Trinuclear and Cyclometallated Organometallic Dinuclear Pt-Pyrazolato Complexes: A Combined Experimental and Theoretical Study

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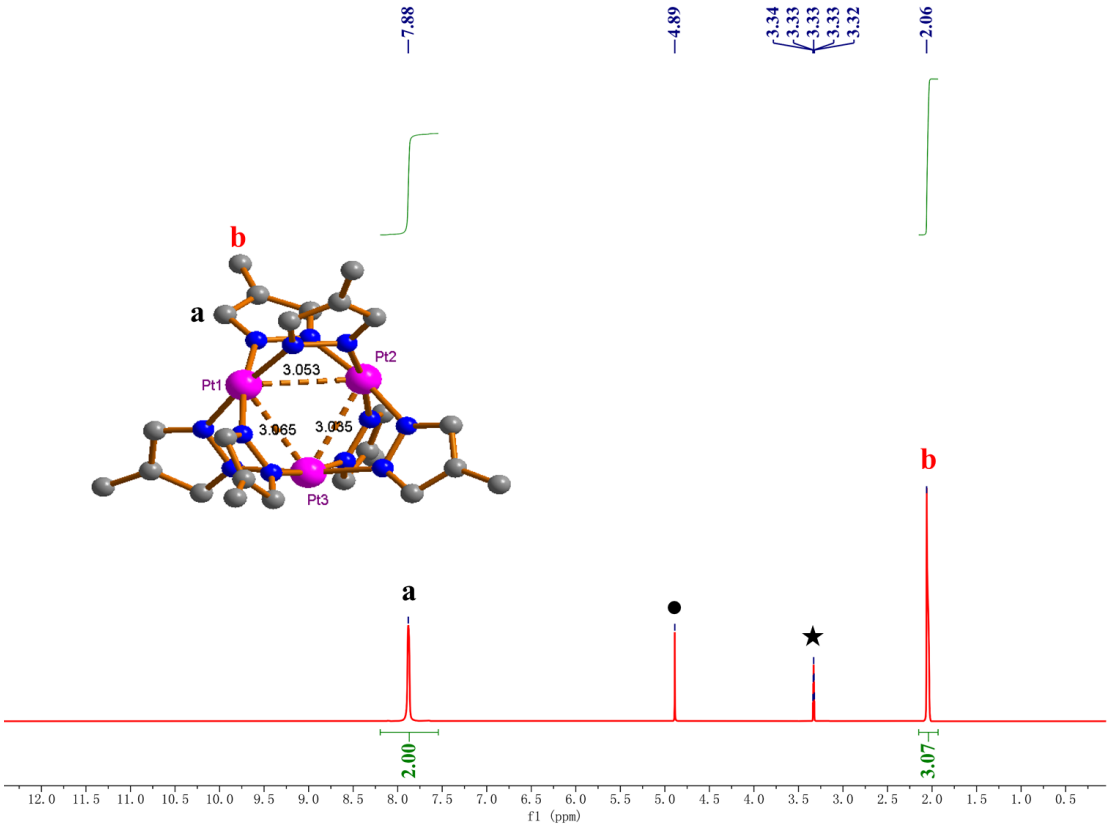

Figure S1. ^{1}H NMR of **1** in CD_3OD solvent at 293 K. Peaks marked by a solid dot or star identify solvent peaks.

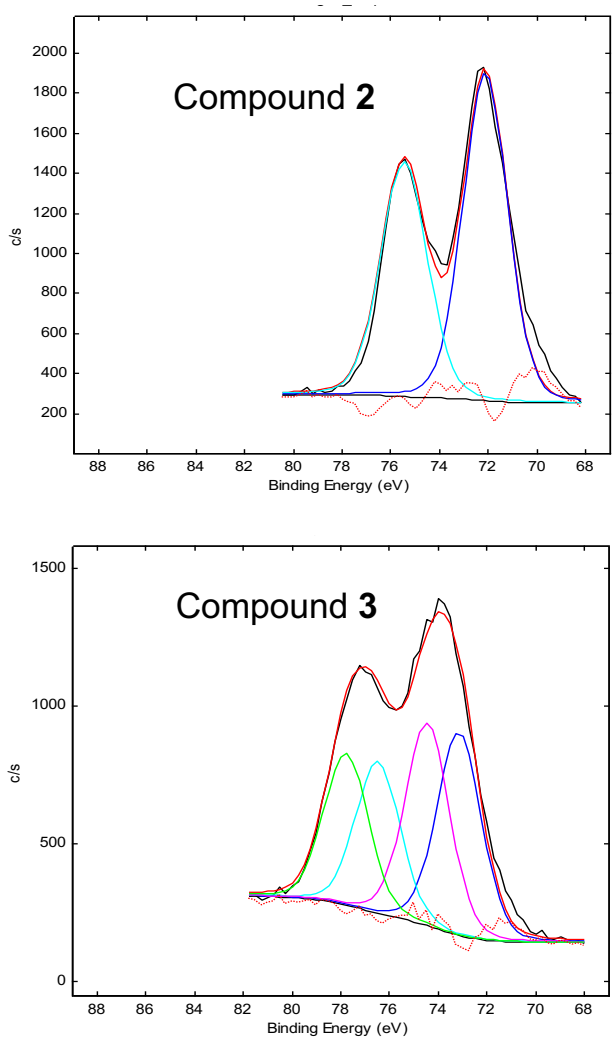

Figure S2. XPS spectra of **2** (top) and **3** (bottom).

