Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Data for Communication

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Supplementary Table 5: Occupancy (n) and energies (a.u) of NBOs involved donor-acceptor interactions for complexes (**1**) to (**5**) and [PdCl(CH_3)(1-tetralone oxime)].

Supplementary Table 6: Selected structural data for (**1**) to (**5**) and [PdCl(CH_3)(1-tetralone oxime)].

Supplementary Table 7: NBO donations (kcal mol^{-1}) for (**1**) to (**5**) and [PdCl(CH_3)(1-tetralone oxime)].

Supplementary Data 1: Computational details for complexes (**1**) to (**6**) and [PdCl(CH_3)(1-tetralone oxime)].

DFT PBE-D3[1] functional based geometry optimizations and vibrational calculations for the complexes (**1**)-(**6**) were performed using the Gaussian09 (G09)[2] software. A triple-zeta high quality basis set (aug-cc-pVTZ-PP)[3] was employed for Pd; aug-cc-pVTZ[4] for the attached ancillary ligands (Cl atoms), agostic hydrogen and nitrogen (attached to Pd) and double-zeta quality basis set (aug-cc-pVDZ)[4] was used for the remainder of atoms. All the structures were energy-minimised as no imaginary frequency was found in the vibrational analysis. For the QTAIM analysis, the input files (.wfx) were obtained from G09[2] and QTAIM calculations were performed with the AIMALL software[5]. The NBO calculations were performed with the NBO6.0 package[6] and NBOView2.0[6] was used to visualize the contours and surfaces of donor-acceptor interactions. The same procedure was used for the ligand calculations.

Supplementary Data 2: Cartesian coordinates and energies for calculated structures (**1**) to (**6**) and [PdCl(CH_3)(1-tetralone oxime)].

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

0 1

Pd	1.33110500	0.05038900	-0.09868200
Cl	2.95379500	-1.43745800	0.54319000
Cl	2.71227200	1.85393100	-0.11694400
C	-1.28543400	-1.19282400	-0.21582800
C	-2.35744000	-2.24306700	-0.17071000
C	-3.74675000	-1.62350800	-0.38995400
H	-2.29873400	-2.75054100	0.81548500
H	-2.13424100	-3.02656200	-0.91910900
C	-3.95155400	-0.38031400	0.49054600
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 = -2572.52350911 a.u)

0 1

Pd	-2.49625200	-0.37269500	-0.06109400
Cl	-4.38623800	0.35300000	0.99942700
Cl	-3.13852000	-2.54649000	-0.13614700
C	-0.54504200	1.75612900	-0.37088800
C	0.06132300	3.12707100	-0.36263300
C	1.51452000	3.07681600	-0.85055100
H	-0.00046800	3.52362800	0.67285300
H	-0.56018700	3.80519800	-0.97712600
C	2.30922500	1.96184600	-0.15530800
H	2.00329400	4.05000700	-0.66653900
H	1.53462400	2.90630700	-1.94472200
H	3.34712100	1.94458300	-0.52379000
H	2.37142300	2.15743500	0.93594200
C	0.25881900	0.54995800	-0.55400300
C	-0.40273200	-0.69955300	-0.75327200
C	1.66165200	0.60902700	-0.36060800
C	0.30488300	-1.90914600	-0.68818500
H	-1.35432400	-0.72570100	-1.40991000
C	2.33003700	-0.63576000	-0.33262400
C	1.68620000	-1.87864300	-0.45887200
H	-0.22845300	-2.85770000	-0.82355000
H	2.27239300	-2.80280700	-0.40219600
N	-1.80496800	1.51950900	-0.10079400
O	-2.58509200	2.59875400	0.18906700
H	-3.43820300	2.15421200	0.48879100
S	4.13991900	-0.73303500	-0.12790700
O	4.82804700	0.25423700	-1.01073700
O	4.55480400	-2.16318500	-0.09256700
Cl	4.33776100	0.00619000	1.89249700

Complex (3): (E = -1816.51594223 a.u)

-1 1

C	-0.12629200	1.72190100	-0.28032700
C	0.51697300	3.07464700	-0.19104900
C	1.98790100	2.99829600	-0.62492600
H	0.43175800	3.42212700	0.86108000
H	-0.06519500	3.79882200	-0.79268500
C	2.72549300	1.84226500	0.06203700
H	2.48862900	3.96095100	-0.40659200
H	2.03365800	2.85143000	-1.72342500
H	3.76114400	1.75175100	-0.31020500
H	2.81421800	2.01863200	1.15431500
C	0.65849400	0.50609800	-0.44470300
C	-0.04024800	-0.72538900	-0.69133300
C	2.03984800	0.51078000	-0.16400400
C	0.65920800	-1.94269400	-0.56207100
H	-0.88228900	-0.71544900	-1.45693100
C	2.75732000	-0.72068600	-0.06359600
C	2.02439400	-1.91933000	-0.24305500
H	0.12440000	-2.88424000	-0.74288500
H	2.58195000	-2.86185600	-0.15014000
N	-1.40530600	1.51449300	-0.08919900
Pd	-2.12591800	-0.36108000	-0.06393300
O	-2.18271600	2.61803700	0.19312000
H	-3.06108800	2.17664800	0.40939900
Cl	-4.15324200	0.45257900	0.77336200
Cl	-2.81556300	-2.54469200	-0.17141700
B	4.36769900	-0.77059500	0.31874600
O	4.79671900	-2.19257000	0.46626700
H	5.56416100	-2.29454000	-0.11997700
O	5.14937400	-0.07592500	-0.75076800
H	5.83400400	0.42343200	-0.27121100
O	4.56423900	-0.04441000	1.62173200
H	4.79570300	-0.73696900	2.26312300

Complex (4): (E = -1962.33595181 a.u)

-1 1

Pd	-1.65064900	-0.28566600	-0.04801200
Cl	-3.69923900	0.78406100	0.62364100
Cl	-2.47208400	-2.43759700	-0.07467500
C	0.48820500	1.63869300	-0.28972700
C	1.24485500	2.92993400	-0.18946000
C	2.73327100	2.69822500	-0.49094400
H	1.10506200	3.33095700	0.83737600
H	0.79311100	3.68198700	-0.86522700
C	3.28448600	1.47966000	0.26337900
H	3.31313100	3.60553700	-0.23372800
H	2.86087000	2.52836000	-1.57934600
H	4.34195700	1.28420500	0.00408300
H	3.28666400	1.67031800	1.35927900
C	1.15538400	0.34891600	-0.41385900
C	0.31255600	-0.79808600	-0.74633200
C	2.48938200	0.22764800	-0.02869400
C	0.90550300	-2.09360800	-0.54742500
H	-0.27257900	-0.69718300	-1.68730800
C	3.07217500	-1.09415500	0.12840000
C	2.20765600	-2.22699900	-0.11190700
H	0.29264600	-2.97883800	-0.76228300
H	2.64393800	-3.22359300	0.03819900
N	-0.80638900	1.52853500	-0.11625500
O	-1.50181200	2.68856100	0.12437200
S	4.70009000	-1.32058300	0.61414100
H	-2.42551300	2.30871800	0.31704900

Complex (5): (E = -1487.44994119 a.u)

0 1

Pd	-0.91641600	-0.23729900	-0.09354300
Cl	-2.91194600	0.68899500	0.55394400
Cl	-1.70618300	-2.36594600	-0.15774700
C	1.21525900	1.74231100	-0.20224200
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
H	2.92196700	3.03484900	-0.45802700
O	-0.83371600	2.73502700	-0.07977200
H	-1.75429100	2.36072800	0.09236300

Complex (6): (E = -1488.45190461 a.u)

0 1

C	-0.68348900	2.11316400	-0.03810400
C	-1.66126600	-0.02605300	0.00761500
C	-2.97855200	0.54925000	-0.00357000
C	-3.09551600	1.96647500	-0.03113500
C	-1.94937700	2.74215600	-0.04840300
H	0.25217800	2.68852100	-0.04665800
C	-1.50302600	-1.44538000	0.03140800
C	-4.11191800	-0.31374500	0.00515600
H	-4.09395400	2.42444200	-0.04031500
H	-1.99499400	3.83740000	-0.07095900
C	-3.94331400	-1.68910100	0.02020500
C	-2.63980300	-2.24842700	0.03136100
H	-5.11551500	0.13163300	-0.00617800
H	-4.81707000	-2.35344200	0.02228900
H	-2.52146300	-3.34038700	0.04283500
N	-0.53429600	0.78468500	-0.01208300
Pd	1.30855100	-0.15081300	-0.02320200
C	-0.12051300	-2.01570000	0.07103200
H	0.49102800	-1.65236300	-0.82477800
H	0.37983400	-1.81880300	1.04402300
H	-0.06835300	-3.10305700	-0.06676000
Cl	2.49492400	1.77474500	0.10255500
Cl	3.22011400	-1.37269600	-0.05402700

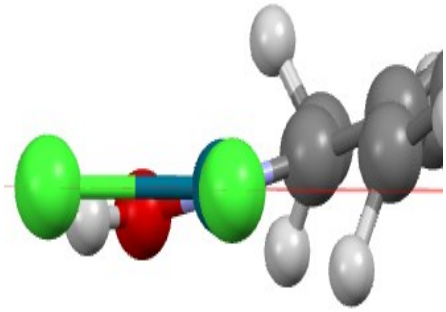
Complex (Cl^1 replaced by CH_3): [PdCl(CH_3)(1-tetralone oxime)]

(E = - -1144.58365822 a.u)

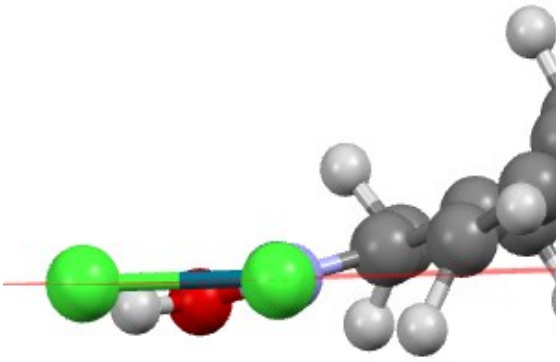
0 1

Pd	1.46746400	0.31339200	-0.11601000
Cl	3.25774200	-0.97818800	0.53084000
C	-1.06246100	-1.23827600	-0.19547300
C	-2.05207400	-2.36884600	-0.15703400
C	-3.48594600	-1.86475200	-0.37876100
H	-1.95871700	-2.87305200	0.82808900
H	-1.76368200	-3.13017700	-0.90626500
C	-3.78621100	-0.64394200	0.50484500
H	-4.20420100	-2.67828100	-0.16887000
H	-3.61758100	-1.58016600	-1.44147800
H	-4.81665100	-0.27961400	0.33442800
H	-3.73360000	-0.93923300	1.57497700
C	-1.49143600	0.16325700	-0.17262400
C	-0.54755600	1.20841600	-0.42321200
C	-2.80387600	0.47977500	0.24755800
C	-0.91303700	2.54950700	-0.21641800
H	0.28005800	1.04281000	-1.22363500
C	-3.14499800	1.83271900	0.43619100
C	-2.20844200	2.85808200	0.22928600
H	-0.18934000	3.34755500	-0.42289200
H	-4.16454800	2.08523300	0.76038300
H	-2.49700900	3.90479100	0.39208700
N	0.23188300	-1.38725600	-0.13573400
O	0.70941200	-2.67028300	-0.06155700
H	1.68176400	-2.49927900	0.09538200
C	2.58054900	2.01461000	-0.14834200
H	3.64526900	1.77076100	-0.23230500
H	2.26368100	2.64139800	-0.99498000
H	2.38407700	2.53017600	0.80373800

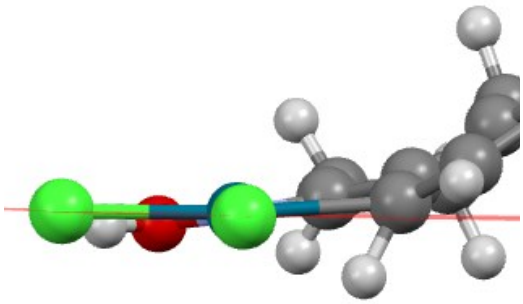
Supplementary Figure 1: Ball and stick diagrams showing the agostic C-H bond in relation to the Pd coordination plane for complexes (**1**) to (**5**)



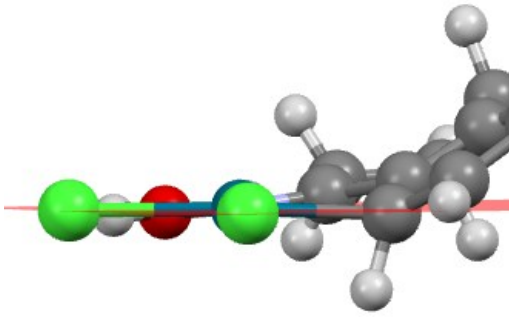
Complex (**1**)



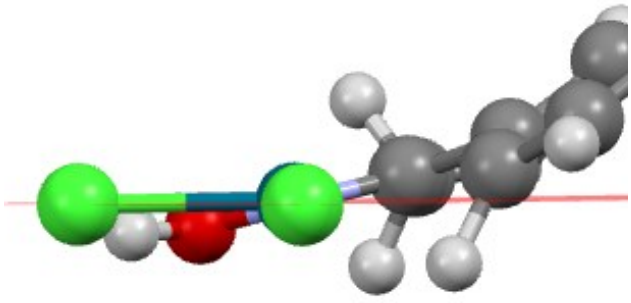
Complex (**2**)



Complex (**3**)



Complex (**4**)



Complex (**5**)

Supplementary Figure 2: NBO electron density and contour plots for the various interactions in complex (**1**)

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

NBOView2.0[6] 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

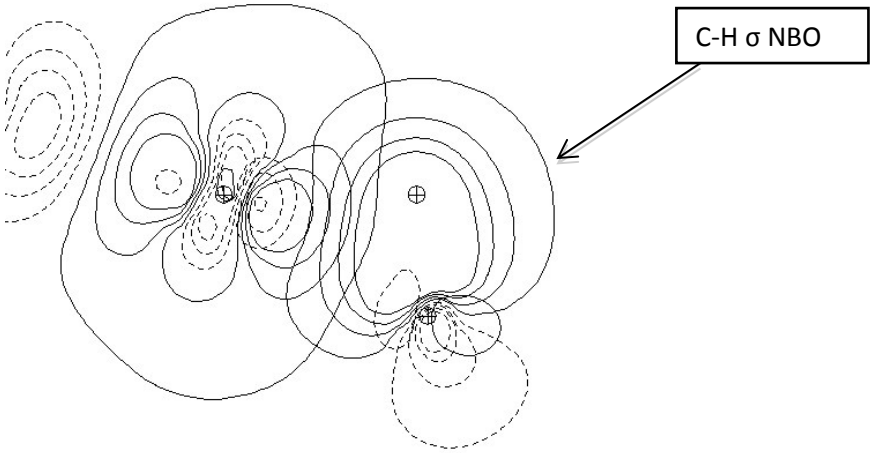
Stepsize: 0.4000

(The outermost value (0.0316 a.u) of the contour corresponds roughly to the empirical van der Waals radius).[6]

