Single Crystal X-Ray Structure Determination of Compounds 8a, 8b and 11a

General:

Preliminary examination and data collection were carried out on an area detecting system (Kappa-CCD; Nonius) using graphite-monochromated Mo K_α radiation (λ = 0.71073 Å) with an Oxford Cryosystems cooling system at the window of a sealed fine-focus X-ray tube. The reflections were integrated. Raw data were corrected for Lorentz, polarization, decay, and absorption effects. The absorption correction was applied using SADABS.[I] After merging, the independent reflections were used for all calculations. The structure was solved by a combination of direct methods[II] and difference Fourier syntheses.[III] All non-hydrogen atom positions were refined with anisotropic displacement parameters. Hydrogen atoms were placed in ideal positions using the SHELXL riding model. Full-matrix least-squares refinements were carried out by minimizing $\Sigma w(F_o^2 - F_c^2)^2$ with the SHELXL-97 weighting scheme and stopped at shift/err < 0.001. Neutral-atom scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were taken from ref V. All calculations were performed with the programs COLLECT,[VI] DIRAX,[VII] EVALCCD,[VIII] SIR92,[II] SADABS,[I] PLATON,[IX] and the SHELXL-97 package.[III,IV] For visualization Mercury[X] and PLATON[IX] and for the preparation of supporting material ENCIFER[XI] and PLATON[IX] were used.

[I] Sheldrick, G. M. SADABS, Version 2.10; University of Göttingen, Göttingen, Germany, 2002.

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[III] Sheldrick, G. M. Acta Crystallogr., Sect. A: Found. Crystallogr. **2008**, A64, 112.

[IV] Sheldrick, G. M. "**SHELXL-97**", University of Göttingen, Göttingen, Germany, (1998).

[V] International Tables for Crystallography, Vol. C, Tables 6.1.1.4 (pp. 500-502), 4.2.6.8 (pp. 219-222), and 4.2.4.2 (pp. 193-199), Wilson, A. J. C., Ed., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1992.

[VI] Hooft, R. W. W. "**COLLECT**" Data Collection Software for Nonius-Kappa CCD; Nonius BV., Delft, The Netherlands, 1999.

[VII] Duisenberg, A. J. M. J. Appl. Crystallogr. **1992**, 25, 92.

[VIII] Duisenberg, A. J. M.; Kroon-Batenburg, L. M. J.; Schreurs, A. M. M., J. Appl. Crystallogr. **2003**, 36, 220.

[IX] Spek, A. L. "**PLATON**", A Multipurpose Crystallographic Tool, Utrecht University, Utrecht, The Netherlands, (2010).

[X] Macrae, C. F.; Bruno, I. J.; Chisholm, J. A.; Edgington, P. R.; McCabe, P.; Pidcock, E.; Rodriguez-Monge, L.; Taylor, R.; van de Streek, J.; Wood, P. A. J. Appl. Crystallogr. **2008**, 41, 466.

[XI] Allen, F. H.; Johnson, O.; Shields, G. P.; Smith, B. R.; Towler, M. J. Appl. Crystallogr. **2004**, 37, 335.

Compound 8a

Table S1 - Crystal Data and Details of the Structure Determination for: **Compound 8a**

Crystal Data			
Formula			C14 H14 Br2 N4 Pd
Formula Weight			504.49
Crystal System			Orthorhombic
Space group		Pna21	(No. 33)
a, b, c [Angstrom]	12.4150(9)	9.508(2)	14.0530(17)
V [Ang**3]			1658.8(4)
Z			4
D(calc) [g/cm**3]			2.020
Mu(MoKa) [/mm]			5.934
F(000)			968
Crystal Size [mm]		0.20 x 0.20 x 0.20	
Data Collection			
Temperature (K)			198
Radiation [Angstrom]		MoKα	0.71073
Theta Min-Max [Deg]			4.8, 25.4
Dataset		-14: 14 ; -11: 11 ; -16: 16	
Tot., Uniq. Data, R(int)		11505, 3005, 0.031	
Observed data [I > 2.0 sigma(I)]			2748
Refinement			
Nref, Npar			3005, 192
R, wR2, S		0.0205, 0.0375, 1.06	
w = 1/[\s^2^(Fo^2^)+(0.0000P)^2^]		where P=(Fo^2^+2Fc^2^)/3	
Max. and Av. Shift/Error			0.01, 0.00
Flack x			0.025(7)
Min. and Max. Resd. Dens. [e/Ang^3]			-0.33, 0.33

