Supplementary Data

Chasing the Agostic interaction in Ligand Assisted cyclometallation reactions of Palladium (II)

M. Arif Sajjad, Kirsten E. Christensen, Nicholas H. Rees, Peter Schwerdtfeger, John A. Harrison and Alastair J. Nielson

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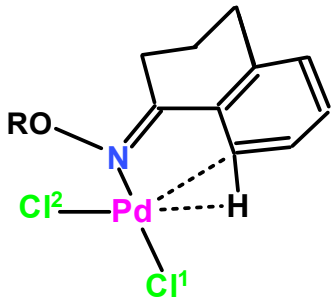
Supplementary scheme 1: Structures of complexes **1-5**



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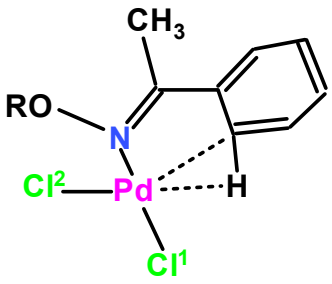
2 R = H



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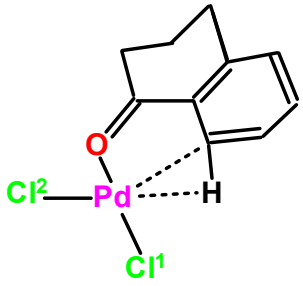
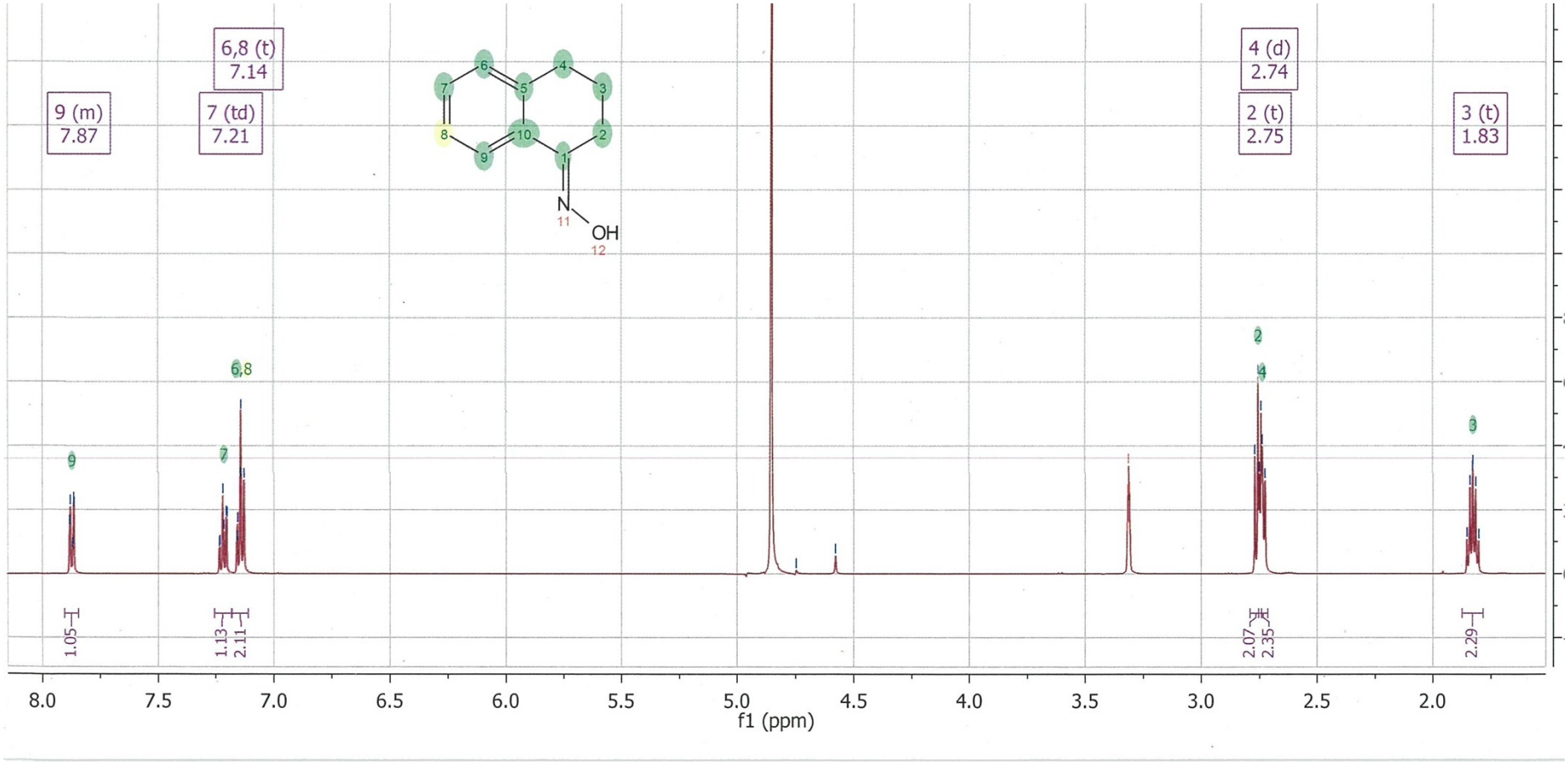
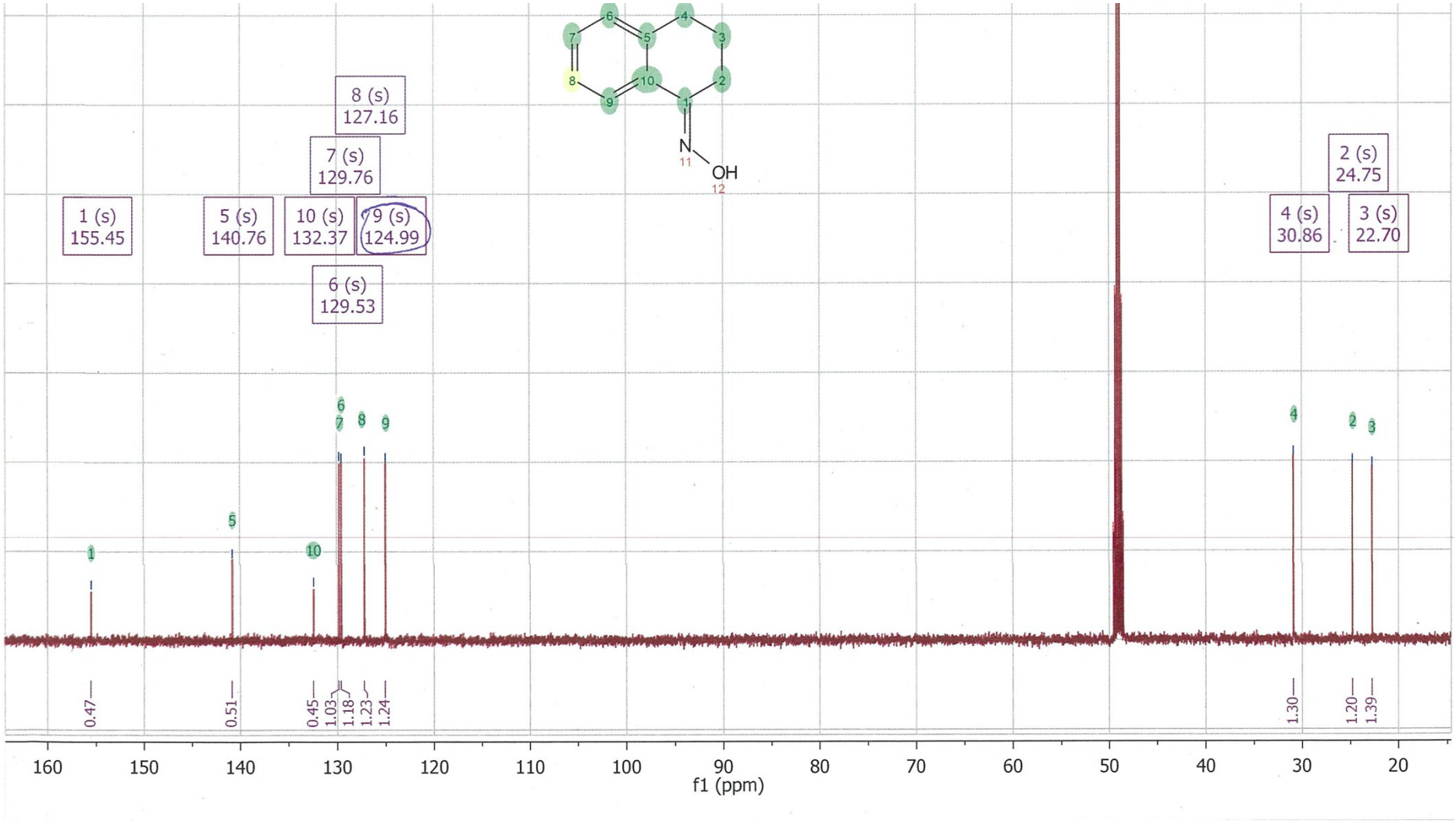


5

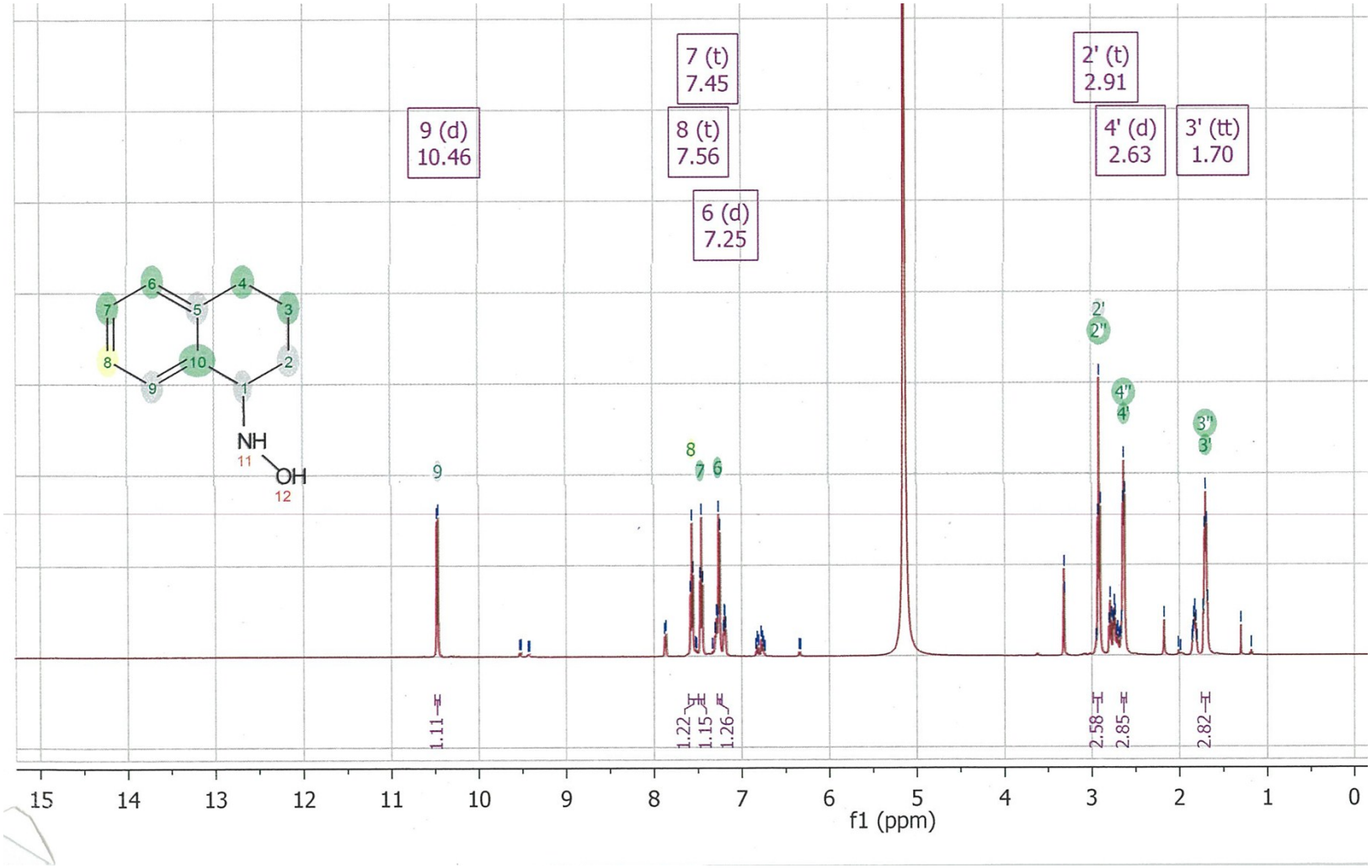
Supplementary figure 1: ^{1}H NMR of 1-tetralone oxime in CD_3OD