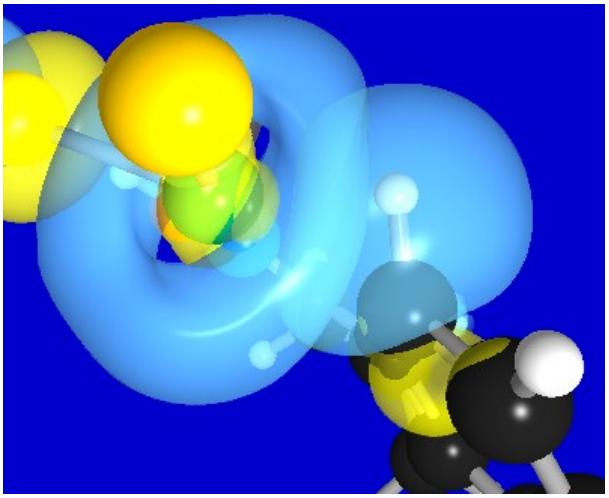
Complex 1: [Pd(Cl)2(1-tetralone oxime)]

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

Contour plot

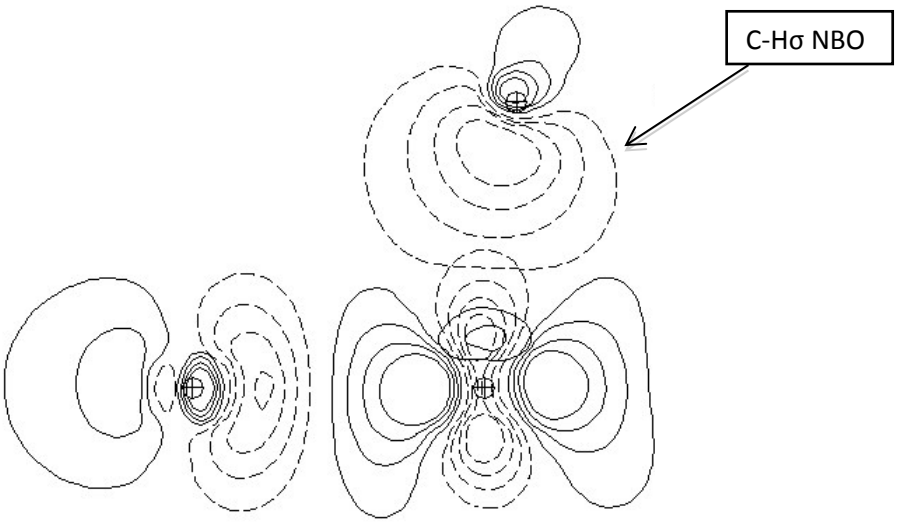


3D Surfaces showing NBOs interaction,

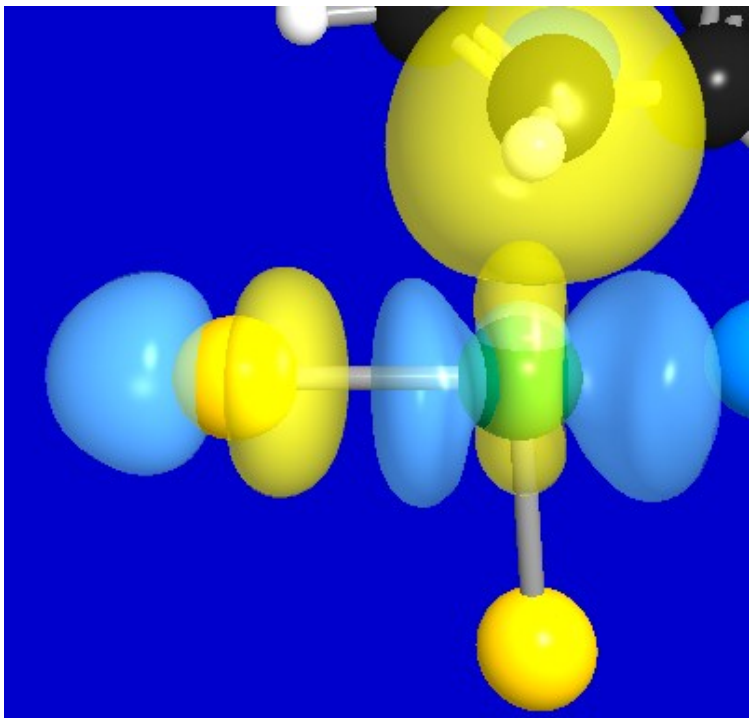


2) C(8)-H(8)σ to Pd-Cl (*cis*)* [agostic donation E(2) = 10.0 kcalmol^{-1}]

Contour plot

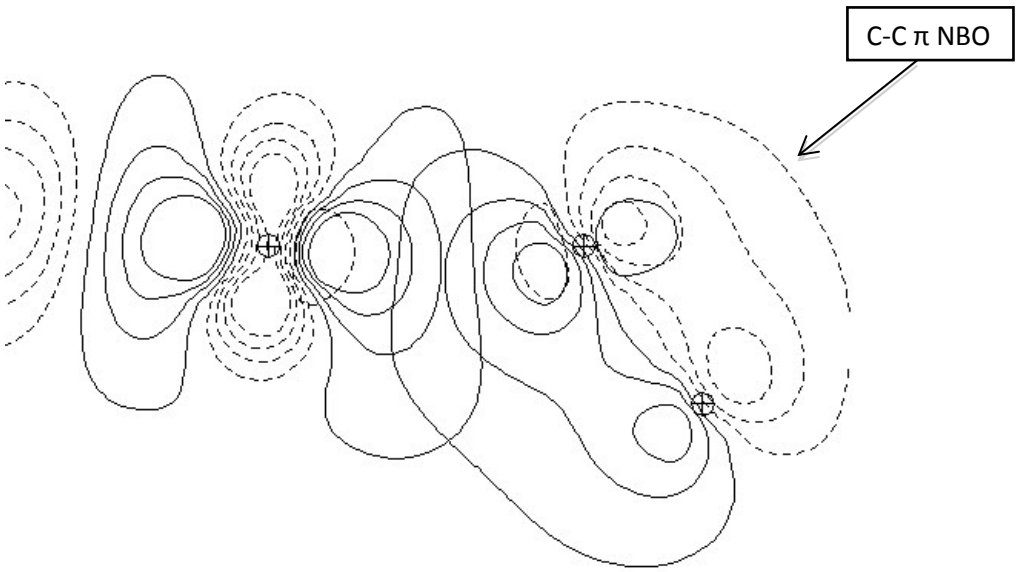


3D Surfaces showing NBOs interaction

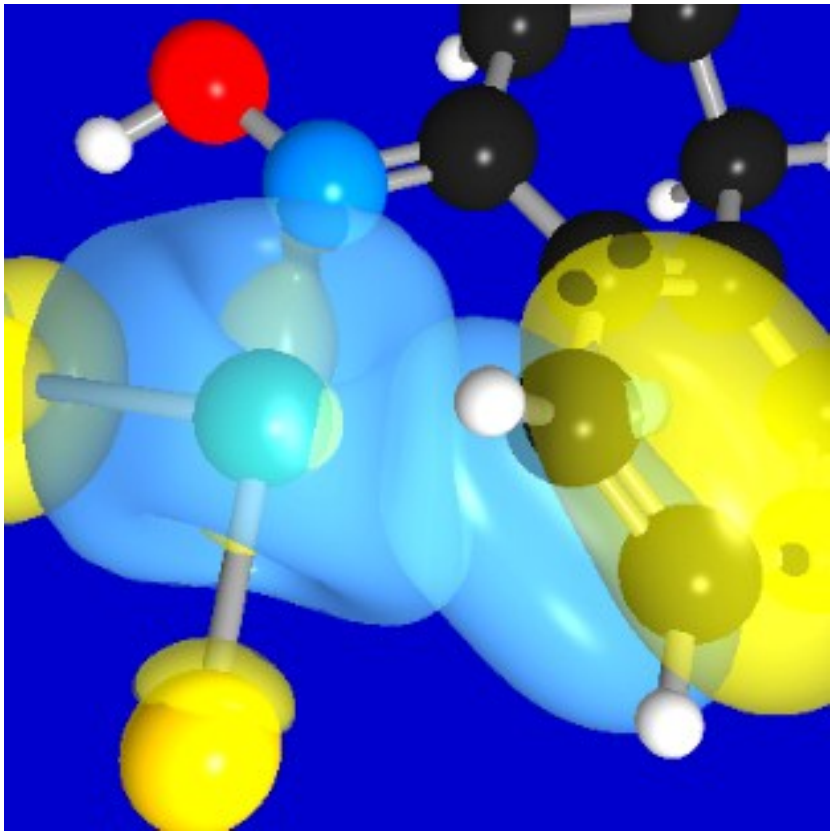


3) C(7)-C(8)π to Pd-Cl (*trans*) σ* [E(2)=20.3 kcalmol^{-1}]

Contour plot

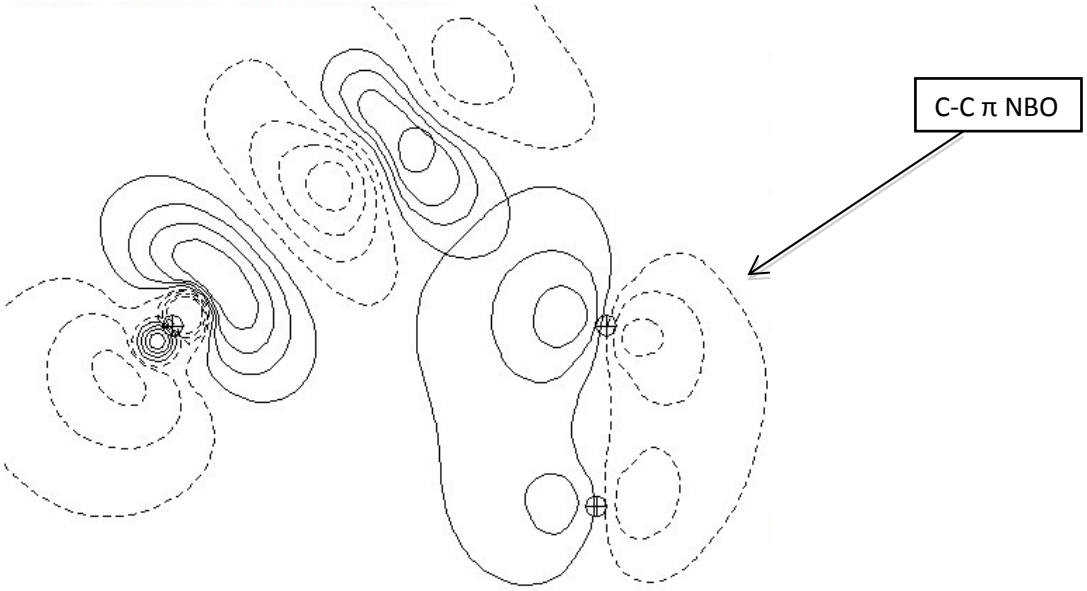


3D Surfaces showing NBOs interaction

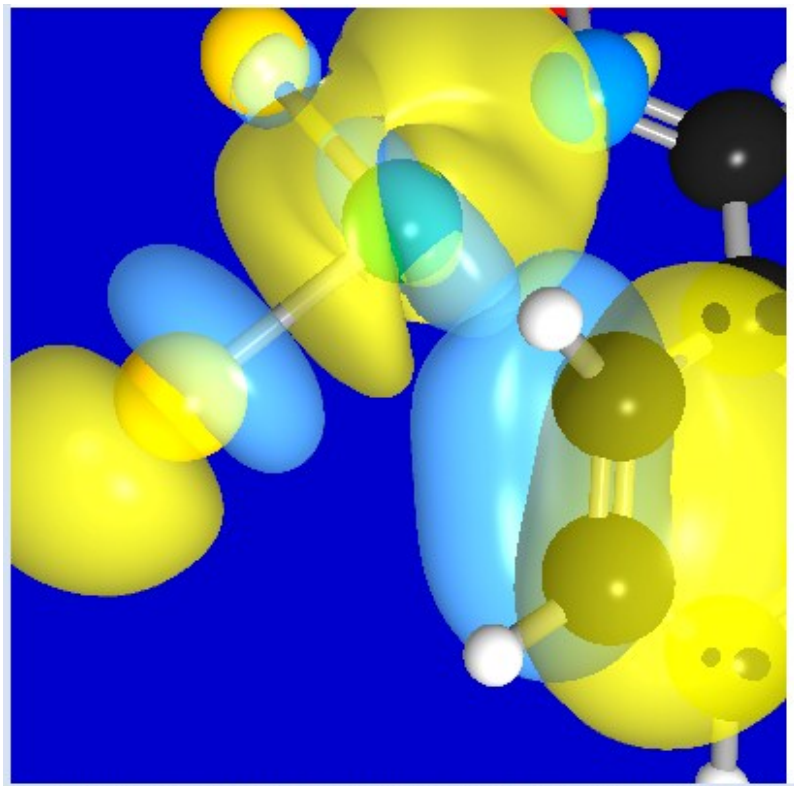


4) C(7)-C(8)π to BD*(1) Pd-Cl (*cis*) σ* (E(2)=6.5 kcalmol^{-1}]

Contour plot

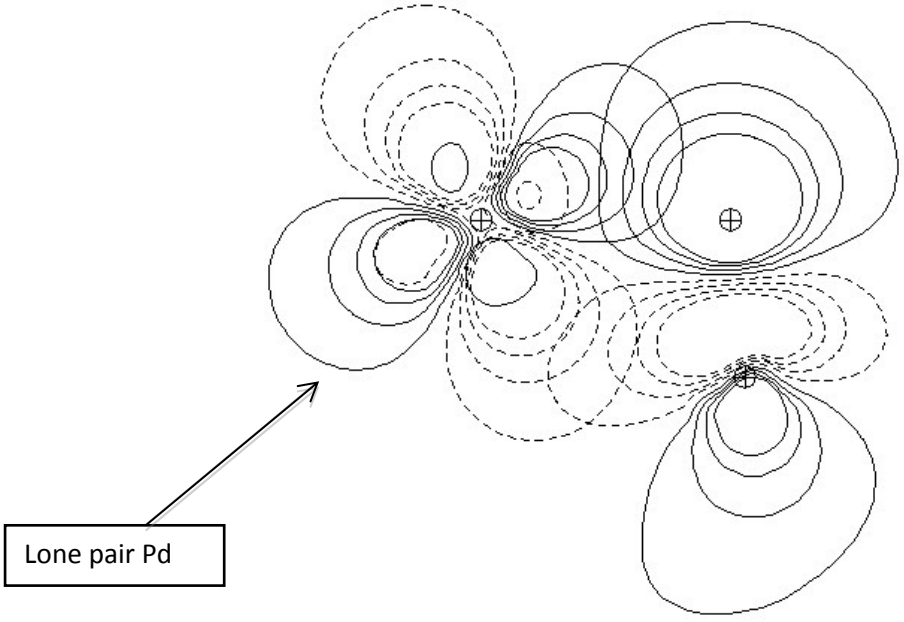


3D Surfaces showing NBOs interaction

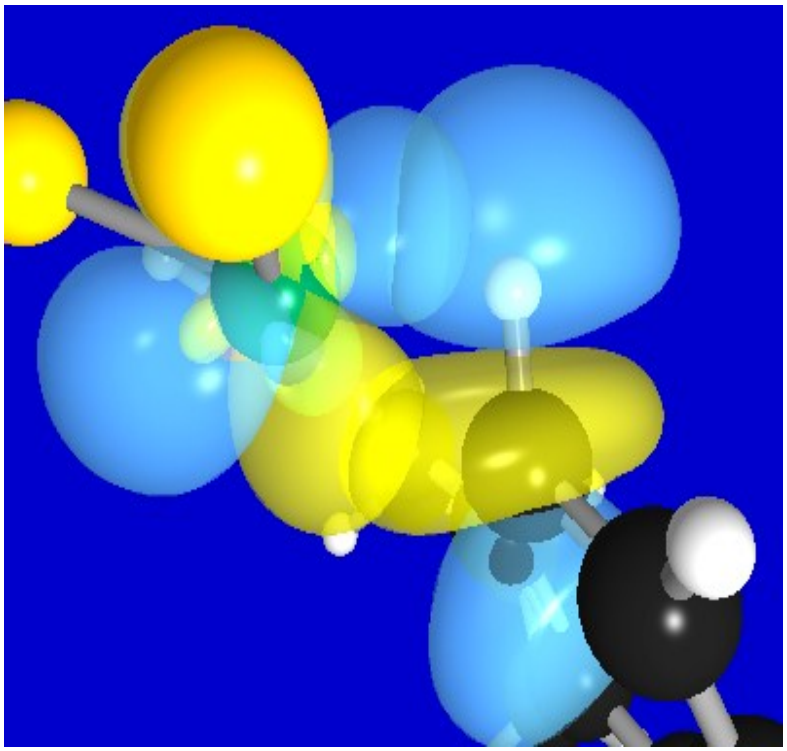


5) Lone pair (4) Pd to C(8)-H(8)σ* [E(2)=4.9 kcalmol^{-1}]

