

Electronic Supplementary Information for:

Reaction of carbon dioxide with a palladium–alkyl complex supported by a bis–NHC framework

Piyal W. G. Ariyananda, Glenn P. A. Yap and Joel Rosenthal*

Department of Chemistry and Biochemistry, University of Delaware, Newark, DE 19716

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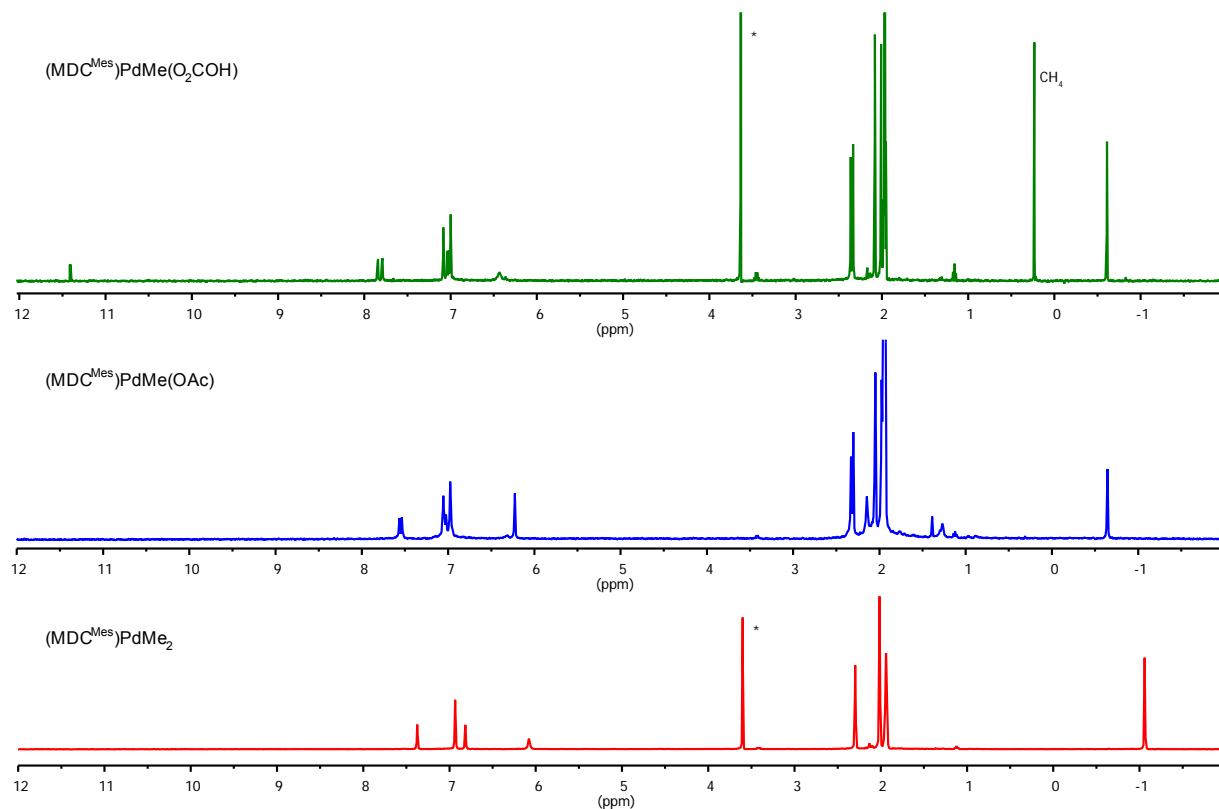


Fig. S-1 Stacked NMR spectra for $(\text{MDC}^{\text{Mes}})\text{PdMe}_2$, $(\text{MDC}^{\text{Mes}})\text{PdMe(OAc)}$, and $(\text{MDC}^{\text{Mes}})\text{PdMe}(\text{O}_2\text{COH})$. Labeled peaks at 3.60 ppm correspond to an internal dioxane standard (*) and peak at 0.22 ppm corresponds to methane coproduct.