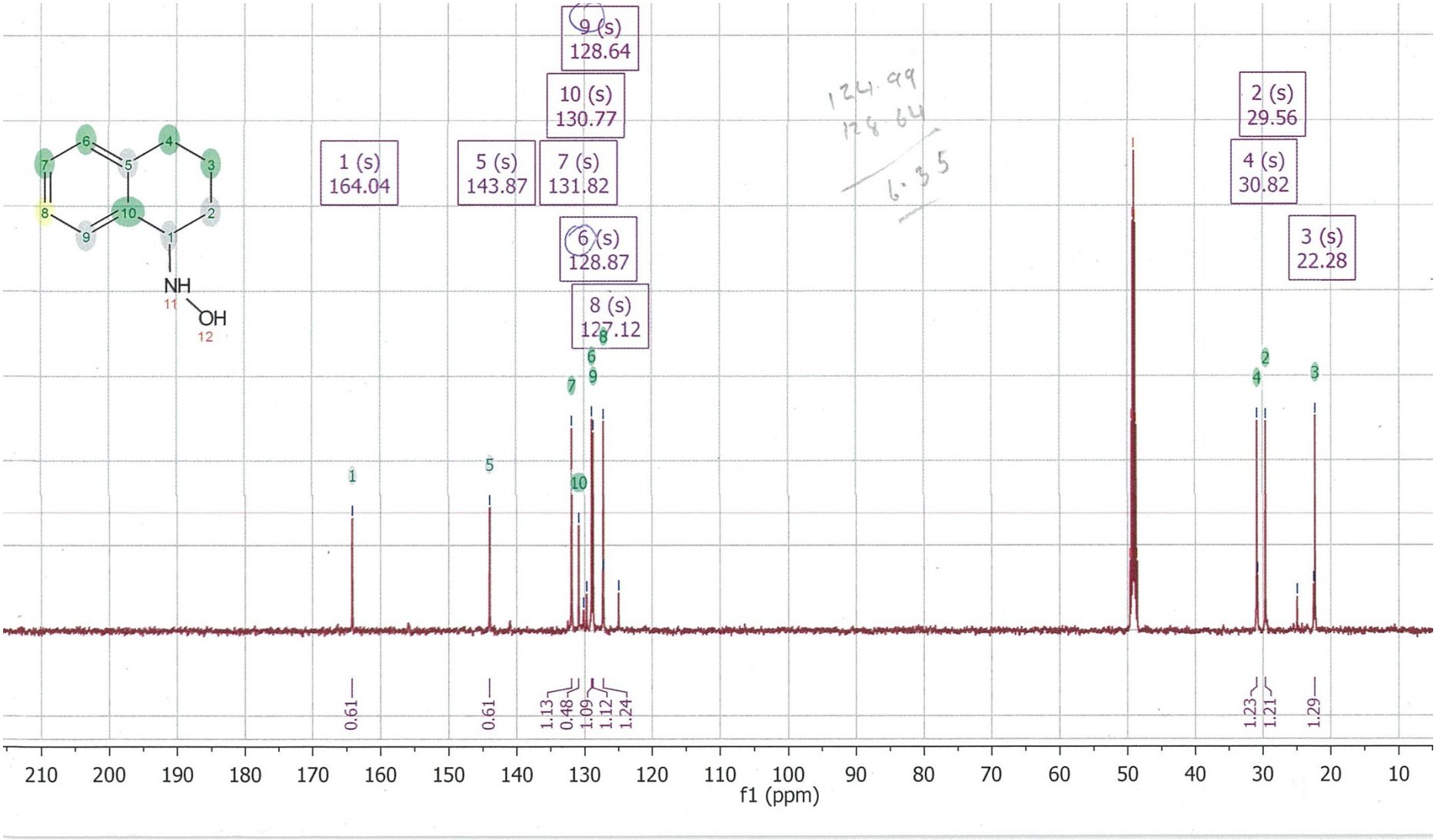
Supplementary figure 2: ^{13}C NMR of 1-tetralone oxime in CD_3OD



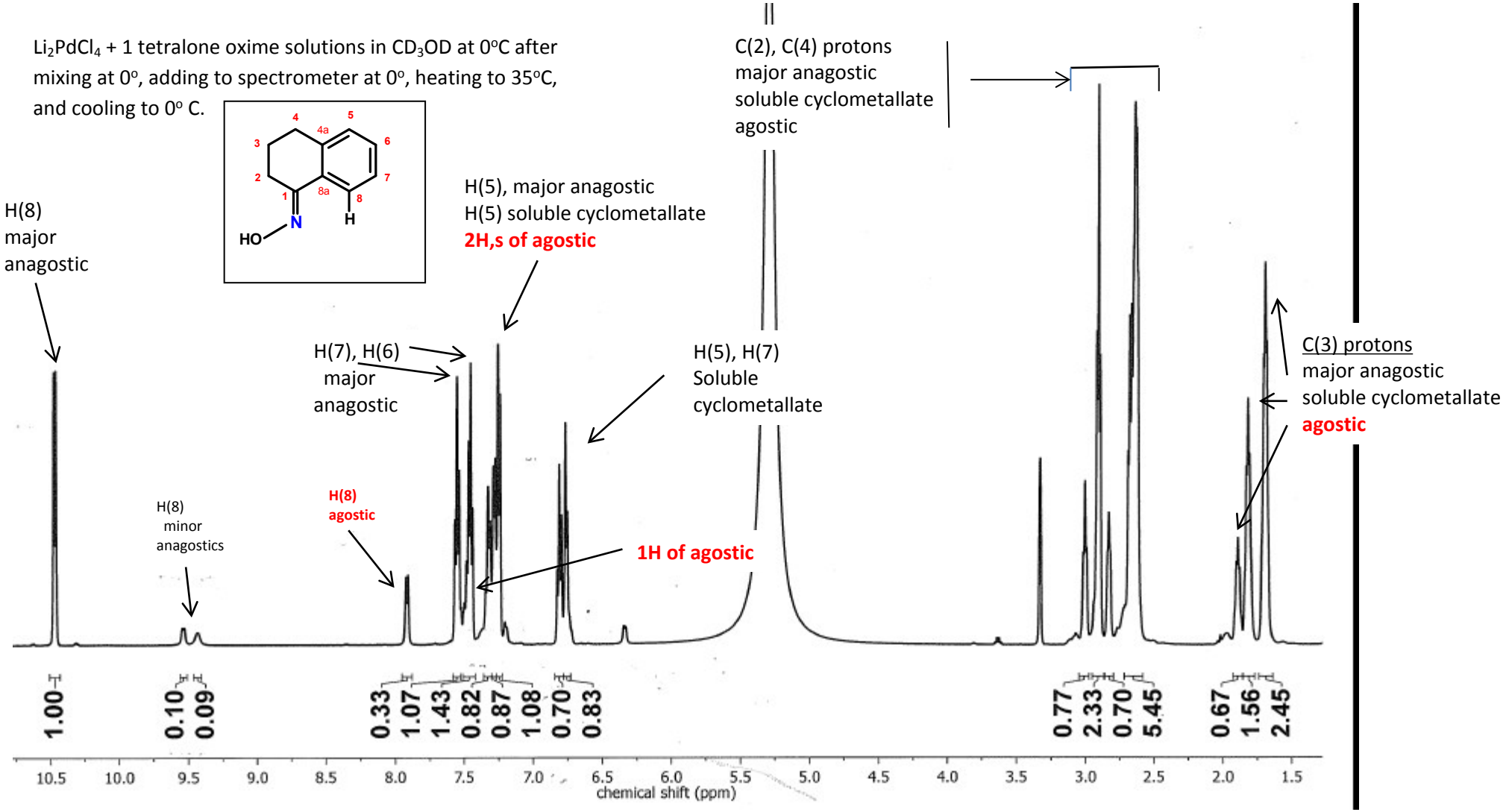
Supplementary figure 3: ^{1}H NMR of Li_2PdCl_4 in CD_3OD and 1-tetralone oxime in CD_3OD mixed at 0°C, at 0° C spectrometer temperature.



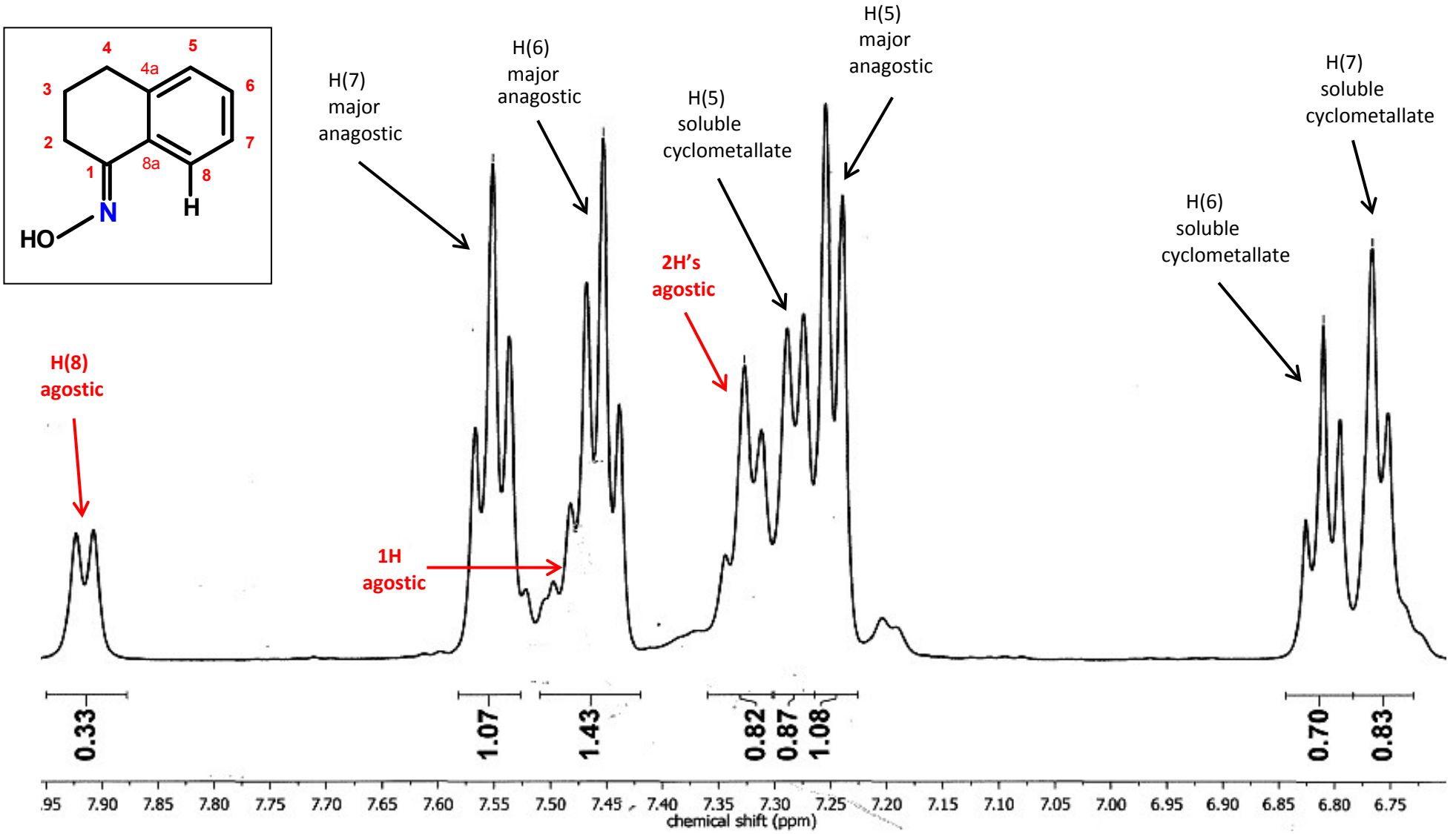
Supplementary figure 4: ^{13}C NMR of Li_2PdCl_4 in CD_3OD and 1-tetralone oxime in CD_3OD mixed at 0°C, at 0° C spectrometer temperature.



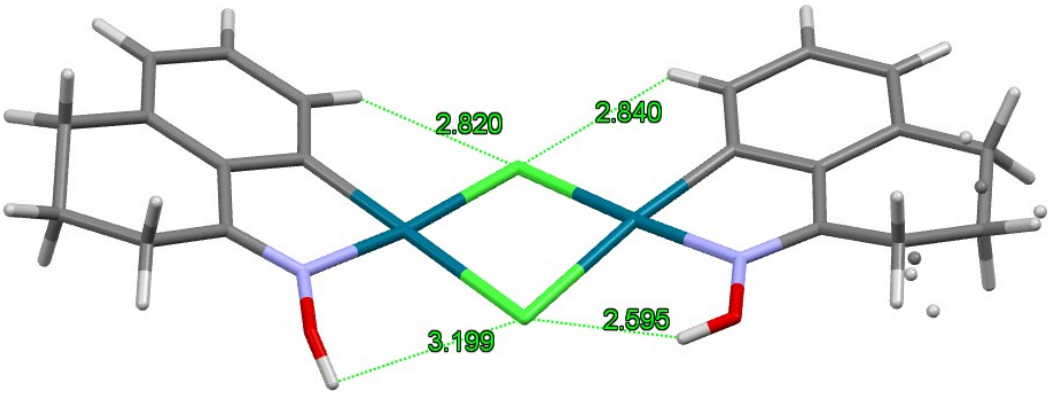
Supplementary figure 5: 1H NMR spectrum of the reaction between $PdCl_4^{2-}$ and 1-tetralone oxime in CD_3OD, mix 0° C, heat 35° C, cool 0°C.