Contour plot

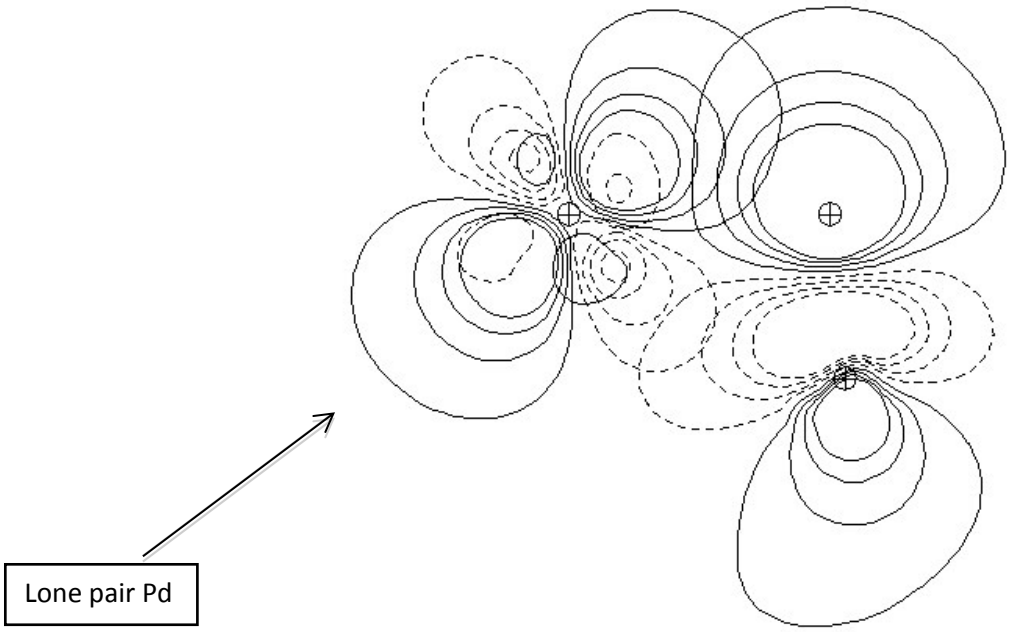


3D Surfaces showing NBOs interaction

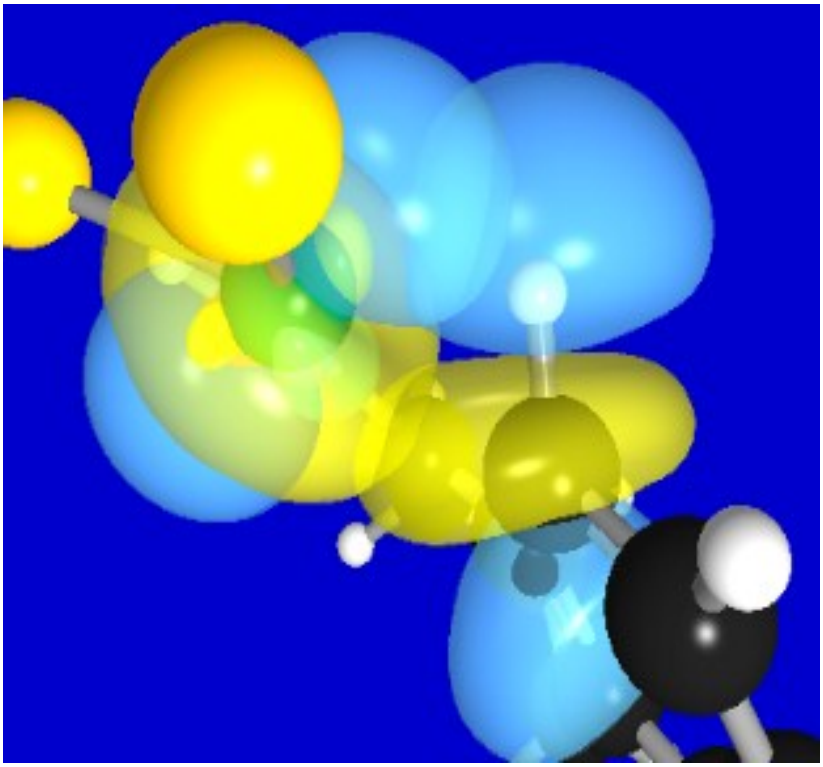


6) Lone pair (3) Pd to C(8)-H(8)σ* [E(2) = 2.9 kcalmol^{-1})

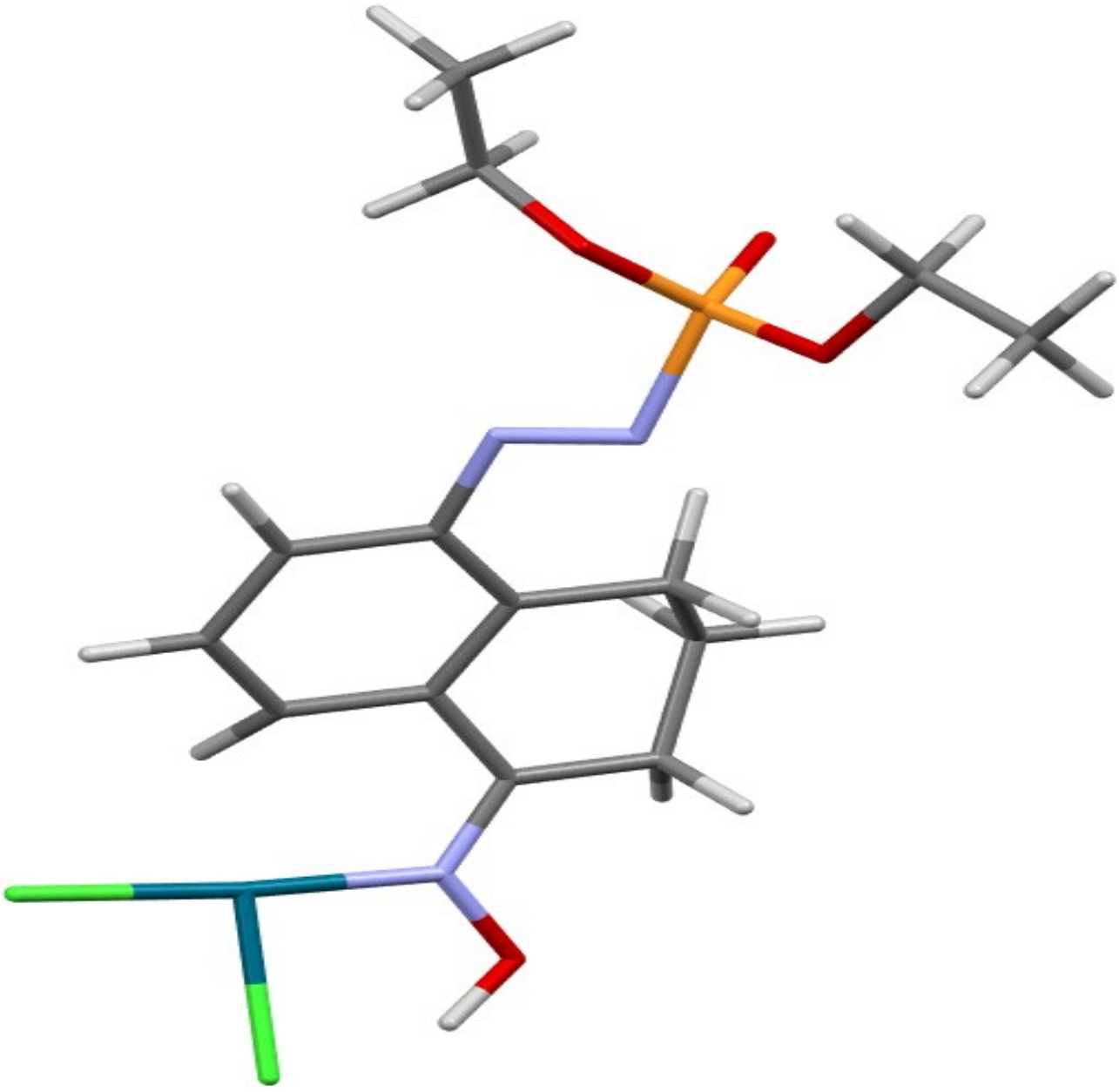
Contour plot



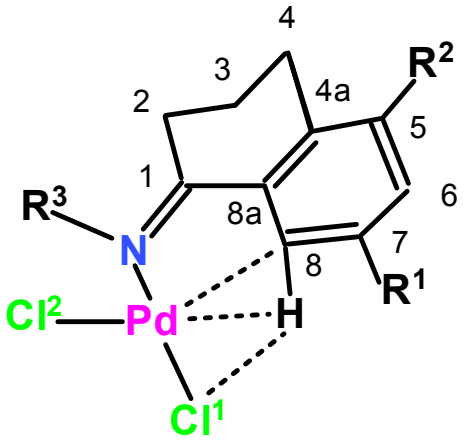
3D Surfaces showing NBOs interaction

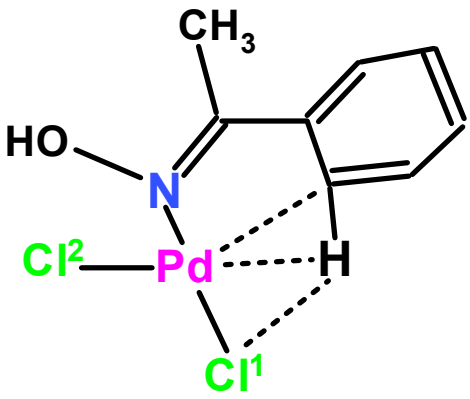


Supplementary Figure 3: Optimised structure of complex with $N{=}NPO(OCH_2CH_3)_2$



Supplementary Table 1: QTAIM aromatic ring C and H atomic charges for complexes (**1**) to (**5**) and [PdCl(CH_3)(1-tetralone oxime)].





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

(2) $R^1 = H$, $R^2 = SO_2Cl$, $R^3 = OH$

(3) $R^1 = H$, $R^2 = B(OH)_3^-$, $R^3 = OH$

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

(5)

(Free ligand values in brackets_

Atom	Complex 1	Complex 2	Complex 3	Complex 4	Complex 5	Cl^1 replaced by CH_3
C4a	-0.003 **(-0.014)**	0.023 **(0.015)**	-0.009 **(-0.022)**	-0.012 **(-0.025)**	-0.005 **(-0.019)**	-0.006 **(-0.014)**
C5	-0.006 **(-0.019)**	-0.094 **(-0.102)**	-0.408 **(-0.444)**	-0.310 **(-0.214)**	0.003 **(-0.011)**	-0.010 **(-0.019)**
C6	-0.002 **(-0.015)**	0.016 **(0.007)**	-0.025 **(-0.038)**	-0.015 **(-0.027)**	-0.000 **(-0.014)**	-0.006 **(-0.015)**
C7	0.012 **(-0.014)**	0.024 **(0.002)**	-0.007 **(-0.041)**	-0.007 **(-0.038)**	0.014 **(-0.011)**	0.005 **(-0.014)**
C8	-0.084 **(0.001)**	-0.073 **(0.015)**	-0.112 **(-0.025)**	-0.089 **(-0.040)**	-0.086 **(0.002)**	-0.080 **(0.001)**
C8a	-0.001 **(-0.015)**	0.009 (-0.004)	-0.017 **(-0.034)**	-0.014 **(-0.029)**	0.015 **(-0.001)**	-0.003 **(-0.015)**
H5	0.026 **(0.006)**	N/A	N/A	N/A	0.037 **(0.015)**	0.020 **(0.006)**
H6	0.038 **(0.014)**	0.102 **(0.086)**	0.051 **(0.020)**	0.021 **(-0.005)**	0.041 **(0.016)**	0.029 **(0.014)**
H7	0.079 **(0.014)**	0.096 **(0.037)**	0.047 **(-0.033)**	0.050 **(-0.035)**	0.083 **(0.016)**	0.043 **(0.014)**
H8	0.056 **(0.040)**	0.060 **(0.057)**	0.053 **(0.001)**	0.051 **(-0.003)**	0.057 **(0.039)**	0.041 **(0.040)**
H4a	N/A	N/A	N/A	N/A	0.029 (**0.011**)	N/A

Supplementary Table 2: QTAIM properties of C(8)-H(8) bond critical point for complexes (**1**) to (**5**) charges for complexes (**1**) to (**5**) and [PdCl(CH_3)(1-tetralone oxime)].

Property	**Complex 1**	**Complex 2**	**Complex 3**	**Complex 4**	**Complex 5**	**Cl^1 replaced by CH_3**
Electron density, ρ(bcp) [e/bohr^3]	0.2333 **(0.2810)**	0.2315 **(0.2825)**	0.2392 **(0.2778)**	0.2566 **(0.2774)**	0.2338 **(0.2810)**	0.2274 **(0.2810)**
Laplacian of electron density, $\nabla^2\rho$(bcp) [e/bohr^5]	–0.6268 **(–0.9458)**	–0.6170 **(–0.9602)**	–0.6582 **(–0.9184)**	–0.7695 **(–0.9117)**	–0.6283 **(–0.9461)**	–0.5886 **(–0.9458)**
Ellipticity, ε(bcp)	0.1059 **(0.0126)**	0.1050 **(0.0087)**	0.1080 **(0.0182)**	0.0704 **(0.0291)**	0.1076 **(0.0132)**	0.1075 **(0.0126)**

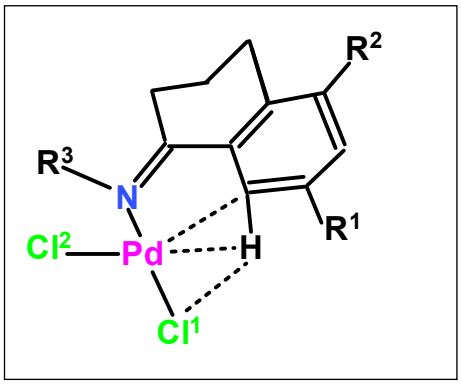
Free ligand values in brackets ( )

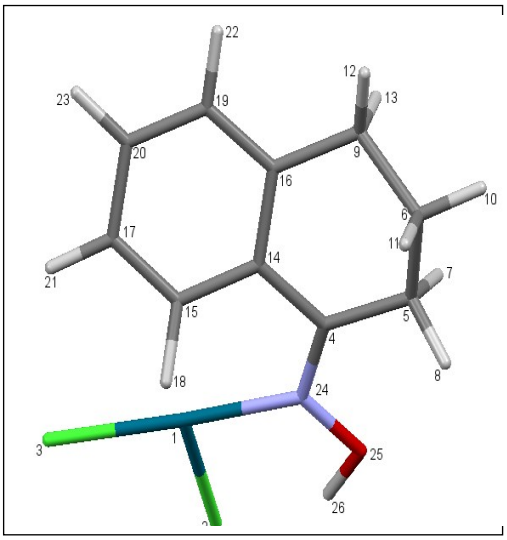
Supplementary Table 3: Second order perturbation energy *E* (2) (kcalmol^{-1}) values for donor-acceptor NBOs interactions for complexes (**1**) to (**6**) and [PdCl(CH_3)(1-tetralone oxime)].