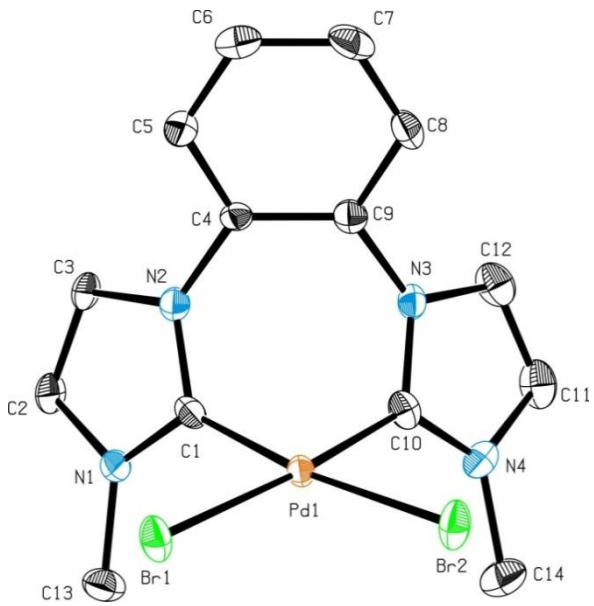
Table S2 - Bond Distances (Angstrom) for: **Compound 8a**

Pd1	-Br1	2.4960(6)	C5	-C6	1.376(5)
Pd1	-Br2	2.4885(8)	C6	-C7	1.380(6)
Pd1	-C1	1.965(4)	C7	-C8	1.385(5)
Pd1	-C10	1.958(3)	C8	-C9	1.385(5)
N1	-C1	1.336(4)	C11	-C12	1.348(6)
N1	-C2	1.386(4)	C2	-H2	0.9500
N1	-C13	1.459(5)	C3	-H3	0.9500
N2	-C1	1.362(5)	C5	-H5	0.9500
N2	-C3	1.399(4)	C6	-H6	0.9500
N2	-C4	1.424(4)	C7	-H7	0.9500
N3	-C9	1.426(4)	C8	-H8	0.9500
N3	-C10	1.359(4)	C11	-H11	0.9500
N3	-C12	1.404(5)	C12	-H12	0.9500
N4	-C10	1.339(4)	C13	-H13A	0.9800
N4	-C11	1.387(5)	C13	-H13B	0.9800
N4	-C14	1.465(5)	C13	-H13C	0.9800
C2	-C3	1.349(5)	C14	-H14A	0.9800
C4	-C5	1.389(5)	C14	-H14B	0.9800
C4	-C9	1.392(5)	C14	-H14C	0.9800

