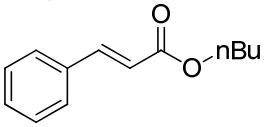
Supporting Information

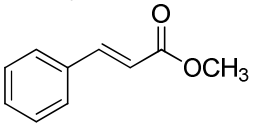
Spectral Data for the phenylated trans-alkene products 12a – 12d.

Butyl cinnamate (12a)



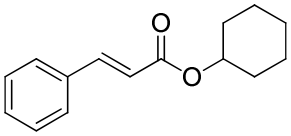
Pale yellow semi-solid; eluent (3% ethyl acetate in hexanes)
^{1}H NMR ($CDCl_3$, 400 MHz):δ7.69 (d, *J*= 16.0Hz, 1 H), 7.54 – 7.52 (m, 2 H), 7.40 – 7.37 (m, 3 H), 6.45 (d, *J*= 16.0Hz, 1 H), 4.22 (t, *J* = 4.0Hz, 2 H), 1.74 – 1.66 (m, 2 H), 1.50 – 1.40 (m, 2 H), 0.97 (t, *J*= 8.0 Hz, 3 H).
^{13}C NMR ($CDCl_3$, 100 MHz):δ167.2, 144.64, 134.5, 130.2, 128.9, 128.1, 118.3, 64.5, 30.8, 19.2, 13.84.
HRMS (ESI): calc. for $[(C_{13}H_{16}O_2)Na]$ $(M+Na)^+$ 227.1048, measured 227.1047.

Methyl cinnamate (12b)



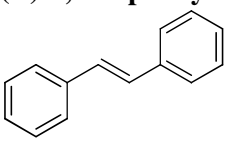
Pale yellow liquid; eluent (3% ethyl acetate in hexanes)
^{1}H NMR ($CDCl_3$, 400 MHz):δ7.71 (d, *J*= 16.0Hz, 1 H), 7.55 – 7.53 (m, 2 H), 7.41 – 7.39 (m, 3 H), 6.46 (d, *J*= 16.0Hz, 1 H), 3.82 (s, 3 H).
^{13}C NMR ($CDCl_3$, 100 MHz):δ167.5, 144.9, 134.4, 130.3, 128.9, 128.1, 117.8, 51.9.
HRMS (ESI): calc. for $[(C_{10}H_{10}O_2)Na]$ $(M+Na)^+$ 185.0578, measured 185.0579.

Cyclohexylcinnamate (12c)



Pale yellow liquid;eluent (3% ethyl acetate in hexanes)
^{1}H NMR ($CDCl_3$, 400 MHz):δ7.68 (d, *J*= 16.0Hz, 1 H), 7.55 – 7.52 (m, 2 H), 7.49 – 7.38 (m, 3 H), 6.44 (d, *J*= 16.0Hz, 1 H), 4.93 – 4.87 (s, 1 H),1.95 – 1.91 (m, 2 H), 1.80 – 1.76 (m, 2 H), 1.60 – 1.54 (m, 1 H), 1.52 – 1.46 (m, 2 H), 1.44 – 1.40 (m, 1 H), 1.34 – 1.26 (m, 2 H).
^{13}C NMR ($CDCl_3$, 100 MHz):δ166.5, 144.3, 134.8, 130.2, 128.9, 128.1, 118.3, 72.8, 31.8, 25.5, 23.9.
HRMS (ESI): calc. for $[(C_{15}H_{18}O_2)Na]$ $(M+Na)^+$ 253.1204, measured 253.1203.

(*E*)-1,2-Diphenylethene (12d)



Pale yellow solid; eluent (3% ethyl acetate in hexanes)
^{1}H NMR ($CDCl_3$, 400 MHz):δ7.59 (d, *J*= 8.0Hz, 4 H), 7.43 (t, *J*= 8.0Hz, 4 H), 7.33 (t, *J*= 8.0Hz, 2 H) 7.19 (s, 2 H).
^{13}C NMR ($CDCl_3$, 100 MHz):δ137.4, 128.2, 127.7, 126.8.
HRMS (ESI): calc. for $[(C_{14}H_{12})]^+$ $(M)^+$ 181.1017, measured 181.1018.

Table S1: Crystallographic Data for **3**-H_3, **5**, **6**.H_2O, **7**.$2H_2O$, **7a**, **7b**.2DMSO, **9**.$2H_2O$ and **10**

Compound	**3-H_3**	**5**	**6.H_2O**	**7.$2H_2O$**
Chemical formula	$C_9H_{24}N_3OP$	$C_{18}H_{36}N_3O_7PPd_3$	$C_{48}H_{86}N_6O_{15}P_2Pd_6$	$C_{31}H_{64}N_6O_{16}P_2Pd_6$
Formula weight	221.28	756.67	1687.57	1477.22
Temperature	296(2)K	100(2)K	100(2)K	100(2)K
Crystal system	Monoclinic	Orthorhombic	Orthorhombic	Monoclinic
Space group	Pnma	Cmc2(1)	C222(1)	C2/c
a (Å); α (°)	9.2210(4); 90	15.899(2); 90	15.31(2); 90	14.8019(16); 90
b (Å); β(°)	18.3933(9); 90	17.194(3); 90	21.694(2); 90	18.678(2); 90.015(4)
c (Å); γ (°)	8.1667(4); 90	9.5281(14); 90	19.245(3); 90	38.140(4); 90
V ($Å^3$); Z	1385.11 (11); 4	2604.8(7); 4	6391.8(14); 4	10545(2); 8
ρ (calc.) mg m^{-3}	1.071	1.929	1.754	1.861
μ(Mo K_α) mm^{-1}	0.179	2.151	1.764	2.125
$2\theta_{max}$ (°)	50	56	56	50
R(int)	0.00859	0.0262	0.1249	0.0792
Completeness to θ	99.6 %	99.8%	99.4%	99.5
Data / param.	1257 / 74	3303 / 164	7897 / 342	9288 / 567
GOF	1.021	1.292	1.001	1.108
R1 [F>4σ(F)]	0.0411	0.0181	0.0603	0.0474
wR2 (all data)	0.1230	0.0650	0.1355	0.0988
max. peak/hole (e.$Å^{-3}$)	0.237/ -0.199	0.482 / -0.524	1.407 /-1.131	1.073 / -1.017
Compound	**7a**	**7b.2DMSO**	**9.$2H_2O$**	**10**
Chemical formula	$C_{28}H_{60}N_6O_{12}P_2Pd_6$	$C_{30}H_{68}N_6O_{14}P_2Pd_6S_2$	$C_{42}H_{81}N_6O_7PPd_3$	$C_{33}H_{69}N_6O_7PPd_3$
Formula weight	1373.16	1501.36	1132.30	1012.11
Temperature	100(2)K	100(2)K	100(2)K	100(2)K
Crystal system	Monoclinic	Monoclinic	Trigonal	Monoclinic
Space group	P2(1)/c	C2/c	P-3c1	P2(1)/n
a (Å); α (°)	11.9132(6); 90	24.812(3); 90	17.0471(16); 90	11.6709(10); 90
b (Å); β(°)	32.9964(14); 115.837	9.7381(14); 120.349	17.0471(16); 90	16.7648(14); 98.24(2)
c (Å); γ (°)	12.2459(5); 90	23.628(3); 90	22.921(3); 120	21.993(2); 90
V ($Å^3$); Z	4332.6(3); 4	4926.7(11); 4	5768(10); 4	4258.7(6); 4
ρ (calc.) mg m^{-3}	2.105	2.024	1.304	1.579
μ(Mo K_α) mm^{-1}	2.571	2.355	0.996	1.339
$2\theta_{max}$ (°)	50	50	56	56
R(int)	0.0469	0.0463	0.1711	0.0671
Completeness to θ	98.9%	96.6%	99.7%	99.7
Data / param.	7577 / 506	4197 / 272	4800 / 181	10546 / 461
GOF	1.017	1.037	0.921	1.021
R1 [F>4σ(F)]	0.0350	0.0373	0.0652	0.0387
wR2 (all data)	0.0672	0.0887	0.2330	0.0847
max. peak/hole (e.$Å^{-3}$)	0.989 / -1.011	1.262 /-0.834	1.099 /-1.060	0.898 / -0.904

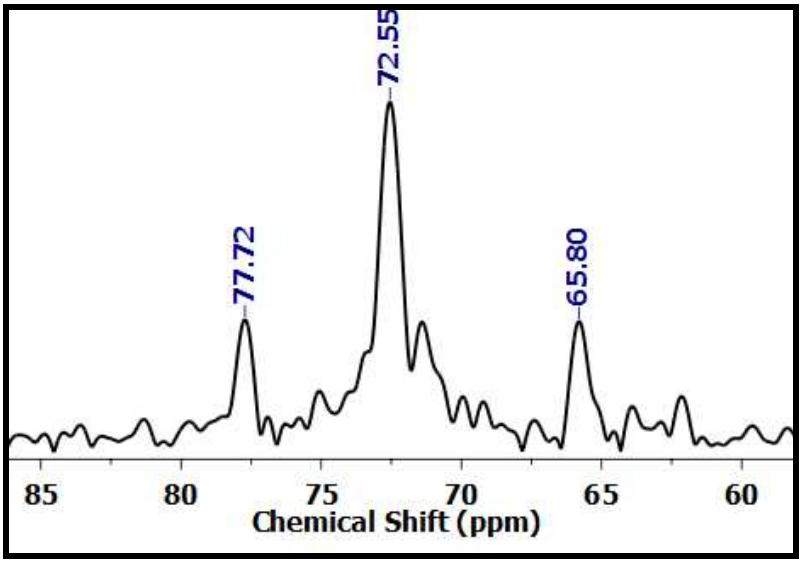


Figure S1: ^{31}P-NMR spectra of a reaction mixture of 3-H_3, $Pd(OAc)_2$ in methanol after 12 hours of stirring

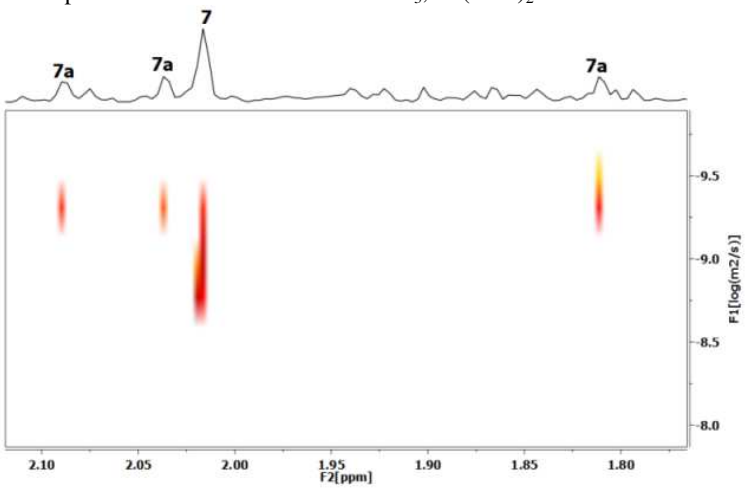


Figure S2: ^{1}H-2D- DOSY NMR spectra of a reaction mixture of 3-H_3, $Pd(OAc)_2$ in methanol after 15 hours of stirring