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

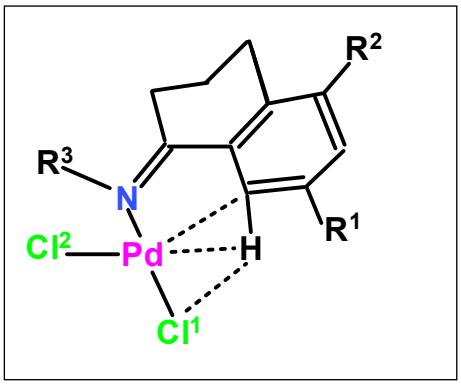


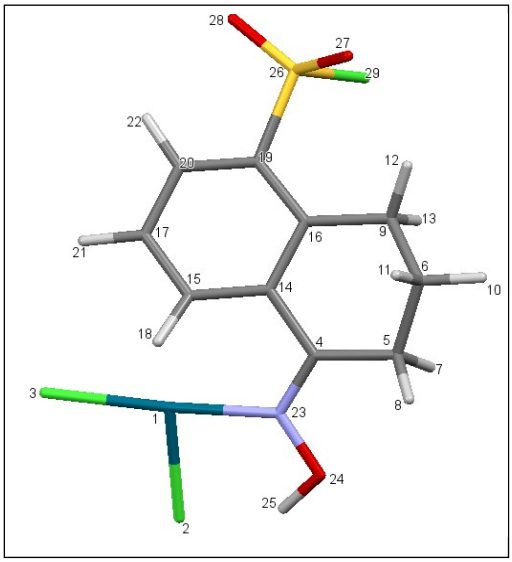


57. BD (2) C 14- C 16	90. BD*(1) C 15- H 18	1.11
57. BD (2) C 14- C 16	95. BD*(2) C 19- C 20	15.14
58. BD (1) C 15- C 17	73. BD*(1) C 4- C 14	2.83
58. BD (1) C 15- C 17	85. BD*(1) C 14- C 15	1.99
58. BD (1) C 15- C 17	90. BD*(1) C 15- H 18	0.52
58. BD (1) C 15- C 17	92. BD*(1) C 17- C 20	1.29
58. BD (1) C 15- C 17	93. BD*(1) C 17- H 21	0.84
58. BD (1) C 15- C 17	97. BD*(1) C 20- H 23	2.07
59. BD (2) C 15- C 17	87. BD*(2) C 14- C 16	15.30
59. BD (2) C 15- C 17	90. BD*(1) C 15- H 18	3.71
59. BD (2) C 15- C 17	95. BD*(2) C 19- C 20	13.50
62. BD (1) C 17- C 20	90. BD*(1) C 15- H 18	2.59
69. BD (1) O 25- H 26	74. BD*(1) C 4- N 24	3.88

Complex (2):

(2) R^1 =H, R^2 = SO_2Cl, R^3 = OH





Donor (L) NBO	Acceptor (NL) NBO	*E* (2) kcalmol^{-1}
39. LP (1)Pd 1	97. BD*(1) C 4- C 14	0.05
39. LP (1)Pd 1	112. BD*(1) C 15- C 17	0.06
39. LP (1)Pd 1	113. BD*(2) C 15- C 17	1.49
40. LP (2)Pd 1	96. BD*(1) C 4- C 5	0.06
40. LP (2)Pd 1	98. BD*(1) C 4- N 23	0.83
40. LP (2)Pd 1	109. BD*(1) C 14- C 15	0.34
40. LP (2)Pd 1	110. BD*(1) C 14- C 16	0.06
40. LP (2)Pd 1	112. BD*(1) C 15- C 17	0.92
40. LP (2)Pd 1	113. BD*(2) C 15- C 17	0.21
40. LP (2)Pd 1	116. BD*(1) C 17- C 20	0.06
40. LP (2)Pd 1	122. BD*(1) N 23- O 24	2.31
41. LP (3)Pd 1	99. BD*(2) C 4- N 23	3.80
41. LP (3)Pd 1	109. BD*(1) C 14- C 15	0.11
41. LP (3)Pd 1	113. BD*(2) C 15- C 17	0.26
41. LP (3)Pd 1	114. BD*(1) C 15- H 18	2.39
41. LP (3)Pd 1	122. BD*(1) N 23- O 24	0.11
42. LP (4)Pd 1	99. BD*(2) C 4- N 23	1.04
42. LP (4)Pd 1	11. BD*(2) C 14- C 16	0.10
42. LP (4)Pd 1	112. BD*(1) C 15- C 17	0.06
42. LP (4)Pd 1	113. BD*(2) C 15- C 17	1.63
42. LP (4)Pd 1	114. BD*(1) C 15- H 18	5.35
42. LP (4)Pd 1	122. BD*(1) N 23- O 24	0.07
43. LP (1)Cl 2	112. BD*(1) C 15- C 17	0.06
43. LP (1)Cl 2	113. BD*(2) C 15- C 17	0.41
43. LP (1)Cl 2	123. BD*(1) O 24- H 25	0.25
44. LP (2)Cl 2	99. BD*(2) C 4- N 23	0.11
44. LP (2)Cl 2	113. BD*(2) C 15- C 17	0.13
44. LP (2)Cl 2	114. BD*(1) C 15- H 18	0.17
45. LP (3)Cl 2	98. BD*(1) C 4- N 23	0.17
45. LP (3)Cl 2	113. BD*(2) C 15- C 17	0.19
45. LP (3)Cl 2	123. BD*(1) O 24- H 25	16.31
46. LP (1)Cl 3	112. BD*(1) C 15- C 17	0.05
46. LP (1)Cl 3	113. BD*(2) C 15- C 17	0.25
46. LP (1)Cl 3	117. BD*(1) C 17- H 21	0.08
46. LP (1)Cl 3	122. BD*(1) N 23- O 24	0.06
47. LP (2)Cl 3	109. BD*(1) C 14- C 15	0.12
47. LP (2)Cl 3	114. BD*(1) C 15- H 18	0.10
47. LP (2)Cl 3	116. BD*(1) C 17- C 20	0.10
47. LP (2)Cl 3	117. BD*(1) C 17- H 21	0.29
47. LP (2)Cl 3	123. BD*(1) O 24- H 25	0.06
48. LP (3)Cl 3	114. BD*(1) C 15- H 18	0.15
48. LP (3)Cl 3	116. BD*(1) C 17- C 20	0.05
48. LP (3)Cl 3	117. BD*(1) C 17- H 21	0.16
61. BD (1)Pd 1-Cl 2	98. BD*(1) C 4- N 23	0.13
61. BD (1)Pd 1-Cl 2	112. BD*(1) C 15- C 17	0.32
61. BD (1)Pd 1-Cl 2	113. BD*(2) C 15- C 17	2.99
61. BD (1)Pd 1-Cl 2	114. BD*(1) C 15- H 18	0.15
61. BD (1)Pd 1-Cl 2	117. BD*(1) C 17- H 21	0.10
61. BD (1)Pd 1-Cl 2	123. BD*(1) O 24- H 25	0.85
62. BD (1)Pd 1-Cl 3	109. BD*(1) C 14- C 15	0.24
62. BD (1)Pd 1-Cl 3	112. BD*(1) C 15- C 17	0.09

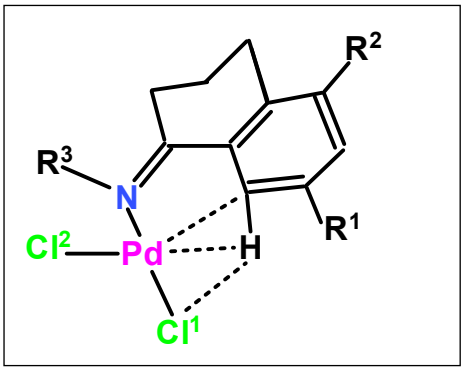
62. BD (1)Pd 1-Cl 3	113. BD*(2) C 15- C 17	1.46
62. BD (1)Pd 1-Cl 3	114. BD*(1) C 15- H 18	0.34
62. BD (1)Pd 1-Cl 3	122. BD*(1) N 23- O 24	0.20
62. BD (1)Pd 1-Cl 3	123. BD*(1) O 24- H 25	0.11
49. LP (1) N 23	94. BD*(1)Pd 1-Cl 2	16.45
49. LP (1) N 23	95. BD*(1)Pd 1-Cl 3	104.63
50. LP (1) O 24	94. BD*(1)Pd 1-Cl 2	0.18
50. LP (1) O 24	95. BD*(1)Pd 1-Cl 3	0.31
63. BD (1) C 4- C 5	94. BD*(1)Pd 1-Cl 2	0.48
63. BD (1) C 4- C 5	95. BD*(1)Pd 1-Cl 3	0.75
65. BD (1) C 4- N 23	94. BD*(1)Pd 1-Cl 2	0.96
65. BD (1) C 4- N 23	95. BD*(1)Pd 1-Cl 3	4.35
66. BD (2) C 4- N 23	95. BD*(1)Pd 1-Cl 3	0.25
76. BD (1) C 14- C 15	94. BD*(1)Pd 1-Cl 2	0.65
76. BD (1) C 14- C 15	95. BD*(1)Pd 1-Cl 3	0.10
79. BD (1) C 15- C 17	94. BD*(1)Pd 1-Cl 2	0.16
79. BD (1) C 15- C 17	95. BD*(1)Pd 1-Cl 3	0.59
80. BD (2) C 15- C 17	94. BD*(1)Pd 1-Cl 2	27.55
80. BD (2) C 15- C 17	95. BD*(1)Pd 1-Cl 3	0.47
81. BD (1) C 15- H 18	94. BD*(1)Pd 1-Cl 2	75.57
81. BD (1) C 15- H 18	95. BD*(1)Pd 1-Cl 3	14.98
83. BD (1) C 17- C 20	94. BD*(1)Pd 1-Cl 2	0.57
83. BD (1) C 17- C 20	95. BD*(1)Pd 1-Cl 3	0.37
49. LP (1) N 23	96. BD*(1) C 4- C 5	7.96
49. LP (1) N 23	97. BD*(1) C 4- C 14	0.82
49. LP (1) N 23	109. BD*(1) C 14- C 15	0.64
49. LP (1) N 23	123. BD*(1) O 24- H 25	0.71
51. LP (2) O 24	99. BD*(2) C 4- N 23	20.11
52. LP (1) O 27	106. BD*(1) C 9- H 12	0.59
52. LP (1) O 27	120. BD*(1) C 19- S 26	0.84
52. LP (1) O 27	125. BD*(1) S 26- O 28	1.38
77. BD (1) C 14- C 16	97. BD*(1) C 4- C 14	1.70
77. BD (1) C 14- C 16	98. BD*(1) C 4- N 23	1.37
77. BD (1) C 14- C 16	106. BD*(1) C 9- H 12	0.64
77. BD (1) C 14- C 16	108. BD*(1) C 9- C 16	1.14
77. BD (1) C 14- C 16	109. BD*(1) C 14- C 15	2.72
77. BD (1) C 14- C 16	114. BD*(1) C 15- H 18	1.85
77. BD (1) C 14- C 16	115. BD*(1) C 16- C 19	2.30
77. BD (1) C 14- C 16	120. BD*(1) C 19- **S** 26	4.46
78. BD (2) C 14- C 16	99. BD*(2) C 4- N 23	20.74
78. BD (2) C 14- C 16	103. BD*(1) C 6- C 9	0.51
78. BD (2) C 14- C 16	106. BD*(1) C 9- H 12	0.91
78. BD (2) C 14- C 16	107. BD*(1) C 9- H 13	2.88
78. BD (2) C 14- C 16	113. BD*(2) C 15- C 17	12.03
78. BD (2) C 14- C 16	114. BD*(1) C 15- H 18	0.92
78. BD (2) C 14- C 16	119. BD*(2) C 19- C 20	14.49
79. BD (1) C 15- C 17	97. BD*(1) C 4- C 14	3.22
79. BD (1) C 15- C 17	109. BD*(1) C 14- C 15	1.62
79. BD (1) C 15- C 17	116. BD*(1) C 17- C 20	1.41
79. BD (1) C 15- C 17	117. BD*(1) C 17- H 21	1.08
79. BD (1) C 15- C 17	121. BD*(1) C 20- H 22	2.27
80. BD (2) C 15- C 17	97. BD*(1) C 4- C 14	0.73
80. BD (2) C 15- C 17	110. BD*(1) C 14- C 16	0.50
80. BD (2) C 15- C 17	111. BD*(2) C 14- C 16	15.96
80. BD (2) C 15- C 17	113. BD*(2) C 15- C 17	0.78
80. **BD (2) C 15- C 17**	**114. BD*(1) C 15- H 18**	**3.16**
80. BD (2) C 15- C 17	119. BD*(2) C 19- C 20	16.82
81. BD (1) C 15- H 18	97. BD*(1) C 4- C 14	0.98

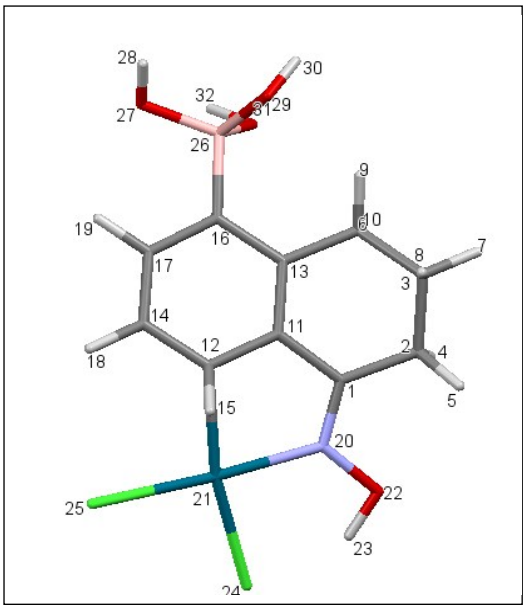
81. BD (1) C 15- H 18	110. BD*(1) C 14- C 16	5.48
81. BD (1) C 15- H 18	113. BD*(2) C 15- C 17	1.68
81. BD (1) C 15- H 18	116. BD*(1) C 17- C 20	4.69
81. BD (1) C 15- H 18	117. BD*(1) C 17- H 21	0.89

Complex (3):