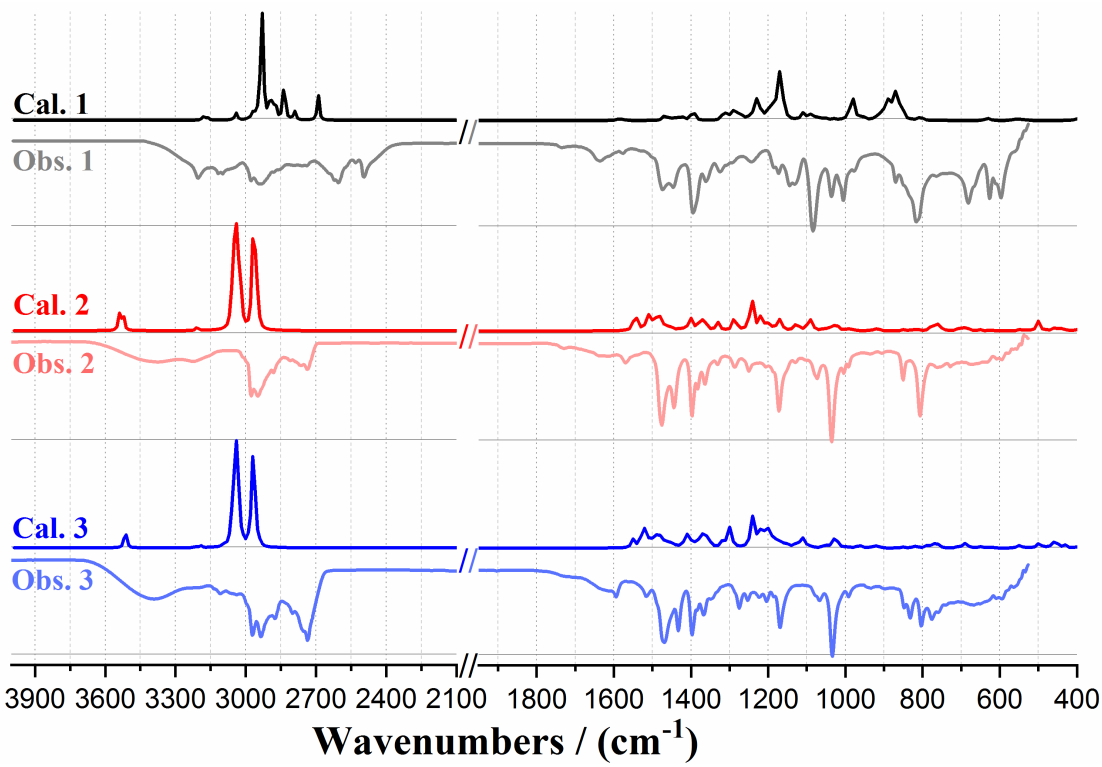

Figure S3. Calculated and observed FT-IR spectra of **1**, **2** and **3**. The intensity on the Y axis is normalized.

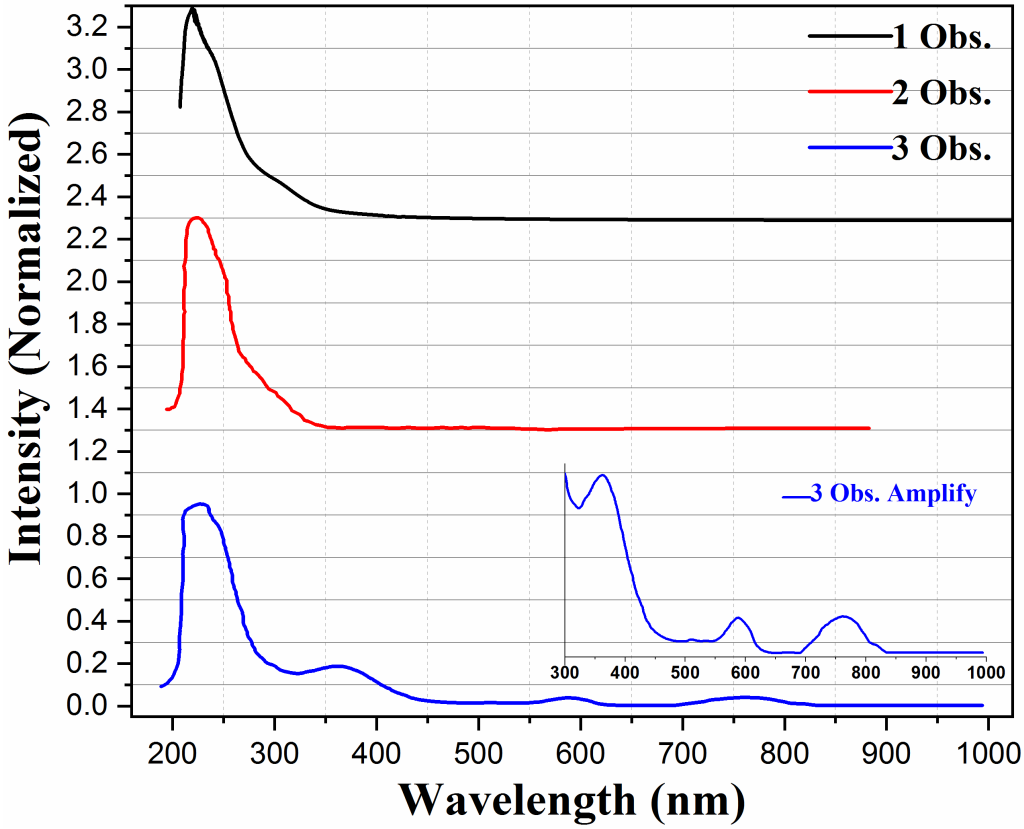

Figure S4. UV-vis-NIR spectra of **1** (black), **2** (red) and **3** (blue), 0.08 mM/CH_2Cl_2.