Table S3 - Bond Angles (Degrees) for: **Compound 8a**

Br1	-Pd1	-Br2	94.10(2)	Pd1	-C10	-N3	124.3(2)
Br1	-Pd1	-C1	91.65(10)	Pd1	-C10	-N4	130.3(3)
Br1	-Pd1	-C10	174.91(13)	N3	-C10	-N4	105.4(2)
Br2	-Pd1	-C1	172.78(8)	N4	-C11	-C12	107.3(3)
Br2	-Pd1	-C10	90.67(12)	N3	-C12	-C11	106.0(3)
C1	-Pd1	-C10	83.45(15)	N1	-C2	-H2	126.00
C1	-N1	-C2	111.0(3)	C3	-C2	-H2	126.00
C1	-N1	-C13	124.4(3)	N2	-C3	-H3	127.00
C2	-N1	-C13	124.7(3)	C2	-C3	-H3	127.00
C1	-N2	-C3	110.2(3)	C4	-C5	-H5	120.00
C1	-N2	-C4	124.9(3)	C6	-C5	-H5	120.00
C3	-N2	-C4	124.9(3)	C5	-C6	-H6	120.00
C9	-N3	-C10	125.0(3)	C7	-C6	-H6	120.00
C9	-N3	-C12	124.5(3)	C6	-C7	-H7	120.00
C10	-N3	-C12	110.3(3)	C8	-C7	-H7	120.00
C10	-N4	-C11	111.0(3)	C7	-C8	-H8	120.00
C10	-N4	-C14	125.2(3)	C9	-C8	-H8	120.00
C11	-N4	-C14	123.7(3)	N4	-C11	-H11	126.00
Pd1	-C1	-N1	129.2(3)	C12	-C11	-H11	126.00
Pd1	-C1	-N2	125.3(2)	N3	-C12	-H12	127.00
N1	-C1	-N2	105.5(3)	C11	-C12	-H12	127.00
N1	-C2	-C3	107.3(3)	N1	-C13	-H13A	110.00
N2	-C3	-C2	106.1(3)	N1	-C13	-H13B	109.00
N2	-C4	-C5	119.1(3)	N1	-C13	-H13C	110.00
N2	-C4	-C9	121.3(3)	H13A	-C13	-H13B	109.00
C5	-C4	-C9	119.7(3)	H13A	-C13	-H13C	109.00
C4	-C5	-C6	120.3(4)	H13B	-C13	-H13C	109.00
C5	-C6	-C7	120.3(4)	N4	-C14	-H14A	109.00
C6	-C7	-C8	119.8(4)	N4	-C14	-H14B	110.00
C7	-C8	-C9	120.4(4)	N4	-C14	-H14C	110.00
N3	-C9	-C4	122.3(3)	H14A	-C14	-H14B	109.00
N3	-C9	-C8	118.1(3)	H14A	-C14	-H14C	109.00
C4	-C9	-C8	119.6(3)	H14B	-C14	-H14C	109.00

Figure F1 – Ortep drawing with 50% ellipsoids for: **Compound 8a**



Compound 8b

Table S4 - Crystal Data and Details of the Structure Determination for: **Compound 8b**

Crystal Data			
Formula	C22 H18 Br2 N4 Pd, 2(C2 H3 N)		
Formula Weight			686.71
Crystal System			Triclinic
Space group		P-1	(No. 2)
a, b, c [Angstrom]	9.7310(12)	10.752(2)	13.9470(7)
alpha, beta, gamma [deg]	96.085(9)	103.753(6)	98.478(15)
V [Ang**3]			1386.7(3)
Z			2
D(calc) [g/cm**3]			1.645
Mu(MoKa) [/mm]			3.576
F(000)			676
Crystal Size [mm]		0.19 x 0.19 x	0.33
Data Collection			
Temperature (K)			198
Radiation [Angstrom]		MoKα	0.71073
Theta Min-Max [Deg]			2.7, 26.4
Dataset		-12: 11 ; -13: 13 ;	0: 17
Tot., Uniq. Data, R(int)		5686, 5686,	0.000
Observed data [I > 2.0 sigma(I)]			4437
Refinement			
Nref, Npar			5686, 320
R, wR2, S		0.0308, 0.0576,	1.05
w = 1/[\s^2^(Fo^2^)+(0.0203P)^2^+1.4433P] where P=(Fo^2^+2Fc^2^)/3			
Max. and Av. Shift/Error			0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]			-0.54, 0.50

The unit cell contains 1 disordered acetonitrile molecule which has been treated as a diffuse contribution to the overall scattering without specific atom positions by SQUEEZE/PLATON.[IX]