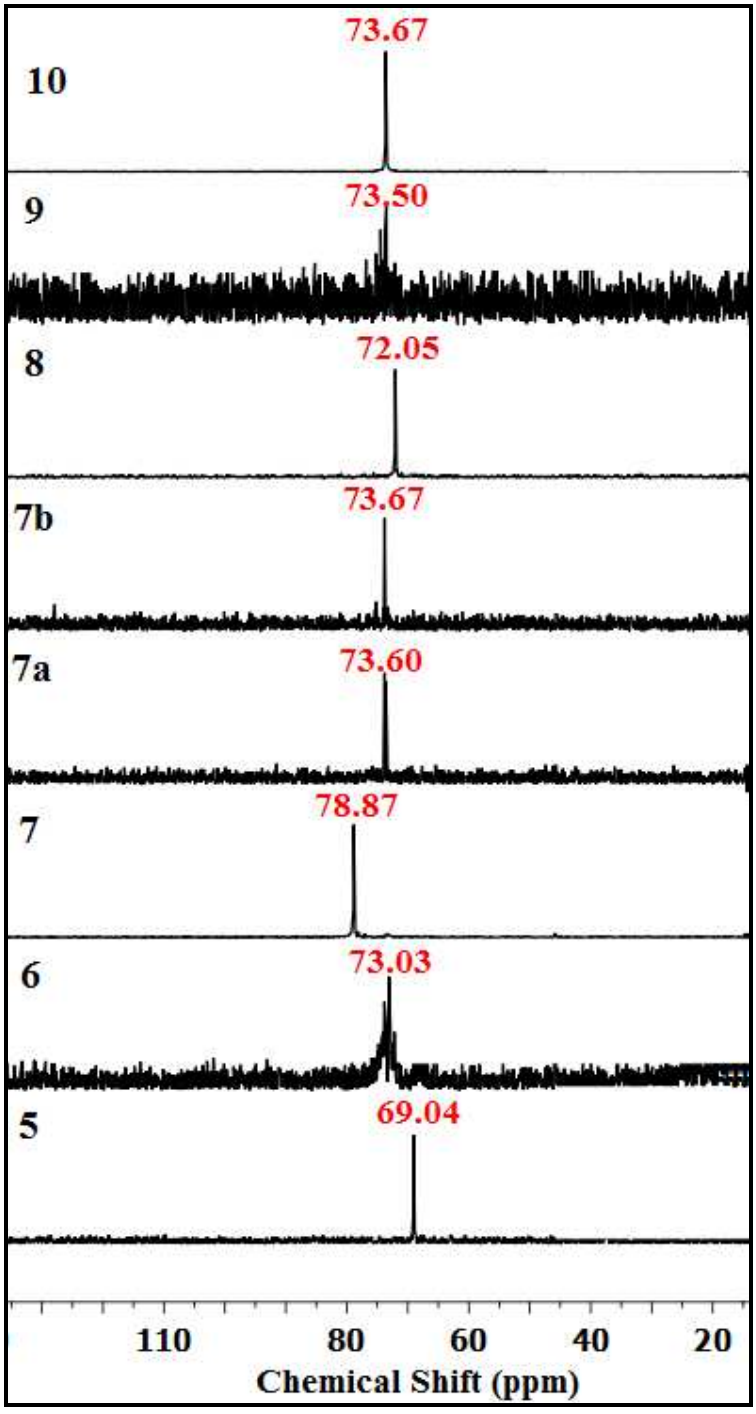


Figure S3: ^{31}P NMR spectra of **5, 6, 7, 7a, 7b, 8, 9, 10**

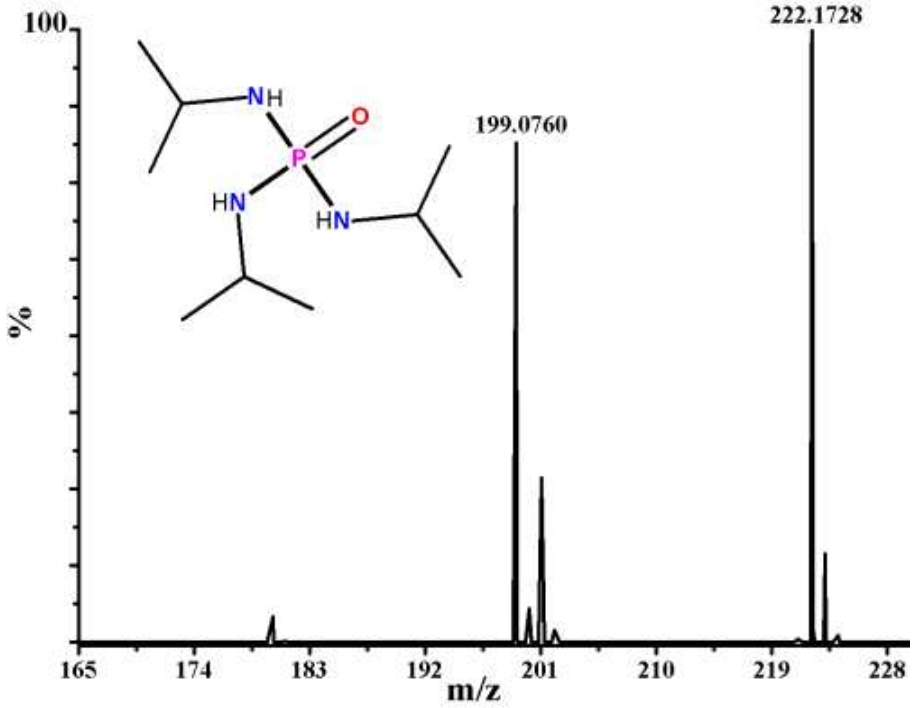


Figure S4: ESI (+) HRMS Mass spectra of **3**-H_3: m/z = 222.

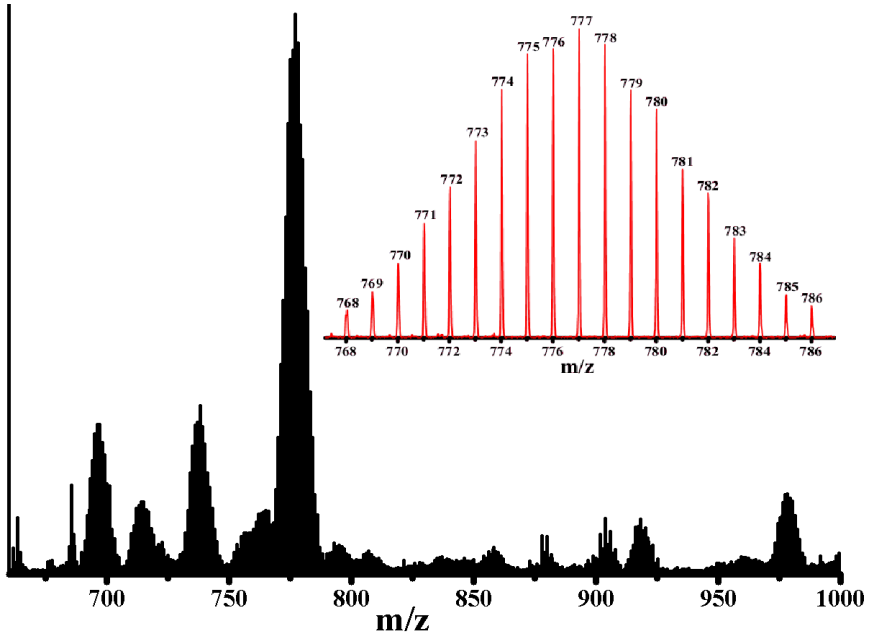


Figure S5: ESI (+) HRMS Mass spectra of **5**: m/z = 755; $[M+Na]^+$ = 778

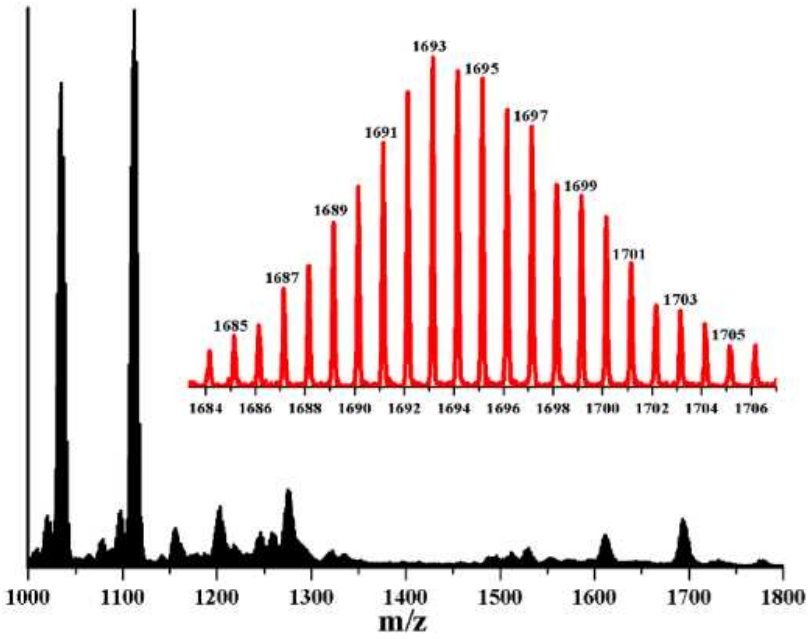


Figure S6: ESI (+)HRMS Mass spectra of **6**.H_2O: m/z = 1671; $[M+Na]^+$ = 1694.

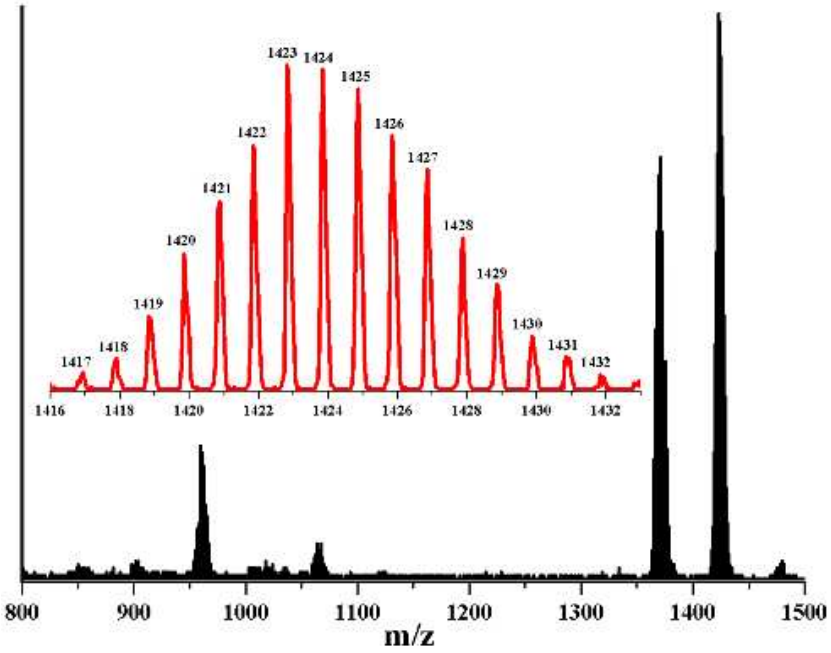


Figure S7: MALDI-TOF Mass spectra of **7**.$2H_2O$: m/z 1423.

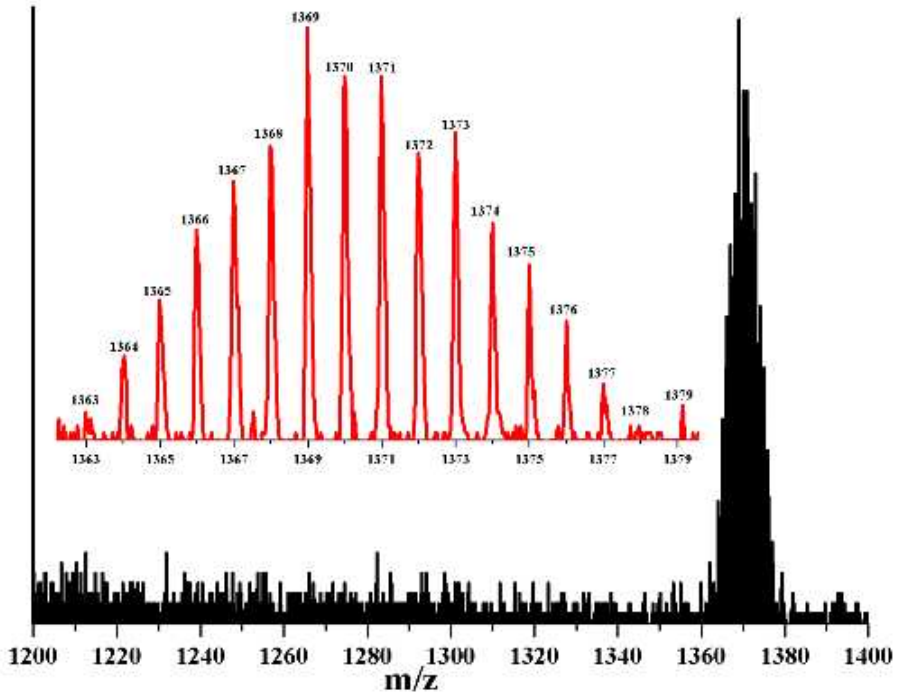


Figure S8: MALDI-TOF Mass spectra of **7a**: m/z = 1369.

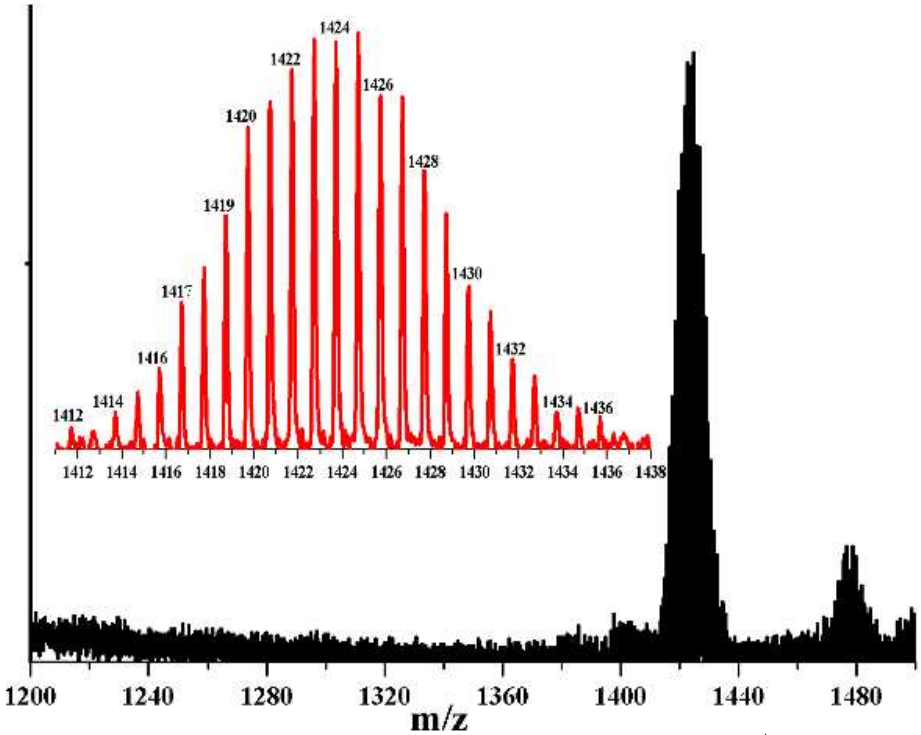


Figure S9: MALDI-TOF Mass spectra of **7b**.2DMSO: $[M+DMSO]^+$ = 1423.

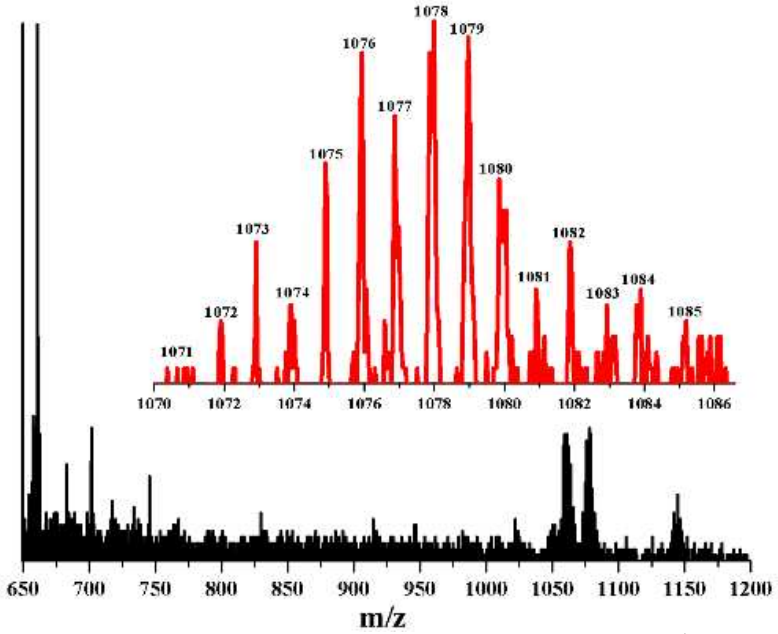


Figure S10: MALDI-TOF Mass spectra of **8**: m/z = 1054; $[M+Na]^+$ = 1077.