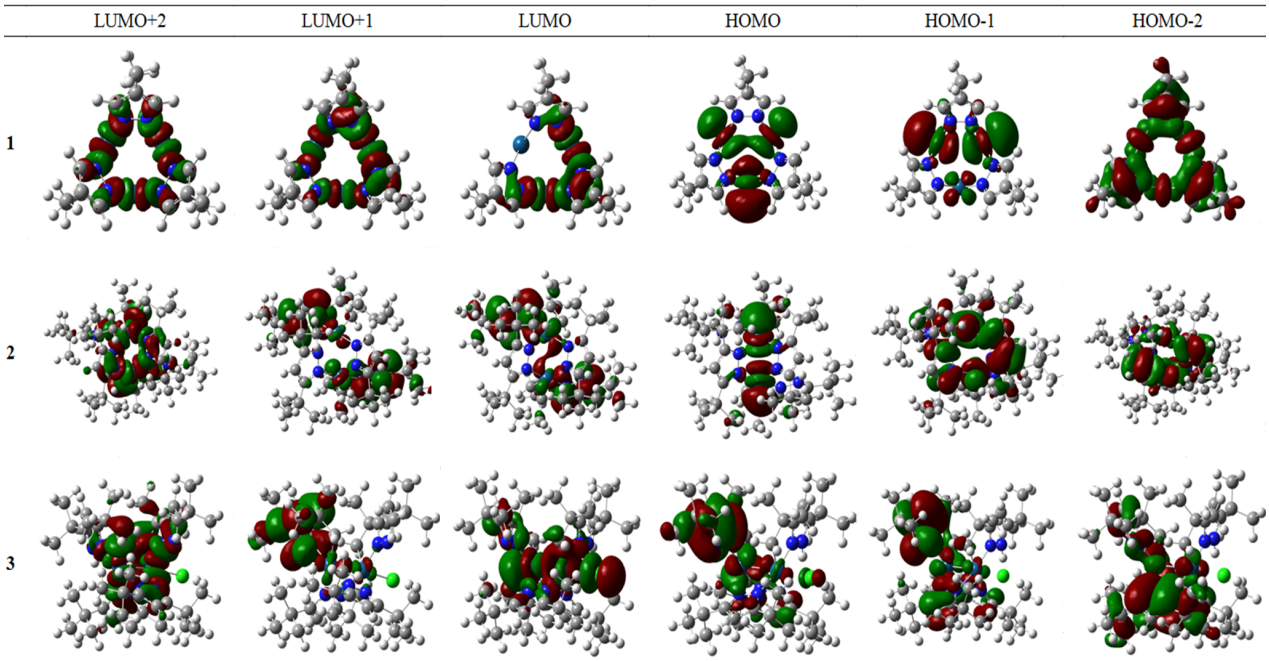

Figure S5. Important molecular orbitals of Pt-complexes **1**, **2** and **3**.

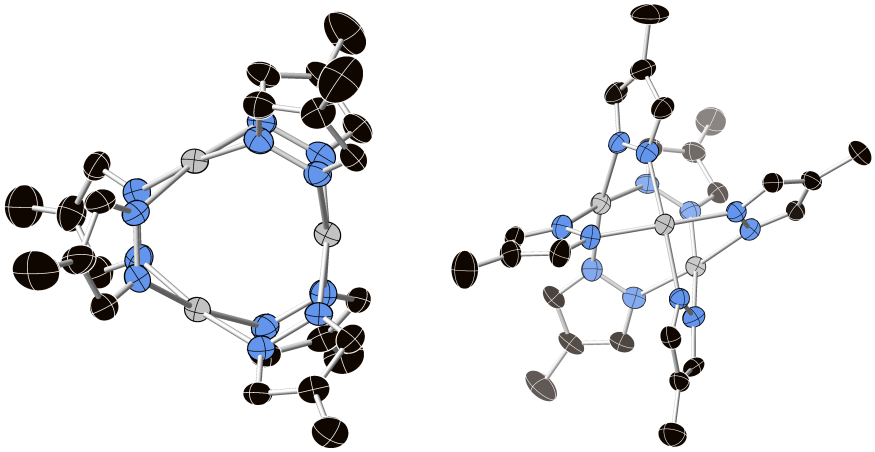

Figure S6. ORTEP diagram of compound **1**. H atoms are omitted for clarity.

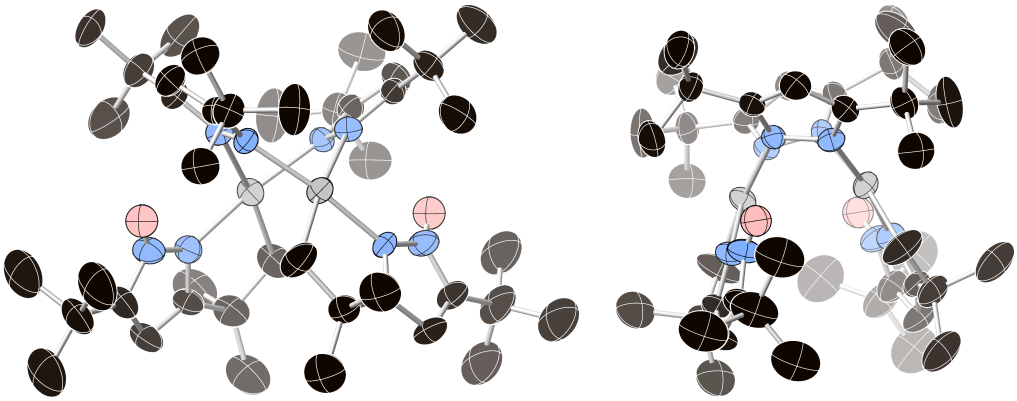

Figure S7. ORTEP diagram of compound **2**. C-H atoms are omitted for clarity.