(3) R^1 = H, R^2 = $B(OH)_3^-$, R^3 = OH

Donor (L) NBO	Acceptor (NL) NBO	*E* (2) kcalmol^{-1}
72. BD (1) C 12- H 15	91. BD*(1) C 1- C 11	0.75
72. BD (1) C 12- H 15	104. BD*(1) C 11- C 13	4.91
72. BD (1) C 12- H 15	105. BD*(2) C 11- C 13	0.73
72. BD (1) C 12- H 15	107. BD*(2) C 12- C 14	1.09
72. BD (1) C 12- H 15	110. BD*(1) C 14- C 17	4.19
72. BD (1) C 12- H 15	111. BD*(1) C 14- H 18	0.67
32. LP (1) N 20	116. BD*(1)Pd 21-Cl 24	18.37
32. LP (1) N 20	117. BD*(1)Pd 21-Cl 25	108.27
54. BD (1) C 1- C 2	116. BD*(1)Pd 21-Cl 24	0.59
54. BD (1) C 1- C 2	117. BD*(1)Pd 21-Cl 25	0.87
56. BD (1) C 1- N 20	116. BD*(1)Pd 21-Cl 24	1.08
56. BD (1) C 1- N 20	117. BD*(1)Pd 21-Cl 25	4.69
67. BD (1) C 11- C 12	116. BD*(1)Pd 21-Cl 24	0.94
67. BD (1) C 11- C 12	117. BD*(1)Pd 21-Cl 25	0.12
68. BD (1) C 11- C 13	116. BD*(1)Pd 21-Cl 24	0.16
68. BD (1) C 11- C 13	117. BD*(1)Pd 21-Cl 25	0.11
69. BD (2) C 11- C 13	116. BD*(1)Pd 21-Cl 24	0.21
69. BD (2) C 11- C 13	117. BD*(1)Pd 21-Cl 25	0.09
70. BD (1) C 12- C 14	116. BD*(1)Pd 21-Cl 24	0.06
70. BD (1) C 12- C 14	117. BD*(1)Pd 21-Cl 25	0.58
71. BD (2) C 12- C 14	116. BD*(1)Pd 21-Cl 24	41.92
71. BD (2) C 12- C 14	117. BD*(1)Pd 21-Cl 25	15.99
72. BD (1) C 12- H 15	116. BD*(1)Pd 21-Cl 24	63.99
72. BD (1) C 12- H 15	117. BD*(1)Pd 21-Cl 25	13.81
74. BD (1) C 14- C 17	116. BD*(1)Pd 21-Cl 24	0.64
74. BD (1) C 14- C 17	117. BD*(1)Pd 21-Cl 25	0.41
33. LP (1)Pd 21	107. BD*(2) C 12- C 14	1.57
34. LP (2)Pd 21	90. BD*(1) C 1- C 2	0.05
34. LP (2)Pd 21	92. BD*(1) C 1- N 20	0.86
34. LP (2)Pd 21	93. BD*(2) C 1- N 20	0.07
34. LP (2)Pd 21	103. BD*(1) C 11- C 12	0.31
34. LP (2)Pd 21	106. BD*(1) C 12- C 14	0.98
34. LP (2)Pd 21	107. BD*(2) C 12- C 14	0.35
34. LP (2)Pd 21	108. BD*(1) C 12- H 15	0.10
34. LP (2)Pd 21	110. BD*(1) C 14- C 17	0.06
34. LP (2)Pd 21	115. BD*(1) N 20- O 22	2.41
35. LP (3)Pd 21	93. BD*(2) C 1- N 20	2.75
35. LP (3)Pd 21	103. BD*(1) C 11- C 12	0.22
35. LP (3)Pd 21	104. BD*(1) C 11- C 13	0.05
35. LP (3)Pd 21	107. BD*(2) C 12- C 14	0.20
35. LP (3)Pd 21	108. BD*(1) C 12- H 15	2.53
35. LP (3)Pd 21	115. BD*(1) N 20- O 22	0.29
36. LP (4)Pd 21	93. BD*(2) C 1- N 20	1.97
36. LP (4)Pd 21	105. BD*(2) C 11- C 13	0.11
36. LP (4)Pd 21	106. BD*(1) C 12- C 14	0.14
36. LP (4)Pd 21	107. BD*(2) C 12- C 14	0.51
36. LP (4)Pd 21	108. BD*(1) C 12- H 15	2.70
39. LP (1)Cl 24	107. BD*(2) C 12- C 14	0.41
39. LP (1)Cl 24	118. BD*(1) O 22- H 23	0.33
41. LP (3)Cl 24	118. BD*(1) O 22- H 23	17.80
44. LP (3)Cl 25	108. BD*(1) C 12- H 15	0.13

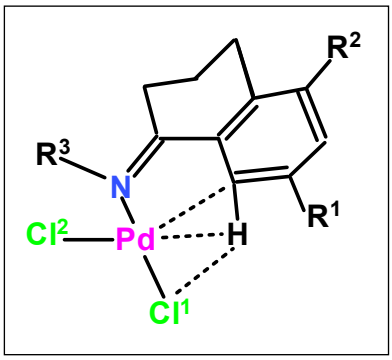


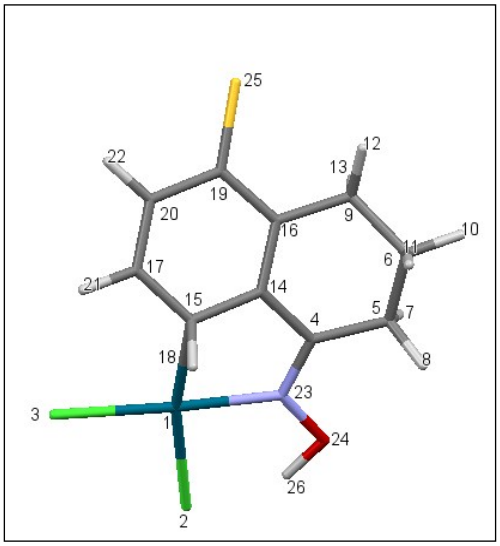


80. BD (1)Pd 21-Cl 24	92. BD*(1) C 1- N 20	0.13
80. BD (1)Pd 21-Cl 24	106. BD*(1) C 12- C 14	0.26
80. BD (1)Pd 21-Cl 24	107. BD*(2) C 12- C 14	2.59
80. BD (1)Pd 21-Cl 24	111. BD*(1) C 14- H 18	0.06
80. BD (1)Pd 21-Cl 24	118. BD*(1) O 22- H 23	1.18
81. BD (1)Pd 21-Cl 25	93. BD*(2) C 1- N 20	0.07
81. BD (1)Pd 21-Cl 25	103. BD*(1) C 11- C 12	0.25
81. BD (1)Pd 21-Cl 25	106. BD*(1) C 12- C 14	0.08
81. BD (1)Pd 21-Cl 25	107. BD*(2) C 12- C 14	1.31
81. BD (1)Pd 21-Cl 25	108. BD*(1) C 12- H 15	0.14
81. BD (1)Pd 21-Cl 25	115. BD*(1) N 20- O 22	0.20
81. BD (1)Pd 21-Cl 25	118. BD*(1) O 22- H 23	0.08

Complex (4):

(4) R^1 = H, R^2 = S^-, R^3 = OH

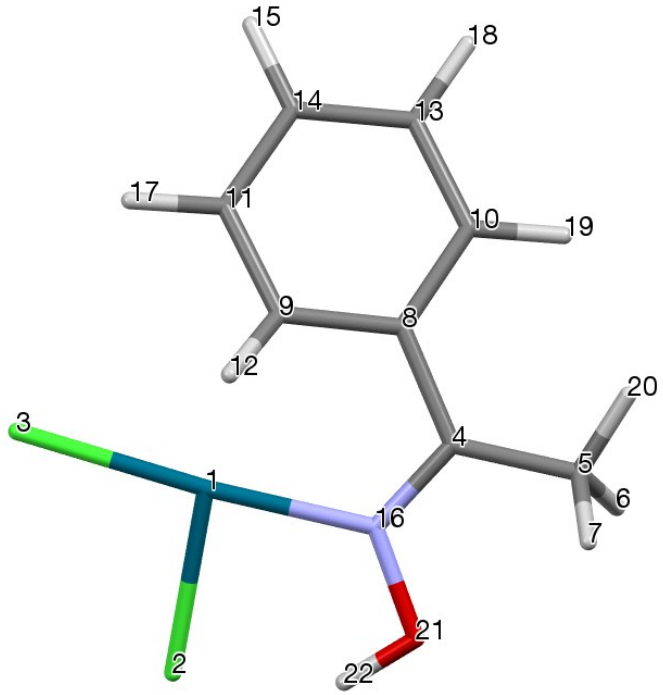


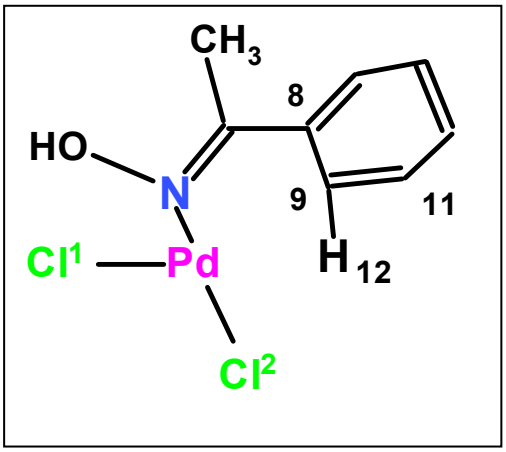


Donor (L) NBO	Acceptor (NL) NBO	*E* (2) kcalmol^{-1}
32. LP (1)Pd 1	79. BD*(1)Pd 1- C 15	2.12
33. LP (2)Pd 1	78. BD*(1)Pd 1-Cl 3	8.39
33. LP (2)Pd 1	79. BD*(1)Pd 1- C 15	7.27
33. LP (2)Pd 1	82. BD*(1) C 4- N 23	0.93
33. LP (2)Pd 1	83. BD*(2) C 4- N 23	0.54
33. LP (2)Pd 1	96. BD*(1) C 15- C 17	0.53
33. LP (2)Pd 1	106. BD*(1) N 23- O 24	2.03
34. LP (3)Pd 1	78. BD*(1)Pd 1-Cl 3	2.77
34. LP (3)Pd 1	79. BD*(1)Pd 1- C 15	0.86
34. LP (3)Pd 1	83. BD*(2) C 4- N 23	0.64
34. LP (3)Pd 1	93. BD*(1) C 14- C 15	0.79
34. LP (3)Pd 1	97. BD*(1) C 15- H 18	0.78
34. LP (3)Pd 1	106. BD*(1) N 23- O 24	1.08
35. LP (4)Pd 1	78. BD*(1)Pd 1-Cl 3	1.58
35. LP (4)Pd 1	79. BD*(1)Pd 1- C 15	0.80
35. LP (4)Pd 1	83. BD*(2) C 4- N 23	4.88
40. LP (1)Cl 3	101. BD*(1) C 17- H 21	0.59
43. LP (1) N 23	78. BD*(1)Pd 1-Cl 3	101.20
43. LP (1) N 23	79. BD*(1)Pd 1- C 15	7.92
43. LP (1) N 23	80. BD*(1) C 4- C 5	9.17
43. LP (1) N 23	81. BD*(1) C 4- C 14	1.50
43. LP (1) N 23	93. BD*(1) C 14- C 15	0.92
43. LP (1) N 23	96. BD*(1) C 15- C 17	0.51
43. LP (1) N 23	107. BD*(1) O 24- H 26	0.51
48. BD (1)Pd 1-Cl 3	78. BD*(1)Pd 1-Cl 3	3.67
48. BD (1)Pd 1-Cl 3	79. BD*(1)Pd 1- C 15	20.91
49. BD (1)Pd 1- C 15	78. BD*(1)Pd 1-Cl 3	56.60
49. BD (1)Pd 1- C 15	79. BD*(1)Pd 1- C 15	12.50
49. BD (1)Pd 1- C 15	81. BD*(1) C 4- C 14	1.10
49. BD (1)Pd 1- C 15	94. BD*(1) C 14- C 16	4.61
49. BD (1)Pd 1- C 15	95. BD*(2) C 14- C 16	11.28
49. BD (1)Pd 1- C 15	97. BD*(1) C 15- H 18	0.51
49. BD (1)Pd 1- C 15	99. BD*(1) C 17- C 20	1.08
49. BD (1)Pd 1- C 15	100. BD*(2) C 17- C 20	14.50
49. BD (1)Pd 1- C 15	106. BD*(1) N 23- O 24	1.46
50. BD (1) C 4- C 5	78. BD*(1)Pd 1-Cl 3	1.52
50. BD (1) C 4- C 5	79. BD*(1)Pd 1- C 15	1.06
50. BD (1) C 4- C 5	81. BD*(1) C 4- C 14	1.02
50. BD (1) C 4- C 5	82. BD*(1) C 4- N 23	0.67
50. BD (1) C 4- C 5	84. BD*(1) C 5- C 6	0.51
50. BD (1) C 4- C 5	88. BD*(1) C 6- H 10	1.39
50. BD (1) C 4- C 5	93. BD*(1) C 14- C 15	2.15
50. BD (1) C 4- C 5	106. BD*(1) N 23- O 24	1.05
51. BD (1) C 4- C 14	80. BD*(1) C 4- C 5	0.80
51. BD (1) C 4- C 14	82. BD*(1) C 4- N 23	1.39
51. BD (1) C 4- C 14	85. BD*(1) C 5- H 7	0.54
51. BD (1) C 4- C 14	86. BD*(1) C 5- H 8	0.64
51. BD (1) C 4- C 14	93. BD*(1) C 14- C 15	1.15
51. BD (1) C 4- C 14	94. BD*(1) C 14- C 16	1.98
51. BD (1) C 4- C 14	96. BD*(1) C 15- C 17	1.72
51. BD (1) C 4- C 14	98. BD*(1) C 16- C 19	3.44
51. BD (1) C 4- C 14	106. BD*(1) N 23- O 24	6.05