Supplementary figure 6: Expansion of the δ 6.5 to 8.0 region of the ^{1}H NMR spectrum in supplementary figure 5.



Supplementary figure 7: Mercury diagram showing the 'butterfly'arrangement for the cyclometallated product (separations in Å)



Supplementary Figure 8: Diagrams showing the agostic C-H bond in relation to the Pd coordination plane for complexes **1-5**

Left-hand image ball and stick looking down the Pd-N bond; right-hand image capped stick looking down the Pd-Cl2 bond

Fig 8.1 Complex **1**

Fig. 8.2 Complex **2**

Fig 8.3 acetophenone oxime complex **3**

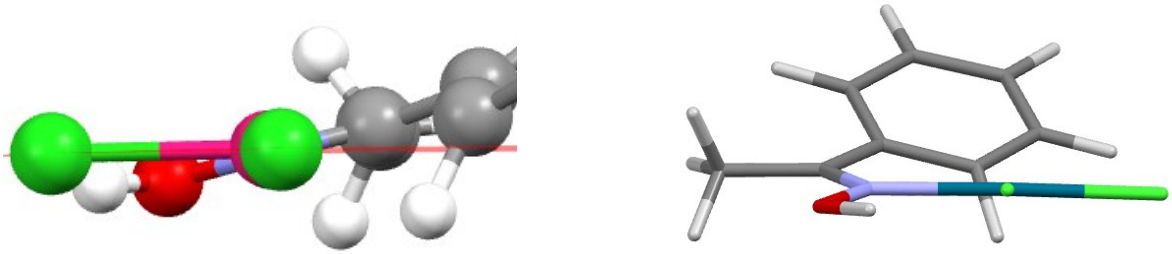
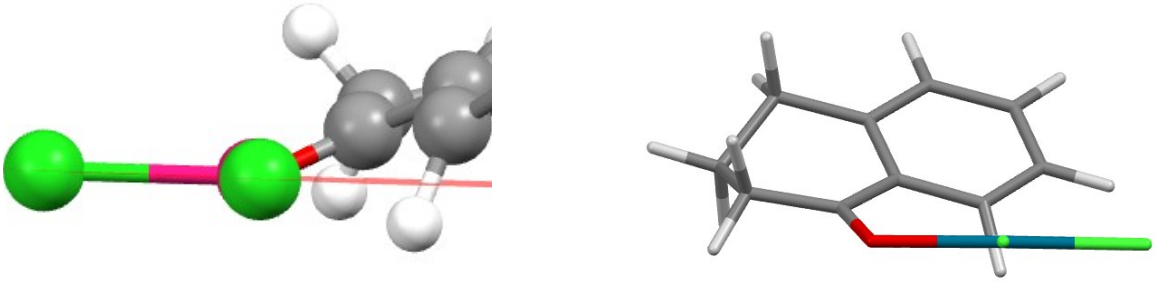


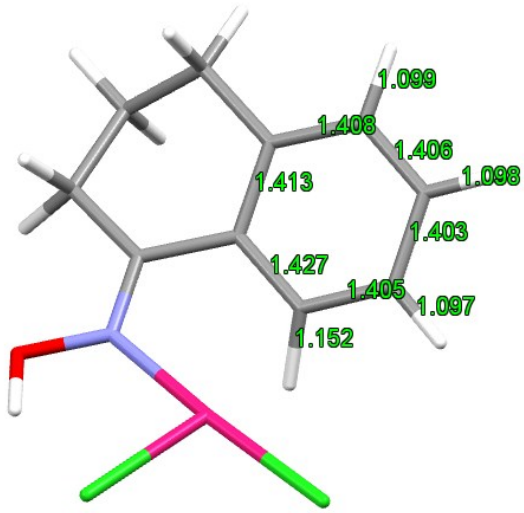
Fig 8.4 (N)-OMe acetophenone oxime complex **4**

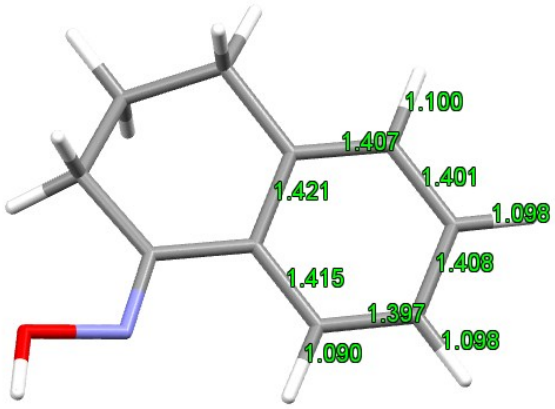
Fig 8.5 1-tetralone complex **5**



Supplementary Figure 9. Comparison of the aromatic ring C-C bond distances (Å) and angles(°) for [$PdCl_2$(1-tetralone oxime)] (**1**) and the free ligand.

A) Aromatic ring C-C bond distances (Å)

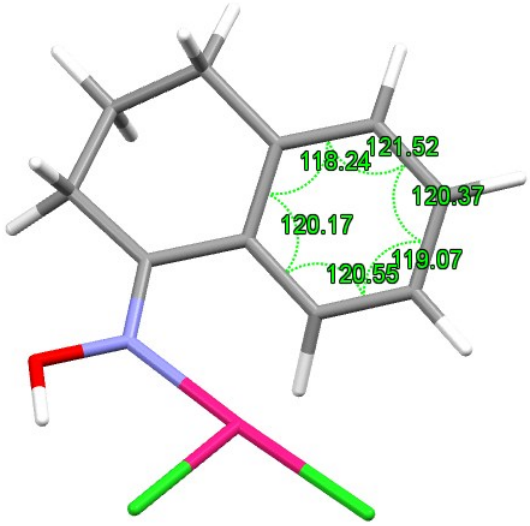


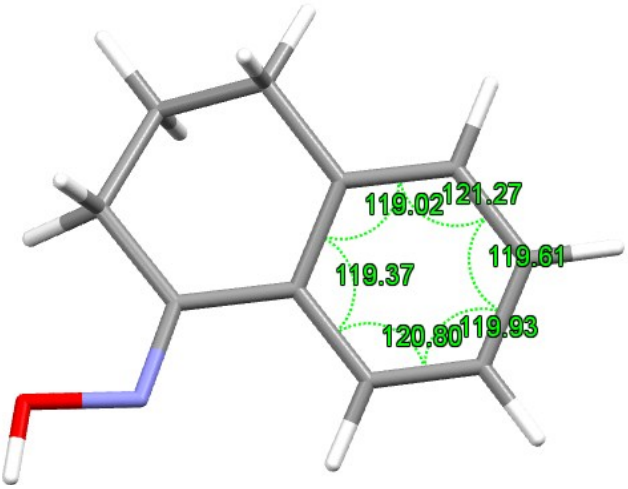


[$PdCl_2$(1-tetralone oxime)] (**1**)

1-tetralone oxime

B) Aromatic ring bond C-C angles (°)





Supplementary Figure 10: NBO electron density and contour plots for the agostic and syndetic donations.

For larger versions of the NBO images click on the image and expand by the normal angular method.)

NBOView2.0 was employed to plot the contours of the donor-acceptor interactions. The default parameter values were used for all the contours:

Contour value: 0.0316

Contour tolerance: 0.0001

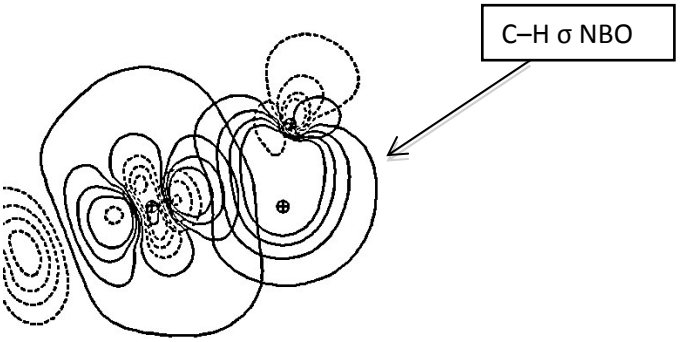
Stepsize: 0.4000

(The outermost value (0.0316 a.u) of the contour corresponds roughly to the empirical van der Waals radius).

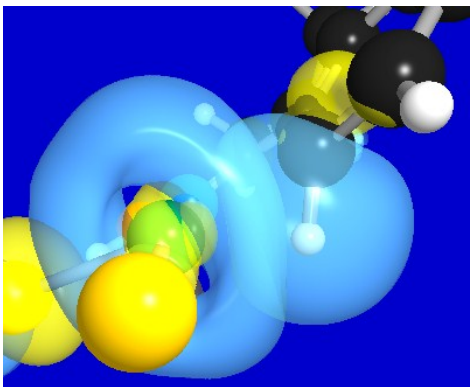
Complex 1: [Pd(Cl)$_2$(1-tetralone oxime)]

1) C(8)–H(8) σ to Pd–Cl σ* (trans) (agostic donation *E*(2) = 58.6 kcal mol^{-1})

Contour plot

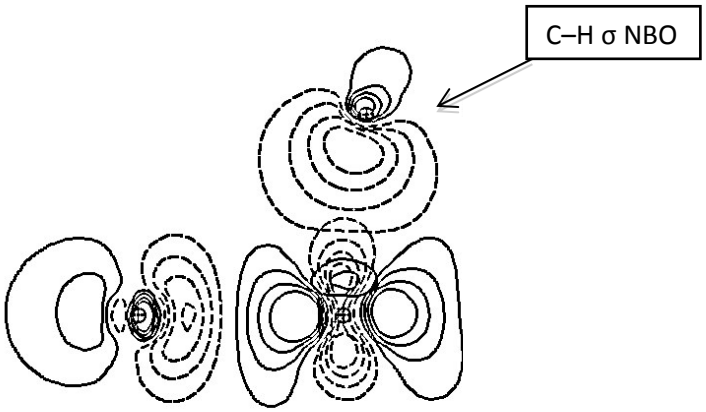


3D Surfaces showing NBOs interaction,

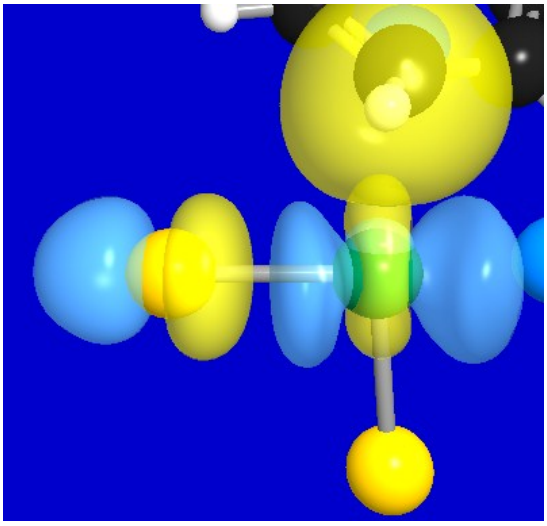


2) C(8)-H(8) σ to Pd-Cl σ* (*cis*) [agostic donation *E*(2) = 10.0 kcal mol^{-1}]

Contour plot

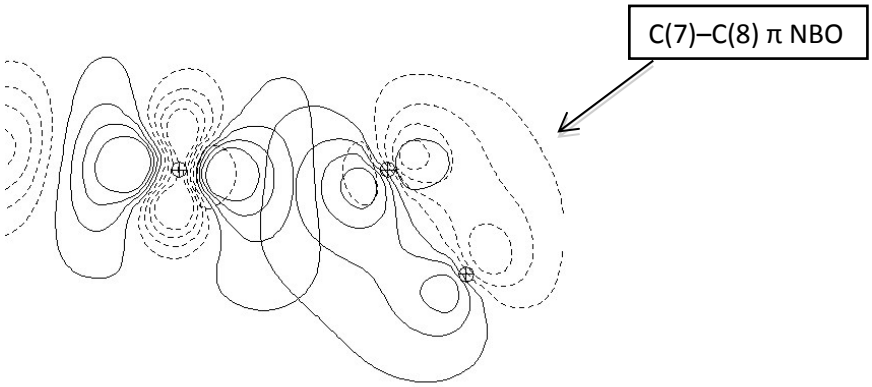


3D Surfaces showing NBOs interaction

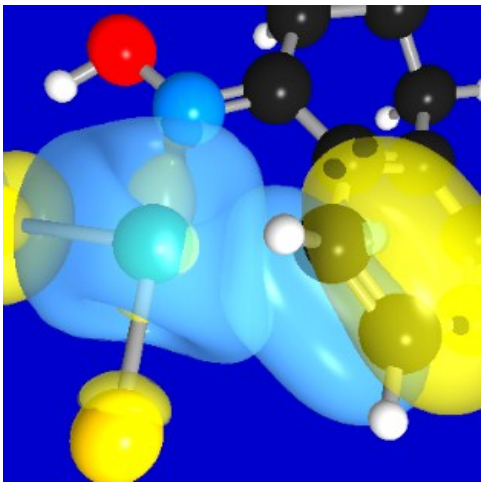


2) C(7)–C(8) π to Pd–Cl σ* (*trans*) [Syndetic donation *E*(2)=20.3 kcal mol^{-1}]