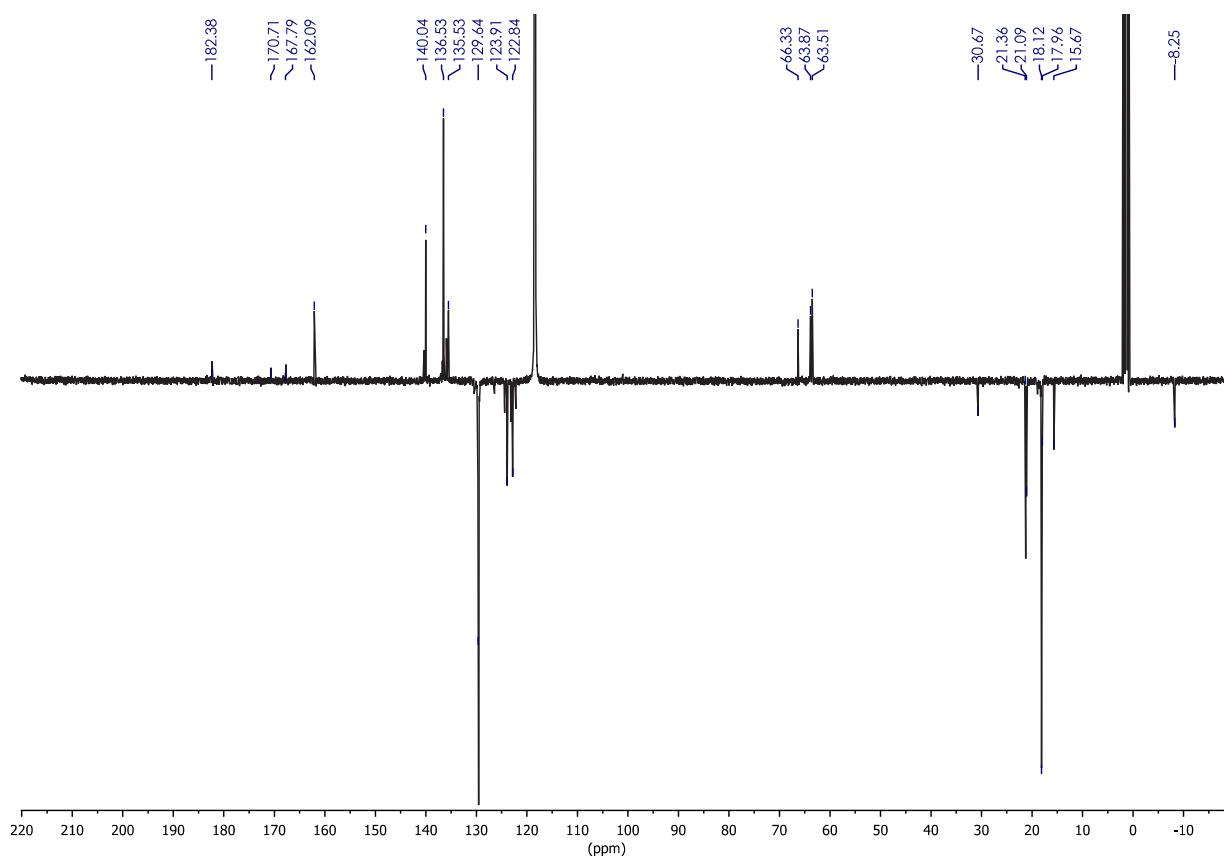


Fig. S-2 APT ¹³C NMR Spectrum for (MDC^{Mes})PdMe(O₂COH).