52. BD (1) C 4- N 23	78. BD*(1)Pd 1-Cl 3	3.90
52. BD (1) C 4- N 23	80. BD*(1) C 4- C 5	1.20
52. BD (1) C 4- N 23	81. BD*(1) C 4- C 14	1.14
52. BD (1) C 4- N 23	84. BD*(1) C 5- C 6	0.59
52. BD (1) C 4- N 23	94. BD*(1) C 14- C 16	1.33
52. BD (1) C 4- N 23	107. BD*(1) O 24- H 26	1.02
53. BD (2) C 4- N 23	83. BD*(2) C 4- N 23	2.27
53. BD (2) C 4- N 23	85. BD*(1) C 5- H 7	1.53
53. BD (2) C 4- N 23	86. BD*(1) C 5- H 8	1.21
53. BD (2) C 4- N 23	95. BD*(2) C 14- C 16	7.72
63. BD (1) C 14- C 15	78. BD*(1)Pd 1-Cl 3	1.86
63. BD (1) C 14- C 15	79. BD*(1)Pd 1- C 15	1.14
63. BD (1) C 14- C 15	80. BD*(1) C 4- C 5	3.25
63. BD (1) C 14- C 15	81. BD*(1) C 4- C 14	1.58
63. BD (1) C 14- C 15	92. BD*(1) C 9- C 16	2.98
63. BD (1) C 14- C 15	94. BD*(1) C 14- C 16	2.26
63. BD (1) C 14- C 15	96. BD*(1) C 15- C 17	1.36
63. BD (1) C 14- C 15	101. BD*(1) C 17- H 21	2.25
65. BD (2) C 14- C 16	79. BD*(1)Pd 1- C 15	1.28
65. BD (2) C 14- C 16	97. BD*(1) C 15- H 18	3.30
67. BD (1) C 15- H 18	78. BD*(1)Pd 1-Cl 3	3.10
67. BD (1) C 15- H 18	79. BD*(1)Pd 1- C 15	2.70
67. BD (1) C 15- H 18	94. BD*(1) C 14- C 16	1.29
67. BD (1) C 15- H 18	95. BD*(2) C 14- C 16	4.27
67. BD (1) C 15- H 18	99. BD*(1) C 17- C 20	2.20
67. BD (1) C 15- H 18	100. BD*(2) C 17- C 20	3.55
69. BD (1) C 17- C 20	79. BD*(1)Pd 1- C 15	1.02
69. BD (1) C 17- C 20	96. BD*(1) C 15- C 17	1.35
69. BD (1) C 17- C 20	97. BD*(1) C 15- H 18	1.35
69. BD (1) C 17- C 20	101. BD*(1) C 17- H 21	0.77
69. BD (1) C 17- C 20	102. BD*(1) C 19- C 20	1.64
69. BD (1) C 17- C 20	103. BD*(1) C 19- S 25	2.72
69. BD (1) C 17- C 20	105. BD*(1) C 20- H 22	0.80
70. BD (2) C 17- C 20	79. BD*(1)Pd 1- C 15	3.95
70. BD (2) C 17- C 20	97. BD*(1) C 15- H 18	2.58
70. BD (2) C 17- C 20	104. BD*(2) C 19- S 25	25.60
37. LP (2)Cl 2	78. BD*(1)Pd 1-Cl 3	3.29
37. **LP (2)Cl 2**	**79. BD*(1)Pd 1- C 15**	**9.27**
37. LP (2)Cl 2	107. BD*(1) O 24- H 26	0.63
38. LP (3)Cl 2	78. BD*(1)Pd 1-Cl 3	1.02
38. **LP (3)Cl 2**	**79. BD*(1)Pd 1- C 15**	**1.86**
38. LP (3)Cl 2	82. BD*(1) C 4- N 23	0.10
38. LP (3)Cl 2	107. BD*(1) O 24- H 26	23.09
39. LP (4)Cl 2	78. BD*(1)Pd 1-Cl 3	39.34
39. **LP (4)Cl 2**	**79. BD*(1)Pd 1- C 15**	**100.63**
39. LP (4)Cl 2	80. BD*(1) C 4- C 5	0.10
39. LP (4)Cl 2	82. BD*(1) C 4- N 23	0.82
39. LP (4)Cl 2	93. BD*(1) C 14- C 15	0.28
39. LP (4)Cl 2	94. BD*(1) C 14- C 16	0.43
39. LP (4)Cl 2	101. BD*(1) C 17- H 21	0.05
39. LP (4)Cl 2	106. BD*(1) N 23- O 24	0.36
39. LP (4)Cl 2	107. BD*(1) O 24- H 26	0.81

Acetophenone oxime complex (5):





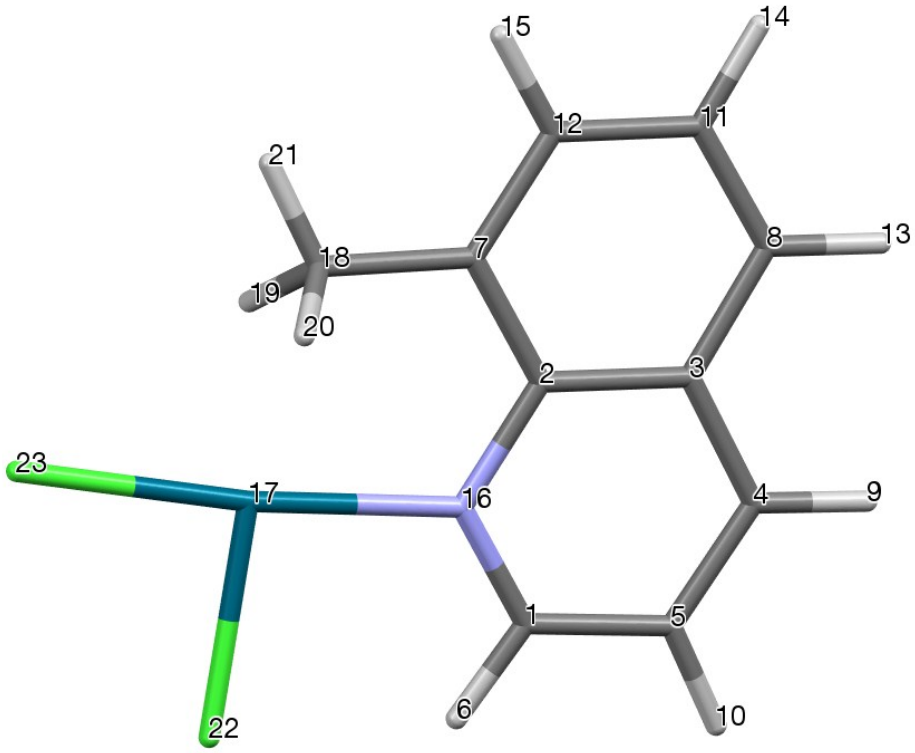
Donor (L) NBO	Acceptor (NL) NBO	*E* (2) kcalmol^{-1}
25. LP (1)Pd 1	63. BD*(1)Pd 1-Cl 2	11.07
25. LP (1)Pd 1	64. BD*(1)Pd 1-Cl 3	9.51
26. LP (2)Pd 1	63. BD*(1)Pd 1-Cl 2	1.72
26. LP (2)Pd 1	64. BD*(1)Pd 1-Cl 3	1.76
28. LP (4)Pd 1	63. BD*(1)Pd 1-Cl 2	1.02
28. LP (4)Pd 1	64. BD*(1)Pd 1-Cl 3	1.19
29. LP (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	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

8-methylquinoline complex (6):



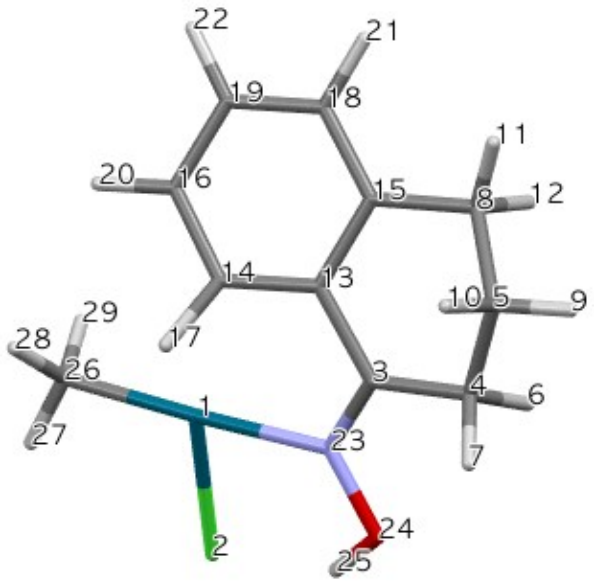
Donor (L) NBO	Acceptor (NL) NBO	*E* (2) kcalmol^{-1}
26. LP (1) N 16	65. BD*(1) C 1- C 5	7.66
26. LP (1) N 16	66. BD*(1) C 1- H 6	4.41
26. LP (1) N 16	69. BD*(1) C 2- C 3	10.34
26. LP (1) N 16	70. BD*(1) C 2- C 7	2.00
26. LP (1) N 16	81. BD*(1) C 7- C 18	0.87
26. LP (1) N 16	90. BD*(1) C 18- H 19	0.84
37. BD (1) C 1- C 5	66. BD*(1) C 1- H 6	0.62
37. BD (1) C 1- C 5	67. BD*(1) C 1- N 16	0.54
37. BD (1) C 1- C 5	76. BD*(1) C 4- C 5	1.40
37. BD (1) C 1- C 5	78. BD*(1) C 4- H 9	2.71
38. BD (1) C 1- H 6	72. BD*(1) C 2- N 16	4.80
38. BD (1) C 1- H 6	76. BD*(1) C 4- C 5	3.40
39. BD (1) C 1- N 16	65. BD*(1) C 1- C 5	0.71
39. BD (1) C 1- N 16	70. BD*(1) C 2- C 7	2.62
39. BD (1) C 1- N 16	72. BD*(1) C 2- N 16	1.11
39. BD (1) C 1- N 16	79. BD*(1) C 5- H 10	1.14
40. BD (2) C 1- N 16	71. BD*(2) C 2- C 7	17.35
40. BD (2) C 1- N 16	77. BD*(2) C 4- C 5	7.15
41. BD (1) C 2- C 3	70. BD*(1) C 2- C 7	2.28
41. BD (1) C 2- C 3	72. BD*(1) C 2- N 16	0.76
41. BD (1) C 2- C 3	73. BD*(1) C 3- C 4	1.77
41. BD (1) C 2- C 3	74. BD*(1) C 3- C 8	1.79
41. BD (1) C 2- C 3	78. BD*(1) C 4- H 9	2.00
41. BD (1) C 2- C 3	81. BD*(1) C 7- C 18	2.50
41. BD (1) C 2- C 3	83. BD*(1) C 8- H 13	1.77

42. BD (1) C 2- C 7	67. BD*(1) C 1- N 16	2.42
42. BD (1) C 2- C 7	69. BD*(1) C 2- C 3	2.01
42. BD (1) C 2- C 7	72. BD*(1) C 2- N 16	1.08
42. BD (1) C 2- C 7	73. BD*(1) C 3- C 4	2.37
42. BD (1) C 2- C 7	80. BD*(1) C 7- C 12	0.99
42. BD (1) C 2- C 7	87. BD*(1) C 12- H 15	2.36
42. BD (1) C 2- C 7	92. BD*(1) C 18- H 21	1.10
43. BD (2) C 2- C 7	68. BD*(2) C 1- N 16	15.36
43. BD (2) C 2- C 7	75. BD*(2) C 3- C 8	14.95
43. BD (2) C 2- C 7	85. BD*(2) C 11- C 12	16.89
43. BD (2) C 2- C 7	90. BD*(1) C 18- H 19	2.19
43. BD (2) C 2- C 7	91. BD*(1) C 18- H 20	2.84
44. BD (1) C 2- N 16	66. BD*(1) C 1- H 6	2.02
44. BD (1) C 2- N 16	67. BD*(1) C 1- N 16	0.97
44. BD (1) C 2- N 16	69. BD*(1) C 2- C 3	1.36
44. BD (1) C 2- N 16	70. BD*(1) C 2- C 7	1.21
44. BD (1) C 2- N 16	74. BD*(1) C 3- C 8	1.63
44. BD (1) C 2- N 16	80. BD*(1) C 7- C 12	0.97
45. BD (1) C 3- C 4	69. BD*(1) C 2- C 3	1.80
45. BD (1) C 3- C 4	70. BD*(1) C 2- C 7	2.40
45. BD (1) C 3- C 4	74. BD*(1) C 3- C 8	2.11
45. BD (1) C 3- C 4	76. BD*(1) C 4- C 5	1.43
45. BD (1) C 3- C 4	78. BD*(1) C 4- H 9	0.50
45. BD (1) C 3- C 4	79. BD*(1) C 5- H 10	2.46
45. BD (1) C 3- C 4	82. BD*(1) C 8- C 11	1.76
46. BD (1) C 3- C 8	69. BD*(1) C 2- C 3	2.03
46. BD (1) C 3- C 8	72. BD*(1) C 2- N 16	3.48
46. BD (1) C 3- C 8	73. BD*(1) C 3- C 4	2.01
46. BD (1) C 3- C 8	76. BD*(1) C 4- C 5	1.69
46. BD (1) C 3- C 8	82. BD*(1) C 8- C 11	1.54
46. BD (1) C 3- C 8	86. BD*(1) C 11- H 14	2.34
47. BD (2) C 3- C 8	71. BD*(2) C 2- C 7 1	4.21
47. BD (2) C 3- C 8	77. BD*(2) C 4- C 5	19.21
47. BD (2) C 3- C 8	85. BD*(2) C 11- C 12	16.81
48. BD (1) C 4- C 5	65. BD*(1) C 1- C 5	1.32
48. BD (1) C 4- C 5	66. BD*(1) C 1- H 6	1.94
48. BD (1) C 4- C 5	73. BD*(1) C 3- C 4	1.47
48. BD (1) C 4- C 5	74. BD*(1) C 3- C 8	3.01
48. BD (1) C 4- C 5	78. BD*(1) C 4- H 9	0.74
48. BD (1) C 4- C 5	79. BD*(1) C 5- H 10	0.83
49. BD (2) C 4- C 5	68. BD*(2) C 1- N 16	23.05
49. BD (2) C 4- C 5	75. BD*(2) C 3- C 8	15.47
50. BD (1) C 4- H 9	65. BD*(1) C 1- C 5	3.44
51. BD (1) C 5- H 10	67. BD*(1) C 1- N 16	4.67
51. BD (1) C 5- H 10	73. BD*(1) C 3- C 4	3.63
51. BD (1) C 5- H 10	93. RY (1) C 1	0.69
52. BD (1) C 7- C 12	70. BD*(1) C 2- C 7	1.14
52. BD (1) C 7- C 12	72. BD*(1) C 2- N 16	4.31
52. BD (1) C 7- C 12	81. BD*(1) C 7- C 18	1.05
52. BD (1) C 7- C 12	84. BD*(1) C 11- C 12	1.80
52. BD (1) C 7- C 12	86. BD*(1) C 11- H 14	1.91
52. BD (1) C 7- C 12	7. BD*(1) C 12- H 15	0.86
52. BD (1) C 7- C 12	90. BD*(1) C 18- H 19	0.65
53. BD (1) C 7- C 18	69. BD*(1) C 2- C 3	3.39
53. BD (1) C 7- C 18	70. BD*(1) C 2- C 7	0.68
53. BD (1) C 7- C 18	80. BD*(1) C 7- C 12	1.36
53. BD (1) C 7- C 18	84. BD*(1) C 11- C 12	3.13