Contour plot

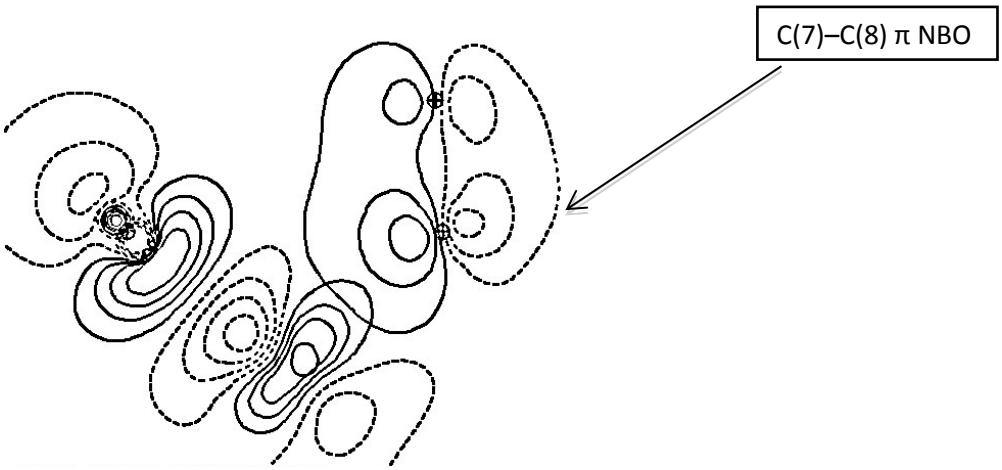


3D Surfaces showing NBOs interaction

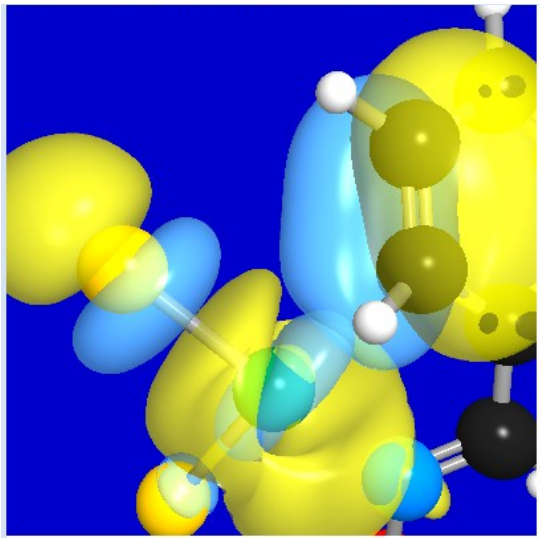


4) C(7)–C(8)π to BD*(1) Pd–Cl σ* (*cis*) (*E*(2)=6.5 kcal mol^{-1}]

Contour plot



3D Surfaces showing NBOs interaction



Supplementary Data 1: **checkCIF/PLATON report**

Structure factors have been supplied for datablock(s) I
THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.
No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

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Bond precision: C-C = 0.0093 A Wavelength=1.54184
Cell: a=7.6451(1) b=17.2164(3) c=15.4658(3)
alpha=90 beta=99.1931(17) gamma=90
Temperature: 150 K
Calculated Reported
Volume 2009.48(6) 2009.48(6)
Space group P 21/n P 21/n
Hall group -P 2yn -P 2yn
Moiety formula C20 H20 Cl2 N2 O2 Pd2 C20 H20 Cl2 N2 O2 Pd2
Sum formula C20 H20 Cl2 N2 O2 Pd2 C20 H20 Cl2 N2 O2 Pd2
Mr 604.08 604.10
Dx,g cm-3 1.997 1.997
Z 4 4
Mu (mm-1) 17.048 17.048
F000 1184.0 1184.0
F000' 1190.48
h,k,lmax 9,21,19 9,21,19
Nref 4209 4191
Tmin,Tmax 0.227,0.360 0.020,0.360
Tmin' 0.145
Correction method= # Reported T Limits: Tmin=0.020 Tmax=0.360
AbsCorr = MULTI-SCAN
Data completeness= 0.996 Theta(max)= 76.205
R(reflections)= 0.0575( 2660) wR2(reflections)= 0.1392( 2882)
S = 1.085 Npar= 260
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The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**.
Click on the hyperlinks for more details of the test.

Alert level B

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PLAT415_ALERT_2_B Short Inter D-H..H-X H121 .. H221 .. 1.95 Ang.
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min) 16 Note
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Alert level C

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PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ............... 0.00926 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H231 .. H242 . 1.99 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.557 5 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 7 Note
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Alert level G

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PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report
PLAT301_ALERT_3_G Main Residue Disorder ..............(Resd 1).. 7 % Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ........... 4 Note
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still 88 % Note
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ 2 Units
PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ... 4 Check
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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9 ALERT level G = General information/check it is not something unexpected
2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
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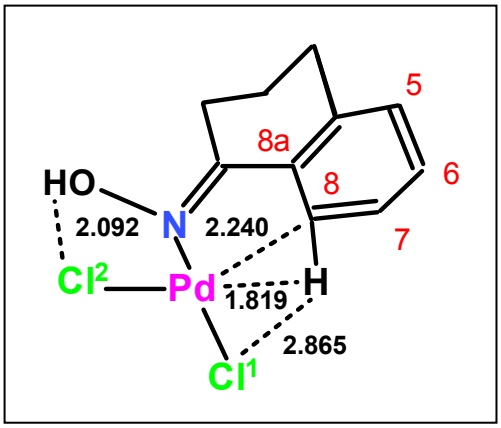
Supplementary Data 2: Cartesian coordinates and energies for calculated structures **1** to **5**

Complex 1: (E = -1564.79211120 a.u.)



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Pd	1.33110500	0.05038900	-0.09868200
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C	-2.35744000	-2.24306700	-0.17071000
C	-3.74675000	-1.62350800	-0.38995400
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H	-2.13424100	-3.02656200	-0.91910900
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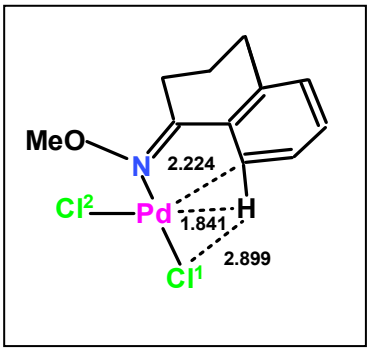
H	-4.52537700	-2.37824900	-0.17708100
H	-3.85678500	-1.33323000	-1.45341900
H	-4.94710100	0.06680500	0.31104900
H	-3.93198600	-0.67509600	1.56179900
C	-1.60137000	0.23089500	-0.19167300
C	-0.57022800	1.18740100	-0.43448300
C	-2.87787300	0.65701400	0.23926100
C	-0.79055000	2.55278500	-0.19006400
H	0.22955200	0.95451600	-1.22977200
C	-3.08571100	2.03399000	0.44710600
C	-2.05400800	2.96987600	0.25821300
H	0.02261700	3.26719100	-0.36688000
H	-4.07503800	2.37857700	0.78011700
H	-2.24251600	4.03532900	0.44391200
N	-0.00443900	-1.45796200	-0.15682800
O	0.35244300	-2.77339300	-0.06665800
H	1.34270600	-2.69732400	0.10367600

Complex 2: (E = -1604.03319674 a.u.)



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C	2.31808900	2.23733200	0.02635400
C	3.74168700	1.67851500	-0.11794100
H	2.17384400	2.69371600	1.02826300
H	2.11565000	3.05093900	-0.69472900
C	3.92305400	0.39478000	0.70706800
H	4.47152800	2.44660700	0.19649600
H	3.94490600	1.45277100	-1.18336400
H	4.94754600	-0.00513400	0.59224000
H	3.79593800	0.62399100	1.78687100
C	1.64814400	-0.24324000	-0.17385200
C	0.67873100	-1.20710800	-0.57969100
C	2.91805800	-0.65757200	0.29349000
C	0.95755500	-2.58081500	-0.47725500
H	-0.10823800	-0.91372400	-1.36709200
C	3.18363100	-2.03603700	0.36371900
C	2.21244000	-2.98674500	-0.00016600
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H	4.16641200	-2.37347900	0.72182500
H	2.44390100	-4.05741000	0.07522600
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C	-1.47707900	3.09062000	-0.90677400
H	-1.24928400	2.94561100	-1.97523500
H	-2.34728900	2.49303300	-0.60075000
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Complex 3: (E = -1487.44994119 a.u.)

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Pd	-0.91641600	-0.23729900	-0.09354300
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C	1.84329300	3.09961500	-0.24684200
H	1.68890100	3.63139400	0.71179600
H	1.35880700	3.71177300	-1.02884600
C	1.94181300	0.46964000	-0.14886100
C	1.22913800	-0.73951200	-0.42526200
C	3.26707700	0.37317500	0.31637000
C	1.81511300	-1.99631300	-0.19103000
H	0.41349600	-0.72995300	-1.23790600
C	3.85339800	-0.88524100	0.52779600
C	3.12946400	-2.06776700	0.29236700
H	3.59453700	-3.04470200	0.47678200
N	-0.08656100	1.59503100	-0.13467900
H	1.22909600	-2.90022000	-0.39897300
H	4.88444800	-0.94195500	0.90136000
H	3.83467300	1.28111300	0.55624200
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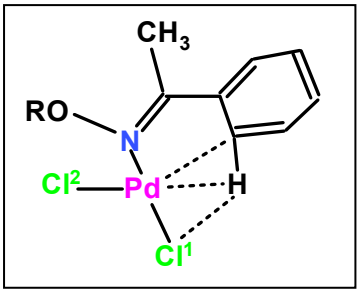
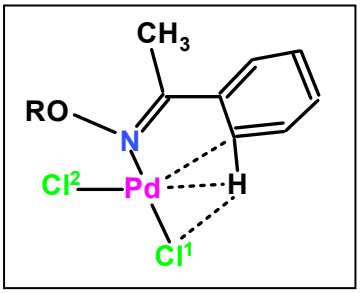


(**3**) R = H

Complex 4: (E = -1526.69076595 a.u.)



(**3**) R = Me

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Pd	-0.74631400	-0.50064600	-0.11063000
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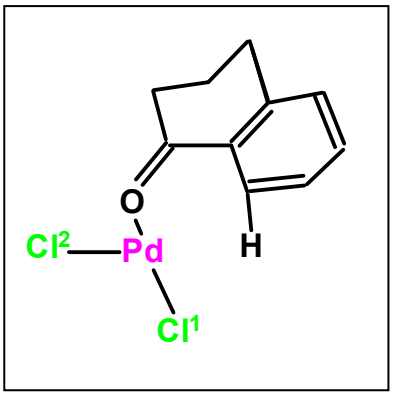
Cl	-0.95660900	-2.76139000	-0.30242400
C	0.92013200	1.87476500	-0.03329400
C	1.31623400	3.31408400	0.07990800
H	1.03430000	3.71846400	1.07082700
H	0.76973700	3.91330400	-0.66947000
C	1.87113700	0.76270400	-0.04474100
C	1.42922600	-0.50124800	-0.54263400
C	3.16642900	0.85995200	0.50246000
C	2.26077000	-1.63440300	-0.46861500
H	0.62272400	-0.53100000	-1.36047300
C	3.99375500	-0.27048400	0.56134800
C	3.54228500	-1.51557800	0.08446800
H	4.19533000	-2.39598300	0.14361200
N	-0.34112900	1.50594100	-0.12439700
H	1.88268400	-2.59459500	-0.83941300
H	4.99607700	-0.18417800	1.00110500
H	3.51736000	1.81101200	0.92216200
H	2.39947400	3.44161100	-0.06975600
O	-1.22669000	2.56535500	-0.06722000
C	-2.39742800	2.33979100	-0.88546200
H	-2.10846200	2.27523300	-1.94676800
H	-2.92418900	1.43147100	-0.56085200
H	-3.01713900	3.22809600	-0.71103400

Complex 5: (E = -1509.49100521 a.u.)