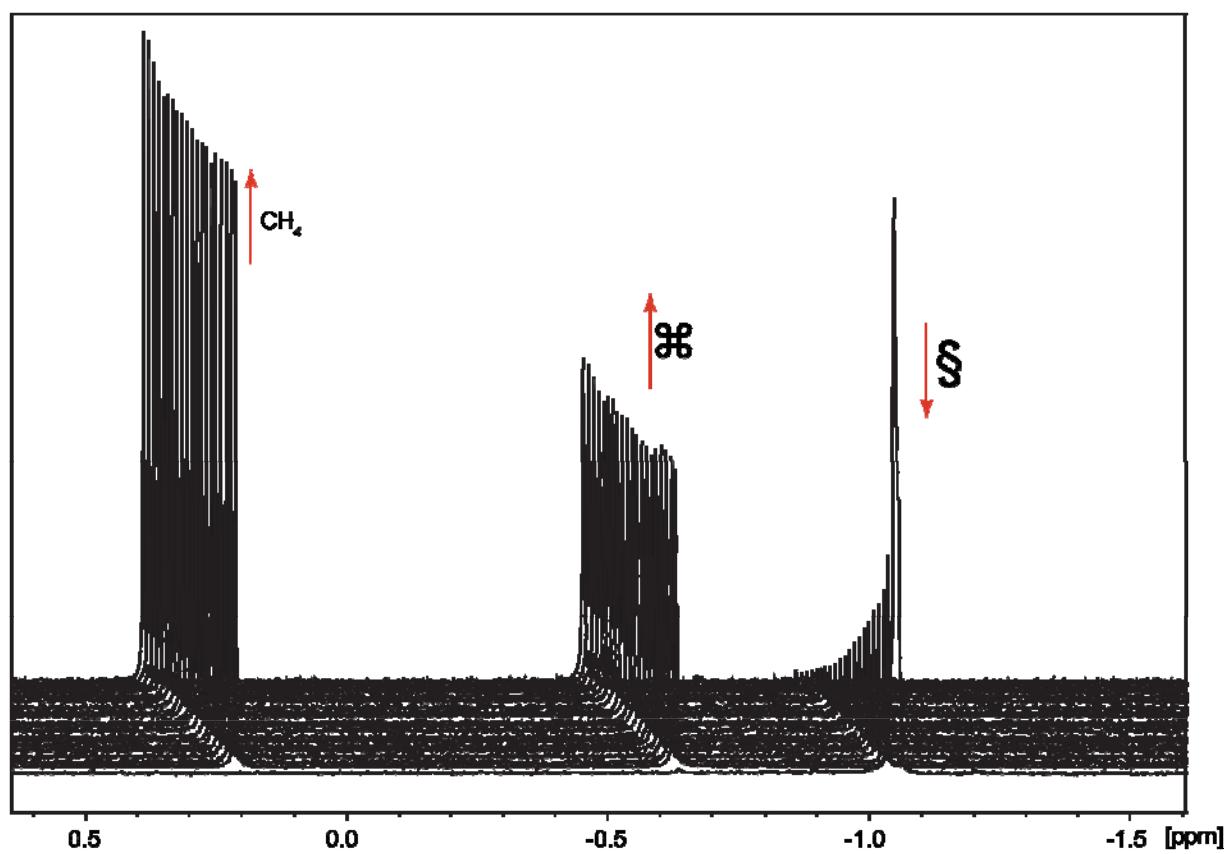


Fig. S-3 ^1H NMR stack plot of the timecourse NMR scale reaction of $(\text{MDC}^{\text{Mes}})\text{PdMe}_2$ with CO_2 in CD_3CN at $25\text{ }^\circ\text{C}$; § corresponds to the Pd–Me resonance of $(\text{MDC}^{\text{Mes}})\text{PdMe}_2$ and □ corresponds to the Pd–Me resonance of $(\text{MDC}^{\text{Mes}})\text{PdMe(O}_2\text{COH)}$. Consumption of $(\text{MDC}^{\text{Mes}})\text{PdMe}_2$ and simultaneous formation of $(\text{MDC}^{\text{Mes}})\text{PdMe(O}_2\text{COH})$ and CH_4 is indicated. Note: Integration of the peak corresponding to CH_4 is complicated by partitioning of this gas between the solution and headspace of the NMR tube. This complication precludes a full kinetic analysis.

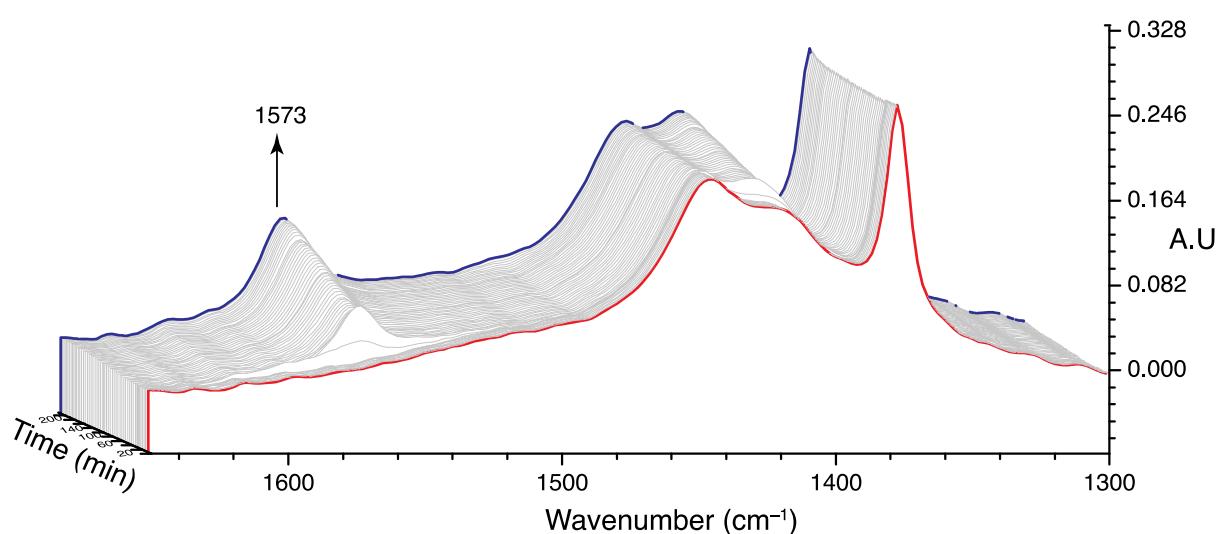


Fig. S-4 React-IR spectra acquired for $(\text{MDC}^{\text{Mes}})\text{PdMe}_2$ upon addition of $\text{CH}_3\text{CO}_2\text{H}$. The peak at 1573 cm^{-1} corresponds to the formation of $(\text{MDC}^{\text{Mes}})\text{Pd(OAc)}_2$ over the course of three hours.

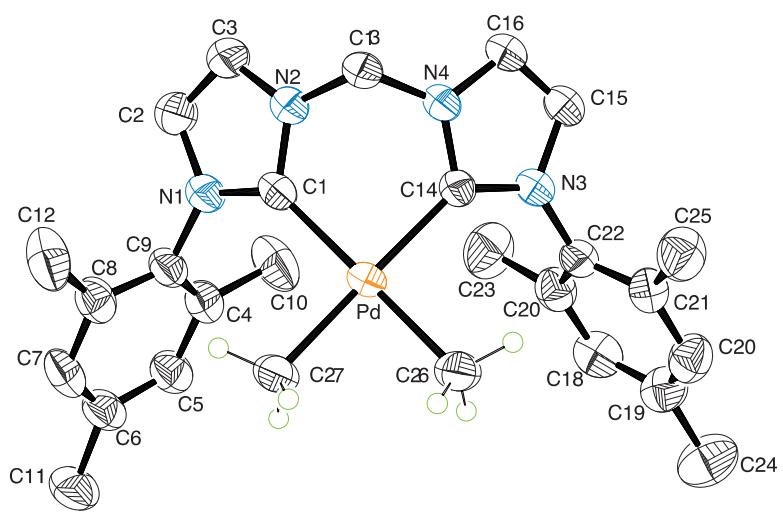


Fig. S-5 Fully labeled thermal ellipsoid plot of the solid-state structure of $(MDC^{Mes})PdMe_2$. Ellipsoids are shown at the 50% probability level and hydrogen atoms are omitted for clarity.