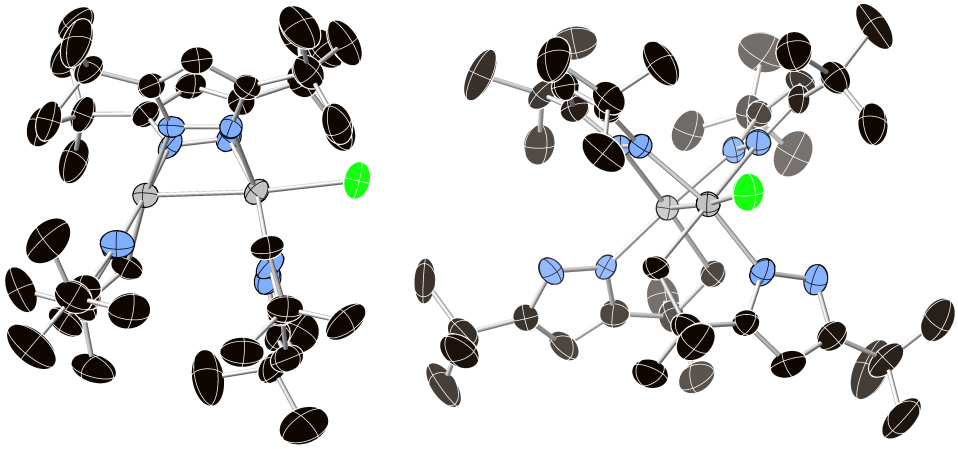

Figure S8. ORTEP diagram of compound **3**. H atoms are omitted for clarity.

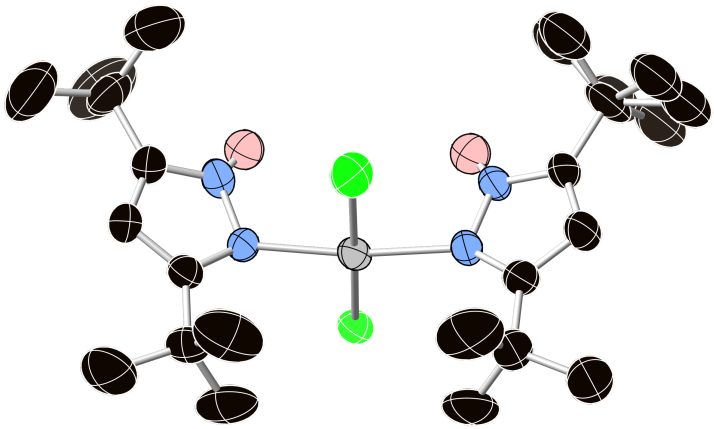

Figure S9. ORTEP diagram of *trans*-**[PtCl$_2$(3,5-^{t}Bu$_2$-pzH)$_2$]**. C-H atoms are omitted for clarity.

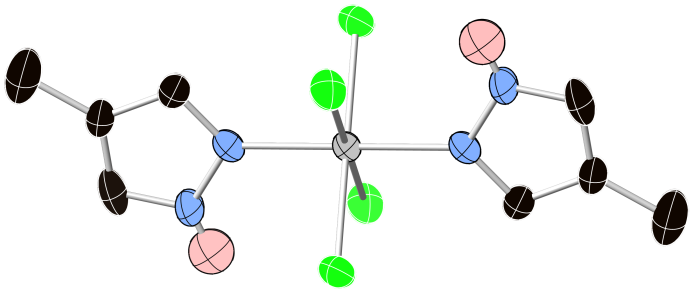

Figure S10. ORTEP diagram of *trans*-[**PtCl$_2$(4-Me-pzH)$_2$]**. C-H atoms are omitted for clarity.

Table S1. Crystallographic data for *trans*-**[PtCl$_2$(3,5-^{t}Bu$_2$-pzH)$_2$]** and *trans*-[**PtCl$_2$(4-Me-pzH)$_2$]**.

	[PtCl$_2$(3,5-^{t}Bu$_2$-pzH)$_2$] ·CHCl$_3$	**[PtCl$_2$(4-Me-pzH)$_2$]**
formula	$C_{23}H_{41}Cl_5N_4Pt$	$C_8H_{16}N_4Cl_4Pt$
crystal size, mm^3	0.40 × 0.25 × 0.16	0.11 × 0.07 × 0.03
fw	745.94	505.14
space group	*C*2/*c* (No. 15)	*Pmna* (No. 53)
a, Å	25.360(5)	7.187(6)
b, Å	12.569(2)	8.144(3)
c, Å	21.115(3)	12.068(10)
α, º	90	90
β, º	105.715(17)	90
γ, º	90	90
V, Å^3	6479(2)	706.4(9)
Z	8	2
T, K	298(2)	298(2)
ρ_{calcd}, g cm^{-3}	1.529	2.375
reflctns collected/2θ_{max}	19813/56.24	3126/46.58
Unique reflctns/I > 2σ(I)	5656/7941	567/552
No. of params/restraints	310/114	51/0
μ(Mo Kα), mm^{-1}	4.761	10.672
F(000)	2960	476
R1[a]/ all data	0.0617/0.1253	0.0189/0.0469
wR2[b] (I > 2σ(I))	0.1406	0.0492
Goodness of fit[c]	1.273	1.101

[a] $I > 2\sigma(I)$. R1 = $\Sigma \, | |F_o| - |F_c| | / \Sigma \, |F_o|$. [b] wR2 = $[\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$, where $w = 1/\sigma^2(F_o^2) + (aP)^2 + bP$, $P = (F_o^2 + 2F_c^2)/3$. [c] GoF = $[\Sigma[w(F_o^2 - F_c^2)^2]/(n - p)]^{1/2}$.

Table S2. Selected bond lengths(Å) and angles(º) for **[PtCl$_2$(3,5-^{t}Bu$_2$-pzH)$_2$]**.

Pt1—Cl1	2.297 (3)	Pt1—N1	2.020 (6)
Pt1—Cl2	2.321 (2)	Pt1—N3	2.004 (6)
Cl1—Pt1—Cl2	176.01 (9)	N3—Pt1—Cl2	92.1 (2)
N1—Pt1—Cl1	87.7 (2)	N3—Pt1—N1	172.4 (3)
N1—Pt1—Cl2	93.2 (2)	N2—N1—Pt1	113.5 (5)
N3—Pt1—Cl1	86.7 (2)	C12—N1—Pt1	136.9 (6)
N4—N3—Pt1	113.7 (5)	C1—N3—Pt1	137.2 (6)

Table S3. Selected bond lengths(Å) and angles(º) for **[$PtCl_2$(4-Me-pzH)$_2$]**.