0 1

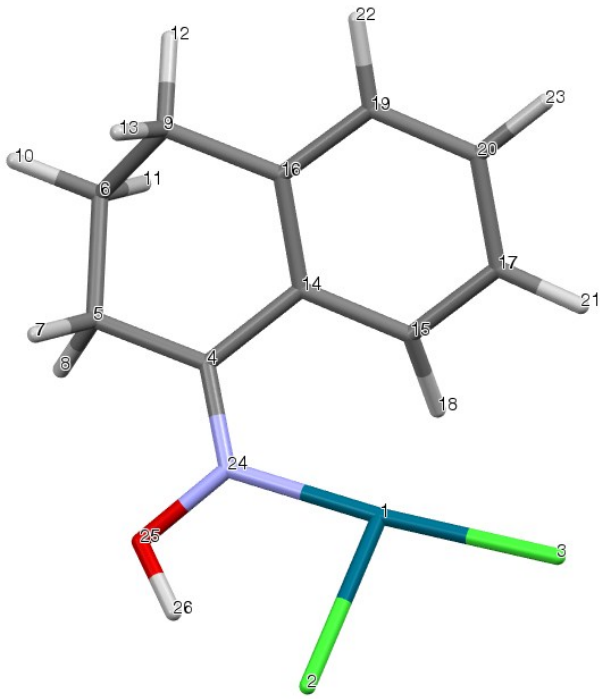
Pd	1.34767000	-0.16651800	-0.16701300
Cl	2.86651700	-1.58158400	0.70663900
Cl	2.78112200	1.58002900	-0.10694100
C	-1.27594400	-1.28511600	-0.25477100
C	-2.40026000	-2.28179300	-0.15992600
C	-3.77391400	-1.62713300	-0.36646600
H	-2.32999300	-2.73697200	0.85161500
H	-2.20376300	-3.10305800	-0.87373100
C	-3.92508700	-0.37877600	0.51658900
H	-4.57315700	-2.35630300	-0.14115800
H	-3.88897100	-1.33620200	-1.42922700
H	-4.89998700	0.11291100	0.34122200
H	-3.91641600	-0.67502200	1.58777000
C	-1.55625600	0.14184000	-0.19189400
C	-0.47518600	1.04490900	-0.43662900
C	-2.80965300	0.61242200	0.27011500
C	-0.64226500	2.41635900	-0.19029500
H	0.30364200	0.78393000	-1.26061600
C	-2.95208000	1.99174900	0.50506700
C	-1.87937000	2.87625400	0.29243300
H	0.19314400	3.10265700	-0.37357300
H	-3.91461400	2.38105700	0.86440100
H	-2.01529000	3.94783700	0.49172300
O	-0.07714600	-1.68735500	-0.30950200



Supplementary Data 3: Second order perturbation energy *E* (2) (kcalmol^{-1}) values for donor-acceptor NBOs interactions for complexes **1** to **5**

Complex 1:

(1) $R^1 = R^2 = H$, $R^3 = OH$

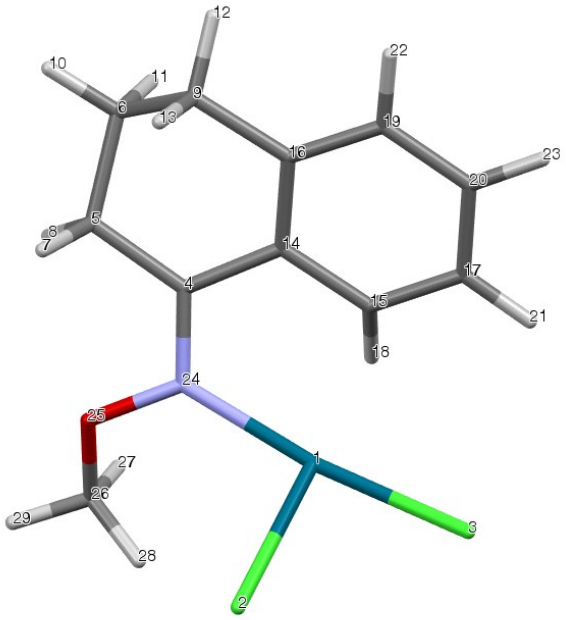


Donor (L) NBO	Acceptor (NL) NBO	*E* (2) kcalmol^{-1}
27. LP (1)Pd 1	89. BD*(2) C 15- C 17	0.67
27. LP (1)Pd 1	90. BD*(1) C 15- H 18	0.15
28. LP (2)Pd 1	87. BD*(2) C 14- C 16	0.07
28. LP (2)Pd 1	88. BD*(1) C 15- C 17	0.60
28. LP (2)Pd 1	89. BD*(2) C 15- C 17	0.12
28. LP (2)Pd 1	90. BD*(1) C 15- H 18	0.13
28. LP (2)Pd 1	98. BD*(1) N 24- O 25	2.60
29. LP (3)Pd 1	90. BD*(1) C 15- H 18	2.85
29. LP (3)Pd 1	98. BD*(1) N 24- O 25	0.13
30. LP (4)Pd 1	75. BD*(2) C 4- N 24	1.34
30. LP (4)Pd 1	87. BD*(2) C 14- C 16	0.09
30. LP (4)Pd 1	89. BD*(2) C 15- C 17	1.60
30. LP (4)Pd 1	90. BD*(1) C 15- H 18	4.87
33. LP (3)Cl 2	99. BD*(1) O 25- H 26	16.63
36. LP (3)Cl 3	90. BD*(1) C 15- H 18	0.22
40. BD (1)Pd 1-Cl 2	89. BD*(2) C 15- C 17	1.97
40. BD (1)Pd 1-Cl 2	90. BD*(1) C 15- H 18	0.49
40. BD (1)Pd 1-Cl 2	98. BD*(1) N 24- O 25	0.11
40. BD (1)Pd 1-Cl 2	99. BD*(1) O 25- H 26	0.93
41. BD (1)Pd 1-Cl 3	89. BD*(2) C 15- C 17	1.01

41. BD (1)Pd 1-Cl 3	90. BD*(1) C 15- H 18	0.68
41. BD (1)Pd 1-Cl 3	98. BD*(1) N 24- O 25	0.32
41. BD (1)Pd 1-Cl 3	99. BD*(1) O 25- H 26	0.12
37. LP (1) N 24	70. BD*(1)Pd 1-Cl 2	17.57
37. LP (1) N 24	71. BD*(1)Pd 1-Cl 3	105.35
38. LP (1) O 25	70. BD*(1)Pd 1-Cl 2	0.19
38. LP (1) O 25	71. BD*(1)Pd 1-Cl 3	0.32
42. BD (1) C 4- C 5	70. BD*(1)Pd 1-Cl 2	0.44
42. BD (1) C 4- C 5	71. BD*(1)Pd 1-Cl 3	0.71
44. BD (1) C 4- N 24	70. BD*(1)Pd 1-Cl 2	1.02
44. BD (1) C 4- N 24	71. BD*(1)Pd 1-Cl 3	4.49
55. BD (1) C 14- C 15	70. BD*(1)Pd 1-Cl 2	1.42
55. BD (1) C 14- C 15	71. BD*(1)Pd 1-Cl 3	0.43
59. BD (2) C 15- C 17	70. BD*(1)Pd 1-Cl 2	20.33
59. BD (2) C 15- C 17	71. BD*(1)Pd 1-Cl 3	6.48
60. BD (1) C 15- H 18	70. BD*(1)Pd 1-Cl 2	58.60
60. BD (1) C 15- H 18	71. BD*(1)Pd 1-Cl 3	9.97
68. BD (1) N 24- O 25	70. BD*(1)Pd 1-Cl 2	0.22
57. BD (2) C 14- C 16	75. BD*(2) C 4- N 24	20.95
57. BD (2) C 14- C 16	79. BD*(1) C 6- C 9	0.59
57. BD (2) C 14- C 16	82. BD*(1) C 9- H 12	1.05
57. BD (2) C 14- C 16	83. BD*(1) C 9- H 13	3.13
57. BD (2) C 14- C 16	89. BD*(2) C 15- C 17	12.54

Complex 2:

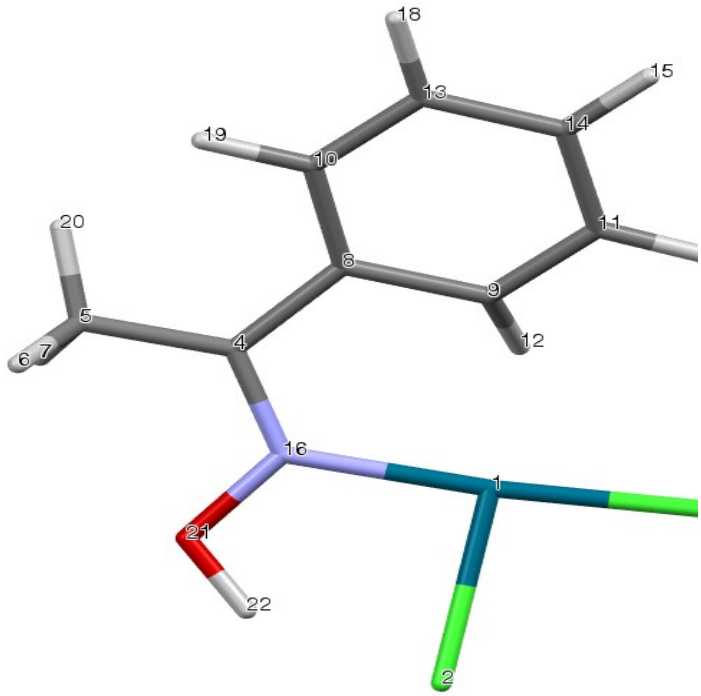
(2) $R^1 = R^2 = H$, $R^3 = OMe$



Donor (L) NBO	Acceptor (NL) NBO	*E* (2) kcalmol^{-1}
28. LP (1)Pd 1	89. BD*(1) C 14- C 15	0.61
28. LP (1)Pd 1	91. BD*(2) C 14- C 16	0.07
28. LP (1)Pd 1	93. BD*(2) C 15- C 17	1.11
28. LP (1)Pd 1	94. BD*(1) C 15- H 18	0.27
29. LP (2)Pd 1	76. BD*(1) C 4- C 5	0.06
29. LP (2)Pd 1	78. BD*(1) C 4- N 24	0.64
29. LP (2)Pd 1	79. BD*(2) C 4- N 24	0.14
29. LP (2)Pd 1	89. BD*(1) C 14- C 15	0.33
29. LP (2)Pd 1	90. BD*(1) C 14- C 16	0.08
29. LP (2)Pd 1	91. BD*(2) C 14- C 16	0.14
29. LP (2)Pd 1	92. BD*(1) C 15- C 17	0.58
29. LP (2)Pd 1	102. BD*(1) N 24- O 25	2.20
29. LP (2)Pd 1	105. BD*(1) C 26- H 28	0.07
29. LP (2)Pd 1	106. BD*(1) C 26- H 29	0.06
30. LP (3)Pd 1	79. BD*(2) C 4- N 24	2.54
30. LP (3)Pd 1	89. BD*(1) C 14- C 15	0.29
30. LP (3)Pd 1	92. BD*(1) C 15- C 17	0.10
30. LP (3)Pd 1	93. BD*(2) C 15- C 17	0.51
30. LP (3)Pd 1	94. BD*(1) C 15- H 18	1.34
31. LP (4)Pd 1	79. BD*(2) C 4- N 24	0.64
31. LP (4)Pd 1	91. BD*(2) C 14- C 16	0.10
31. LP (4)Pd 1	93. BD*(2) C 15- C 17	2.38
31. LP (4)Pd 1	94. BD*(1) C 15- H 18	5.69
34. LP (3)Cl 2	93. BD*(2) C 15- C 17	0.12
34. LP (3)Cl 2	94. BD*(1) C 15- H 18	0.10
34. LP (3)Cl 2	105. BD*(1) C 26- H 28	3.75
41. BD (1)Pd 1-Cl 2	78. BD*(1) C 4- N 24	0.14
41. BD (1)Pd 1-Cl 2	79. BD*(2) C 4- N 24	0.38
41. BD (1)Pd 1-Cl 2	89. BD*(1) C 14- C 15	0.21
41. BD (1)Pd 1-Cl 2	93. BD*(2) C 15- C 17	2.70
41. BD (1)Pd 1-Cl 2	94. BD*(1) C 15- H 18	0.29

41. BD (1)Pd 1-Cl 2	103. BD*(1) O 25- C 26	0.12
41. BD (1)Pd 1-Cl 2	105. BD*(1) C 26- H 28	0.46
41. BD (1)Pd 1-Cl 2	106. BD*(1) C 26- H 29	0.09
42. BD (1)Pd 1-Cl 3	79. BD*(2) C 4- N 24	0.32
42. BD (1)Pd 1-Cl 3	93. BD*(2) C 15- C 17	1.27
42. BD (1)Pd 1-Cl 3	94. BD*(1) C 15- H 18	0.39
42. BD (1)Pd 1-Cl 3	102. BD*(1) N 24- O 25	0.28
38. LP (1) N 24	74. BD*(1)Pd 1-Cl 2	18.80
38. LP (1) N 24	75. BD*(1)Pd 1-Cl 3	96.31
43. BD (1) C 4- C 5	74. BD*(1)Pd 1-Cl 2	0.60
43. BD (1) C 4- C 5	75. BD*(1)Pd 1-Cl 3	0.87
45. BD (1) C 4- N 24	74. BD*(1)Pd 1-Cl 2	1.28
45. BD (1) C 4- N 24	75. BD*(1)Pd 1-Cl 3	4.75
46. BD (2) C 4- N 24	74. BD*(1)Pd 1-Cl 2	0.15
46. BD (2) C 4- N 24	75. BD*(1)Pd 1-Cl 3	2.17
56. BD (1) C 14- C 15	74. BD*(1)Pd 1-Cl 2	1.69
56. BD (1) C 14- C 15	75. BD*(1)Pd 1-Cl 3	0.51
60. BD (2) C 15- C 17	74. BD*(1)Pd 1-Cl 2	18.94
60. BD (2) C 15- C 17	75. BD*(1)Pd 1-Cl 3	5.95
61. BD (1) C 15- H 18	74. BD*(1)Pd 1-Cl 2	57.68
61. BD (1) C 15- H 18	75. BD*(1)Pd 1-Cl 3	9.45

Complex 3:



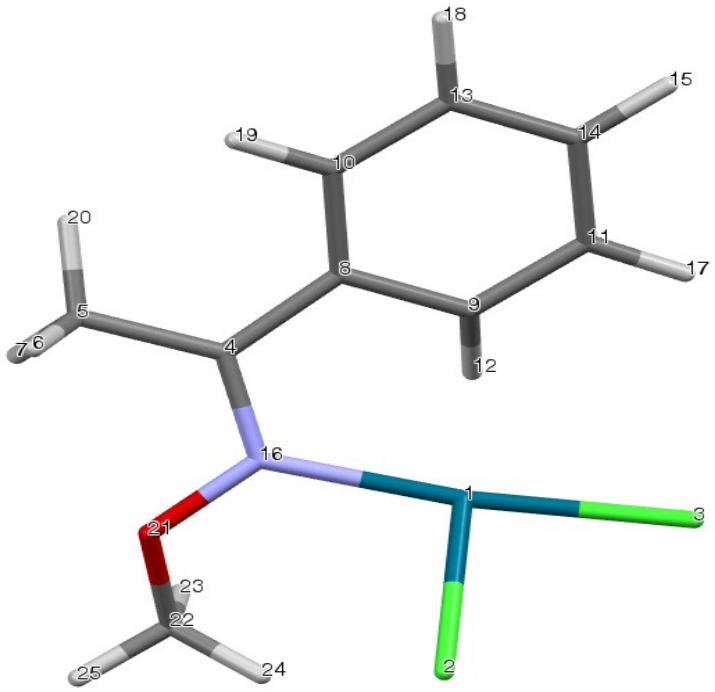
Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal mol^{-1}
25. LP (1)Pd 1	63. BD*(1)Pd 1-Cl 2	11.07
25. LP (1)Pd 1	64. BD*(1)Pd 1-Cl 3	9.51
26. LP (2)Pd 1	63. BD*(1)Pd 1-Cl 2	1.72
26. LP (2)Pd 1	64. BD*(1)Pd 1-Cl 3	1.76
28. LP (4)Pd 1	63. BD*(1)Pd 1-Cl 2	1.02
28. LP (4)Pd 1	64. BD*(1)Pd 1-Cl 3	1.19
29. LP (1)Cl 2	63. BD*(1)Pd 1-Cl 2	2.82
29. LP (1)Cl 2	64. BD*(1)Pd 1-Cl 3	3.26
31. LP (3)Cl 2	63. BD*(1)Pd 1-Cl 2	1.45
31. LP (3)Cl 2	64. BD*(1)Pd 1-Cl 3	1.86
32. LP (1)Cl 3	63. BD*(1)Pd 1-Cl 2	2.85
32. LP (1)Cl 3	64. BD*(1)Pd 1-Cl 3	1.84
33. LP (2)Cl 3	63. BD*(1)Pd 1-Cl 2	3.51
33. LP (2)Cl 3	64. BD*(1)Pd 1-Cl 3	2.04
34. LP (3)Cl 3	63. BD*(1)Pd 1-Cl 2	0.72
34. LP (3)Cl 3	64. BD*(1)Pd 1-Cl 3	0.55
38. BD (1)Pd 1-Cl 2	63. BD*(1)Pd 1-Cl 2	11.01
38. BD (1)Pd 1-Cl 2	64. BD*(1)Pd 1-Cl 3	32.78
39. BD (1)Pd 1-Cl 3	63. BD*(1)Pd 1-Cl 2	23.01
39. BD (1)Pd 1-Cl 3	64. BD*(1)Pd 1-Cl 3	3.69
25. LP (1)Pd 1	72. BD*(1) C 8- C 9	0.13
25. LP (1)Pd 1	73. BD*(2) C 8- C 9	0.69
25. LP (1)Pd 1	76. BD*(1) C 9- H 12	0.15
26. LP (2)Pd 1	67. BD*(1) C 4- N 16	0.87
26. LP (2)Pd 1	72. BD*(1) C 8- C 9	0.59
26. LP (2)Pd 1	74. BD*(1) C 8- C 10	0.08
26. LP (2)Pd 1	75. BD*(1) C 9- C 11	0.78

26. LP (2)Pd 1	76. BD*(1) C 9- H 12	0.14
26. LP (2)Pd 1	86. BD*(1) N 16- O 21	2.51
27. LP (3)Pd 1	68. BD*(2) C 4- N 16	3.56
27. LP (3)Pd 1	72. BD*(1) C 8- C 9	0.10
27. LP (3)Pd 1	73. BD*(2) C 8- C 9	0.49
27. LP (3)Pd 1	76. BD*(1) C 9- H 12	2.90
27. LP (3)Pd 1	86. BD*(1) N 16- O 21	0.10
28. LP (4)Pd 1	68. BD*(2) C 4- N 16	1.56
28. LP (4)Pd 1	73. BD*(2) C 8- C 9	0.78
28. LP (4)Pd 1	76. BD*(1) C 9- H 12	5.00
29. LP (1)Cl 2	73. BD*(2) C 8- C 9	0.27
29. LP (1)Cl 2	76. BD*(1) C 9- H 12	0.08
29. LP (1)Cl 2	87. BD*(1) O 21- H 22	0.28
30. LP (2)Cl 2	68. BD*(2) C 4- N 16	0.12
30. LP (2)Cl 2	73. BD*(2) C 8- C 9	0.06
30. LP (2)Cl 2	76. BD*(1) C 9- H 12	0.13
31. LP (3)Cl 2	67. BD*(1) C 4- N 16	0.17
31. LP (3)Cl 2	73. BD*(2) C 8- C 9	0.16
31. LP (3)Cl 2	86. BD*(1) N 16- O 21	0.05
31. LP (3)Cl 2	87. BD*(1) O 21- H 22	17.18
32. LP (1)Cl 3	73. BD*(2) C 8- C 9	0.17
32. LP (1)Cl 3	76. BD*(1) C 9- H 12	0.06
32. LP (1)Cl 3	82. BD*(1) C 11- H 17	0.11
32. LP (1)Cl 3	86. BD*(1) N 16- O 21	0.08
33. LP (2)Cl 3	72. BD*(1) C 8- C 9	0.20
33. LP (2)Cl 3	80. BD*(1) C 11- C 14	0.09
33. LP (2)Cl 3	82. BD*(1) C 11- H 17	0.32
33. LP (2)Cl 3	87. BD*(1) O 21- H 22	0.06
34. LP (3)Cl 3	76. BD*(1) C 9- H 12	0.21
34. LP (3)Cl 3	81. BD*(2) C 11- C 14	0.07
34. LP (3)Cl 3	82. BD*(1) C 11- H 17	0.10
38. BD (1)Pd 1-Cl 2	67. BD*(1) C 4- N 16	0.13
38. BD (1)Pd 1-Cl 2	73. BD*(2) C 8- C 9	1.97
38. BD (1)Pd 1-Cl 2	75. BD*(1) C 9- C 11	0.10
38. BD (1)Pd 1-Cl 2	76. BD*(1) C 9- H 12	0.42
38. BD (1)Pd 1-Cl 2	82. BD*(1) C 11- H 17	0.06
38. BD (1)Pd 1-Cl 2	86. BD*(1) N 16- O 21	0.06
38. BD (1)Pd 1-Cl 2	87. BD*(1) O 21- H 22	0.97
39. BD (1)Pd 1-Cl 3	73. BD*(2) C 8- C 9	1.20
39. BD (1)Pd 1-Cl 3	76. BD*(1) C 9- H 12	0.59
39. BD (1)Pd 1-Cl 3	86. BD*(1) N 16- O 21	0.25
39. BD (1)Pd 1-Cl 3	87. BD*(1) O 21- H 22	0.11
35. LP (1) N 16	63. BD*(1)Pd 1-Cl 2	17.35
35. LP (1) N 16	64. BD*(1)Pd 1-Cl 3	106.97
36. LP (1) O 21	63. BD*(1)Pd 1-Cl 2	0.19
36. LP (1) O 21	64. BD*(1)Pd 1-Cl 3	0.32
40. BD (1) C 4- C 5	63. BD*(1)Pd 1-Cl 2	0.53
40. BD (1) C 4- C 5	64. BD*(1)Pd 1-Cl 3	0.84
41. BD (1) C 4- C 8	63. BD*(1)Pd 1-Cl 2	0.06
42. BD (1) C 4- N 16	63. BD*(1)Pd 1-Cl 2	0.84
42. BD (1) C 4- N 16	64. BD*(1)Pd 1-Cl 3	3.99

43. BD (2) C 4- N 16	64. BD*(1)Pd 1-Cl 3	0.17
47. BD (1) C 8- C 9	63. BD*(1)Pd 1-Cl 2	1.47
47. BD (1) C 8- C 9	64. BD*(1)Pd 1-Cl 3	0.42
48. BD (2) C 8- C 9	63. BD*(1)Pd 1-Cl 2	20.25
48. BD (2) C 8- C 9	64. BD*(1)Pd 1-Cl 3	6.75
50. BD (1) C 9- C 11	64. BD*(1)Pd 1-Cl 3	0.08
51. BD (1) C 9- H 12	63. BD*(1)Pd 1-Cl 2	56.92
51. BD (1) C 9- H 12	64. BD*(1)Pd 1-Cl 3	8.92
55. BD (1) C 11- C 14	63. BD*(1)Pd 1-Cl 2	0.08
56. BD (2) C 11- C 14	63. BD*(1)Pd 1-Cl 2	0.11
56. BD (2) C 11- C 14	64. BD*(1)Pd 1-Cl 3	0.06
61. BD (1) N 16- O 21	63. BD*(1)Pd 1-Cl 2	0.20
35. LP (1) N 16	65. BD*(1) C 4- C 5	8.31
35. LP (1) N 16	66. BD*(1) C 4- C 8	1.58
35. LP (1) N 16	87. BD*(1) O 21- H 22	0.68
37. LP (2) O 21	68. BD*(2) C 4- N 16	20.27
40. BD (1) C 4- C 5	66. BD*(1) C 4- C 8	1.12
40. BD (1) C 4- C 5	67. BD*(1) C 4- N 16	0.68
40. BD (1) C 4- C 5	72. BD*(1) C 8- C 9	2.22
40. BD (1) C 4- C 5	86. BD*(1) N 16- O 21	1.05
41. BD (1) C 4- C 8	65. BD*(1) C 4- C 5	0.83
41. BD (1) C 4- C 8	67. BD*(1) C 4- N 16	0.88
41. BD (1) C 4- C 8	72. BD*(1) C 8- C 9	1.51
41. BD (1) C 4- C 8	74. BD*(1) C 8- C 10	1.41
41. BD (1) C 4- C 8	75. BD*(1) C 9- C 11	1.98
41. BD (1) C 4- C 8	77. BD*(1) C 10- C 13	1.84
41. BD (1) C 4- C 8	86. BD*(1) N 16- O 21	5.51
42. BD (1) C 4- N 16	65. BD*(1) C 4- C 5	0.93
42. BD (1) C 4- N 16	66. BD*(1) C 4- C 8	0.94
42. BD (1) C 4- N 16	74. BD*(1) C 8- C 10	1.92
42. BD (1) C 4- N 16	87. BD*(1) O 21- H 22	1.05
43. BD (2) C 4- N 16	68. BD*(2) C 4- N 16	2.52
43. BD (2) C 4- N 16	69. BD*(1) C 5- H 6	1.61
43. BD (2) C 4- N 16	70. BD*(1) C 5- H 7	0.99
43. BD (2) C 4- N 16	73. BD*(2) C 8- C 9	7.93
44. BD (1) C 5- H 6	66. BD*(1) C 4- C 8	1.53
44. BD (1) C 5- H 6	68. BD*(2) C 4- N 16	5.94
45. BD (1) C 5- H 7	66. BD*(1) C 4- C 8	2.77
45. BD (1) C 5- H 7	68. BD*(2) C 4- N 16	4.15
46. BD (1) C 5- H 20	67. BD*(1) C 4- N 16	4.90
47. BD (1) C 8- C 9	65. BD*(1) C 4- C 5	2.82
47. BD (1) C 8- C 9	66. BD*(1) C 4- C 8	1.77
47. BD (1) C 8- C 9	74. BD*(1) C 8- C 10	2.29
47. BD (1) C 8- C 9	75. BD*(1) C 9- C 11	1.77
47. BD (1) C 8- C 9	79. BD*(1) C 10- H 19	2.15
47. BD (1) C 8- C 9	82. BD*(1) C 11- H 17	1.81
48. BD (2) C 8- C 9	65. BD*(1) C 4- C 5	0.63
48. BD (2) C 8- C 9	67. BD*(1) C 4- N 16	0.55
48. BD (2) C 8- C 9	68. BD*(2) C 4- N 16	15.44
48. BD (2) C 8- C 9	76. BD*(1) C 9- H 12	3.30
48. BD (2) C 8- C 9	78. BD*(2) C 10- C 13	13.43