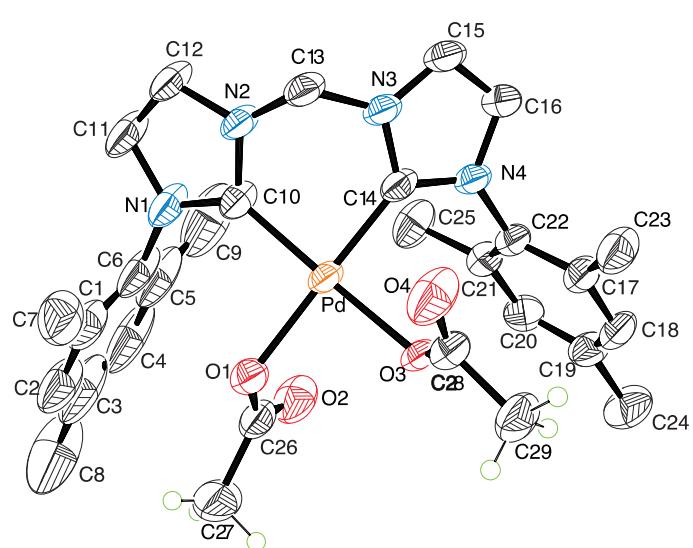


Fig. S-6 Fully labeled thermal ellipsoid plot of the solid-state structure of $(\text{MDC}^{\text{Mes}})\text{Pd}(\text{OAc})_2$. Ellipsoids are shown at the 50% probability level and hydrogen atoms are omitted for clarity.

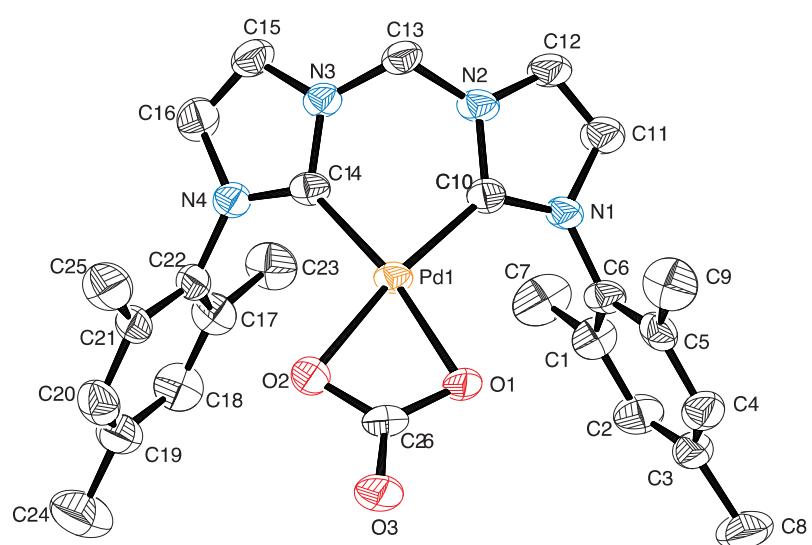


Fig. S-7 Fully labeled thermal ellipsoid plot of the solid-state structure of $(\text{MDC}^{\text{Mes}})\text{Pd}(\text{CO}_3)$. Ellipsoids are shown at the 50% probability level and hydrogen atoms are omitted for clarity.

Table S-1. Bond Lengths (\AA) for $(\text{MDC}^{\text{Mes}})\text{PdMe}_2$.

Pd-C(1)	2.065(4)
Pd-C(14)	2.072(4)
Pd-C(27)	2.075(4)
Pd-C(26)	2.079(4)
N(1)-C(1)	1.374(5)
N(1)-C(2)	1.390(6)
N(1)-C(9)	1.449(5)
N(2)-C(1)	1.364(5)
N(2)-C(3)	1.377(6)
N(2)-C(13)	1.460(5)
N(3)-C(14)	1.369(5)
N(3)-C(15)	1.390(5)
N(3)-C(22)	1.431(5)
N(4)-C(14)	1.367(5)
N(4)-C(16)	1.379(5)
N(4)-C(13)	1.452(5)
C(2)-C(3)	1.339(6)
C(4)-C(9)	1.374(6)
C(4)-C(5)	1.397(6)
C(4)-C(10)	1.513(7)
C(5)-C(6)	1.389(7)
C(6)-C(7)	1.382(7)
C(6)-C(11)	1.513(6)
C(7)-C(8)	1.396(6)
C(8)-C(9)	1.389(6)
C(8)-C(12)	1.512(7)
C(15)-C(16)	1.334(7)
C(17)-C(18)	1.392(7)
C(17)-C(22)	1.395(6)
C(17)-C(23)	1.517(7)
C(18)-C(19)	1.377(7)
C(19)-C(20)	1.370(7)
C(19)-C(24)	1.522(7)
C(20)-C(21)	1.406(7)

C(21)-C(22)	1.390(6)
C(21)-C(25)	1.506(7)
O(1)-C(31)	1.399(8)
O(1)-C(28)	1.433(7)
C(28)-C(29)	1.474(9)
C(29)-C(30)	1.495(9)
C(30)-C(31)	1.455(9)
O(2)-C(32)	1.444(12)
O(2)-C(35)	1.471(14)
C(32)-C(33)	1.404(13)
C(33)-C(34)	1.490(14)
<u>C(34)-C(35)</u>	<u>1.422(15)</u>

Table S-2. Bond angles ($^{\circ}$) of $\text{MDC}^{\text{Mes}}\text{PdMe}_2$.