Pt1—Cl1^{i}	2.3181 (15)	Pt1—Cl1^{iii}	2.3181 (15)
Pt1—Cl1^{ii}	2.3181 (15)	Pt1—N1^{iii}	2.019 (5)
Pt1—Cl1	2.3181 (15)	Pt1—N1	2.019 (5)
Cl1^{i}—Pt1—Cl1	89.01 (8)	N1^{iii}—Pt1—Cl1^{iii}	90.11 (10)
Cl1^{i}—Pt1—Cl1^{ii}	180.00 (5)	N1^{iii}—Pt1—Cl1	89.89 (10)
Cl1—Pt1—Cl1^{iii}	180.0	N1^{iii}—Pt1—Cl1^{i}	89.89 (10)
Cl1—Pt1—Cl1^{ii}	90.99 (8)	N1—Pt1—Cl1	90.11 (10)
Cl1^{i}—Pt1—Cl1^{iii}	90.99 (8)	N1^{iii}—Pt1—Cl1^{ii}	90.11 (10)
Cl1^{iii}—Pt1—Cl1^{ii}	89.01 (8)	N1—Pt1—Cl1^{iii}	89.89 (10)
N1—Pt1—Cl1^{i}	90.11 (10)	N1^{iii}—Pt1—N1	180.00 (15)
N1—Pt1—Cl1^{ii}	89.89 (10)	N2—N1—Pt1	122.6 (4)
C1—N1—Pt1	131.7 (5)	N1^{iii}—Pt1—N1—N2	0.0 (6)
Pt1—N1—N2—C3	180.000 (2)	N1^{iii}—Pt1—N1—C1	180.0 (6)
Pt1—N1—C1—C2	180.000 (2)	Cl1^{i}—Pt1—N1—C1	−44.50 (4)
Cl1^{i}—Pt1—N1—N2	135.50 (4)	Cl1^{iii}—Pt1—N1—C1	−135.50 (4)
Cl1—Pt1—N1—N2	−135.50 (4)	Cl1^{ii}—Pt1—N1—C1	135.50 (4)
Cl1^{iii}—Pt1—N1—N2	44.50 (4)	Cl1—Pt1—N1—C1	44.50 (4)
Cl1^{ii}—Pt1—N1—N2	−44.50 (4)		

Symmetry codes: (i) −*x*, *y*, *z*; (ii) *x*, −*y*+1, −*z*; (iii) −*x*, −*y*+1, −*z*

Table S4. Computed NBA charges and natural electron configurations of the selected atoms **1**, 2 and **3** at BP86/6-31G*~dz.

	1		**2**		**3**	
Atom	Natural Charge	Natural Electron Configuration	Natural Charge	Natural Electron Configuration	Natural Charge	Natural Electron Configuration
Pt	0.47 |e|	$6s^{0.54}5d^{8.66}6p^{0.33}$	0.35 |e|	$6s^{0.58}5d^{8.78}6p^{0.29}$	0.56 |e|	$6s^{0.51}5d^{8.60}6p^{0.33}$
Pt	0.44 |e|	$6s^{0.54}5d^{8.68}6p^{0.33}$	0.35 |e|	$6s^{0.58}5d^{8.79}6p^{0.29}$	0.46 |e|	$6s^{0.46}5d^{8.50}6p^{0.57}$
Pt	0.43 |e|	$6s^{0.54}5d^{8.70}6p^{0.33}$	–	–	–	–
Cl	–	–	–	–	-0.30 |e|	$3s^{1.88}3p^{5.42}$
N	-0.28 |e|	$2s^{1.33}2p^{3.94}$	-0.33 |e|	$2s^{1.33}2p^{3.98}$	-0.24 |e|	$2s^{1.26}2p^{3.96}$
N	-0.35 |e|	$2s^{1.37}2p^{3.96}$	-0.29 |e|	$2s^{1.29}2p^{3.98}$	-0.30 |e|	$2s^{1.31}2p^{3.96}$
N	-0.26 |e|	$2s^{1.31}2p^{3.93}$	-0.29 |e|	$2s^{1.29}2p^{3.98}$	-0.32 |e|	$2s^{1.33}2p^{3.96}$
N	-0.31 |e|	$2s^{1.32}2p^{3.96}$	-0.33 |e|	$2s^{1.33}2p^{3.98}$	-0.29v	$2s^{1.29}2p^{3.98}$
N	-0.26 |e|	$2s^{1.34}2p^{3.89}$	-0.26 |e|	$2s^{1.28}2p^{3.95}$	-0.29 |e|	$2s^{1.27}2p^{4.00}$
N	-0.25 |e|	$2s^{1.34}2p^{3.89}$	-0.31 |e|	$2s^{1.20}2p^{4.09}$	-0.31v	$2s^{1.41}2p^{3.88}$
N	-0.28 |e|	$2s^{1.36}2p^{3.89}$	-0.26 |e|	$2s^{1.28}2p^{3.95}$	-0.23 |e|	$2s^{1.26}2p^{3.95}$
N	-0.25 |e|	$2s^{1.32}2p^{3.91}$	-0.31 |e|	$2s^{1.20}2p^{4.09}$	-0.31 |e|	$2s^{1.20}2p^{4.09}$
N	-0.31 |e|	$2s^{1.32}2p^{3.96}$	–	–	–	–
N	-0.30 |e|	$2s^{1.36}2p^{3.92}$	–	–	–	–
N	-0.29 |e|	$2s^{1.35}2p^{3.92}$	–	–	–	–
N	-0.27 |e|	$2s^{1.30}2p^{3.95}$	–	–	–	–
C	–	–	-0.64 |e|	$2s^{1.12}2p^{3.50}$	-0.62 |e|	$2s^{1.11}2p^{3.49}$
C	–	–	-0.64 |e|	$2s^{1.12}2p^{3.50}$	-0.50 |e|	$2s^{1.10}2p^{3.38}$

Table S5. Computed WBI Pt-Pt/Pt-N/Pt-C/Pt-Cl bonds in the three simplified Pt Complexes at BP86/6-31G*~dz.