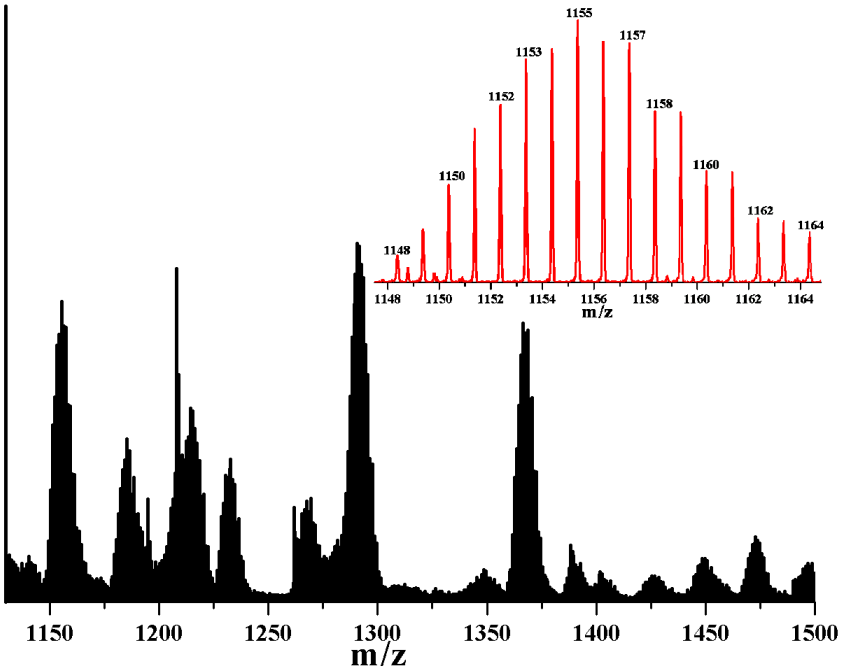


Figure S11: ESI (+) HRMS Mass spectra of **9**.$2H_2O$: m/z = 1133; $[M+Na]^+$ = 1154.

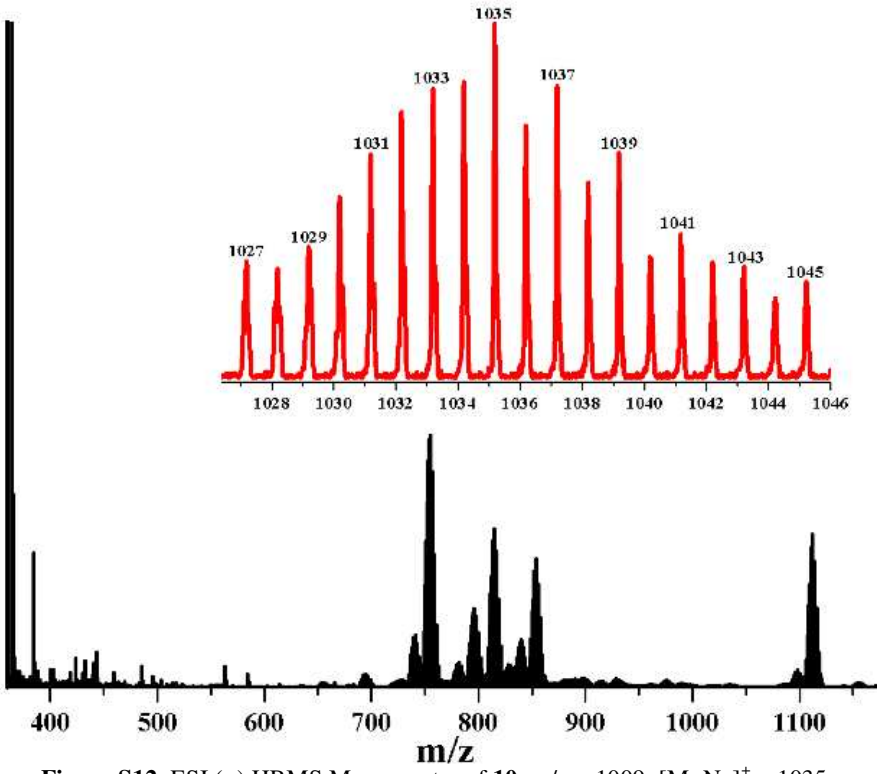


Figure S12: ESI (+) HRMS Mass spectra of **10**: m/z = 1009; $[M+Na]^+$ = 1035.

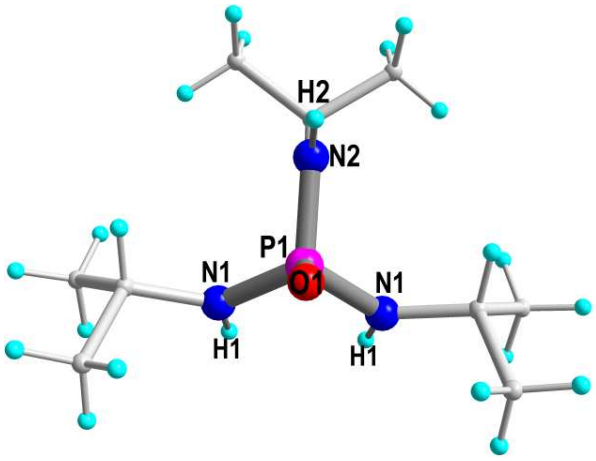


Figure S13: Crystal Structure of **3**.H_3.

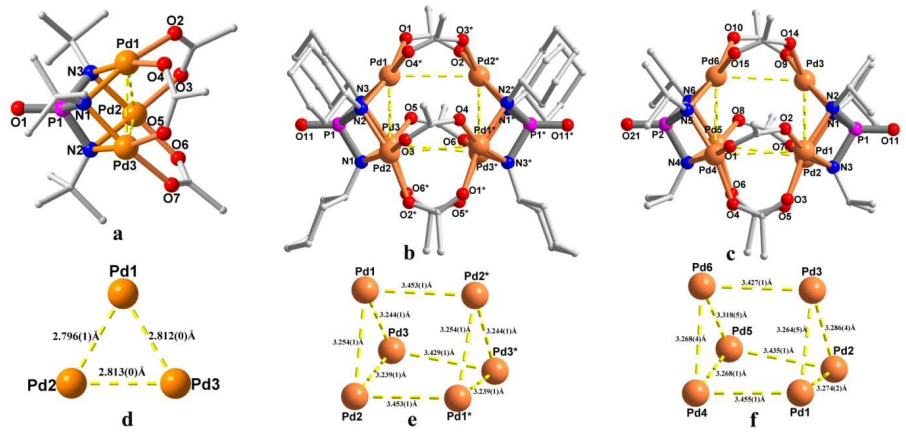


Figure S14: Crystal structures of **5, 6** and **7**

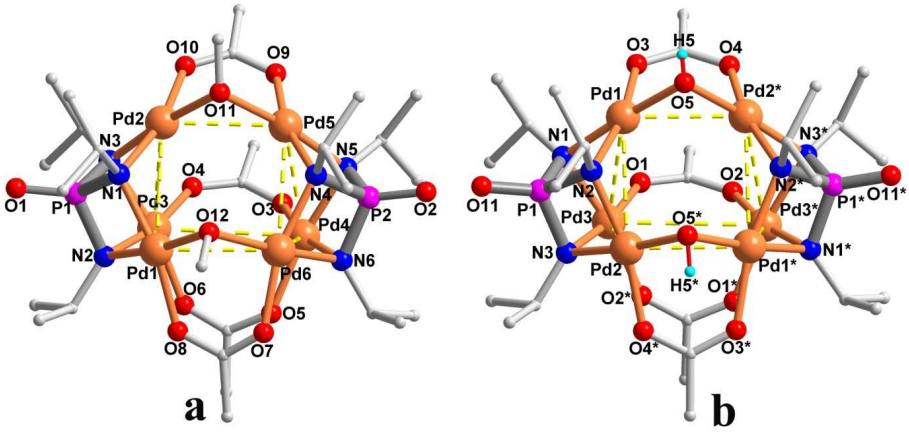


Figure S15: Core molecular view for the hexameric structures in **7a** and **7b**.2DMSO

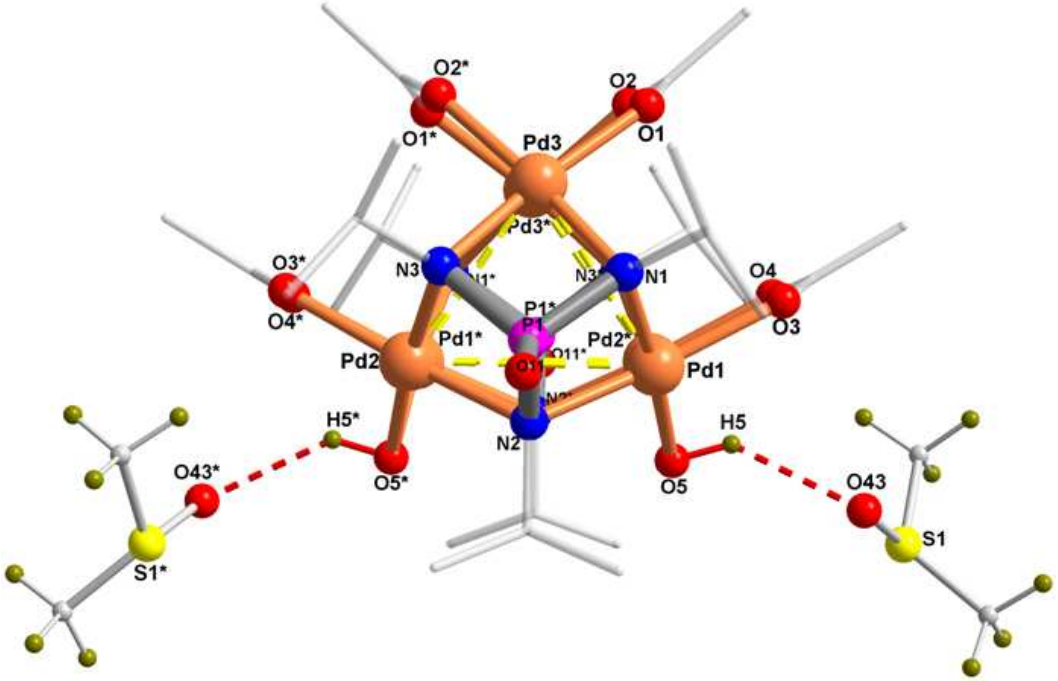


Figure S16: Eclipsed view of the structure of **7b**.2DMSO containing two H-bonded DMSO molecules

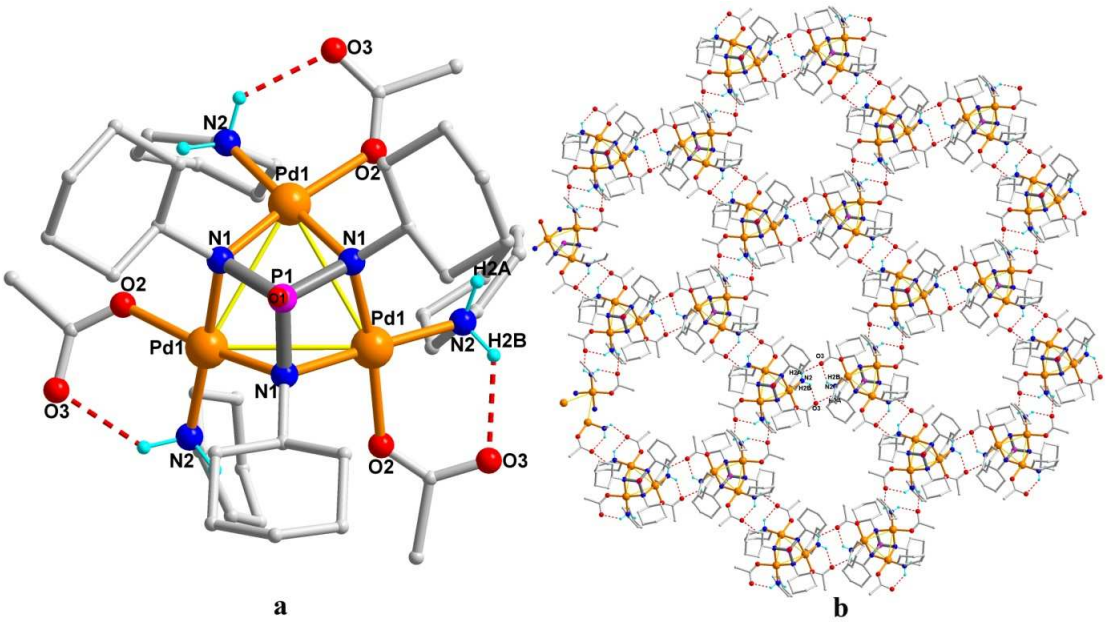


Figure S17: Crystal structure (a) and formation of a hexagonal 2D-structure (b) in **9**.2H_2O.