C(1)-Pd-C(14)	86.86(15)
C(1)-Pd-C(27)	94.71(17)
C(14)-Pd-C(27)	177.52(17)
C(1)-Pd-C(26)	178.76(18)
C(14)-Pd-C(26)	93.80(17)
C(27)-Pd-C(26)	84.60(19)
C(1)-N(1)-C(2)	111.3(3)
C(1)-N(1)-C(9)	125.1(4)
C(2)-N(1)-C(9)	123.4(4)
C(1)-N(2)-C(3)	113.3(3)
C(1)-N(2)-C(13)	121.7(3)
C(3)-N(2)-C(13)	125.0(4)
C(14)-N(3)-C(15)	111.2(4)
C(14)-N(3)-C(22)	126.3(3)
C(15)-N(3)-C(22)	122.4(4)
C(14)-N(4)-C(16)	112.9(4)
C(14)-N(4)-C(13)	122.5(3)
C(16)-N(4)-C(13)	124.6(4)
N(2)-C(1)-N(1)	102.1(3)
N(2)-C(1)-Pd	121.2(3)
N(1)-C(1)-Pd	136.5(3)
C(3)-C(2)-N(1)	107.4(4)
C(2)-C(3)-N(2)	105.8(4)
C(9)-C(4)-C(5)	118.1(4)
C(9)-C(4)-C(10)	121.5(4)
C(5)-C(4)-C(10)	120.5(5)
C(6)-C(5)-C(4)	121.9(5)
C(7)-C(6)-C(5)	117.6(4)
C(7)-C(6)-C(11)	121.3(5)
C(5)-C(6)-C(11)	121.0(5)
C(6)-C(7)-C(8)	122.3(4)
C(9)-C(8)-C(7)	117.6(5)
C(9)-C(8)-C(12)	122.6(4)
C(7)-C(8)-C(12)	119.8(5)

C(4)-C(9)-C(8)	122.2(4)
C(4)-C(9)-N(1)	118.8(4)
C(8)-C(9)-N(1)	119.0(4)
N(4)-C(13)-N(2)	110.7(3)
N(4)-C(14)-N(3)	102.4(3)
N(4)-C(14)-Pd	120.5(3)
N(3)-C(14)-Pd	137.1(3)
C(16)-C(15)-N(3)	107.6(4)
C(15)-C(16)-N(4)	105.9(4)
C(18)-C(17)-C(22)	118.0(5)
C(18)-C(17)-C(23)	121.6(5)
C(22)-C(17)-C(23)	120.4(5)
C(19)-C(18)-C(17)	122.2(5)
C(20)-C(19)-C(18)	118.6(5)
C(20)-C(19)-C(24)	120.2(5)
C(18)-C(19)-C(24)	121.2(5)
C(19)-C(20)-C(21)	122.0(5)
C(22)-C(21)-C(20)	117.8(4)
C(22)-C(21)-C(25)	122.2(4)
C(20)-C(21)-C(25)	120.0(4)
C(21)-C(22)-C(17)	121.3(4)
C(21)-C(22)-N(3)	119.2(4)
C(17)-C(22)-N(3)	119.3(4)
C(31)-O(1)-C(28)	107.4(5)
O(1)-C(28)-C(29)	104.4(6)
C(28)-C(29)-C(30)	103.7(6)
C(31)-C(30)-C(29)	102.7(6)
O(1)-C(31)-C(30)	110.1(6)
C(32)-O(2)-C(35)	109.6(10)
C(33)-C(32)-O(2)	98.9(10)
C(32)-C(33)-C(34)	107.3(12)
C(35)-C(34)-C(33)	98.1(13)
C(34)-C(35)-O(2)	93.9(13)

Table S-3. Bond Lengths (\AA) for $(\text{MDC}^{\text{Mes}})\text{Pd}(\text{OAc})_2$.

Pd-C(14)	1.955(3)
Pd-C(10)	1.977(3)
Pd-O(3)	2.069(2)
Pd-O(1)	2.077(3)
N(1)-C(10)	1.362(4)
N(1)-C(11)	1.394(5)
N(1)-C(6)	1.442(5)
N(2)-C(10)	1.362(4)
N(2)-C(12)	1.386(4)
N(2)-C(13)	1.452(5)
N(3)-C(14)	1.347(4)
N(3)-C(15)	1.386(5)
N(3)-C(13)	1.451(4)
N(4)-C(14)	1.361(4)
N(4)-C(16)	1.391(4)
N(4)-C(22)	1.450(4)
O(1)-C(26)	1.271(5)
O(2)-C(26)	1.233(6)
O(3)-C(28)	1.241(5)
O(4)-C(28)	1.247(4)
C(1)-C(6)	1.387(7)
C(1)-C(2)	1.393(6)
C(1)-C(7)	1.502(7)
C(2)-C(3)	1.390(10)
C(3)-C(4)	1.346(11)
C(3)-C(8)	1.533(8)
C(4)-C(5)	1.399(9)
C(5)-C(6)	1.396(7)
C(5)-C(9)	1.501(9)
C(11)-C(12)	1.345(6)
C(15)-C(16)	1.350(5)
C(17)-C(18)	1.392(5)
C(17)-C(22)	1.399(5)
C(17)-C(23)	1.504(5)

C(18)-C(19)	1.388(5)
C(19)-C(20)	1.381(5)
C(19)-C(24)	1.520(5)
C(20)-C(21)	1.398(5)
C(21)-C(22)	1.391(5)
C(21)-C(25)	1.509(5)
C(26)-C(27)	1.524(6)
C(28)-C(29)	1.535(5)
N(5)-C(30)	1.135(5)
C(30)-C(31)	1.455(6)
N(6)-C(32)	1.116(10)
C(32)-C(33)	1.456(15)
N(6')-C(32')	1.134(12)
<u>C(32')-C(33')</u>	<u>1.459(15)</u>

Table S-4. Bond angles ($^{\circ}$) of $\text{MDC}^{\text{Mes}}\text{Pd(OAc)}_2$.