48. BD (2) C 8- C 9	81. BD*(2) C 11- C 14	16.64
49. BD (1) C 8- C 10	66. BD*(1) C 4- C 8	1.74
49. BD (1) C 8- C 10	67. BD*(1) C 4- N 16	1.35
49. BD (1) C 8- C 10	68. BD*(2) C 4- N 16	0.53
49. BD (1) C 8- C 10	72. BD*(1) C 8- C 9	2.32
49. BD (1) C 8- C 10	76. BD*(1) C 9- H 12	2.46
49. BD (1) C 8- C 10	77. BD*(1) C 10- C 13	1.47
49. BD (1) C 8- C 10	79. BD*(1) C 10- H 19	0.71
49. BD (1) C 8- C 10	84. BD*(1) C 13- H 18	1.88
50. BD (1) C 9- C 11	66. BD*(1) C 4- C 8	2.70
50. BD (1) C 9- C 11	72. BD*(1) C 8- C 9	1.89
50. BD (1) C 9- C 11	80. BD*(1) C 11- C 14	1.26
50. BD (1) C 9- C 11	82. BD*(1) C 11- H 17	0.79
50. BD (1) C 9- C 11	85. BD*(1) C 14- H 15	2.07
51. BD (1) C 9- H 12	73. BD*(2) C 8- C 9	0.57
51. BD (1) C 9- H 12	74. BD*(1) C 8- C 10	3.78
51. BD (1) C 9- H 12	80. BD*(1) C 11- C 14	3.65
51. BD (1) C 9- H 12	82. BD*(1) C 11- H 17	0.55
52. BD (1) C 10- C 13	66. BD*(1) C 4- C 8	3.21
52. BD (1) C 10- C 13	74. BD*(1) C 8- C 10	1.67
52. BD (1) C 10- C 13	79. BD*(1) C 10- H 19	0.74
52. BD (1) C 10- C 13	83. BD*(1) C 13- C 14	1.37
52. BD (1) C 10- C 13	84. BD*(1) C 13- H 18	0.53
52. BD (1) C 10- C 13	85. BD*(1) C 14- H 15	2.00
53. BD (2) C 10- C 13	73. BD*(2) C 8- C 9	17.28
53. BD (2) C 10- C 13	81. BD*(2) C 11- C 14	13.32
54. BD (1) C 10- H 19	72. BD*(1) C 8- C 9	4.47
54. BD (1) C 10- H 19	83. BD*(1) C 13- C 14	3.48
55. BD (1) C 11- C 14	75. BD*(1) C 9- C 11	1.40
55. BD (1) C 11- C 14	76. BD*(1) C 9- H 12	2.44
55. BD (1) C 11- C 14	82. BD*(1) C 11- H 17	0.65
55. BD (1) C 11- C 14	83. BD*(1) C 13- C 14	1.24
55. BD (1) C 11- C 14	84. BD*(1) C 13- H 18	2.10
55. BD (1) C 11- C 14	85. BD*(1) C 14- H 15	0.60
56. BD (2) C 11- C 14	73. BD*(2) C 8- C 9	13.51
56. BD (2) C 11- C 14	76. BD*(1) C 9- H 12	0.60
56. BD (2) C 11- C 14	78. BD*(2) C 10- C 13	16.65
57. BD (1) C 11- H 17	72. BD*(1) C 8- C 9	3.80
57. BD (1) C 11- H 17	83. BD*(1) C 13- C 14	3.45
58. BD (1) C 13- C 14	77. BD*(1) C 10- C 13	1.36
58. BD (1) C 13- C 14	79. BD*(1) C 10- H 19	2.18
58. BD (1) C 13- C 14	80. BD*(1) C 11- C 14	1.27
58. BD (1) C 13- C 14	82. BD*(1) C 11- H 17	2.20
58. BD (1) C 13- C 14	84. BD*(1) C 13- H 18	0.55
58. BD (1) C 13- C 14	85. BD*(1) C 14- H 15	0.60
59. BD (1) C 13- H 18	74. BD*(1) C 8- C 10	3.67
59. BD (1) C 13- H 18	80. BD*(1) C 11- C 14	3.52
60. BD (1) C 14- H 15	75. BD*(1) C 9- C 11	3.68
60. BD (1) C 14- H 15	77. BD*(1) C 10- C 13	3.60
61. BD (1) N 16- O 21	66. BD*(1) C 4- C 8	3.11

Complex 4:

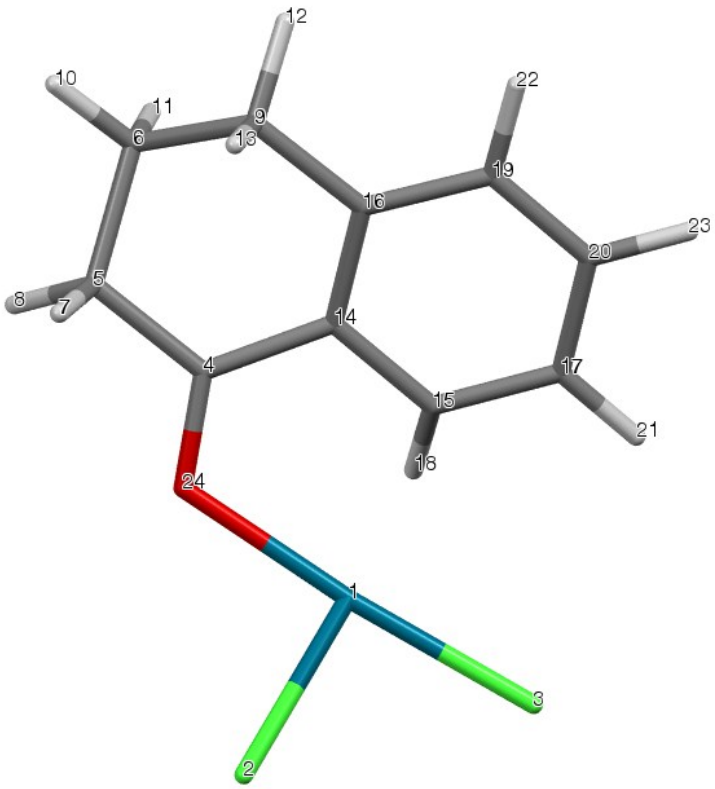


Donor (L) NBO	Acceptor (NL) NBO	*E*(2) kcalmol^{-1}
26. LP (1)Pd 1	76. BD*(1) C 8- C 9	0.19
26. LP (1)Pd 1	77. BD*(2) C 8- C 9	0.59
26. LP (1)Pd 1	80. BD*(1) C 9- H 12	0.27
26. LP (1)Pd 1	94. BD*(1) C 22- H 25	0.06
27. LP (2)Pd 1	69. BD*(1) C 4- C 5	0.07
27. LP (2)Pd 1	71. BD*(1) C 4- N 16	0.71
27. LP (2)Pd 1	72. BD*(2) C 4- N 16	0.12
27. LP (2)Pd 1	76. BD*(1) C 8- C 9	0.29
27. LP (2)Pd 1	77. BD*(2) C 8- C 9	0.35
27. LP (2)Pd 1	78. BD*(1) C 8- C 10	0.08
27. LP (2)Pd 1	79. BD*(1) C 9- C 11	0.63
27. LP (2)Pd 1	90. BD*(1) N 16- O 21	2.28
27. LP (2)Pd 1	93. BD*(1) C 22- H 24	0.07
27. LP (2)Pd 1	94. BD*(1) C 22- H 25	0.08
28. LP (3)Pd 1	72. BD*(2) C 4- N 16	2.74
28. LP (3)Pd 1	76. BD*(1) C 8- C 9	0.27
28. LP (3)Pd 1	77. BD*(2) C 8- C 9	0.59
28. LP (3)Pd 1	79. BD*(1) C 9- C 11	0.11
28. LP (3)Pd 1	80. BD*(1) C 9- H 12	1.36
28. LP (3)Pd 1	90. BD*(1) N 16- O 21	0.23
29. LP (4)Pd 1	72. BD*(2) C 4- N 16	0.84
29. LP (4)Pd 1	77. BD*(2) C 8- C 9	1.42
29. LP (4)Pd 1	80. BD*(1) C 9- H 12	5.53
30. LP (1)Cl 2	77. BD*(2) C 8- C 9	0.19
30. LP (1)Cl 2	93. BD*(1) C 22- H 24	0.07
31. LP (2)Cl 2	77. BD*(2) C 8- C 9	0.28
31. LP (2)Cl 2	80. BD*(1) C 9- H 12	0.18
31. LP (2)Cl 2	93. BD*(1) C 22- H 24	0.48

32. LP (3)Cl 2	77. BD*(2) C 8- C 9	0.11
32. LP (3)Cl 2	80. BD*(1) C 9- H 12	0.09
32. LP (3)Cl 2	93. BD*(1) C 22- H 24	4.05
33. LP (1)Cl 3	77. BD*(2) C 8- C 9	0.12
33. LP (1)Cl 3	80. BD*(1) C 9- H 12	0.08
33. LP (1)Cl 3	86. BD*(1) C 11- H 17	0.06
34. LP (2)Cl 3	76. BD*(1) C 8- C 9	0.22
34. LP (2)Cl 3	77. BD*(2) C 8- C 9	0.07
34. LP (2)Cl 3	84. BD*(1) C 11- C 14	0.18
34. LP (2)Cl 3	85. BD*(2) C 11- C 14	0.17
34. LP (2)Cl 3	86. BD*(1) C 11- H 17	0.60
35. LP (3)Cl 3	72. BD*(2) C 4- N 16	0.10
35. LP (3)Cl 3	77. BD*(2) C 8- C 9	0.07
35. LP (3)Cl 3	80. BD*(1) C 9- H 12	0.08
39. BD (1)Pd 1-Cl 2	71. BD*(1) C 4- N 16	0.10
39. BD (1)Pd 1-Cl 2	72. BD*(2) C 4- N 16	0.27
39. BD (1)Pd 1-Cl 2	77. BD*(2) C 8- C 9	2.59
39. BD (1)Pd 1-Cl 2	79. BD*(1) C 9- C 11	0.09
39. BD (1)Pd 1-Cl 2	80. BD*(1) C 9- H 12	0.25
39. BD (1)Pd 1-Cl 2	86. BD*(1) C 11- H 17	0.06
39. BD (1)Pd 1-Cl 2	91. BD*(1) O 21- C 22	0.12
39. BD (1)Pd 1-Cl 2	93. BD*(1) C 22- H 24	0.47
39. BD (1)Pd 1-Cl 2	94. BD*(1) C 22- H 25	0.11
40. BD (1)Pd 1-Cl 3	72. BD*(2) C 4- N 16	0.19
40. BD (1)Pd 1-Cl 3	77. BD*(2) C 8- C 9	1.54
40. BD (1)Pd 1-Cl 3	80. BD*(1) C 9- H 12	0.33
40. BD (1)Pd 1-Cl 3	90. BD*(1) N 16- O 21	0.20
36. LP (1) N 16	67. BD*(1)Pd 1-Cl 2	17.70
36. LP (1) N 16	68. BD*(1)Pd 1-Cl 3	96.46
37. LP (1) O 21	67. BD*(1)Pd 1-Cl 2	0.34
37. LP (1) O 21	68. BD*(1)Pd 1-Cl 3	0.56
38. LP (2) O 21	67. BD*(1)Pd 1-Cl 2	0.18
38. LP (2) O 21	68. BD*(1)Pd 1-Cl 3	0.27
41. BD (1) C 4- C 5	67. BD*(1)Pd 1-Cl 2	0.55
41. BD (1) C 4- C 5	68. BD*(1)Pd 1-Cl 3	0.84
43. BD (1) C 4- N 16	67. BD*(1)Pd 1-Cl 2	0.86
43. BD (1) C 4- N 16	68. BD*(1)Pd 1-Cl 3	3.84
44. BD (2) C 4- N 16	67. BD*(1)Pd 1-Cl 2	0.08
44. BD (2) C 4- N 16	68. BD*(1)Pd 1-Cl 3	1.51
48. BD (1) C 8- C 9	67. BD*(1)Pd 1-Cl 2	1.65
48. BD (1) C 8- C 9	68. BD*(1)Pd 1-Cl 3	0.45
49. BD (2) C 8- C 9	67. BD*(1)Pd 1-Cl 2	19.05
49. BD (2) C 8- C 9	68. BD*(1)Pd 1-Cl 3	6.46
52. BD (1) C 9- H 12	67. BD*(1)Pd 1-Cl 2	53.70
52. BD (1) C 9- H 12	68. BD*(1)Pd 1-Cl 3	8.04
56. BD (1) C 11- C 14	67. BD*(1)Pd 1-Cl 2	0.09
57. BD (2) C 11- C 14	67. BD*(1)Pd 1-Cl 2	0.14
57. BD (2) C 11- C 14	68. BD*(1)Pd 1-Cl 3	0.08
62. BD (1) N 16- O 21	67. BD*(1)Pd 1-Cl 2	0.16
63. BD (1) O 21- C 22	67. BD*(1)Pd 1-Cl 2	0.06
65. BD (1) C 22- H 24	67. BD*(1)Pd 1-Cl 2	0.15
65. BD (1) C 22- H 24	68. BD*(1)Pd 1-Cl 3	0.33
36. LP (1) N 16	69. BD*(1) C 4- C 5	7.91
36. LP (1) N 16	70. BD*(1) C 4- C 8	1.33
37. LP (1) O 21	75. BD*(1) C 5- H 20	0.54