1		**2**		**3**	
Bond	WBI	Bond	WBI	Bond	WBI
Pt1-Pt2	0.0843	Pt1-Pt2	0.0621	Pt1-Pt2	0.2769
Pt1-Pt3	0.0863	Pt1-N4	0.3064	Pt1-N5	0.1804
Pt2-Pt3	0.0912	Pt1-N6	0.2247	Pt1-N7	0.2706
Pt1-N4	0.3285	Pt1-N7	0.2973	Pt1-N8	0.3691
Pt1-N6	0.2880	Pt2-N3	0.2247	Pt2-N4	0.3630
Pt1-N13	0.3973	Pt2-N5	0.3064	Pt2-N6	0.1774
Pt1-N15	0.3035	Pt2-N10	0.2973	Pt2-N10	0.2867
Pt2-N5	0.3516	Pt1-C33	0.6135	Pt1-C33	0.5326
Pt2-N7	0.3049	Pt2-C44	0.6135	Pt2-C44	0.5694
Pt2-N8	0.3300			Pt2-Cl3	0.0936
Pt2-N10	0.3165				
Pt3-N9	0.2880				
Pt3-N11	0.2767				
Pt3-N12	0.2982				
Pt3-N14	0.3608				

Table S6. Selected bond lengths(Å)and bond angles(º)of compound **1**.

Pt1—Pt2	3.0525 (6)	Pt4—Pt5	3.0397 (6)
Pt1—Pt3	3.0648 (6)	Pt4—Pt6	3.0758 (6)
Pt1—N1	2.007 (5)	Pt4—N13	2.017 (5)
Pt1—N3	2.013 (5)	Pt4—N15	2.012 (5)
Pt1—N10	2.012 (5)	Pt4—N22	2.023 (6)
Pt1—N12	2.006 (6)	Pt4—N24	2.007 (5)
Pt2—Pt3	3.0355 (5)	Pt5—Pt6	3.0384 (7)
Pt2—N2	2.015 (5)	Pt5—N14	2.009 (6)
Pt2—N4	2.018 (5)	Pt5—N16	2.009 (5)
Pt2—N5	2.017 (5)	Pt5—N17	2.015 (6)
Pt2—N7	2.017 (6)	Pt5—N19	2.013 (6)
Pt3—N6	2.008 (5)	Pt6—N18	2.017 (5)
Pt3—N8	2.020 (5)	Pt6—N20	2.025 (5)
Pt3—N9	2.016 (6)	Pt6—N21	2.014 (6)
Pt3—N11	2.012 (5)	Pt6—N23	2.018 (5)
Pt2—Pt1—Pt3	59.501 (13)	Pt3—Pt2—Pt1	60.451 (12)
N1—Pt1—Pt2	65.31 (15)	N2—Pt2—Pt1	65.11 (15)
N1—Pt1—Pt3	107.89 (15)	N2—Pt2—Pt3	107.87 (15)
N1—Pt1—N3	87.5 (2)	N2—Pt2—N4	88.2 (2)
N1—Pt1—N10	91.8 (2)	N2—Pt2—N5	91.3 (2)
N3—Pt1—Pt2	65.33 (15)	N2—Pt2—N7	172.1 (2)
N3—Pt1—Pt3	106.53 (16)	N4—Pt2—Pt1	65.05 (15)
N10—Pt1—Pt2	106.39 (15)	N4—Pt2—Pt3	106.78 (15)
N10—Pt1—Pt3	65.29 (15)	N5—Pt2—Pt1	107.03 (14)
N10—Pt1—N3	171.1 (2)	N5—Pt2—Pt3	65.23 (15)
N12—Pt1—Pt2	108.08 (16)	N5—Pt2—N4	171.4 (2)
N12—Pt1—Pt3	65.35 (16)	N5—Pt2—N7	89.1 (2)
N12—Pt1—N1	172.8 (2)	N7—Pt2—Pt1	107.24 (15)
N12—Pt1—N3	92.1 (2)	N7—Pt2—Pt3	65.18 (15)
N12—Pt1—N10	87.4 (2)	N7—Pt2—N4	90.2 (2)
Pt2—Pt3—Pt1	60.049 (14)	Pt5—Pt4—Pt6	59.578 (16)
N6—Pt3—Pt1	107.62 (15)	N13—Pt4—Pt5	65.78 (16)
N6—Pt3—Pt2	65.53 (15)	N13—Pt4—Pt6	108.21 (16)
N6—Pt3—N8	88.8 (2)	N13—Pt4—N22	91.4 (2)
N6—Pt3—N9	90.7 (2)	N15—Pt4—Pt5	65.62 (15)
N6—Pt3—N11	172.1 (2)	N15—Pt4—Pt6	106.01 (15)
N8—Pt3—Pt1	107.14 (15)	N15—Pt4—N13	88.9 (2)