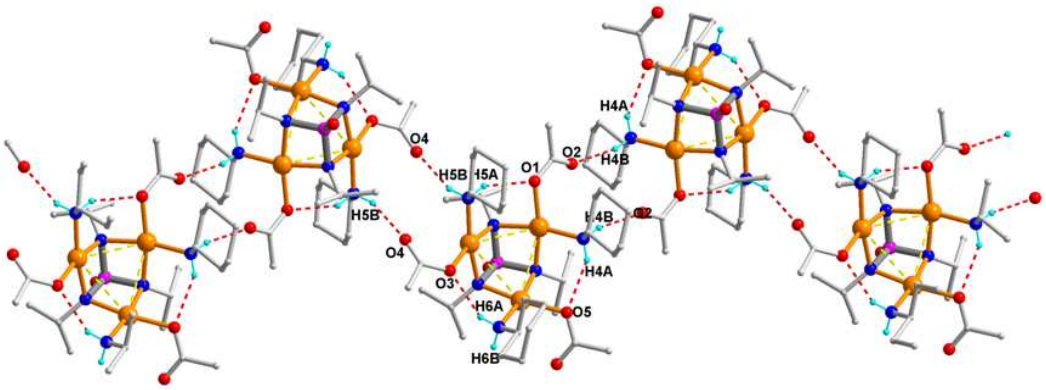


Figure S18: Formation of a 1D-chain structure in **10**

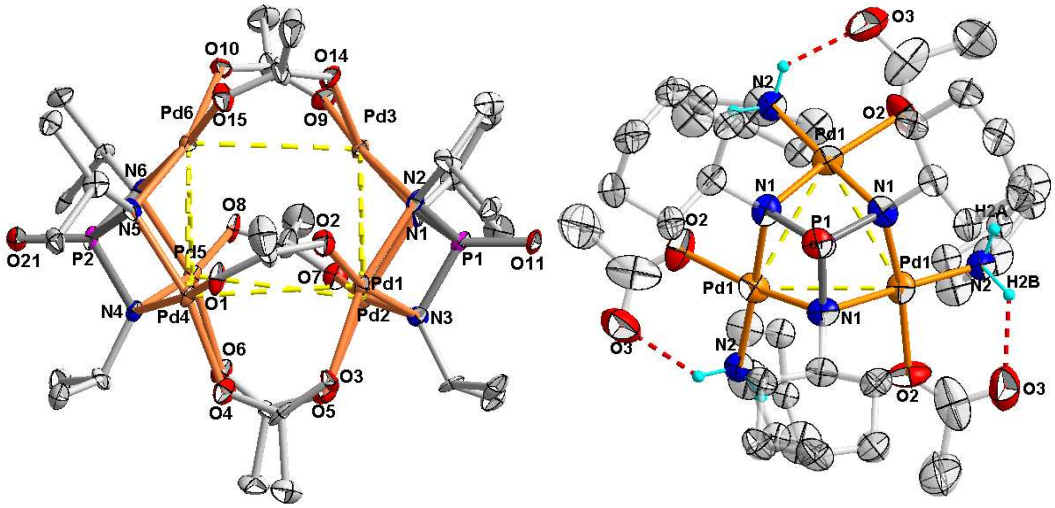


Figure S19: Thermal Ellipsoid plots at 50% probability for **7**.2H_2O and **9**.2H_2O

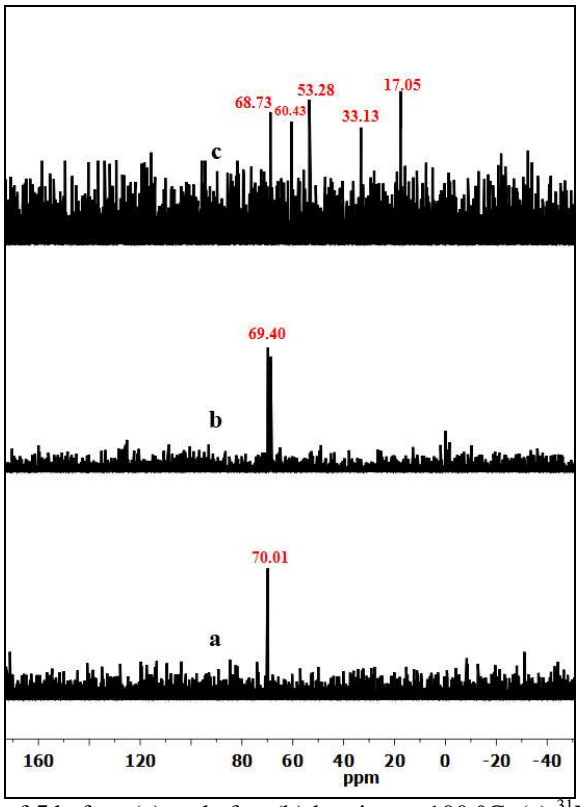


Figure S20: ^{31}P-NMR spectra of **5** before (a) and after (b) heating at 100 °C. (c) ^{31}P-NMR of the reaction mixture after 4 hours of refluxing under the conditions of the catalytic reactions with 11a as a substrate. The noisy baseline in this spectrum is due to the turbid nature of the reaction mixture and smaller amounts of the catalyst (10 mol %) present in it.

We have checked the ^{31}P-NMR spectra of the complex **5** in DMF before and after heating it to 100 °C. The ^{31}P-NMR did not show any significant change in peak position indicating the stability of the complex at elevated temperatures. However, under the conditions of the catalytic reactions (with 11a as a substrate) the complex undergoes various reactions as indicated by the ^{31}P-NMR of the reaction mixture (after 4 hours of refluxing) showing peaks at the regions of trianionic, dianionic, monoanionic and neutral ligands (please see the figure below) with the peak at δ 68.73 can be attributed to the presence of un-cleaved catalyst in the mixture. Based on this, we believe that these complexes (**5**, **6** or **7a**) act as active catalysts in the M-H type coupling reaction although they may degrade to certain extent during the course of the reaction.

Table S2: Selected bond-lengths and angles for **3**-H_3, **5**, **6**.H_2O**, 7**.2H_2O**, 7a, 7b**.2DMSO**, 9**.2H_2O and **10**

Compound	Bond lengths	Bond Angles
3-H_3	P(1)-O(1): 1.482(2) P(1)-N(2): 1.628(3) P(1)-N(1): 1.6319(17) P(1)-N(1)#1: 1.6319(17)	O(1)-P(1)-N(2): 105.61(13) O(1)-P(1)-N(1): 116.58(8) N(2)-P(1)-N(1): 108.98(9) O(1)-P(1)-N(1)#1: 116.57(8) N(2)-P(1)-N(1)#1: 108.98(9) N(1)-P(1)-N(1)#1: 99.88(12)
5	Pd(1)-O(3): 2.043(3) Pd(1)-O(4): 2.057(3) Pd(1)-N(2): 2.061(3) Pd(1)-N(1): 2.061(3) Pd(1)-P(1): 2.7356(12) Pd(1)-Pd(1)#1: 2.7958(6) Pd(1)-Pd(2): 2.8128(5) Pd(2)-N(1): 2.052(3) Pd(2)-N(1)#1: 2.052(3) Pd(2)-O(2)#1: 2.055(3) Pd(2)-O(2): 2.055(3) Pd(2)-P(1): 2.7296(13) Pd(2)-Pd(1)#1: 2.8128(5) P(1)-O(1): 1.468(4) P(1)-N(1): 1.696(3) P(1)-N(1)#1: 1.696(3) P(1)-N(2): 1.700(5) P(1)-Pd(1)#1: 2.7357(12) N(2)-Pd(1)#1: 2.061(3)	O(3)-Pd(1)-O(4): 84.70(12) O(3)-Pd(1)-N(2): 169.08(14) O(4)-Pd(1)-N(2): 99.34(16) O(3)-Pd(1)-N(1): 97.61(12) O(4)-Pd(1)-N(1): 167.99(12) N(2)-Pd(1)-N(1):76.37(16) O(3)-Pd(1)-P(1): 134.26(9) O(4)-Pd(1)-P(1): 135.54(9) N(2)-Pd(1)-P(1): 38.36(15) N(1)-Pd(1)-P(1): 38.25(9) O(3)-Pd(1)-Pd(1)#1: 124.05(9) O(4)-Pd(1)-Pd(1)#1: 82.52(9) N(2)-Pd(1)-Pd(1)#1: 47.29(7) N(1)-Pd(1)-Pd(1)#1: 86.46(8) P(1)-Pd(1)-Pd(1)#1: 59.270(16) O(3)-Pd(1)-Pd(2): 82.84(9) O(4)-Pd(1)-Pd(2): 122.44(9) N(2)-Pd(1)-Pd(2): 86.45(12) N(1)-Pd(1)-Pd(2): 46.73(8) P(1)-Pd(1)-Pd(2): 58.92(3) Pd(1)#1-Pd(1)-Pd(2): 60.201(8) N(1)-Pd(2)-N(1)#1: 76.51(17) N(1)-Pd(2)-O(2)#1: 168.17(14) N(1)#1-Pd(2)-O(2)#1: 97.58(12) N(1)-Pd(2)-O(2): 97.58(12) N(1)#1-Pd(2)-O(2): 168.17(14) O(2)#1-Pd(2)-O(2): 86.30(17) N(1)-Pd(2)-P(1): 38.35(8) N(1)#1-Pd(2)-P(1): 38.35(8) O(2)#1-Pd(2)-P(1): 134.20(8) O(2)-Pd(2)-P(1): 134.20(8)

		N(1)-Pd(2)-Pd(1): 46.99(9) N(1)#1-Pd(2)-Pd(1): 86.17(9) O(2)#1-Pd(2)-Pd(1): 123.16(11) O(2)-Pd(2)-Pd(1): 82.37(10) P(1)-Pd(2)-Pd(1): 59.13(2) N(1)-Pd(2)-Pd(1)#1: 86.17(9) N(1)#1-Pd(2)-Pd(1)#1: 46.99(9) O(2)#1-Pd(2)-Pd(1)#1: 82.37(10) O(2)-Pd(2)-Pd(1)#1: 123.16(11) P(1)-Pd(2)-Pd(1)#1: 59.13(2) Pd(1)-Pd(2)-Pd(1)#1: 59.600(17) O(1)-P(1)-N(1): 120.52(15) O(1)-P(1)-N(1)#1: 120.52(15) N(1)-P(1)-N(1)#1: 97.1(2) O(1)-P(1)-N(2): 118.9(2) N(1)-P(1)-N(2): 97.26(15) N(1)#1-P(1)-N(2): 97.26(15) O(1)-P(1)-Pd(2): 144.3(2) N(1)-P(1)-Pd(2): 48.67(11) N(1)#1-P(1)-Pd(2): 48.67(11) N(2)-P(1)-Pd(2): 96.81(13) O(1)-P(1)-Pd(1): 143.32(10) N(1)-P(1)-Pd(1): 48.80(12) N(1)#1-P(1)-Pd(1): 96.15(12) N(2)-P(1)-Pd(1): 48.80(9) Pd(2)-P(1)-Pd(1): 61.95(3) O(1)-P(1)-Pd(1)#1: 143.32(10) N(1)-P(1)-Pd(1)#1: 96.15(12) N(1)#1-P(1)-Pd(1)#1: 48.80(12) N(2)-P(1)-Pd(1)#1: 48.80(9) Pd(2)-P(1)-Pd(1)#1: 61.95(3) Pd(1)-P(1)-Pd(1)#1: 61.46(3) P(1)-N(1)-Pd(2): 92.99(13) P(1)-N(1)-Pd(1): 92.95(15) Pd(2)-N(1)-Pd(1): 86.28(12) P(1)-N(2)-Pd(1): 92.84(17) C(21)-N(2)-Pd(1)#1: 126.5(2) P(1)-N(2)-Pd(1)#1: 92.84(17) Pd(1)-N(2)-Pd(1)#1: 85.43(14)

6.H_2O	Pd(1)-N(2): 2.014(7) Pd(1)-N(3): 2.046(8) Pd(1)-O(4)#1: 2.048(7) Pd(1)-O(1): 2.059(7) Pd(1)-P(1): 2.719(3) Pd(1)-Pd(3): 3.2442(9) Pd(1)-Pd(2): 3.2539(10) Pd(2)-N(1): 2.028(7) Pd(2)-N(2): 2.030(7) Pd(2)-O(2)#1: 2.053(7) Pd(2)-O(3): 2.060(8) Pd(2)-P(1): 2.720(3) Pd(2)-Pd(3): 3.2386(9) Pd(3)-N(3): 2.019(8) Pd(3)-N(1): 2.030(7) Pd(3)-O(5): 2.041(7) Pd(3)-O(6)#1: 2.071(7) Pd(3)-P(1): 2.712(3) P(1)-O(11): 1.424(7) P(1)-N(1): 1.685(7) P(1)-N(2): 1.692(8) P(1)-N(3): 1.699(8)	N(2)-Pd(1)-N(3): 76.8(3) N(2)-Pd(1)-O(4)#1: 91.2(3) N(3)-Pd(1)-O(4)#1: 166.7(3) N(2)-Pd(1)-O(1): 164.7(3) N(3)-Pd(1)-O(1): 93.8(3) O(4)#1-Pd(1)-O(1): 96.6(3) N(2)-Pd(1)-P(1): 38.4(2) N(3)-Pd(1)-P(1): 38.6(2) O(4)#1-Pd(1)-P(1): 128.8(2) O(1)-Pd(1)-P(1): 130.4(2) N(2)-Pd(1)-Pd(3): 79.27(19) N(3)-Pd(1)-Pd(3): 36.8(2) O(4)#1-Pd(1)-Pd(3): 147.1(2) O(1)-Pd(1)-Pd(3): 100.6(2) P(1)-Pd(1)-Pd(3): 53.22(5) N(2)-Pd(1)-Pd(2): 36.6(2) N(3)-Pd(1)-Pd(2): 79.7(2) O(4)#1-Pd(1)-Pd(2): 94.2(2) O(1)-Pd(1)-Pd(2): 154.3(2) P(1)-Pd(1)-Pd(2): 53.27(6) Pd(3)-Pd(1)-Pd(2): 59.79(2) N(1)-Pd(2)-N(2): 76.4(3) N(1)-Pd(2)-O(2)#1: 91.9(3) N(2)-Pd(2)-O(2)#1: 166.9(3) N(1)-Pd(2)-O(3): 164.4(3) N(2)-Pd(2)-O(3): 93.2(3) O(2)#1-Pd(2)-O(3): 97.0(3) N(1)-Pd(2)-P(1): 38.2(2) N(2)-Pd(2)-P(1): 38.4(2) O(2)#1-Pd(2)-P(1): 129.3(2) O(3)-Pd(2)-P(1): 129.7(2) N(1)-Pd(2)-Pd(3): 37.1(2) N(2)-Pd(2)-Pd(3): 79.2(2) O(2)#1-Pd(2)-Pd(3): 95.0(2) O(3)-Pd(2)-Pd(3): 153.1(2) P(1)-Pd(2)-Pd(3): 53.28(6) N(1)-Pd(2)-Pd(1): 79.54(19) N(2)-Pd(2)-Pd(1): 36.2(2) O(2)#1-Pd(2)-Pd(1): 147.9(2) O(3)-Pd(2)-Pd(1): 99.1(2)