54. BD (1) C 8- C 11	73. BD*(1) C 3- C 4	2.98	
54. BD (1) C 8- C 11	74. BD*(1) C 3- C 8	1.58	
54. BD (1) C 8- C 11	83. BD*(1) C 8- H 13	0.85	
54. BD (1) C 8- C 11	84. BD*(1) C 11- C 12	1.36	
54. BD (1) C 8- C 11	86. BD*(1) C 11- H 14	0.77	
54. BD (1) C 8- C 11	87. BD*(1) C 12- H 15	2.03	
55. BD (1) C 8- H 13	69. BD*(1) C 2- C 3	3.95	
55. BD (1) C 8- H 13	84. BD*(1) C 11- C 12	3.64	
56. BD (1) C 11- C 12	80. BD*(1) C 7- C 12	1.52	
56. BD (1) C 11- C 12	81. BD*(1) C 7- C 18	2.99	
56. BD (1) C 11- C 12	82. BD*(1) C 8- C 11	1.48	
56. BD (1) C 11- C 12	83. BD*(1) C 8- H 13	2.51	
56. BD (1) C 11- C 12	87. BD*(1) C 12- H 15	0.54	
57. BD (2) C 11- C 12	71. BD*(2) C 2- C 7	14.66	
57. BD (2) C 11- C 12	75. BD*(2) C 3- C 8	15.94	
58. BD (1) C 11- H 14	74. BD*(1) C 3- C 8	3.81	
58. BD (1) C 11- H 14	80. BD*(1) C 7- C 12	3.27	
59. BD (1) C 12- H 15	70. BD*(1) C 2- C 7	3.68	
59. BD (1) C 12- H 15	82. BD*(1) C 8- C 11	3.36	
62. BD (1) C 18- H 19	71. BD*(2) C 2- C 7	2.54	
62. BD (1) C 18- H 19	80. BD*(1) C 7- C 12	1.12	
63. BD (1) C 18- H 20	71. BD*(2) C 2- C 7	3.67	
63. BD (1) C 18- H 20	80. BD*(1) C 7- C 12	0.82	
64. BD (1) C 18- H 21	70. BD*(1) C 2- C 7	3.42	
26. LP (1) N 16	88. BD*(1)Pd 17-Cl 22	25.53	
37. BD (1) C 1- C 5	88. BD*(1)Pd 17-Cl 22	0.16	
37. BD (1) C 1- C 5	89. BD*(1)Pd 17-Cl 23	0.30	
39. BD (1) C 1- N 16	88. BD*(1)Pd 17-Cl 22	0.07	
39. BD (1) C 1- N 16	89. BD*(1)Pd 17-Cl 23	0.66	
41. BD (1) C 2- C 3	88. BD*(1)Pd 17-Cl 22	0.84	
41. BD (1) C 2- C 3	89. BD*(1)Pd 17-Cl 23	1.13	
44. BD (1) C 2- N 16	88. BD*(1)Pd 17-Cl 22	0.55	
44. BD (1) C 2- N 16	89. BD*(1)Pd 17-Cl 23	2.37	
52. BD (1) C 7- C 12	88. BD*(1)Pd 17-Cl 22	0.50	
52. BD (1) C 7- C 12	89. BD*(1)Pd 17-Cl 23	0.44	
53. BD (1) C 7- C 18	88. BD*(1)Pd 17-Cl 22	0.50	
53. BD (1) C 7- C 18	89. BD*(1)Pd 17-Cl 23	0.20	
62. BD (1) C 18- H 19	88. BD*(1)Pd 17-Cl 22	43.98	
62. BD (1) C 18- H 19	89. BD*(1)Pd 17-Cl 23	9.05	
63. BD (1) C 18- H 20	88. BD*(1)Pd 17-Cl 22	16.63	
63. BD (1) C 18- H 20	89. BD*(1)Pd 17-Cl 23	3.71	
64. BD (1) C 18- H 21	88. BD*(1)Pd 17-Cl 22	1.46	
64. BD (1) C 18- H 21	89. BD*(1)Pd 17-Cl 23	0.40	
27. LP (1)Pd 17	65. BD*(1) C 1- C 5	0.07	
27. LP (1)Pd 17	67. BD*(1) C 1- N 16	0.60	
27. LP (1)Pd 17	72. BD*(1) C 2- N 16	0.83	
27. LP (1)Pd 17	80. BD*(1) C 7- C 12	0.35	
27. LP (1)Pd 17	81. BD*(1) C 7- C 18	0.17	
27. LP (1)Pd 17	90. BD*(1) C 18- H 19	0.36	
27. LP (1)Pd 17	91. BD*(1) C 18- H 20	0.10	*
27. LP (1)Pd 17	92. BD*(1) C 18- H 21	0.92	
28. LP (2)Pd 17	67. BD*(1) C 1- N 16	0.10	
28. LP (2)Pd 17	69. BD*(1) C 2- C 3	0.18	
28. LP (2)Pd 17	72. BD*(1) C 2- N 16	0.06	
28. LP (2)Pd 17	81. BD*(1) C 7- C 18	0.17	
28. LP (2)Pd 17	90. BD*(1) C 18- H 19	0.27	
29. LP (3)Pd 17	68. BD*(2) C 1- N 16	0.20	

29. LP (3)Pd 17	90. BD*(1) C 18- H 19	5.96
29. LP (3)Pd 17	91. BD*(1) C 18- H 20	0.09
29. LP (3)Pd 17	92. BD*(1) C 18- H 21	0.09
30. LP (4)Pd 17	68. BD*(2) C 1- N 16	4.04
30. LP (4)Pd 17	71. BD*(2) C 2- C 7	0.09
30. LP (4)Pd 17	90. BD*(1) C 18- H 19	0.43
31. LP (1)Cl 22	90. BD*(1) C 18- H 19	0.13
31. LP (1)Cl 22	92. BD*(1) C 18- H 21	0.20
32. LP (2)Cl 22	90. BD*(1) C 18- H 19	0.23
33. LP (3)Cl 22	65. BD*(1) C 1- C 5	0.37
33. LP (3)Cl 22	66. BD*(1) C 1- H 6	4.64
33. LP (3)Cl 22	2. BD*(1) C 2- N 16	0.13
33. LP (3)Cl 22	90. BD*(1) C 18- H 19	0.12
34. LP (1)Cl 23	81. BD*(1) C 7- C 18	0.10
34. LP (1)Cl 23	90. BD*(1) C 18- H 19	0.13
34. LP (1)Cl 23	92. BD*(1) C 18- H 21	0.06
35. LP (2)Cl 23	66. BD*(1) C 1- H 6	0.05
35. LP (2)Cl 23	81. BD*(1) C 7- C 18	0.08
35. LP (2)Cl 23	90. BD*(1) C 18- H 19	0.06
35. LP (2)Cl 23	92. BD*(1) C 18- H 21	0.06
36. LP (3)Cl 23	68. BD*(2) C 1- N 16	0.06
36. LP (3)Cl 23	90. BD*(1) C 18- H 19	0.24
36. LP (3)Cl 23	91. BD*(1) C 18- H 20	0.09
60. BD (1)Pd 17-Cl 22	65. BD*(1) C 1- C 5	0.12
60. BD (1)Pd 17-Cl 22	66. BD*(1) C 1- H 6	0.33
60. BD (1)Pd 17-Cl 22	67. BD*(1) C 1- N 16	0.06
60. BD (1)Pd 17-Cl 22	69. BD*(1) C 2- C 3	0.14
60. BD (1)Pd 17-Cl 22	72. BD*(1) C 2- N 16	0.10
60. BD (1)Pd 17-Cl 22	80. BD*(1) C 7- C 12	0.12
60. BD (1)Pd 17-Cl 22	90. BD*(1) C 18- H 19	1.01
60. BD (1)Pd 17-Cl 22	91. BD*(1) C 18- H 20	0.07
60. BD (1)Pd 17-Cl 22	92. BD*(1) C 18- H 21	0.86
61. BD (1)Pd 17-Cl 23	66. BD*(1) C 1- H 6	0.21
61. BD (1)Pd 17-Cl 23	69. BD*(1) C 2- C 3	0.07
61. BD (1)Pd 17-Cl 23	81. BD*(1) C 7- C 18	0.24
61. BD (1)Pd 17-Cl 23	90. BD*(1) C 18- H 19	1.01
61. BD (1)Pd 17-Cl 23	91. BD*(1) C 18- H 20	0.13
61. BD (1)Pd 17-Cl 23	92. BD*(1) C 18- H 21	0.38
27. LP (1)Pd 17	88. BD*(1)Pd 17-Cl 22	8.59
27. LP (1)Pd 17	89. BD*(1)Pd 17-Cl 23	7.35
28. LP (2)Pd 17	88. BD*(1)Pd 17-Cl 22	7.31
28. LP (2)Pd 17	89. BD*(1)Pd 17-Cl 23	7.39
29. LP (3)Pd 17	88. BD*(1)Pd 17-Cl 22	0.98
29. LP (3)Pd 17	89. BD*(1)Pd 17-Cl 23	1.11
31. LP (1)Cl 22	88. BD*(1)Pd 17-Cl 22	3.53
31. LP (1)Cl 22	89. BD*(1)Pd 17-Cl 23	3.73
33. LP (3)Cl 22	88. BD*(1)Pd 17-Cl 22	2.29
33. LP (3)Cl 22	89. BD*(1)Pd 17-Cl 23	2.61
34. LP (1)Cl 23	88. BD*(1)Pd 17-Cl 22	1.36
34. LP (1)Cl 23	89. BD*(1)Pd 17-Cl 23	0.98
35. LP (2)Cl 23	88. BD*(1)Pd 17-Cl 22	5.63
35. LP (2)Cl 23	89. BD*(1)Pd 17-Cl 23	4.16
60. BD (1)Pd 17-Cl 22	88. BD*(1)Pd 17-Cl 22	14.64
60. BD (1)Pd 17-Cl 22	89. BD*(1)Pd 17-Cl 23	39.44
61. BD (1)Pd 17-Cl 23	88. BD*(1)Pd 17-Cl 22	26.41
61. BD (1)Pd 17-Cl 23	89. BD*(1)Pd 17-Cl 23	5.99

Complex (Cl^1 replaced by CH3): [$PdCl(CH_3)$(1-tetralone oxime)].



Donor (L) NBO	Acceptor (NL) NBO	*E* (2) kcalmol^{-1}
24. LP (2)Pd 1	96. BD*(1) C 26- H 27	1.24
25. LP (3)Pd 1	97. BD*(1) C 26- H 28	0.70
25. LP (3)Pd 1	98. BD*(1) C 26- H 29	0.79
33. BD (1)Pd 1-Cl 2	67. BD*(1)Pd 1- C 26	44.68
33. BD (1)Pd 1-Cl 2	97. BD*(1) C 26- H 28	0.68
23. LP (1)Pd 1	81. BD*(1) C 13- C 14	0.20
23. LP (1)Pd 1	82. BD*(2) C 13- C 14	2.29
24. LP (2)Pd 1	70. BD*(1) C 3- N 23	0.65
24. LP (2)Pd 1	71. BD*(2) C 3- N 23	0.17
24. LP (2)Pd 1	81. BD*(1) C 13- C 14	0.55
24. LP (2)Pd 1	83. BD*(1) C 13- C 15	0.08
24. LP (2)Pd 1	84. BD*(1) C 14- C 16	0.83
24. LP (2)Pd 1	94. BD*(1) N 23- O 24	1.77
25. LP (3)Pd 1	71. BD*(2) C 3- N 23	3.32
25. LP (3)Pd 1	81. BD*(1) C 13- C 14	0.09
25. LP (3)Pd 1	84. BD*(1) C 14- C 16	0.05
25. LP (3)Pd 1	85. BD*(1) C 14- H 17	1.51
25. LP (3)Pd 1	94. BD*(1) N 23- O 24	0.06
26. LP (4)Pd 1	71. BD*(2) C 3- N 23	0.43
26. LP (4)Pd 1	82. BD*(2) C 13- C 14	0.93
26. LP (4)Pd 1	84. BD*(1) C 14- C 16	0.06
26. LP (4)Pd 1	85. BD*(1) C 14- H 17	7.18
27. LP (1)Cl 2	82. BD*(2) C 13- C 14	0.32
28. LP (2)Cl 2	71. BD*(2) C 3- N 23	0.08
28. LP (2)Cl 2	85. BD*(1) C 14- H 17	0.20
29. LP (3)Cl 2	70. BD*(1) C 3- N 23	0.20
29. LP (3)Cl 2	82. BD*(2) C 13- C 14	0.30
29. LP (3)Cl 2	94. BD*(1) N 23- O 24	0.07
29. LP (3)Cl 2	95. BD*(1) O 24- H 25	9.77
33. BD (1)Pd 1-Cl 2	81. BD*(1) C 13- C 14	0.11
33. BD (1)Pd 1-Cl 2	82. BD*(2) C 13- C 14	3.19
33. BD (1)Pd 1-Cl 2	84. BD*(1) C 14- C 16	0.36
33. BD (1)Pd 1-Cl 2	85. BD*(1) C 14- H 17	0.09

33. BD (1)Pd 1-Cl 2	90. BD*(1) C 16- H 20	0.06
33. BD (1)Pd 1-Cl 2	94. BD*(1) N 23- O 24	0.21
33. BD (1)Pd 1-Cl 2	95. BD*(1) O 24- H 25	0.73
34. BD (1)Pd 1- C 26	70. BD*(1) C 3- N 23	0.10
34. BD (1)Pd 1- C 26	82. BD*(2) C 13- C 14	4.45
34. BD (1)Pd 1- C 26	84. BD*(1) C 14- C 16	0.26
34. BD (1)Pd 1- C 26	85. BD*(1) C 14- H 17	0.40
34. BD (1)Pd 1- C 26	94. BD*(1) N 23- O 24	0.89
34. BD (1)Pd 1- C 26	95. BD*(1) O 24- H 25	0.37
63. BD (1) C 26- H 27	90. BD*(1) C 16- H 20	0.05
64. BD (1) C 26- H 28	81. BD*(1) C 13- C 14	0.05
64. BD (1) C 26- H 28	85. BD*(1) C 14- H 17	0.11
64. BD (1) C 26- H 28	90. BD*(1) C 16- H 20	0.10
30. LP (1) N 23	66. BD*(1)Pd 1-Cl 2	18.97
30. LP (1) N 23	67. BD*(1)Pd 1- C 26	76.47
31. LP (1) O 24	66. BD*(1)Pd 1-Cl 2	0.13
31. LP (1) O 24	67. BD*(1)Pd 1- C 26	0.19
35. BD (1) C 3- C 4	66. BD*(1)Pd 1-Cl 2	0.61
35. BD (1) C 3- C 4	67. BD*(1)Pd 1- C 26	0.71
36. BD (1) C 3- C 13	66. BD*(1)Pd 1-Cl 2	0.37
36. BD (1) C 3- C 13	67. BD*(1)Pd 1- C 26	0.13
37. BD (1) C 3- N 23	66. BD*(1)Pd 1-Cl 2	1.29
37. BD (1) C 3- N 23	67. BD*(1)Pd 1- C 26	3.23
48. BD (1) C 13- C 14	66. BD*(1)Pd 1-Cl 2	0.64
48. BD (1) C 13- C 14	67. BD*(1)Pd 1- C 26	0.10
49. BD (2) C 13- C 14	66. BD*(1)Pd 1-Cl 2	22.61
49. BD (2) C 13- C 14	67. BD*(1)Pd 1- C 26	6.05
49. BD (2) C 13- C 14	98. BD*(1) C 26- H 29	0.06
50. BD (1) C 13- C 15	66. BD*(1)Pd 1-Cl 2	0.12
50. BD (1) C 13- C 15	67. BD*(1)Pd 1- C 26	0.06
51. BD (1) C 14- C 16	66. BD*(1)Pd 1-Cl 2	0.15
51. BD (1) C 14- C 16	67. BD*(1)Pd 1- C 26	0.31
52. BD (1) C 14- H 17	66. BD*(1)Pd 1-Cl 2	73.83
52. BD (1) C 14- H 17	67. BD*(1)Pd 1- C 26	8.56
52. BD (1) C 14- H 17	97. BD*(1) C 26- H 28	0.15
55. BD (1) C 16- C 19	66. BD*(1)Pd 1-Cl 2	0.54
55. BD (1) C 16- C 19	67. BD*(1)Pd 1- C 26	0.24
56. BD (2) C 16- C 19	66. BD*(1)Pd 1-Cl 2	0.26
56. BD (2) C 16- C 19	67. BD*(1)Pd 1- C 26	0.14
61. BD (1) N 23- O 24	66. BD*(1)Pd 1-Cl 2	0.26
30. LP (1) N 23	68. BD*(1) C 3- C 4	8.74
30. LP (1) N 23	69. BD*(1) C 3- C 13	1.54
30. LP (1) N 23	95. BD*(1) O 24- H 25	0.88
32. LP (2) O 24	71. BD*(2) C 3- N 23	19.72
35. BD (1) C 3- C 4	69. BD*(1) C 3- C 13	0.96
35. BD (1) C 3- C 4	70. BD*(1) C 3- N 23	0.73
35. BD (1) C 3- C 4	76. BD*(1) C 5- H 9	1.32
35. BD (1) C 3- C 4	81. BD*(1) C 13- C 14	2.43
35. BD (1) C 3- C 4	94. BD*(1) N 23- O 24	1.00
36. BD (1) C 3- C 13	68. BD*(1) C 3- C 4	0.66
36. BD (1) C 3- C 13	70. BD*(1) C 3- N 23	1.39
36. BD (1) C 3- C 13	74. BD*(1) C 4- H 7	0.51
36. BD (1) C 3- C 13	81. BD*(1) C 13- C 14	1.80
36. BD (1) C 3- C 13	83. BD*(1) C 13- C 15	1.55
36. BD (1) C 3- C 13	84. BD*(1) C 14- C 16	1.64
36. BD (1) C 3- C 13	86. BD*(1) C 15- C 18	2.54
36. BD (1) C 3- C 13	94. BD*(1) N 23- O 24	6.16
37. BD (1) C 3- N 23	68. BD*(1) C 3- C 4	1.29