C(14)-Pd-C(10)	86.76(14)
C(14)-Pd-O(3)	92.08(11)
C(10)-Pd-O(3)	174.08(12)
C(14)-Pd-O(1)	178.21(11)
C(10)-Pd-O(1)	94.59(13)
O(3)-Pd-O(1)	86.46(9)
C(10)-N(1)-C(11)	110.3(3)
C(10)-N(1)-C(6)	127.8(3)
C(11)-N(1)-C(6)	121.8(3)
C(10)-N(2)-C(12)	111.4(3)
C(10)-N(2)-C(13)	123.2(3)
C(12)-N(2)-C(13)	125.2(3)
C(14)-N(3)-C(15)	112.1(3)
C(14)-N(3)-C(13)	121.6(3)
C(15)-N(3)-C(13)	126.4(3)
C(14)-N(4)-C(16)	110.6(3)
C(14)-N(4)-C(22)	126.1(3)
C(16)-N(4)-C(22)	123.1(3)
C(26)-O(1)-Pd	110.8(3)
C(28)-O(3)-Pd	117.7(2)
C(6)-C(1)-C(2)	117.3(5)
C(6)-C(1)-C(7)	121.3(4)
C(2)-C(1)-C(7)	121.4(6)
C(3)-C(2)-C(1)	121.5(7)
C(4)-C(3)-C(2)	119.4(6)
C(4)-C(3)-C(8)	120.4(8)
C(2)-C(3)-C(8)	120.2(9)
C(3)-C(4)-C(5)	122.1(7)
C(6)-C(5)-C(4)	117.4(7)
C(6)-C(5)-C(9)	122.1(6)
C(4)-C(5)-C(9)	120.6(6)
C(1)-C(6)-C(5)	122.2(5)
C(1)-C(6)-N(1)	119.6(4)
C(5)-C(6)-N(1)	118.0(5)

N(1)-C(10)-N(2)	104.5(3)
N(1)-C(10)-Pd	134.1(3)
N(2)-C(10)-Pd	121.4(2)
C(12)-C(11)-N(1)	107.5(3)
C(11)-C(12)-N(2)	106.4(3)
N(2)-C(13)-N(3)	109.3(3)
N(3)-C(14)-N(4)	104.3(3)
N(3)-C(14)-Pd	124.0(2)
N(4)-C(14)-Pd	131.6(2)
C(16)-C(15)-N(3)	106.0(3)
C(15)-C(16)-N(4)	107.0(3)
C(18)-C(17)-C(22)	117.1(3)
C(18)-C(17)-C(23)	121.2(3)
C(22)-C(17)-C(23)	121.7(3)
C(19)-C(18)-C(17)	122.5(3)
C(20)-C(19)-C(18)	118.4(3)
C(20)-C(19)-C(24)	120.9(4)
C(18)-C(19)-C(24)	120.7(4)
C(19)-C(20)-C(21)	121.7(3)
C(22)-C(21)-C(20)	117.9(3)
C(22)-C(21)-C(25)	122.0(3)
C(20)-C(21)-C(25)	120.0(3)
C(21)-C(22)-C(17)	122.3(3)
C(21)-C(22)-N(4)	119.1(3)
C(17)-C(22)-N(4)	118.6(3)
O(2)-C(26)-O(1)	124.6(4)
O(2)-C(26)-C(27)	120.0(4)
O(1)-C(26)-C(27)	115.4(4)
O(3)-C(28)-O(4)	126.8(3)
O(3)-C(28)-C(29)	114.9(3)
O(4)-C(28)-C(29)	118.3(4)
N(5)-C(30)-C(31)	178.6(5)
N(6)-C(32)-C(33)	177.4(13)
<u>N(6')-C(32')-C(33')</u>	<u>178.8(19)</u>

Table S-5. Bond Lengths (\AA) for $(\text{MDC}^{\text{Mes}})\text{Pd}(\text{CO}_3)$.