		P(1)-Pd(2)-Pd(1): 53.24(6) Pd(3)-Pd(2)-Pd(1): 59.96(2) N(3)-Pd(3)-N(1): 77.0(3) N(3)-Pd(3)-O(5): 90.7(3) N(1)-Pd(3)-O(5): 166.7(3) N(3)-Pd(3)-O(6)#1: 163.5(3) N(1)-Pd(3)-O(6)#1: 93.8(3) O(5)-Pd(3)-O(6)#1: 97.0(3) N(3)-Pd(3)-P(1): 38.7(2) N(1)-Pd(3)-P(1): 38.3(2) O(5)-Pd(3)-P(1): 128.9(2) O(6)#1-Pd(3)-P(1): 129.95(19) N(3)-Pd(3)-Pd(2): 80.4(2) N(1)-Pd(3)-Pd(2): 37.0(2) O(5)-Pd(3)-Pd(2): 146.3(2) O(6)#1-Pd(3)-Pd(2): 100.48(19) P(1)-Pd(3)-Pd(2): 53.52(6) N(3)-Pd(3)-Pd(1): 37.4(2) N(1)-Pd(3)-Pd(1): 79.8(2) O(5)-Pd(3)-Pd(1): 93.5(2) O(6)#1-Pd(3)-Pd(1): 155.1(2) P(1)-Pd(3)-Pd(1): 53.42(5) Pd(2)-Pd(3)-Pd(1): 60.26(2) O(11)-P(1)-N(1): 120.4(4) O(11)-P(1)-N(2): 122.3(4) N(1)-P(1)-N(2): 96.0(4) O(11)-P(1)-N(3): 119.8(4) N(1)-P(1)-N(3): 96.2(3) N(2)-P(1)-N(3): 96.1(4) O(11)-P(1)-Pd(3): 135.6(3) N(1)-P(1)-Pd(3): 48.4(2) N(2)-P(1)-Pd(3): 102.1(3) N(3)-P(1)-Pd(3): 48.0(3) O(11)-P(1)-Pd(1): 136.5(3) N(1)-P(1)-Pd(1): 103.1(3) N(2)-P(1)-Pd(1): 47.6(3) N(3)-P(1)-Pd(1): 48.8(3) Pd(3)-P(1)-Pd(1): 73.36(7) O(11)-P(1)-Pd(2): 137.0(3) N(1)-P(1)-Pd(2): 48.1(3)

		N(2)-P(1)-Pd(2): 48.1(3) N(3)-P(1)-Pd(2): 103.1(3) Pd(3)-P(1)-Pd(2): 73.20(6) Pd(1)-P(1)-Pd(2): 73.49(6) P(1)-N(1)-Pd(2): 93.8(3) P(1)-N(1)-Pd(3): 93.3(3) Pd(2)-N(1)-Pd(3): 105.9(3)
7.2H_2O	Pd(1)-N(2): 2.028(9) Pd(1)-O(2): 2.029(7) Pd(1)-O(3): 2.039(7) Pd(1)-N(3): 2.043(9) Pd(1)-P(1): 2.710(3) Pd(2)-N(3): 2.022(8) Pd(2)-N(1): 2.034(9) Pd(2)-O(5): 2.045(7) Pd(2)-O(7): 2.051(7) Pd(2)-P(1): 2.738(3) Pd(3)-O(9): 2.042(6) Pd(3)-N(2): 2.044(8) Pd(3)-N(1): 2.051(7) Pd(3)-O(14): 2.060(7) Pd(3)-P(1): 2.717(2) Pd(4)-O(4): 2.024(7) Pd(4)-N(5): 2.042(8) Pd(4)-N(4): 2.051(8) Pd(4)-O(1): 2.073(7) Pd(4)-P(2): 2.724(2) Pd(5)-N(4): 2.028(8) Pd(5)-O(8): 2.051(7) Pd(5)-N(6): 2.057(7) Pd(5)-O(6): 2.060(7) Pd(5)-P(2): 2.724(2) Pd(6)-N(5): 2.021(8) Pd(6)-N(6): 2.027(8) Pd(6)-O(15): 2.035(7) Pd(6)-O(10): 2.045(7) Pd(6)-P(2): 2.713(3) P(1)-O(11): 1.452(6) P(1)-N(1): 1.701(9)	O(2)-Pd(1)-O(3): 95.1(3) N(2)-Pd(1)-N(3): 77.8(3) O(2)-Pd(1)-N(3): 167.6(3) O(3)-Pd(1)-N(3): 93.1(3) N(2)-Pd(1)-P(1): 39.0(2) O(2)-Pd(1)-P(1): 130.3(3) O(3)-Pd(1)-P(1): 130.37(19) N(3)-Pd(1)-P(1): 38.9(2) N(3)-Pd(2)-N(1): 76.6(3) N(3)-Pd(2)-O(5): 92.3(3) N(1)-Pd(2)-O(5): 168.2(3) N(3)-Pd(2)-O(7): 163.6(3) N(1)-Pd(2)-O(7): 94.9(3) O(5)-Pd(2)-O(7): 94.9(3) N(3)-Pd(2)-P(1): 38.4(2) N(1)-Pd(2)-P(1): 38.3(2) O(5)-Pd(2)-P(1): 130.3(2) O(7)-Pd(2)-P(1): 130.9(2) O(9)-Pd(3)-N(2): 167.3(3) O(9)-Pd(3)-N(1): 91.6(3) N(2)-Pd(3)-N(1): 77.5(3) O(9)-Pd(3)-O(14): 95.8(3) N(2)-Pd(3)-O(14): 93.2(3) N(1)-Pd(3)-O(14): 163.2(3) O(9)-Pd(3)-P(1): 129.5(2) N(2)-Pd(3)-P(1): 38.9(2) N(1)-Pd(3)-P(1): 38.7(2) O(14)-Pd(3)-P(1): 129.6(2) O(4)-Pd(4)-N(5): 165.8(3) O(4)-Pd(4)-N(4): 89.7(3) N(5)-Pd(4)-N(4): 77.3(3) O(4)-Pd(4)-O(1): 96.4(3)

	P(1)-N(3): 1.704(8) P(1)-N(2): 1.709(7) P(2)-O(21): 1.470(6) P(2)-N(6): 1.695(9) P(2)-N(4): 1.702(7) P(2)-N(5): 1.707(8)	N(5)-Pd(4)-O(1): 95.0(3) N(4)-Pd(4)-O(1): 165.1(3) O(4)-Pd(4)-P(2): 127.8(2) N(5)-Pd(4)-P(2): 38.8(2) N(4)-Pd(4)-P(2): 38.61(19) O(1)-Pd(4)-P(2): 131.7(2) N(4)-Pd(5)-O(8): 168.2(3) N(4)-Pd(5)-N(6): 76.8(3) O(8)-Pd(5)-N(6): 93.9(3) N(4)-Pd(5)-O(6): 92.3(3) O(8)-Pd(5)-O(6): 95.0(3) N(6)-Pd(5)-O(6): 164.0(3) N(4)-Pd(5)-P(2): 38.59(19) O(8)-Pd(5)-P(2): 131.32(19) N(6)-Pd(5)-P(2): 38.4(2) O(6)-Pd(5)-P(2): 129.0(2) N(5)-Pd(6)-N(6): 77.4(3) N(5)-Pd(6)-O(15): 92.4(3) N(6)-Pd(6)-O(15): 168.3(3) N(5)-Pd(6)-O(10): 165.2(3) N(6)-Pd(6)-O(10): 94.1(3) O(15)-Pd(6)-O(10): 94.6(3) N(5)-Pd(6)-P(2): 38.9(2) N(6)-Pd(6)-P(2): 38.6(2) O(15)-Pd(6)-P(2): 130.6(2) O(10)-Pd(6)-P(2): 130.7(2) O(11)-P(1)-N(1): 120.3(4) O(11)-P(1)-N(3): 119.7(4) N(1)-P(1)-N(3): 95.1(4) O(11)-P(1)-N(2): 121.4(4) N(1)-P(1)-N(2): 97.5(3) N(3)-P(1)-N(2): 97.0(4) O(11)-P(1)-Pd(1): 136.2(3) N(1)-P(1)-Pd(1): 103.4(3) N(3)-P(1)-Pd(1): 48.9(3) N(2)-P(1)-Pd(1): 48.4(3) O(11)-P(1)-Pd(3): 137.0(3) N(1)-P(1)-Pd(3): 49.0(3) N(3)-P(1)-Pd(3): 103.3(2) N(2)-P(1)-Pd(3): 48.7(3)

		Pd(1)-P(1)-Pd(3): 73.97(6) O(11)-P(1)-Pd(2): 134.7(3) N(1)-P(1)-Pd(2): 47.8(3) N(3)-P(1)-Pd(2): 47.4(3) N(2)-P(1)-Pd(2): 103.8(3) Pd(1)-P(1)-Pd(2): 73.88(7) Pd(3)-P(1)-Pd(2): 74.09(6) O(21)-P(2)-N(6): 121.4(4) O(21)-P(2)-N(4): 119.1(4) N(6)-P(2)-N(4): 96.7(4) O(21)-P(2)-N(5): 120.7(4) N(6)-P(2)-N(5): 96.1(4) N(4)-P(2)-N(5): 97.1(4) O(21)-P(2)-Pd(6): 136.4(3) N(6)-P(2)-Pd(6): 48.3(3) N(4)-P(2)-Pd(6): 104.5(3) N(5)-P(2)-Pd(6): 48.1(3) O(21)-P(2)-Pd(5): 135.3(3) N(6)-P(2)-Pd(5): 49.0(3) N(4)-P(2)-Pd(5): 48.0(3) N(5)-P(2)-Pd(5): 104.1(3) Pd(6)-P(2)-Pd(5): 75.22(6) O(21)-P(2)-Pd(4): 135.7(3) N(6)-P(2)-Pd(4): 102.8(3) N(4)-P(2)-Pd(4): 48.8(3) N(5)-P(2)-Pd(4): 48.5(3) Pd(6)-P(2)-Pd(4): 73.88(6) Pd(5)-P(2)-Pd(4): 73.72(6) P(1)-N(1)-Pd(2): 93.8(4) P(1)-N(1)-Pd(3): 92.3(4) Pd(2)-N(1)-Pd(3): 107.1(4) P(1)-N(2)-Pd(1): 92.6(4) P(1)-N(2)-Pd(3): 92.3(3) Pd(1)-N(2)-Pd(3): 106.6(4) P(1)-N(3)-Pd(2): 94.2(4) P(1)-N(3)-Pd(1): 92.2(4) Pd(2)-N(3)-Pd(1): 107.3(3) P(2)-N(4)-Pd(5): 93.4(4) P(2)-N(4)-Pd(4): 92.6(4) Pd(5)-N(4)-Pd(4): 106.5(3)

		P(2)-N(5)-Pd(6): 93.0(4) P(2)-N(5)-Pd(4): 92.8(4) Pd(6)-N(5)-Pd(4): 107.1(3) P(2)-N(6)-Pd(5): 92.6(4) Pd(6)-N(6)-Pd(5): 108.6(3)
7a	Pd(1)-N(2): 2.032(4) Pd(1)-N(1): 2.048(5) Pd(1)-O(8): 2.064(4) Pd(1)-O(12): 2.119(4) Pd(1)-P(1): 2.7316(16) Pd(1)-Pd(6): 3.0144(6) Pd(1)-Pd(3): 3.1161(6) Pd(2)-N(3): 2.018(4) Pd(2)-N(1): 2.051(4) Pd(2)-O(10): 2.059(4) Pd(2)-O(11): 2.115(4) Pd(2)-P(1): 2.7299(14) Pd(2)-Pd(5): 3.0213(6) Pd(2)-Pd(3): 3.1321(6) Pd(3)-N(2): 2.035(4) Pd(3)-N(3): 2.042(4) Pd(3)-O(6): 2.052(4) Pd(3)-O(4): 2.055(4) Pd(3)-P(1): 2.7250(14) Pd(4)-N(5): 2.040(4) Pd(4)-N(6): 2.041(5) Pd(4)-O(3): 2.047(4) Pd(4)-O(5): 2.052(4) Pd(4)-P(2): 2.7232(16) Pd(4)-Pd(6): 3.0748(6) Pd(4)-Pd(5): 3.1133(6) Pd(5)-N(5): 2.038(4) Pd(5)-N(4): 2.041(5) Pd(5)-O(9): 2.048(4) Pd(5)-O(11): 2.105(3) Pd(5)-P(2): 2.7269(17) Pd(6)-N(6): 2.019(4) Pd(6)-O(7): 2.044(4) Pd(6)-N(4): 2.046(4) Pd(6)-O(12): 2.092(4) Pd(6)-P(2): 2.7328(15)	N(2)-Pd(1)-N(1): 76.43(17) N(2)-Pd(1)-O(8): 90.25(17) N(1)-Pd(1)-O(8): 166.00(17) N(2)-Pd(1)-O(12): 173.07(16) N(1)-Pd(1)-O(12): 96.95(16) O(8)-Pd(1)-O(12): 96.50(16) N(2)-Pd(1)-P(1): 38.32(12) N(1)-Pd(1)-P(1): 38.36(13) O(8)-Pd(1)-P(1): 127.91(12) O(12)-Pd(1)-P(1): 135.22(11) N(2)-Pd(1)-Pd(6): 137.41(11) N(1)-Pd(1)-Pd(6): 116.62(12) O(8)-Pd(1)-Pd(6): 76.17(11) O(12)-Pd(1)-Pd(6): 43.93(10) P(1)-Pd(1)-Pd(6): 142.09(3) N(2)-Pd(1)-Pd(3): 40.02(11) N(1)-Pd(1)-Pd(3): 78.72(12) O(8)-Pd(1)-Pd(3): 93.91(12) O(12)-Pd(1)-Pd(3): 137.34(10) P(1)-Pd(1)-Pd(3): 55.08(3) Pd(6)-Pd(1)-Pd(3): 99.980(16) N(3)-Pd(2)-N(1): 76.09(17) N(3)-Pd(2)-O(10): 93.14(16) N(1)-Pd(2)-O(10): 165.06(18) N(3)-Pd(2)-O(11): 172.56(17) N(1)-Pd(2)-O(11): 98.96(15) O(10)-Pd(2)-O(11): 92.69(14) N(3)-Pd(2)-P(1): 38.00(12) N(1)-Pd(2)-P(1): 38.40(13) O(10)-Pd(2)-P(1): 129.23(12) O(11)-Pd(2)-P(1): 137.36(10) N(3)-Pd(2)-Pd(5): 132.91(12) N(1)-Pd(2)-Pd(5): 115.77(14) O(10)-Pd(2)-Pd(5): 79.14(12)