N8—Pt3—Pt2	65.66 (15)	N15—Pt4—N22	170.3 (2)
N9—Pt3—Pt1	64.38 (16)	N22—Pt4—Pt5	105.82 (16)
N9—Pt3—Pt2	105.91 (15)	N22—Pt4—Pt6	64.75 (16)
N9—Pt3—N8	170.9 (2)	N24—Pt4—Pt5	106.93 (16)
N11—Pt3—Pt1	64.72 (17)	N24—Pt4—Pt6	64.56 (16)
N11—Pt3—Pt2	107.60 (16)	N24—Pt4—N13	172.2 (2)
N11—Pt3—N8	91.7 (2)	N24—Pt4—N15	90.4 (2)
N11—Pt3—N9	87.5 (2)	N24—Pt4—N22	88.0 (2)
Pt6—Pt5—Pt4	60.801 (15)	Pt5—Pt6—Pt4	59.621 (13)
N14—Pt5—Pt4	65.24 (15)	N18—Pt6—Pt4	107.99 (16)
N14—Pt5—Pt6	107.95 (15)	N18—Pt6—Pt5	65.54 (16)
N14—Pt5—N16	89.2 (2)	N18—Pt6—N20	86.6 (2)
N14—Pt5—N17	92.4 (2)	N18—Pt6—N23	172.7 (2)
N14—Pt5—N19	172.3 (2)	N20—Pt6—Pt4	107.82 (16)
N16—Pt5—Pt4	64.75 (16)	N20—Pt6—Pt5	65.60 (16)
N16—Pt5—Pt6	106.25 (16)	N21—Pt6—Pt4	64.51 (17)
N16—Pt5—N17	171.6 (2)	N21—Pt6—Pt5	105.87 (16)
N16—Pt5—N19	90.5 (2)	N21—Pt6—N18	91.7 (2)
N17—Pt5—Pt4	108.57 (15)	N21—Pt6—N20	171.2 (2)
N17—Pt5—Pt6	65.42 (16)	N21—Pt6—N23	87.6 (2)
N19—Pt5—Pt4	107.76 (15)	N23—Pt6—Pt4	65.17 (15)
N19—Pt5—Pt6	64.80 (15)	N23—Pt6—Pt5	107.66 (15)
N19—Pt5—N17	86.8 (2)	N23—Pt6—N20	93.0 (2)
N2—N1—Pt1	114.8 (4)	N1—N2—Pt2	114.7 (4)
C3—N1—Pt1	137.9 (5)	C1—N2—Pt2	137.2 (5)
N4—N3—Pt1	114.7 (4)	N3—N4—Pt2	115.0 (4)
C7—N3—Pt1	137.4 (5)	C5—N4—Pt2	136.3 (5)
N6—N5—Pt2	114.6 (4)	N5—N6—Pt3	114.6 (4)
C11—N5—Pt2	136.7 (5)	C9—N6—Pt3	135.8 (5)
N8—N7—Pt2	115.2 (4)	N7—N8—Pt3	113.9 (4)
C15—N7—Pt2	135.7 (5)	C13—N8—Pt3	136.6 (5)
N10—N9—Pt3	116.0 (4)	N9—N10—Pt1	114.3 (4)
C19—N9—Pt3	135.7 (5)	C17—N10—Pt1	136.9 (5)
N12—N11—Pt3	115.4 (4)	N11—N12—Pt1	114.5 (4)
C23—N11—Pt3	136.7 (5)	C21—N12—Pt1	137.4 (5)
N14—N13—Pt4	113.6 (4)	N13—N14—Pt5	115.4 (4)
C27—N13—Pt4	137.7 (5)	C25—N14—Pt5	136.8 (5)
N16—N15—Pt4	113.7 (4)	N15—N16—Pt5	115.9 (4)

C31—N15—Pt4	136.6 (5)	C29—N16—Pt5	134.8 (5)
N18—N17—Pt5	114.8 (4)	N17—N18—Pt6	114.3 (4)
C35—N17—Pt5	137.4 (5)	C33—N18—Pt6	138.4 (5)
N20—N19—Pt5	116.2 (4)	N19—N20—Pt6	113.4 (4)
C39—N19—Pt5	134.9 (5)	C37—N20—Pt6	139.0 (5)
N22—N21—Pt6	116.0 (4)	N21—N22—Pt4	114.8 (4)
C43—N21—Pt6	135.3 (5)	C41—N22—Pt4	136.7 (5)
N24—N23—Pt6	114.0 (4)	N23—N24—Pt4	116.3 (4)
C47—N23—Pt6	138.0 (5)	C45—N24—Pt4	136.2 (5)

Table S7. Selected bond lengths(Å)and bond angles(º)of compound **2**.

Pt1—Pt2	2.9290 (5)	Pt2—N1	2.151 (7)
Pt1—N2	2.034 (7)	Pt2—N3	2.026 (7)
Pt1—N4	2.157 (7)	Pt2—N7	1.961 (8)
Pt1—N5	1.961 (7)	Pt2—C44	2.034 (10)
Pt1—C33	2.048 (10)		
N2—Pt1—Pt2	71.0 (2)	N1—Pt2—Pt1	64.94 (19)
N2—Pt1—N4	89.2 (3)	N3—Pt2—Pt1	71.2 (2)
N2—Pt1—C33	98.7 (4)	N3—Pt2—N1	89.3 (3)
N4—Pt1—Pt2	64.7 (2)	N3—Pt2—C44	98.6 (4)
N5—Pt1—Pt2	102.2 (2)	N7—Pt2—Pt1	102.5 (2)
N5—Pt1—N2	172.2 (3)	N7—Pt2—N1	91.9 (3)
N5—Pt1—N4	91.2 (3)	N7—Pt2—N3	172.3 (3)
N5—Pt1—C33	80.1 (4)	N7—Pt2—C44	79.3 (4)
C33—Pt1—Pt2	111.8 (5)	C33—Pt1—N4	169.9 (4)
C44—Pt2—Pt1	110.7 (4)	N2—N1—Pt2	112.8 (5)
C44—Pt2—N1	169.2 (4)	C3—N1—Pt2	138.3 (6)
N1—N2—Pt1	108.9 (5)	N4—N3—Pt2	109.0 (5)
C1—N2—Pt1	142.1 (7)	C14—N3—Pt2	141.9 (7)
N3—N4—Pt1	112.8 (5)	C12—N4—Pt1	137.5 (6)
N6—N5—Pt1	129.8 (6)	N8—N7—Pt2	130.1 (6)
C25—N5—Pt1	120.6 (6)	C36—N7—Pt2	120.7 (7)
Pt1—N2—C1—C2	172.4 (8)	Pt2—N1—N2—Pt1	16.6 (6)
Pt1—N2—C1—C4	−9.8 (17)	Pt2—N1—N2—C1	−167.7 (6)
Pt1—N4—C12—C13	162.3 (7)	Pt2—N1—C3—C2	163.6 (7)
Pt1—N4—C12—C15	−23.2 (14)	Pt2—N1—C3—C8	−21.2 (15)

