	0.031593
0.39083	0.011923	0.017543	0.023266	0.040145
0.4690	0.013838	0.018477	0.025096	0.040551
0.54717			0.031612	0.051571

$[Pt]_0 = 3 \times 10^{-4}$ M, Estimated errors in k_{obs} values are ±5 %.

Table S4. k_{obs} (s^{-1}) values at varying [ethyl chloroacetate] and T in benzene

C_M ($mol.L^{-1}$)	k_{obs} (s^{-1}) T = 10 °C	k_{obs} (s^{-1}) T = 15 °C
0.15433	0.0027048	0.0032216
0.2345	0.0048840	0.0044782
0.31267		0.011719
0.39083	0.0072058	0.018311
0.4690	0.0087723	
0.54717	0.011386	
0.62533	0.013894	

$[Pt]_0 = 3 \times 10^{-4}$ M, Estimated errors in k_{obs} values are ±5 %.