	P(1)-O(1): 1.463(4) P(1)-N(3): 1.686(4) P(1)-N(2): 1.697(4) P(1)-N(1): 1.698(5) P(2)-O(2): 1.468(4) P(2)-N(6): 1.684(4) P(2)-N(5): 1.701(5) P(2)-N(4): 1.705(5)	O(11)-Pd(2)-Pd(5): 44.15(9) P(1)-Pd(2)-Pd(5): 138.73(4) N(3)-Pd(2)-Pd(3): 39.81(13) N(1)-Pd(2)-Pd(3): 78.28(11) O(10)-Pd(2)-Pd(3): 100.20(11) O(11)-Pd(2)-Pd(3): 134.24(10) P(1)-Pd(2)-Pd(3): 54.88(3) Pd(5)-Pd(2)-Pd(3): 95.458(16) N(2)-Pd(3)-N(3): 76.56(17) N(2)-Pd(3)-O(6): 93.99(16) N(3)-Pd(3)-O(6): 167.90(16) N(2)-Pd(3)-O(4): 167.71(17) N(3)-Pd(3)-O(4): 91.88(16) O(6)-Pd(3)-O(4): 96.88(15) N(2)-Pd(3)-P(1): 38.45(12) N(3)-Pd(3)-P(1): 38.15(12) O(6)-Pd(3)-P(1): 132.23(11) O(4)-Pd(3)-P(1): 130.00(12) N(2)-Pd(3)-Pd(1): 39.96(12) N(3)-Pd(3)-Pd(1): 83.92(12) O(6)-Pd(3)-Pd(1): 93.70(12) O(4)-Pd(3)-Pd(1): 144.15(11) P(1)-Pd(3)-Pd(1): 55.27(3) N(2)-Pd(3)-Pd(2): 84.30(11) N(3)-Pd(3)-Pd(2): 39.25(12) O(6)-Pd(3)-Pd(2): 148.64(12) O(4)-Pd(3)-Pd(2): 89.35(10) P(1)-Pd(3)-Pd(2): 55.03(3) Pd(1)-Pd(3)-Pd(2): 65.235(14) N(5)-Pd(4)-N(6): 76.56(18) N(5)-Pd(4)-O(3): 93.03(18) N(6)-Pd(4)-O(3): 166.08(16) N(5)-Pd(4)-O(5): 167.72(19) N(6)-Pd(4)-O(5): 91.84(18) O(3)-Pd(4)-O(5): 97.72(17) N(5)-Pd(4)-P(2): 38.59(14) N(6)-Pd(4)-P(2): 38.11(12) O(3)-Pd(4)-P(2): 131.42(12) O(5)-Pd(4)-P(2): 129.95(13) N(5)-Pd(4)-Pd(6): 85.74(13)

		N(6)-Pd(4)-Pd(6): 40.51(12) O(3)-Pd(4)-Pd(6): 149.39(11) O(5)-Pd(4)-Pd(6): 87.99(11) P(2)-Pd(4)-Pd(6): 55.85(3) N(5)-Pd(4)-Pd(5): 40.19(12) N(6)-Pd(4)-Pd(5): 84.70(12) O(3)-Pd(4)-Pd(5): 93.32(12) O(5)-Pd(4)-Pd(5): 144.03(11) P(2)-Pd(4)-Pd(5): 55.22(4) Pd(6)-Pd(4)-Pd(5): 66.438(14) N(5)-Pd(5)-N(4): 76.72(18) N(5)-Pd(5)-O(9): 92.19(17) N(4)-Pd(5)-O(9): 165.36(17) N(5)-Pd(5)-O(11): 171.71(16) N(4)-Pd(5)-O(11): 97.07(16) O(9)-Pd(5)-O(11): 94.81(15) N(5)-Pd(5)-P(2): 38.52(14) N(4)-Pd(5)-P(2): 38.63(13) O(9)-Pd(5)-P(2): 128.74(12) O(11)-Pd(5)-P(2): 135.68(11) N(5)-Pd(5)-Pd(2): 133.57(13) N(4)-Pd(5)-Pd(2): 116.50(12) O(9)-Pd(5)-Pd(2): 78.07(12) O(11)-Pd(5)-Pd(2): 44.41(11) P(2)-Pd(5)-Pd(2): 140.62(3) N(5)-Pd(5)-Pd(4): 40.25(12) N(4)-Pd(5)-Pd(4): 77.65(12) O(9)-Pd(5)-Pd(4): 100.16(11) O(11)-Pd(5)-Pd(4): 133.52(10) P(2)-Pd(5)-Pd(4): 55.11(3) Pd(2)-Pd(5)-Pd(4): 96.392(16) N(6)-Pd(6)-O(7): 91.39(17) N(6)-Pd(6)-N(4): 76.12(17) O(7)-Pd(6)-N(4): 163.79(18) N(6)-Pd(6)-O(12): 172.48(18) O(7)-Pd(6)-O(12): 93.21(15) N(4)-Pd(6)-O(12): 100.34(16) N(6)-Pd(6)-P(2): 37.88(12) O(7)-Pd(6)-P(2): 127.47(12) N(4)-Pd(6)-P(2): 38.53(13)

		O(12)-Pd(6)-P(2): 138.86(11) N(6)-Pd(6)-Pd(1): 130.74(13) O(7)-Pd(6)-Pd(1): 80.25(12) N(4)-Pd(6)-Pd(1): 115.70(14) O(12)-Pd(6)-Pd(1): 44.65(11) P(2)-Pd(6)-Pd(1): 137.17(4) N(6)-Pd(6)-Pd(4): 41.03(14) O(7)-Pd(6)-Pd(4): 98.94(11) N(4)-Pd(6)-Pd(4): 78.53(12) O(12)-Pd(6)-Pd(4): 132.10(12) P(2)-Pd(6)-Pd(4): 55.55(3) Pd(1)-Pd(6)-Pd(4): 92.125(17) O(1)-P(1)-N(3): 120.8(3) O(1)-P(1)-N(2): 120.6(2) N(3)-P(1)-N(2): 96.6(2) O(1)-P(1)-N(1): 121.1(2) N(3)-P(1)-N(1): 95.7(2) N(2)-P(1)-N(1): 96.0(2) O(1)-P(1)-Pd(3): 142.06(17) N(3)-P(1)-Pd(3): 48.43(15) N(2)-P(1)-Pd(3): 48.19(14) N(1)-P(1)-Pd(3): 96.83(15) O(1)-P(1)-Pd(2): 134.70(17) N(3)-P(1)-Pd(2): 47.48(15) N(2)-P(1)-Pd(2): 104.69(15) N(1)-P(1)-Pd(2): 48.62(14) Pd(3)-P(1)-Pd(2): 70.08(3) O(1)-P(1)-Pd(1): 135.24(18) N(3)-P(1)-Pd(1): 104.00(17) N(2)-P(1)-Pd(1): 47.94(15) N(1)-P(1)-Pd(1): 48.47(16) Pd(3)-P(1)-Pd(1): 69.65(4) Pd(2)-P(1)-Pd(1): 76.15(4) O(2)-P(2)-N(6): 120.5(3) O(2)-P(2)-N(5): 121.1(2) N(6)-P(2)-N(5): 96.6(2) O(2)-P(2)-N(4): 121.1(2) N(6)-P(2)-N(4): 95.4(2) N(5)-P(2)-N(4): 96.0(2) O(2)-P(2)-Pd(4): 143.89(19)

		N(6)-P(2)-Pd(4): 48.42(17) N(5)-P(2)-Pd(4): 48.42(14) N(4)-P(2)-Pd(4): 95.05(16) O(2)-P(2)-Pd(5): 134.29(18) N(6)-P(2)-Pd(5): 105.24(18) N(5)-P(2)-Pd(5): 48.25(15) N(4)-P(2)-Pd(5): 48.36(17) Pd(4)-P(2)-Pd(5): 69.67(4) O(2)-P(2)-Pd(6): 134.43(19) N(6)-P(2)-Pd(6): 47.43(15) N(5)-P(2)-Pd(6): 104.46(15) N(4)-P(2)-Pd(6): 48.40(14) Pd(4)-P(2)-Pd(6): 68.61(4) Pd(5)-P(2)-Pd(6): 76.77(4) P(1)-N(1)-Pd(1): 93.17(19) P(1)-N(1)-Pd(2): 93.0(2) Pd(1)-N(1)-Pd(2): 110.50(19)
7b	Pd(1)-N(1)#1: 2.015(5) Pd(1)-O(5): 2.045(4) Pd(1)-O(3): 2.051(4) Pd(1)-N(2)#1: 2.059(5) Pd(1)-P(1)#1: 2.7169(15) Pd(1)-Pd(2): 2.9609(6) Pd(1)-Pd(3)#1: 3.0588(8) Pd(1)-H(5): 2.15(9) Pd(2)-N(3): 2.024(5) Pd(2)-O(4): 2.043(4) Pd(2)-O(5): 2.047(4) Pd(2)-N(2): 2.061(5) Pd(2)-P(1): 2.7151(15) Pd(2)-Pd(3): 3.1071(8) Pd(3)-O(2)#1: 2.032(4) Pd(3)-O(1): 2.036(4) Pd(3)-N(3): 2.041(5) Pd(3)-N(1): 2.043(5) Pd(3)-P(1): 2.7272(18) Pd(3)-Pd(1)#1: 3.0588(8) P(1)-O(11): 1.463(4) P(1)-N(1): 1.685(5)	N(1)#1-Pd(1)-O(5): 174.69(17) N(1)#1-Pd(1)-O(3): 91.74(19) O(5)-Pd(1)-O(3): 93.35(17) N(1)#1-Pd(1)-N(2)#1: 76.6(2) O(5)-Pd(1)-N(2)#1: 98.46(18) O(3)-Pd(1)-N(2)#1: 166.92(17) N(1)#1-Pd(1)-P(1)#1: 38.22(15) O(5)-Pd(1)-P(1)#1: 137.07(12) O(3)-Pd(1)-P(1)#1: 128.88(13) N(2)#1-Pd(1)-P(1)#1: 38.75(14) N(1)#1-Pd(1)-Pd(2): 136.21(15) O(5)-Pd(1)-Pd(2): 43.69(12) O(3)-Pd(1)-Pd(2): 80.09(11) N(2)#1-Pd(1)-Pd(2): 112.43(12) P(1)#1-Pd(1)-Pd(2): 138.44(4) N(1)#1-Pd(1)-Pd(3)#1: 41.43(14) O(5)-Pd(1)-Pd(3)#1: 136.12(12) O(3)-Pd(1)-Pd(3)#1: 96.83(15) N(2)#1-Pd(1)-Pd(3)#1: 78.49(15) P(1)#1-Pd(1)-Pd(3)#1: 55.97(4) Pd(2)-Pd(1)-Pd(3)#1: 96.511(19) N(3)-Pd(2)-O(4): 91.46(19)

	P(1)-N(3): 1.686(5) P(1)-N(2): 1.702(5) P(1)-Pd(1)#1: 2.7170(15)	N(3)-Pd(2)-O(5): 174.29(17) O(4)-Pd(2)-O(5): 94.07(18) N(3)-Pd(2)-N(2): 76.5(2) O(4)-Pd(2)-N(2): 166.31(17) O(5)-Pd(2)-N(2): 98.14(18) N(3)-Pd(2)-P(1): 38.29(14) O(4)-Pd(2)-P(1): 128.25(13) O(5)-Pd(2)-P(1): 136.65(12) N(2)-Pd(2)-P(1): 38.79(14) N(3)-Pd(2)-Pd(1): 136.58(15) O(4)-Pd(2)-Pd(1): 79.69(11) O(5)-Pd(2)-Pd(1): 43.63(12) N(2)-Pd(2)-Pd(1): 113.53(12) P(1)-Pd(2)-Pd(1): 140.50(4) N(3)-Pd(2)-Pd(3): 40.36(14) O(4)-Pd(2)-Pd(3): 97.89(16) O(5)-Pd(2)-Pd(3): 136.98(11) N(2)-Pd(2)-Pd(3): 77.28(15) P(1)-Pd(2)-Pd(3): 55.37(4) Pd(1)-Pd(2)-Pd(3): 98.440(19) O(2)#1-Pd(3)-O(1): 92.6(2) O(2)#1-Pd(3)-N(3): 95.5(2) O(1)-Pd(3)-N(3): 170.30(18) O(2)#1-Pd(3)-N(1): 169.01(17) O(1)-Pd(3)-N(1): 95.4(2) N(3)-Pd(3)-N(1): 75.87(19) O(2)#1-Pd(3)-P(1): 133.55(14) O(1)-Pd(3)-P(1): 133.50(15) N(3)-Pd(3)-P(1): 38.09(14) N(1)-Pd(3)-P(1): 38.08(14) O(2)#1-Pd(3)-Pd(1)#1: 146.93(13) O(1)-Pd(3)-Pd(1)#1: 90.16(16) N(3)-Pd(3)-Pd(1)#1: 86.00(15) N(1)-Pd(3)-Pd(1)#1: 40.74(14) P(1)-Pd(3)-Pd(1)#1: 55.66(4) O(2)#1-Pd(3)-Pd(2): 92.07(16) O(1)-Pd(3)-Pd(2): 145.16(14) N(3)-Pd(3)-Pd(2): 39.95(14) N(1)-Pd(3)-Pd(2): 85.59(15) P(1)-Pd(3)-Pd(2): 55.00(4)