Pt1—N5—N6—C23	−166.4 (7)	Pt2—N3—N4—Pt1	16.5 (6)
Pt1—N5—C25—C24	168.0 (7)	Pt2—N3—N4—C12	−176.1 (5)
Pt1—N5—C25—C30	−8.8 (12)	Pt2—N3—C14—C13	174.3 (8)
Pt2—N7—N8—C34	−166.0 (8)	Pt2—N3—C14—C19	−7.6 (17)
Pt2—N7—C36—C35	167.9 (7)	C3—N1—N2—Pt1	−174.4 (6)
Pt2—N7—C36—C41	−9.4 (13)	C14—N3—N4—Pt1	−166.8 (6)
C25—C30—C33—Pt1	−9.2 (13)	C36—C41—C44—Pt2	−13.0 (14)
C31—C30—C33—Pt1	−144.6 (15)	C42—C41—C44—Pt2	−153.1 (17)
C32—C30—C33—Pt1	97.9 (14)	C43—C41—C44—Pt2	92.5 (14)
C43A—C41—C44—Pt2	114.2 (16)	C31A—C30—C33—Pt1	−119.0 (13)
C42A—C41—C44—Pt2	−129.2 (14)	C32A—C30—C33—Pt1	122.7 (16)

Table S8. Selected bond lengths(Å)and bond angles(º)of compound **3**.

Pt1—Pt2	2.584 (3)	Pt3—Pt4	2.5858 (18)
Pt1—N1	2.124 (7)	Pt3—Cl2	2.346 (3)
Pt1—N3	2.025 (7)	Pt3—N10	2.054 (7)
Pt1—N7	1.992 (7)	Pt3—N12	2.220 (7)
Pt1—C44	2.060 (8)	Pt3—N13	2.015 (7)
Pt2—Cl1	2.352 (3)	Pt3—C77	2.064 (9)
Pt2—N2	2.053 (7)	Pt4—N9	2.138 (7)
Pt2—N4	2.221 (7)	Pt4—N11	2.031 (7)
Pt2—N5	1.988 (7)	Pt4—N15	1.972 (7)
Pt2—C33	2.078 (9)	Pt4—C88	2.068 (9)
N1—Pt1—Pt2	70.5 (2)	C44—Pt1—Pt2	104.8 (3)
N3—Pt1—Pt2	74.9 (2)	C44—Pt1—N1	174.6 (3)
N3—Pt1—N1	88.2 (3)	Cl1—Pt2—Pt1	174.92 (7)
N3—Pt1—C44	93.2 (3)	N2—Pt2—Pt1	76.4 (2)
N7—Pt1—Pt2	106.8 (2)	N2—Pt2—Cl1	102.4 (2)
N7—Pt1—N1	98.4 (3)	N2—Pt2—N4	89.5 (3)
N7—Pt1—N3	173.3 (3)	N2—Pt2—C33	91.3 (3)
N7—Pt1—C44	80.1 (3)	N4—Pt2—Pt1	71.79 (19)
N4—Pt2—Cl1	103.3 (2)	C33—Pt2—Pt1	97.8 (3)
N5—Pt2—Pt1	95.7 (2)	C33—Pt2—Cl1	87.2 (3)
N5—Pt2—Cl1	86.1 (2)	C33—Pt2—N4	169.0 (3)
N5—Pt2—N2	168.4 (3)	Cl2—Pt3—Pt4	174.70 (8)

N5—Pt2—N4	96.2 (3)	N5—Pt2—C33	81.2 (3)
N10—Pt3—Pt4	76.59 (19)	N12—Pt3—Pt4	71.6 (2)
N10—Pt3—Cl2	101.5 (2)	N12—Pt3—Cl2	103.6 (2)
N10—Pt3—N12	89.0 (3)	N13—Pt3—Pt4	95.6 (2)
N10—Pt3—C77	91.2 (3)	N13—Pt3—Cl2	87.1 (2)
C77—Pt3—Pt4	98.0 (3)	N13—Pt3—N10	168.1 (3)
C77—Pt3—Cl2	86.9 (3)	N13—Pt3—N12	97.1 (3)
C77—Pt3—N12	169.3 (4)	N13—Pt3—C77	80.9 (3)
N9—Pt4—Pt3	70.18 (19)	Pt1—C44—H44A	109.4
N11—Pt4—Pt3	75.1 (2)	Pt1—C44—H44B	109.4
N11—Pt4—N9	87.6 (3)	C41—C44—Pt1	111.3 (6)
N11—Pt4—C88	95.3 (3)	N10—N9—Pt4	109.2 (5)
N15—Pt4—Pt3	109.1 (2)	C47—N9—Pt4	142.9 (6)
N15—Pt4—N9	97.3 (3)	N9—N10—Pt3	103.9 (5)
N15—Pt4—N11	174.3 (3)	C45—N10—Pt3	146.8 (6)
N15—Pt4—C88	80.0 (3)	N12—N11—Pt4	110.9 (5)
C88—Pt4—Pt3	105.3 (3)	C58—N11—Pt4	139.1 (6)
C88—Pt4—N9	173.9 (3)	N11—N12—Pt3	102.4 (5)
N2—N1—Pt1	109.2 (5)	C56—N12—Pt3	150.2 (6)
C3—N1—Pt1	141.8 (6)	N14—N13—Pt3	133.7 (6)
N1—N2—Pt2	103.9 (5)	C69—N13—Pt3	118.5 (6)
C1—N2—Pt2	147.7 (6)	Pt4—N15—H15	90.7
N4—N3—Pt1	111.6 (5)	N16—N15—Pt4	132.0 (6)
C14—N3—Pt1	139.6 (6)	N6—N5—Pt2	133.0 (5)
N3—N4—Pt2	101.7 (5)	C25—N5—Pt2	119.6 (5)
C12—N4—Pt2	149.5 (6)	N8—N7—Pt1	131.0 (5)
C36—N7—Pt1	118.2 (6)		