Pd(1)-C(10)	1.980(5)
Pd(1)-C(14)	1.986(5)
Pd(1)-O(1)	2.064(3)
Pd(1)-O(2)	2.069(4)
Pd(1)-C(26)	2.466(5)
Pd(2)-C(36)	1.981(5)
Pd(2)-C(40)	1.988(5)
Pd(2)-O(5)	2.051(3)
Pd(2)-O(4)	2.067(3)
Pd(2)-C(52)	2.453(5)
O(1)-C(26)	1.307(6)
O(2)-C(26)	1.346(6)
O(3)-C(26)	1.244(6)
O(4)-C(52)	1.310(6)
O(5)-C(52)	1.319(6)
O(6)-C(52)	1.250(6)
N(1)-C(10)	1.363(6)
N(1)-C(11)	1.405(7)
N(1)-C(6)	1.446(6)
N(2)-C(10)	1.368(6)
N(2)-C(12)	1.379(7)
N(2)-C(13)	1.455(6)
N(3)-C(14)	1.352(6)
N(3)-C(15)	1.393(6)
N(3)-C(13)	1.451(6)
N(4)-C(14)	1.360(6)
N(4)-C(16)	1.408(7)
N(4)-C(22)	1.460(7)
N(5)-C(36)	1.350(6)
N(5)-C(37)	1.394(6)
N(5)-C(32)	1.470(6)
N(6)-C(36)	1.350(6)
N(6)-C(38)	1.387(6)
N(6)-C(39)	1.475(6)

N(7)-C(40)	1.350(6)
N(7)-C(41)	1.386(6)
N(7)-C(39)	1.456(6)
N(8)-C(40)	1.363(6)
N(8)-C(42)	1.404(6)
N(8)-C(48)	1.455(6)
C(1)-C(6)	1.392(7)
C(1)-C(2)	1.406(8)
C(1)-C(7)	1.509(8)
C(2)-C(3)	1.366(8)
C(3)-C(4)	1.397(8)
C(3)-C(8)	1.522(8)
C(4)-C(5)	1.396(7)
C(5)-C(6)	1.393(7)
C(5)-C(9)	1.512(8)
C(11)-C(12)	1.329(8)
C(15)-C(16)	1.332(8)
C(17)-C(18)	1.371(8)
C(17)-C(22)	1.395(7)
C(17)-C(23)	1.523(8)
C(18)-C(19)	1.431(9)
C(19)-C(20)	1.363(8)
C(19)-C(24)	1.513(9)
C(20)-C(21)	1.404(8)
C(21)-C(22)	1.398(7)
C(21)-C(25)	1.487(8)
C(27)-C(32)	1.375(8)
C(27)-C(28)	1.395(8)
C(27)-C(33)	1.518(8)
C(28)-C(29)	1.406(9)
C(29)-C(30)	1.365(9)
C(29)-C(34)	1.531(8)
C(30)-C(31)	1.383(8)
C(31)-C(32)	1.398(7)
C(31)-C(35)	1.505(8)
C(37)-C(38)	1.341(7)

C(41)-C(42)	1.325(7)
C(43)-C(48)	1.389(8)
C(43)-C(44)	1.391(8)
C(43)-C(49)	1.513(8)
C(44)-C(45)	1.388(9)
C(45)-C(46)	1.391(9)
C(45)-C(50)	1.508(9)
C(46)-C(47)	1.415(8)
C(47)-C(48)	1.397(7)
<u>C(47)-C(51)</u>	<u>1.480(8)</u>

Table S-6. Bond Lengths (\AA) for $(\text{MDC}^{\text{Mes}})\text{Pd}(\text{CO}_3)$.

C(10)-Pd(1)-C(14)	84.9(2)
C(10)-Pd(1)-O(1)	105.44(18)
C(14)-Pd(1)-O(1)	169.49(17)
C(10)-Pd(1)-O(2)	169.94(17)
C(14)-Pd(1)-O(2)	104.63(17)
O(1)-Pd(1)-O(2)	64.96(14)
C(10)-Pd(1)-C(26)	137.09(19)
C(14)-Pd(1)-C(26)	137.50(19)
O(1)-Pd(1)-C(26)	32.01(15)
O(2)-Pd(1)-C(26)	33.08(15)
C(36)-Pd(2)-C(40)	85.25(19)
C(36)-Pd(2)-O(5)	169.81(16)
C(40)-Pd(2)-O(5)	104.08(17)
C(36)-Pd(2)-O(4)	105.81(17)
C(40)-Pd(2)-O(4)	168.74(17)
O(5)-Pd(2)-O(4)	64.74(13)
C(36)-Pd(2)-C(52)	137.74(19)
C(40)-Pd(2)-C(52)	136.49(19)
O(5)-Pd(2)-C(52)	32.54(15)
O(4)-Pd(2)-C(52)	32.28(15)
C(26)-O(1)-Pd(1)	91.2(3)
C(26)-O(2)-Pd(1)	89.9(3)
C(52)-O(4)-Pd(2)	90.3(3)
C(52)-O(5)-Pd(2)	90.7(3)
C(10)-N(1)-C(11)	110.1(4)
C(10)-N(1)-C(6)	126.5(4)
C(11)-N(1)-C(6)	123.3(4)
C(10)-N(2)-C(12)	110.9(4)
C(10)-N(2)-C(13)	121.7(4)
C(12)-N(2)-C(13)	127.3(4)
C(14)-N(3)-C(15)	110.6(4)
C(14)-N(3)-C(13)	122.9(4)
C(15)-N(3)-C(13)	126.5(4)
C(14)-N(4)-C(16)	110.1(4)