		Pd(1)#1-Pd(3)-Pd(2): 68.147(19) O(11)-P(1)-N(1): 120.3(2) O(11)-P(1)-N(3): 120.2(2) N(1)-P(1)-N(3): 96.3(3) O(11)-P(1)-N(2): 121.1(3) N(1)-P(1)-N(2): 96.4(2) N(3)-P(1)-N(2): 96.6(2) O(11)-P(1)-Pd(2): 132.91(19) N(1)-P(1)-Pd(2): 106.78(16) N(3)-P(1)-Pd(2): 48.07(19) N(2)-P(1)-Pd(2): 49.36(16) O(11)-P(1)-Pd(1)#1: 134.38(19) N(1)-P(1)-Pd(1)#1: 47.71(18) N(3)-P(1)-Pd(1)#1: 105.37(16) N(2)-P(1)-Pd(1)#1: 49.22(16) Pd(2)-P(1)-Pd(1)#1: 78.99(4) O(11)-P(1)-Pd(3): 144.3(2) N(1)-P(1)-Pd(3): 48.40(17) N(3)-P(1)-Pd(3): 48.33(18) N(2)-P(1)-Pd(3): 94.63(18) Pd(2)-P(1)-Pd(3): 69.63(4) Pd(1)#1-P(1)-Pd(3): 68.37(4) Pd(1)-O(5)-Pd(2): 92.7(2)
9.2H_2O	Pd(1)-N(1)#1: 2.036(7) Pd(1)-N(2): 2.057(13) Pd(1)-N(1): 2.067(6) Pd(1)-O(2): 2.103(6) Pd(1)-N(2'): 2.131(14) Pd(1)-P(1): 2.736(2) Pd(1)-Pd(1)#1: 3.2049(11) Pd(1)-Pd(1)#2: 3.2049(11) P(1)-O(1): 1.460(8) P(1)-N(1)#2: 1.698(7) P(1)-N(1)#1: 1.698(7) P(1)-N(1): 1.698(7) P(1)-Pd(1)#1: 2.736(2) P(1)-Pd(1)#2: 2.736(2) N(1)-C(11): 1.485(10) N(1)-Pd(1)#2: 2.036(7)	N(1)#1-Pd(1)-N(2): 102.3(5) N(1)#1-Pd(1)-N(1): 76.6(4) N(2)-Pd(1)-N(1): 176.6(4) N(1)#1-Pd(1)-O(2): 169.4(3) N(2)-Pd(1)-O(2): 87.7(5) N(1)-Pd(1)-O(2): 93.2(3) N(1)#1-Pd(1)-N(2'): 89.7(5) N(2)-Pd(1)-N(2'): 16.6(4) N(1)-Pd(1)-N(2'): 164.4(5) O(2)-Pd(1)-N(2'): 100.8(5) N(1)#1-Pd(1)-P(1): 38.28(18) N(2)-Pd(1)-P(1): 140.4(4) N(1)-Pd(1)-P(1): 38.32(18) O(2)-Pd(1)-P(1): 131.4(2) N(2')-Pd(1)-P(1): 127.8(4) N(1)#1-Pd(1)-Pd(1)#1: 38.98(18)

		N(2)-Pd(1)-Pd(1)#1: 100.7(5) N(1)-Pd(1)-Pd(1)#1: 80.50(18) O(2)-Pd(1)-Pd(1)#1: 143.1(2) N(2')-Pd(1)-Pd(1)#1: 84.2(5) P(1)-Pd(1)-Pd(1)#1: 54.14(3) N(1)#1-Pd(1)-Pd(1)#2: 80.90(18) N(2)-Pd(1)-Pd(1)#2: 145.0(4) N(1)-Pd(1)-Pd(1)#2: 38.30(18) O(2)-Pd(1)-Pd(1)#2: 93.0(2) N(2')-Pd(1)-Pd(1)#2: 133.0(4) P(1)-Pd(1)-Pd(1)#2: 54.14(3) Pd(1)#1-Pd(1)-Pd(1)#2: 60.0 O(1)-P(1)-N(1)#2: 120.2(2) O(1)-P(1)-N(1)#1: 120.2(2) N(1)#2-P(1)-N(1)#1: 96.9(3) O(1)-P(1)-N(1): 120.2(2) N(1)#2-P(1)-N(1): 96.9(3) N(1)#1-P(1)-N(1): 96.9(3) O(1)-P(1)-Pd(1): 137.44(4) N(1)#2-P(1)-Pd(1): 102.4(2) N(1)#1-P(1)-Pd(1): 48.0(2) N(1)-P(1)-Pd(1): 49.0(2) O(1)-P(1)-Pd(1)#1: 137.44(4) N(1)#2-P(1)-Pd(1)#1: 48.0(2) N(1)#1-P(1)-Pd(1)#1: 49.0(2) N(1)-P(1)-Pd(1)#1: 102.3(2) Pd(1)-P(1)-Pd(1)#1: 71.71(7) O(1)-P(1)-Pd(1)#2: 137.44(4) N(1)#2-P(1)-Pd(1)#2: 49.0(2) N(1)#1-P(1)-Pd(1)#2: 102.4(2) N(1)-P(1)-Pd(1)#2: 48.0(2) Pd(1)-P(1)-Pd(1)#2: 71.71(7) Pd(1)#1-P(1)-Pd(1)#2: 71.71(7) P(1)-N(1)-Pd(1)#2: 93.8(3) P(1)-N(1)-Pd(1): 92.7(3) Pd(1)#2-N(1)-Pd(1): 102.7(3)
10	Pd(1)-N(1): 2.045(3) Pd(1)-N(2): 2.045(3) Pd(1)-O(1): 2.046(2) Pd(1)-N(4): 2.086(3)	N(1)-Pd(1)-N(2): 76.45(12) N(1)-Pd(1)-O(1): 168.78(11) N(2)-Pd(1)-O(1): 92.47(11) N(1)-Pd(1)-N(4): 94.55(12)

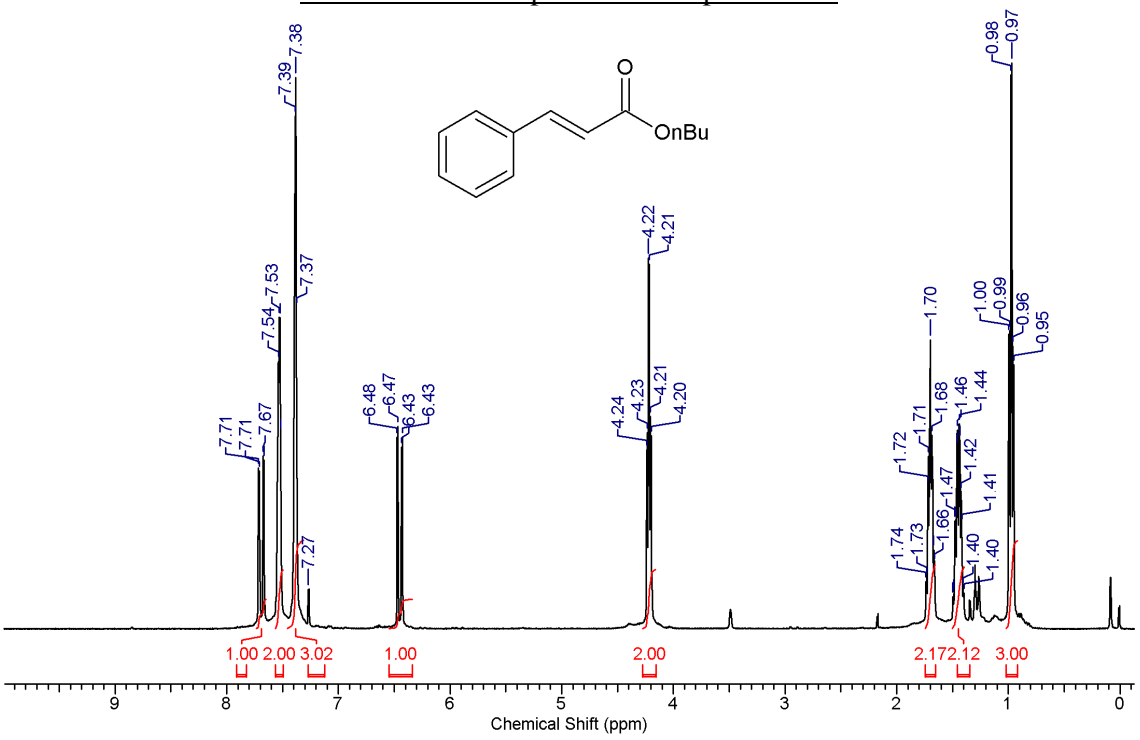
	Pd(1)-P(1): 2.7307(10) Pd(1)-Pd(2): 3.0439(5) Pd(1)-Pd(3): 3.1484(4) Pd(2)-O(3): 2.045(3) Pd(2)-N(3): 2.053(3) Pd(2)-N(2): 2.054(3) Pd(2)-N(5): 2.065(3) Pd(2)-P(1): 2.7314(10) Pd(2)-Pd(3): 3.1582(4) Pd(3)-N(1): 2.029(3) Pd(3)-N(3): 2.042(3) Pd(3)-O(5): 2.046(3) Pd(3)-N(6): 2.087(3) Pd(3)-P(1): 2.7359(10) P(1)-O(11): 1.466(3) P(1)-N(2): 1.689(3) P(1)-N(3): 1.692(3) P(1)-N(1): 1.696(3)	N(2)-Pd(1)-N(4): 168.52(12) O(1)-Pd(1)-N(4): 96.66(11) N(1)-Pd(1)-P(1): 38.31(9) N(2)-Pd(1)-P(1): 38.13(8) O(1)-Pd(1)-P(1): 130.59(7) N(4)-Pd(1)-P(1): 132.45(9) N(1)-Pd(1)-Pd(2): 82.58(8) N(2)-Pd(1)-Pd(2): 42.17(8) O(1)-Pd(1)-Pd(2): 90.38(7) N(4)-Pd(1)-Pd(2): 130.49(8) P(1)-Pd(1)-Pd(2): 56.14(2) N(1)-Pd(1)-Pd(3): 39.22(8) N(2)-Pd(1)-Pd(3): 82.75(8) O(1)-Pd(1)-Pd(3): 142.19(7) N(4)-Pd(1)-Pd(3): 85.76(8) P(1)-Pd(1)-Pd(3): 54.91(2) Pd(2)-Pd(1)-Pd(3): 61.302(9) O(3)-Pd(2)-N(3): 91.90(11) O(3)-Pd(2)-N(2): 167.69(11) N(3)-Pd(2)-N(2): 76.35(11) O(3)-Pd(2)-N(5): 98.88(12) N(3)-Pd(2)-N(5): 168.58(12) N(2)-Pd(2)-N(5): 92.63(12) O(3)-Pd(2)-P(1): 130.01(8) N(3)-Pd(2)-P(1): 38.21(8) N(2)-Pd(2)-P(1): 38.14(8) N(5)-Pd(2)-P(1): 130.70(9) O(3)-Pd(2)-Pd(1): 133.86(8) N(3)-Pd(2)-Pd(1): 82.52(8) N(2)-Pd(2)-Pd(1): 41.95(8) N(5)-Pd(2)-Pd(1): 87.27(9) P(1)-Pd(2)-Pd(1): 56.12(2) O(3)-Pd(2)-Pd(3): 86.20(7) N(3)-Pd(2)-Pd(3): 39.42(8) N(2)-Pd(2)-Pd(3): 82.37(8) N(5)-Pd(2)-Pd(3): 137.18(9) P(1)-Pd(2)-Pd(3): 54.78(2) Pd(1)-Pd(2)-Pd(3): 60.980(10) N(1)-Pd(3)-N(3): 76.21(12) N(1)-Pd(3)-O(5): 93.88(11) N(3)-Pd(3)-O(5): 170.08(11)

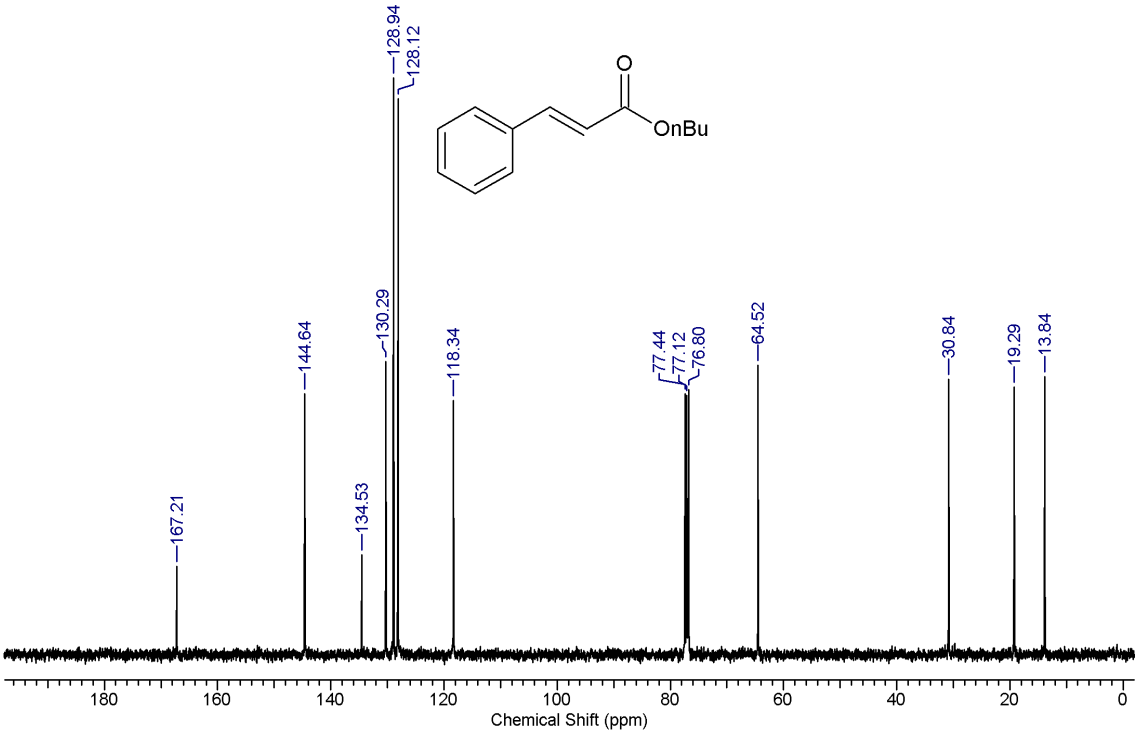
		N(1)-Pd(3)-N(6): 171.46(12) N(3)-Pd(3)-N(6): 96.31(12) O(5)-Pd(3)-N(6): 93.60(11) N(1)-Pd(3)-P(1): 38.19(9) N(3)-Pd(3)-P(1): 38.11(8) O(5)-Pd(3)-P(1): 131.98(8) N(6)-Pd(3)-P(1): 134.41(9) N(1)-Pd(3)-Pd(1): 39.58(8) N(3)-Pd(3)-Pd(1): 80.02(8) O(5)-Pd(3)-Pd(1): 92.57(7) N(6)-Pd(3)-Pd(1): 135.82(9) P(1)-Pd(3)-Pd(1): 54.76(2) N(1)-Pd(3)-Pd(2): 79.88(8) N(3)-Pd(3)-Pd(2): 39.68(8) O(5)-Pd(3)-Pd(2): 139.73(8) N(6)-Pd(3)-Pd(2): 91.74(9) P(1)-Pd(3)-Pd(2): 54.65(2) Pd(1)-Pd(3)-Pd(2): 57.718(10) O(11)-P(1)-N(2): 120.58(16) O(11)-P(1)-N(3): 120.09(15) N(2)-P(1)-N(3): 97.33(14) O(11)-P(1)-N(1): 120.62(15) N(2)-P(1)-N(1): 96.77(14) N(3)-P(1)-N(1): 95.74(15) O(11)-P(1)-Pd(1): 140.34(11) N(2)-P(1)-Pd(1): 48.39(10) N(3)-P(1)-Pd(1): 99.56(10) N(1)-P(1)-Pd(1): 48.39(9) O(11)-P(1)-Pd(2): 140.03(12) N(2)-P(1)-Pd(2): 48.68(10) N(3)-P(1)-Pd(2): 48.65(10) N(1)-P(1)-Pd(2): 99.34(10) Pd(1)-P(1)-Pd(2): 67.74(2) O(11)-P(1)-Pd(3): 136.08(12) N(2)-P(1)-Pd(3): 103.34(10) N(3)-P(1)-Pd(3): 48.14(10) N(1)-P(1)-Pd(3): 47.72(10) Pd(1)-P(1)-Pd(3): 70.33(2) Pd(2)-P(1)-Pd(3): 70.57(2)