37. BD (1) C 3- N 23	69. BD*(1) C 3- C 13	1.18
37. BD (1) C 3- N 23	72. BD*(1) C 4- C 5	0.58
37. BD (1) C 3- N 23	83. BD*(1) C 13- C 15	1.73
37. BD (1) C 3- N 23	95. BD*(1) O 24- H 25	0.91
38. BD (2) C 3- N 23	71. BD*(2) C 3- N 23	2.11
38. BD (2) C 3- N 23	73. BD*(1) C 4- H 6	1.57
38. BD (2) C 3- N 23	74. BD*(1) C 4- H 7	1.07
38. BD (2) C 3- N 23	82. BD*(2) C 13- C 14	8.01
39. BD (1) C 4- C 5	68. BD*(1) C 3- C 4	0.67
39. BD (1) C 4- C 5	70. BD*(1) C 3- N 23	3.83
39. BD (1) C 4- C 5	78. BD*(1) C 8- H 11	1.68
40. BD (1) C 4- H 6	69. BD*(1) C 3- C 13	1.38
40. BD (1) C 4- H 6	71. BD*(2) C 3- N 23	6.14
40. BD (1) C 4- H 6	77. BD*(1) C 5- H 10	2.50
41. BD (1) C 4- H 7	69. BD*(1) C 3- C 13	2.49
41. BD (1) C 4- H 7	71. BD*(2) C 3- N 23	3.77
41. BD (1) C 4- H 7	75. BD*(1) C 5- C 8	2.73
42. BD (1) C 5- C 8	74. BD*(1) C 4- H 7	1.69
42. BD (1) C 5- C 8	80. BD*(1) C 8- C 15	0.65
42. BD (1) C 5- C 8	86. BD*(1) C 15- C 18	2.61
42. BD (1) C 5- C 8	87. BD*(2) C 15- C 18	0.83
43. BD (1) C 5- H 9	68. BD*(1) C 3- C 4	2.82
43. BD (1) C 5- H 9	80. BD*(1) C 8- C 15	2.81
44. BD (1) C 5- H 10	73. BD*(1) C 4- H 6	2.61
44. BD (1) C 5- H 10	79. BD*(1) C 8- H 12	2.72
45. BD (1) C 8- H 11	72. BD*(1) C 4- C 5	2.78
45. BD (1) C 8- H 11	83. BD*(1) C 13- C 15	3.35
45. BD (1) C 8- H 11	87. BD*(2) C 15- C 18	1.06
46. BD (1) C 8- H 12	77. BD*(1) C 5- H 10	2.61
46. BD (1) C 8- H 12	87. BD*(2) C 15- C 18	5.10
47. BD (1) C 8- C 15	76. BD*(1) C 5- H 9	1.39
47. BD (1) C 8- C 15	81. BD*(1) C 13- C 14	3.22
47. BD (1) C 8- C 15	83. BD*(1) C 13- C 15	1.15
47. BD (1) C 8- C 15	86. BD*(1) C 15- C 18	1.35
47. BD (1) C 8- C 15	91. BD*(1) C 18- C 19	2.24
48. BD (1) C 13- C 14	68. BD*(1) C 3- C 4	2.30
48. BD (1) C 13- C 14	69. BD*(1) C 3- C 13	2.10
48. BD (1) C 13- C 14	80. BD*(1) C 8- C 15	2.77
48. BD (1) C 13- C 14	83. BD*(1) C 13- C 15	2.86
48. BD (1) C 13- C 14	84. BD*(1) C 14- C 16	1.69
48. BD (1) C 13- C 14	90. BD*(1) C 16- H 20	1.99
49. BD (2) C 13- C 14	70. BD*(1) C 3- N 23	0.67
49. BD (2) C 13- C 14	71. BD*(2) C 3- N 23	15.93
49. BD (2) C 13- C 14	85. BD*(1) C 14- H 17	2.28
49. BD (2) C 13- C 14	87. BD*(2) C 15- C 18	14.92
49. BD (2) C 13- C 14	89. BD*(2) C 16- C 19	17.75
50. BD (1) C 13- C 15	69. BD*(1) C 3- C 13	1.84
50. BD (1) C 13- C 15	70. BD*(1) C 3- N 23	1.43
50. BD (1) C 13- C 15	78. BD*(1) C 8- H 11	0.65
50. BD (1) C 13- C 15	80. BD*(1) C 8- C 15	0.98
50. BD (1) C 13- C 15	81. BD*(1) C 13- C 14	2.49
50. BD (1) C 13- C 15	85. BD*(1) C 14- H 17	2.20
50. BD (1) C 13- C 15	86. BD*(1) C 15- C 18	1.95
50. BD (1) C 13- C 15	92. BD*(1) C 18- H 21	2.04
51. BD (1) C 14- C 16	69. BD*(1) C 3- C 13	3.06
51. BD (1) C 14- C 16	81. BD*(1) C 13- C 14	1.54
51. BD (1) C 14- C 16	88. BD*(1) C 16- C 19	1.48
51. BD (1) C 14- C 16	90. BD*(1) C 16- H 20	1.04

51. BD (1) C 14- C 16	93. BD*(1) C 19- H 22	2.19
52. BD (1) C 14- H 17	82. BD*(2) C 13- C 14	1.31
52. BD (1) C 14- H 17	83. BD*(1) C 13- C 15	4.58
52. BD (1) C 14- H 17	88. BD*(1) C 16- C 19	4.61
52. BD (1) C 14- H 17	90. BD*(1) C 16- H 20	0.63
53. BD (1) C 15- C 18	69. BD*(1) C 3- C 13	2.71
53. BD (1) C 15- C 18	75. BD*(1) C 5- C 8	0.81
53. BD (1) C 15- C 18	80. BD*(1) C 8- C 15	1.30
53. BD (1) C 15- C 18	83. BD*(1) C 13- C 15	2.23
53. BD (1) C 15- C 18	91. BD*(1) C 18- C 19	1.66
53. BD (1) C 15- C 18	92. BD*(1) C 18- H 21	0.63
53. BD (1) C 15- C 18	93. BD*(1) C 19- H 22	1.90
54. BD (2) C 15- C 18	75. BD*(1) C 5- C 8	1.13
54. BD (2) C 15- C 18	79. BD*(1) C 8- H 12	3.21
54. BD (2) C 15- C 18	82. BD*(2) C 13- C 14	16.13
54. BD (2) C 15- C 18	89. BD*(2) C 16- C 19	15.16
55. BD (1) C 16- C 19	84. BD*(1) C 14- C 16	1.51
55. BD (1) C 16- C 19	85. BD*(1) C 14- H 17	2.35
55. BD (1) C 16- C 19	90. BD*(1) C 16- H 20	0.60
55. BD (1) C 16- C 19	91. BD*(1) C 18- C 19	1.35
55. BD (1) C 16- C 19	92. BD*(1) C 18- H 21	2.16
55. BD (1) C 16- C 19	93. BD*(1) C 19- H 22	0.57
56. BD (2) C 16- C 19	82. BD*(2) C 13- C 14	12.83
56. BD (2) C 16- C 19	87. BD*(2) C 15- C 18	14.86
57. BD (1) C 16- H 20	81. BD*(1) C 13- C 14	3.32
57. BD (1) C 16- H 20	91. BD*(1) C 18- C 19	3.48
58. BD (1) C 18- C 19	80. BD*(1) C 8- C 15	3.23
58. BD (1) C 18- C 19	86. BD*(1) C 15- C 18	1.75
58. BD (1) C 18- C 19	88. BD*(1) C 16- C 19	1.29
58. BD (1) C 18- C 19	90. BD*(1) C 16- H 20	2.22
58. BD (1) C 18- C 19	92. BD*(1) C 18- H 21	0.61
58. BD (1) C 18- C 19	93. BD*(1) C 19- H 22	0.63
59. BD (1) C 18- H 21	83. BD*(1) C 13- C 15	4.22
59. BD (1) C 18- H 21	88. BD*(1) C 16- C 19	3.53
60. BD (1) C 19- H 22	84. BD*(1) C 14- C 16	3.64
60. BD (1) C 19- H 22	86. BD*(1) C 15- C 18	3.59
61. BD (1) N 23- O 24	69. BD*(1) C 3- C 13	3.20

Supplementary Table 4: Overlap matrix for complexes (**1**) to (**5**) and [PdCl(CH_3)(1-tetralone oxime)].

		(1)	(2)	(3)	(4)	(5)	Cl^1 replaced by CH_3
C-Hσ	**Pd-Cl* (trans)**	0.4488	0.4512	0.4287	-	0.4522	0.5248
	Pd-Cl* (cis)	0.0788	0.0736	0.0783	0.1072	0.0811	0.0106‡
C(7)-C(8)π	**Pd-Cl* (trans)**	0.1764	0.1731	0.2050	-	-	0.1711
	Pd-Cl* (cis)	0.0497	0.0502	0.0494	-	-	0.0287‡
C(8)-C(8a)σ	**Pd-Cl* (trans)**	0.1651	0.1642	0.1811	-	0.1749	0.2048
	Pd-Cl* (cis)	0.0968	0.1004	0.1019	0.1229	0.1069	0.0997‡
C(8)-C(8a)π	**Pd-Cl* (trans)**	-	-	-	-	0.1741	-
	Pd-Cl* (cis)	-	-	-	-	0.0699	-‡

‡ Value is for the Pd-Cσ*(*cis*) orbital for the [PdCl(CH_3)(1-tetralone oxime)] complex.

Supplementary Table 5: Occupancy (n) and Energy (a.u) of NBOs involved in donor-acceptor interactions for complexes (**1**) to (**5**) and [PdCl(CH_3)(1-tetralone oxime)].

	(**1**)	(**2**)	(**3**)	(**4**)	(**5**)	**Cl^1 replaced by CH_3**
C-Hσ						
Occupancy (n)	1.8457	1.8375	1.8511	1.9013	1.8444	1.8406
Energy (a.u)	-0.4451	-0.4513	-0.3212	-0.3184	-0.4496	-0.4155
C(7)-C(8)π						
Occupancy (n)	1.6494	1.6309	1.6344	-	-	1.5985
Energy (a.u)	-0.2574	-0.2730	-0.1227	-	-	-0.2382
C(8)-C(8a)σ						
Occupancy (n)	1.9677	1.9626	1.9611	1.9617	1.9671	1.9622
Energy (a.u)	-0.5625	-0.5832	-0.4307	-0.4077	-0.5666	-0.5459
C(8)-C(8a) π						
Occupancy (n)	-	-	-	-	1.6009	-
Energy (a.u)	-	-	-	-	-0.2613	-
Pd-Cl* (*cis*)						
Occupancy (n)	0.3980	0.3984	0.4181	0.3590	0.3966	0.3090‡
Energy (a.u)	0.2146	0.1761	0.3115	0.4442	0.2001	0.2054‡
Pd-Cl* (*trans*)						
Occupancy (n)	0.3208	0.3131	0.3888	-	0.3215	0.3117
Energy (a.u)	0.2970	0.2607	0.3969	-	0.2789	0.5630

‡ Value is for the Pd-Cσ*(*cis*) orbital for the [PdCl(CH_3)(1-tetralone oxime)] complex.

Supplementary Table 6. Selected structural data for (**1**) to (**5**) and [PdCl(CH_3)(1-tetralone oxime)].

	(**1**)	(**2**)	(**3**)	(**4**)	(**5**)	Cl^1 replaced by CH_3
Distances (Å)[a]						
Pd····H	1.819	1.802	1.901	2.180	1.822	1.780
Pd····C	2.240	2.229	2.208	2.146	2.228	2.226
Cl(cis)····H	2.865	2.850	2.957	3.235	2.887	2.720
C-H	1.152	1.156	1.138	1.113	1.152	1.164
	(1.081)	(1.089)	(1.090)	(1.090)	(1.090)	(1.081)
Angles (°)						
Pd-N-C	119.9	120.2	120.0	119.8	120.8	119.4
Pd····C-H	54.0	53.7	59.4	76.8	54.6	52.7
Pd····H-C	95.2	95.3	89.6	73.4	94.4	96.0
Cl(trans)-Pd····H	157.7	159.0	153.4	146.3	157.2	157.5
Cl(trans)-Pd····C	166.3	165.3	167.8	167.3	166.2	165.7
Dihedrals (°)						
Cl(trans)-Pd-N-C	165.8	165.5	168.3	171.4	166.3	166.3
Ar-Plane/CP[b]	34.5	35.6	33.0	33.4	36.1	33.6
N-C-C-C	15.1	15.1	14.0	18.5	18.0	15.4
C-H deform (°)	-27.2	-27.6	-31.1	-43.7	-27.1	-26.6

[a] Free ligand values in brackets. [b] Angle between the aromatic ring plane and the coordination plane.

Supplementary Table 7. NBO donations (kcal mol^{-1}) for (**1**) to (**5**) and [PdCl(CH_3)(1-tetralone oxime)].

	(**1**)	(**2**)	(**3**)	(**4**)	(**5**)	Cl^1 replaced by CH_3
C-Hσ to						
Pd-Clσ*(*trans*)	58.6	75.6	64.0	-	56.9	73.8
Pd-Clσ*(*cis*)	10.0	15.0	13.8	3.1	8.9	8.6‡
C(7)-C(8)π to						
Pd-Clσ*(*trans*)	20.3	27.6	41.9	-	0.1	22.6
Pd-Clσ*(*cis*)	6.5	10.5	13.8	-	-	6.1‡
C(8)-C(8a)σ to						
Pd-Clσ*(*trans*)	1.4	0.7	0.1	-	1.5	0.6
Pd-Clσ*(*cis*)	0.4	0.1	0.9	1.9	0.4	0.1‡
C(8)-C(8a)π to						
Pd-Clσ*(*trans*)	-	-	-	-	20.3	-
Pd-Clσ*(*cis*)	-	-	-	-	6.8	-

‡ Value is for the Pd-Cσ*(*cis*) orbital for the [PdCl(CH_3)(1-tetralone oxime)] complex.

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