C(14)-N(4)-C(22)	126.6(4)
C(16)-N(4)-C(22)	123.0(4)
C(36)-N(5)-C(37)	110.9(4)
C(36)-N(5)-C(32)	125.2(4)
C(37)-N(5)-C(32)	123.9(4)
C(36)-N(6)-C(38)	111.8(4)
C(36)-N(6)-C(39)	123.2(4)
C(38)-N(6)-C(39)	124.9(4)
C(40)-N(7)-C(41)	111.2(4)
C(40)-N(7)-C(39)	123.0(4)
C(41)-N(7)-C(39)	125.8(4)
C(40)-N(8)-C(42)	109.5(4)
C(40)-N(8)-C(48)	125.1(4)
C(42)-N(8)-C(48)	125.0(4)
C(6)-C(1)-C(2)	117.1(5)
C(6)-C(1)-C(7)	120.9(5)
C(2)-C(1)-C(7)	121.9(5)
C(3)-C(2)-C(1)	122.2(6)
C(2)-C(3)-C(4)	119.1(5)
C(2)-C(3)-C(8)	120.4(6)
C(4)-C(3)-C(8)	120.5(6)
C(5)-C(4)-C(3)	121.2(5)
C(6)-C(5)-C(4)	117.9(5)
C(6)-C(5)-C(9)	121.8(5)
C(4)-C(5)-C(9)	120.3(5)
C(1)-C(6)-C(5)	122.5(5)
C(1)-C(6)-N(1)	118.9(5)
C(5)-C(6)-N(1)	118.5(5)
N(1)-C(10)-N(2)	104.4(4)
N(1)-C(10)-Pd(1)	130.8(4)
N(2)-C(10)-Pd(1)	124.7(4)
C(12)-C(11)-N(1)	107.1(5)
C(11)-C(12)-N(2)	107.5(5)
N(3)-C(13)-N(2)	108.4(4)
N(3)-C(14)-N(4)	105.2(4)
N(3)-C(14)-Pd(1)	124.3(4)

N(4)-C(14)-Pd(1)	130.5(4)
C(16)-C(15)-N(3)	107.5(5)
C(15)-C(16)-N(4)	106.6(5)
C(18)-C(17)-C(22)	118.6(5)
C(18)-C(17)-C(23)	120.8(6)
C(22)-C(17)-C(23)	120.6(5)
C(17)-C(18)-C(19)	121.2(6)
C(20)-C(19)-C(18)	117.4(6)
C(20)-C(19)-C(24)	122.5(6)
C(18)-C(19)-C(24)	120.1(6)
C(19)-C(20)-C(21)	124.0(5)
C(22)-C(21)-C(20)	116.0(5)
C(22)-C(21)-C(25)	121.7(5)
C(20)-C(21)-C(25)	122.3(5)
C(17)-C(22)-C(21)	122.8(5)
C(17)-C(22)-N(4)	119.1(5)
C(21)-C(22)-N(4)	118.1(5)
O(3)-C(26)-O(1)	125.0(5)
O(3)-C(26)-O(2)	121.5(5)
O(1)-C(26)-O(2)	113.5(4)
O(3)-C(26)-Pd(1)	174.9(4)
O(1)-C(26)-Pd(1)	56.8(2)
O(2)-C(26)-Pd(1)	57.0(2)
C(32)-C(27)-C(28)	117.9(6)
C(32)-C(27)-C(33)	122.2(5)
C(28)-C(27)-C(33)	119.9(6)
C(27)-C(28)-C(29)	120.9(6)
C(30)-C(29)-C(28)	118.5(6)
C(30)-C(29)-C(34)	120.5(6)
C(28)-C(29)-C(34)	120.9(7)
C(29)-C(30)-C(31)	122.9(6)
C(30)-C(31)-C(32)	116.9(5)
C(30)-C(31)-C(35)	121.9(5)
C(32)-C(31)-C(35)	121.3(5)
C(27)-C(32)-C(31)	123.0(5)
C(27)-C(32)-N(5)	119.7(5)

C(31)-C(32)-N(5)	117.3(5)
N(5)-C(36)-N(6)	104.2(4)
N(5)-C(36)-Pd(2)	131.4(4)
N(6)-C(36)-Pd(2)	124.4(3)
C(38)-C(37)-N(5)	107.0(5)
C(37)-C(38)-N(6)	106.0(5)
N(7)-C(39)-N(6)	109.1(4)
N(7)-C(40)-N(8)	104.9(4)
N(7)-C(40)-Pd(2)	124.8(3)
N(8)-C(40)-Pd(2)	130.3(4)
C(42)-C(41)-N(7)	106.9(5)
C(41)-C(42)-N(8)	107.6(4)
C(48)-C(43)-C(44)	117.4(6)
C(48)-C(43)-C(49)	122.0(5)
C(44)-C(43)-C(49)	120.7(6)
C(45)-C(44)-C(43)	122.6(6)
C(44)-C(45)-C(46)	118.3(6)
C(44)-C(45)-C(50)	121.0(7)
C(46)-C(45)-C(50)	120.7(7)
C(45)-C(46)-C(47)	121.8(6)
C(48)-C(47)-C(46)	116.7(6)
C(48)-C(47)-C(51)	123.2(5)
C(46)-C(47)-C(51)	120.1(5)
C(43)-C(48)-C(47)	123.2(5)
C(43)-C(48)-N(8)	118.3(5)
C(47)-C(48)-N(8)	118.5(5)
O(6)-C(52)-O(4)	123.3(5)
O(6)-C(52)-O(5)	122.7(5)
O(4)-C(52)-O(5)	114.0(4)
O(6)-C(52)-Pd(2)	176.9(4)
O(4)-C(52)-Pd(2)	57.4(2)
O(5)-C(52)-Pd(2)	56.7(2)