Table S3: H-bonding data for **3**-H_3, **9**.$2H_2O$ and **10**

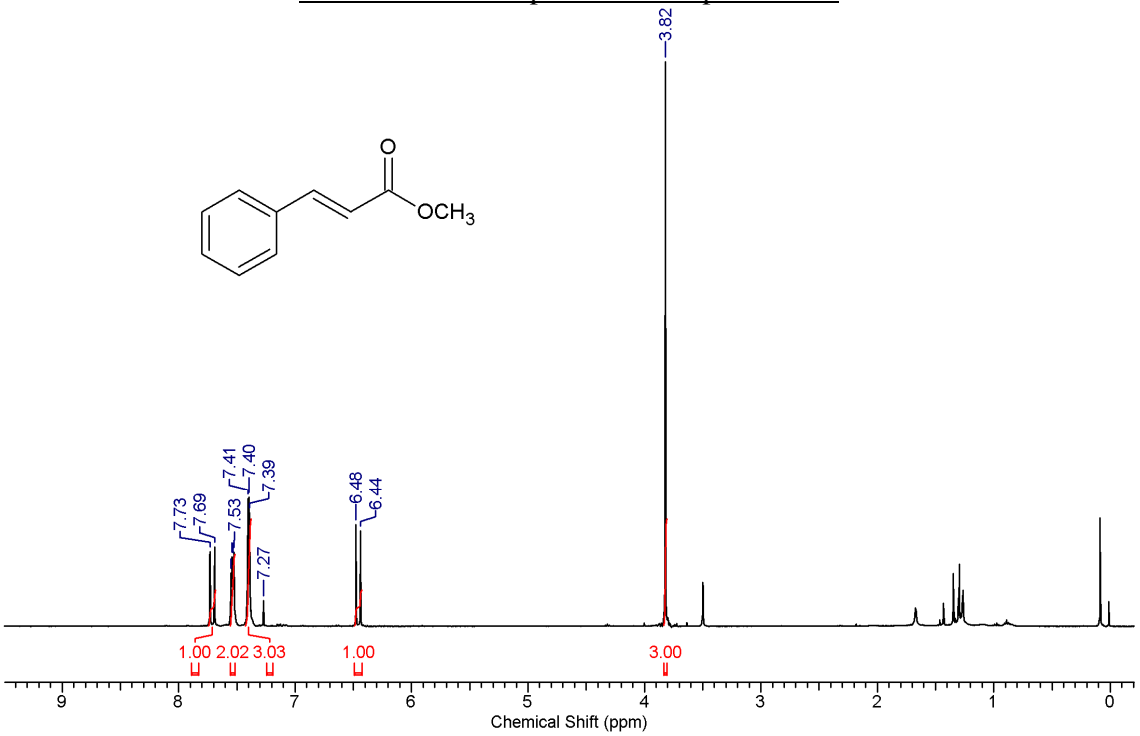
Compound	D-H...A	d(H...A)Å	d(D...A)Å	<(DHA)°
3-H_3	N(1)-H(1)...O(1)#2	2.27	3.043(3)	149.9
	Symmetry transformations used to generate equivalent atoms:			
	#1 x,-y+1/2,z #2 x-1/2,-y+1/2,-z+1/2			
9.$2H_2O$	N(2)-H(2A)...O(3)#3	2.23	2.793(16)	118.6
	N(2)-H(2B)...O(3)	2.06	2.73(2)	128.4
	N(2')-H(2'2)...O(3)#3	2.12	2.894(15)	141.3
	Symmetry transformations used to generate equivalent atoms:			
	#1 -y+1,x-y,z #2 -x+y+1,-x+1,z #3 -x+1,-y+1,-z			
10	N(4)-H(4A)...O(5)	2.32	3.105(4)	145.6
	N(4)-H(4B)...O(2)#1	2.03	2.908(4)	163.5
	N(5)-H(5A)...O(1)	2.16	2.962(4)	148.5
	N(5)-H(5B)...O(4)#2	2.06	2.917(4)	157.6
	N(6)-H(6A)...O(3)	2.28	3.086(4)	149.3
	Symmetry transformations used to generate equivalent atoms:			
	#1 -x+1,-y+1,-z #2 -x+1,-y+2,-z			

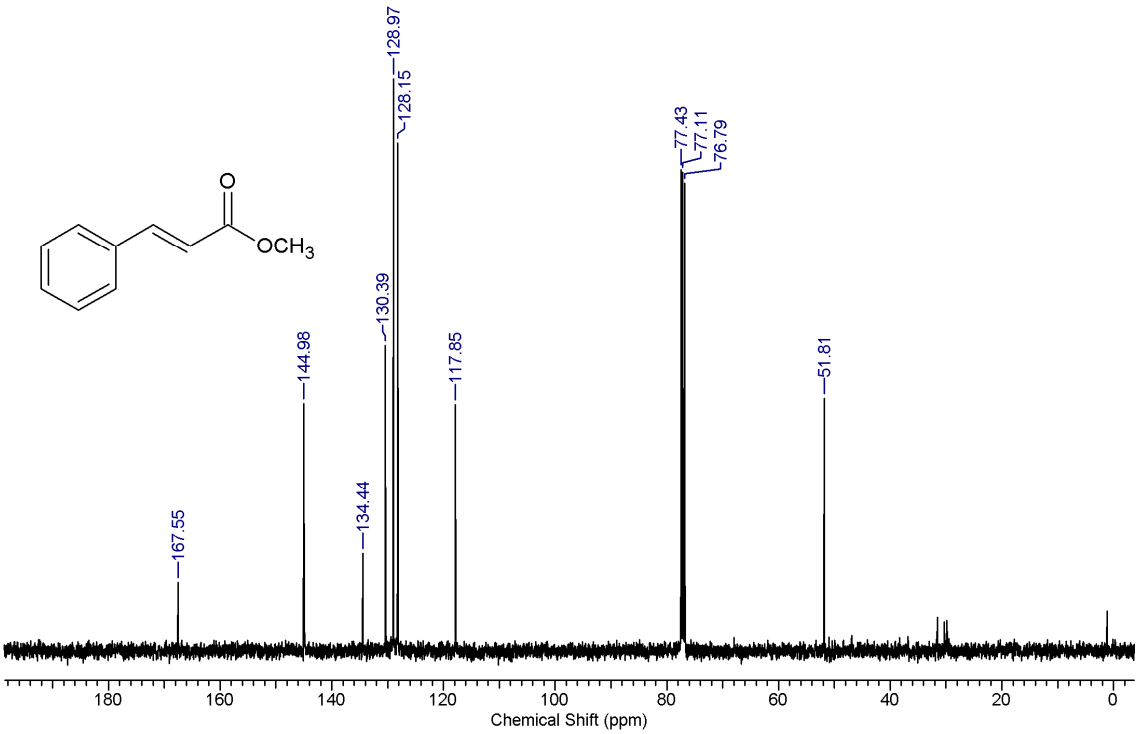
^{1}H and ^{13}C NMR Spectra of Compound **12a.**



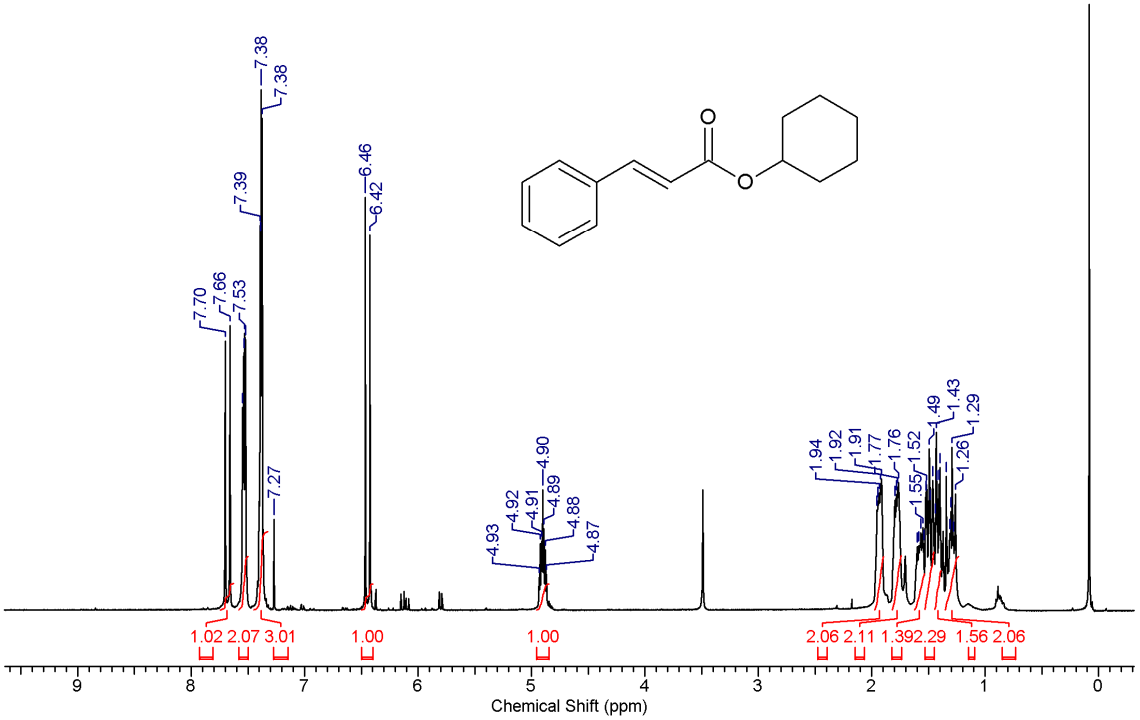


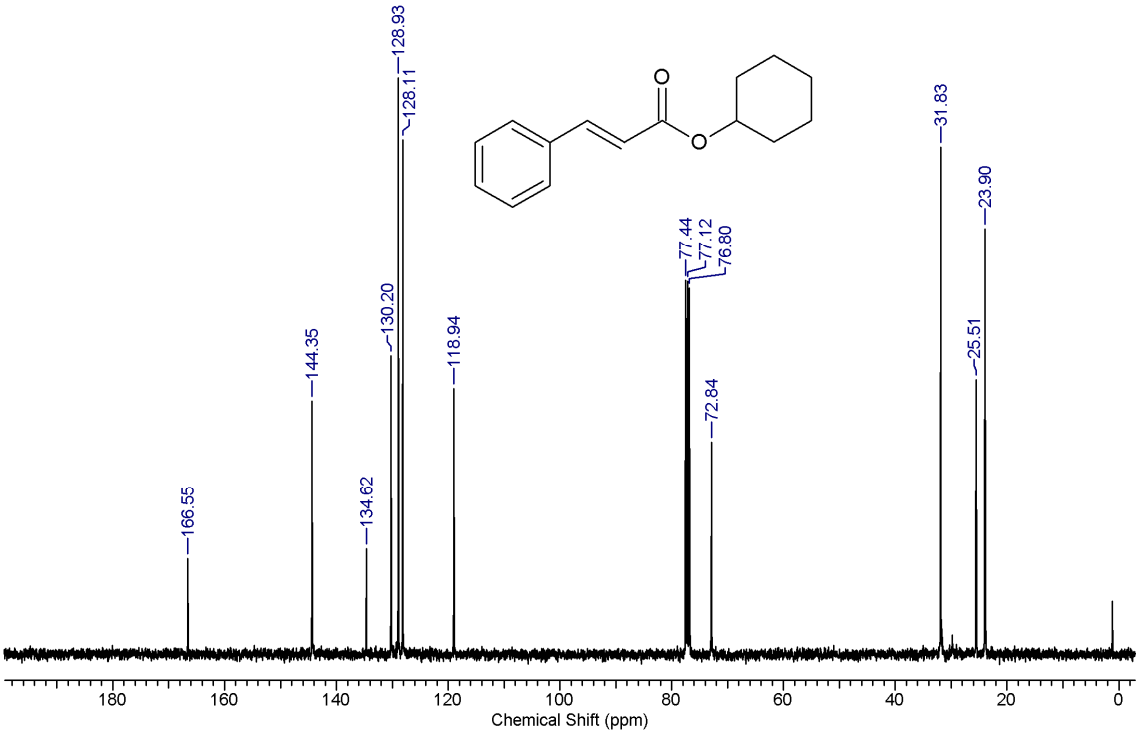
^{1}H and ^{13}C NMR Spectra of Compound **12b.**





^{1}H and ^{13}C NMR Spectra of Compound **12c.**





^{1}H and ^{13}C NMR Spectra of Compound **12d.**