37. LP (1) O 21	93. BD*(1) C 22- H 24	0.81
37. LP (1) O 21	94. BD*(1) C 22- H 25	1.17
38. LP (2) O 21	71. BD*(1) C 4- N 16	1.19
38. LP (2) O 21	72. BD*(2) C 4- N 16	13.41
38. LP (2) O 21	92. BD*(1) C 22- H 23	4.64
38. LP (2) O 21	93. BD*(1) C 22- H 24	3.18

Complex 5:



Donor (L) NBO	Acceptor (NL) NBO	*E*(2) kcalmol^{-1}
26. LP (1)Pd 1	66. BD*(1)Pd 1-Cl 2	5.01
26. LP (1)Pd 1	67. BD*(1)Pd 1-Cl 3	3.95
27. LP (2)Pd 1	66. BD*(1)Pd 1-Cl 2	6.20
27. LP (2)Pd 1	67. BD*(1)Pd 1-Cl 3	4.54
28. LP (3)Pd 1	213. RY (1)Cl 3	1.01
29. LP (4)Pd 1	66. BD*(1)Pd 1-Cl 2	0.57
29. LP (4)Pd 1	67. BD*(1)Pd 1-Cl 3	0.50
30. LP (1)Cl 2	66. BD*(1)Pd 1-Cl 2	0.55
31. LP (2)Cl 2	66. BD*(1)Pd 1-Cl 2	4.96
31. LP (2)Cl 2	67. BD*(1)Pd 1-Cl 3	5.44
33. LP (1)Cl 3	66. BD*(1)Pd 1-Cl 2	2.09
33. LP (1)Cl 3	67. BD*(1)Pd 1-Cl 3	1.58
34. LP (2)Cl 3	66. BD*(1)Pd 1-Cl 2	3.37
34. LP (2)Cl 3	67. BD*(1)Pd 1-Cl 3	2.43
38. BD (1)Pd 1-Cl 2	66. BD*(1)Pd 1-Cl 2	7.58
38. BD (1)Pd 1-Cl 2	67. BD*(1)Pd 1-Cl 3	29.66
39. BD (1)Pd 1-Cl 3	66. BD*(1)Pd 1-Cl 2	22.92
39. BD (1)Pd 1-Cl 3	67. BD*(1)Pd 1-Cl 3	3.75
26. LP (1)Pd 1	68. BD*(1) C 4- C 5	0.06
26. LP (1)Pd 1	71. BD*(2) C 4- O 24	0.09
26. LP (1)Pd 1	84. BD*(1) C 15- C 17	0.33
26. LP (1)Pd 1	85. BD*(2) C 15- C 17	0.51
26. LP (1)Pd 1	86. BD*(1) C 15- H 18	0.16
27. LP (2)Pd 1	68. BD*(1) C 4- C 5	0.11
27. LP (2)Pd 1	70. BD*(1) C 4- O 24	0.24
27. LP (2)Pd 1	81. BD*(1) C 14- C 15	0.64

27. LP (2)Pd 1	82. BD*(1) C 14- C 16	0.09
27. LP (2)Pd 1	83. BD*(2) C 14- C 16	0.09
27. LP (2)Pd 1	84. BD*(1) C 15- C 17	0.53
27. LP (2)Pd 1	85. BD*(2) C 15- C 17	0.57
27. LP (2)Pd 1	86. BD*(1) C 15- H 18	0.21
28. LP (3)Pd 1	71. BD*(2) C 4- O 24	1.85
28. LP (3)Pd 1	81. BD*(1) C 14- C 15	0.12
28. LP (3)Pd 1	84. BD*(1) C 15- C 17	0.08
28. LP (3)Pd 1	85. BD*(2) C 15- C 17	0.11
28. LP (3)Pd 1	86. BD*(1) C 15- H 18	1.05
29. LP (4)Pd 1	71. BD*(2) C 4- O 24	0.06
29. LP (4)Pd 1	83. BD*(2) C 14- C 16	0.06
29. LP (4)Pd 1	85. BD*(2) C 15- C 17	2.98
29. LP (4)Pd 1	86. BD*(1) C 15- H 18	8.08
30. LP (1)Cl 2	70. BD*(1) C 4- O 24	0.13
30. LP (1)Cl 2	85. BD*(2) C 15- C 17	0.13
31. LP (2)Cl 2	70. BD*(1) C 4- O 24	0.07
31. LP (2)Cl 2	85. BD*(2) C 15- C 17	0.41
32. LP (3)Cl 2	85. BD*(2) C 15- C 17	0.19
32. LP (3)Cl 2	86. BD*(1) C 15- H 18	0.16
33. LP (1)Cl 3	85. BD*(2) C 15- C 17	0.14
33. LP (1)Cl 3	86. BD*(1) C 15- H 18	0.09
33. LP (1)Cl 3	89. BD*(1) C 17- H 21	0.07
34. LP (2)Cl 3	81. BD*(1) C 14- C 15	0.22
34. LP (2)Cl 3	88. BD*(1) C 17- C 20	0.09
34. LP (2)Cl 3	89. BD*(1) C 17- H 21	0.25
35. LP (3)Cl 3	86. BD*(1) C 15- H 18	0.16
35. LP (3)Cl 3	88. BD*(1) C 17- C 20	0.06
35. LP (3)Cl 3	89. BD*(1) C 17- H 21	0.18
38. BD (1)Pd 1-Cl 2	70. BD*(1) C 4- O 24	0.13
38. BD (1)Pd 1-Cl 2	84. BD*(1) C 15- C 17	0.14
38. BD (1)Pd 1-Cl 2	85. BD*(2) C 15- C 17	2.60
38. BD (1)Pd 1-Cl 2	86. BD*(1) C 15- H 18	0.35
38. BD (1)Pd 1-Cl 2	89. BD*(1) C 17- H 21	0.06
39. BD (1)Pd 1-Cl 3	81. BD*(1) C 14- C 15	0.06
39. BD (1)Pd 1-Cl 3	85. BD*(2) C 15- C 17	1.24
39. BD (1)Pd 1-Cl 3	86. BD*(1) C 15- H 18	0.51
36. LP (1) O 24	66. BD*(1)Pd 1-Cl 2	0.99
36. LP (1) O 24	67. BD*(1)Pd 1-Cl 3	10.69
37. LP (2) O 24	66. BD*(1)Pd 1-Cl 2	6.03
37. LP (2) O 24	67. BD*(1)Pd 1-Cl 3	58.22
40. BD (1) C 4- C 5	66. BD*(1)Pd 1-Cl 2	0.17
40. BD (1) C 4- C 5	67. BD*(1)Pd 1-Cl 3	0.38
41. BD (1) C 4- C 14	66. BD*(1)Pd 1-Cl 2	0.16
41. BD (1) C 4- C 14	67. BD*(1)Pd 1-Cl 3	0.28
42. BD (1) C 4- O 24	66. BD*(1)Pd 1-Cl 2	0.42
42. BD (1) C 4- O 24	67. BD*(1)Pd 1-Cl 3	2.79
43. BD (2) C 4- O 24	67. BD*(1)Pd 1-Cl 3	0.57
53. BD (1) C 14- C 15	66. BD*(1)Pd 1-Cl 2	1.28
53. BD (1) C 14- C 15	67. BD*(1)Pd 1-Cl 3	0.37
56. BD (1) C 15- C 17	66. BD*(1)Pd 1-Cl 2	0.05
57. BD (2) C 15- C 17	66. BD*(1)Pd 1-Cl 2	17.91
57. BD (2) C 15- C 17	67. BD*(1)Pd 1-Cl 3	5.38
58. BD (1) C 15- H 18	66. BD*(1)Pd 1-Cl 2	64.37
58. BD (1) C 15- H 18	67. BD*(1)Pd 1-Cl 3	9.33
60. BD (1) C 17- C 20	66. BD*(1)Pd 1-Cl 2	0.14
60. BD (1) C 17- C 20	67. BD*(1)Pd 1-Cl 3	0.07

36. LP (1) O 24	69. BD*(1) C 4- C 14	6.26
37. LP (2) O 24	68. BD*(1) C 4- C 5	14.14
37. LP (2) O 24	69. BD*(1) C 4- C 14	6.34
40. BD (1) C 4- C 5	76. BD*(1) C 6- H 10	1.32
40. BD (1) C 4- C 5	81. BD*(1) C 14- C 15	2.65
41. BD (1) C 4- C 14	74. BD*(1) C 5- H 8	0.61
41. BD (1) C 4- C 14	81. BD*(1) C 14- C 15	1.58
41. BD (1) C 4- C 14	82. BD*(1) C 14- C 16	1.91
41. BD (1) C 4- C 14	84. BD*(1) C 15- C 17	2.01
41. BD (1) C 4- C 14	87. BD*(1) C 16- C 19	2.39
42. BD (1) C 4- O 24	69. BD*(1) C 4- C 14	0.61
42. BD (1) C 4- O 24	72. BD*(1) C 5- C 6	0.66
42. BD (1) C 4- O 24	82. BD*(1) C 14- C 16	1.40
43. BD (2) C 4- O 24	73. BD*(1) C 5- H 7	0.99
43. BD (2) C 4- O 24	83. BD*(2) C 14- C 16	5.03
44. BD (1) C 5- C 6	70. BD*(1) C 4- O 24	3.56
44. BD (1) C 5- C 6	78. BD*(1) C 9- H 12	1.70
45. BD (1) C 5- H 7	69. BD*(1) C 4- C 14	0.99
45. BD (1) C 5- H 7	71. BD*(2) C 4- O 24	7.89
45. BD (1) C 5- H 7	77. BD*(1) C 6- H 11	2.56
46. BD (1) C 5- H 8	69. BD*(1) C 4- C 14	2.46
46. BD (1) C 5- H 8	71. BD*(2) C 4- O 24	3.70
46. BD (1) C 5- H 8	75. BD*(1) C 6- C 9	2.63
47. BD (1) C 6- C 9	74. BD*(1) C 5- H 8	1.78
47. BD (1) C 6- C 9	80. BD*(1) C 9- C 16	0.62
47. BD (1) C 6- C 9	83. BD*(2) C 14- C 16	0.76
47. BD (1) C 6- C 9	87. BD*(1) C 16- C 19	2.69
48. BD (1) C 6- H 10	68. BD*(1) C 4- C 5	2.93
48. BD (1) C 6- H 10	80. BD*(1) C 9- C 16	2.87
49. BD (1) C 6- H 11	73. BD*(1) C 5- H 7	2.66
49. BD (1) C 6- H 11	79. BD*(1) C 9- H 13	2.69
50. BD (1) C 9- H 12	72. BD*(1) C 5- C 6	2.75

Supplementary Table 1: QTAIM properties of Pd-X(8) bond crtical point for complexes **1** to **5**[a]

Property	Complex 1	Complex 2	Complex 3	Complex 4	Complex 5
Bcp properties:					
Pd–X(8) bcp	Pd····H(8)	Pd····C(8)	Pd·····H(8)	Pd····C(8)	Pd····C(8)
Ellipticity, ε(bcp)	5.3365	2.2016	12.4515	1.5120	13.7800
Potential energy density, V	-0.1078	-0.1015	-0.1076	-0.1007	-0.1156
Kinetic energy density, G	0.0868	0.0771	0.0859	0.0753	0.0907
Total energy density, H	-0.0210	-0.0244	-0.0217	-0.0254	-0.0249
-V/G	1.2419	1.3165	1.2526	1.3373	1.2745
C–H(8) bcp					
Laplacian of electron density, $\nabla^2\rho$(bcp)	-0.6268 (-0.9458)	-0.6350 (-0.9460)	-0.6282 (-0.9461)	-0.6443 (-0.9464)	-0.5984 (-0.9500)
Atomic basin properties:					
H8 atom					
Charge, q(H8)	0.056 (0.040)	0.044 (0.040)	0.057 (0.039)	0.044 (0.039)	0.050 (0.055)
Total energy, E(H8)	-0.631 (-0.609)	-0.633 (-0.609)	-0.632 (-0.610)	-0.635 (-0.610)	-0.634 (-0.602)
Dipolarisation, M(H8)	0.099 (0.129)	0.108 (0.130)	0.101 (0.130)	0.110 (0.130)	0.105 (0.128)
Volume, V(H8)[b]	36.0 (46.5)	37.2 (46.5)	36.1 (46.7)	37.4 (46.7)	36.5 (45.7)
C8 atom					
Charge, q(C8)	-0.084 (0.001)	-0.070 (0.001)	-0.086 (0.002)	-0.072 (0.002)	-0.066 (0.002)
Total energy, E(C8)	-40.06 (-38.07)	-40.00 (-38.07)	-40.17 (-38.07)	-40.11 (-38.07)	-40.12 (-38.08)
Dipolarisation, M(C8)	0.142 (0.115)	0.113 (0.116)	0.136 (0.114)	0.105 (0.114)	0.138 (0.114)
Volume, V(C8)[a]	69.1 (82.3)	67.4 (82.4)	68.5 (82.4)	67.1 (82.4)	67.6 (81.9)

[a] Free ligand values in brackets ( )

[b] 0.001 isosurface

Atomic Units:
ρ(bcp) = e/bohr^3
$\nabla^2\rho$(bcp) = e/bohr^5
H, G, V = Hartree/bohr^3
ε(bcp) = Dimensionless
Atomic charge, q = e
Atomic energy, E =Hartree
Atomic dipolaisation, M= e*bohr
Atomic volume, V =1/bohr^3