Table S5 - Bond Distances (Angstrom) for: **Compound 8b**

Pd1	-Br1	2.4705(6)	C14	-C15	1.405(4)
Pd1	-Br2	2.4924(6)	C15	-C16	1.374(4)
Pd1	-C1	1.957(3)	C17	-C18	1.368(6)
Pd1	-C10	1.964(3)	C18	-C19	1.388(6)
N1	-C1	1.339(3)	C19	-C20	1.390(5)
N1	-C2	1.397(4)	C5	-H5	0.9500
N1	-C21	1.461(4)	C6	-H6	0.9500
N2	-C1	1.361(4)	C7	-H7	0.9500
N2	-C3	1.408(4)	C8	-H8	0.9500
N2	-C4	1.425(3)	C13	-H13	0.9500
N3	-C9	1.427(4)	C14	-H14	0.9500
N3	-C10	1.359(4)	C15	-H15	0.9500
N3	-C12	1.402(4)	C16	-H16	0.9500
N4	-C10	1.342(4)	C17	-H17	0.9500
N4	-C11	1.389(4)	C18	-H18	0.9500
N4	-C22	1.458(5)	C19	-H19	0.9500
N5	-C24	1.128(5)	C20	-H20	0.9500
N6	-C26	1.124(6)	C21	-H21C	0.9800
C2	-C13	1.384(4)	C21	-H21A	0.9800

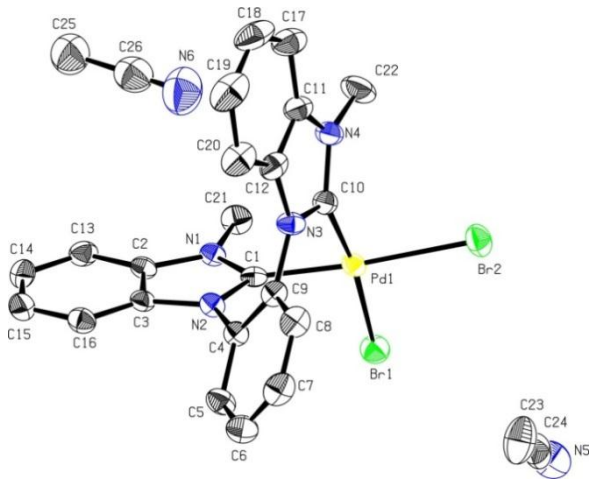
C2	-C3	1.389(4)	C21	-H21B	0.9800
C3	-C16	1.379(4)	C22	-H22C	0.9800
C4	-C9	1.396(4)	C22	-H22A	0.9800
C4	-C5	1.384(4)	C22	-H22B	0.9800
C5	-C6	1.386(4)	C23	-C24	1.462(6)
C6	-C7	1.381(4)	C23	-H23B	0.9800
C7	-C8	1.375(4)	C23	-H23C	0.9800
C8	-C9	1.386(4)	C23	-H23A	0.9800
C11	-C12	1.396(5)	C25	-C26	1.458(6)
C11	-C17	1.379(5)	C25	-H25A	0.9800
C12	-C20	1.385(5)	C25	-H25B	0.9800
C13	-C14	1.374(4)	C25	-H25C	0.9800

Table S6 - Bond Angles (Degrees) for: **Compound 8b**

Br1	-Pd1	-Br2	94.52(2)	C18	-C19	-C20	121.8(4)
Br1	-Pd1	-C1	90.53(9)	C12	-C20	-C19	116.0(3)
Br1	-Pd1	-C10	172.66(9)	C4	-C5	-H5	120.00
Br2	-Pd1	-C1	174.83(10)	C6	-C5	-H5	120.00
Br2	-Pd1	-C10	92.54(9)	C5	-C6	-H6	120.00
C1	-Pd1	-C10	82.45(13)	C7	-C6	-H6	120.00
C1	-N1	-C2	110.8(2)	C6	-C7	-H7	120.00
C1	-N1	-C21	124.8(2)	C8	-C7	-H7	120.00
C2	-N1	-C21	124.4(2)	C7	-C8	-H8	120.00
C1	-N2	-C3	110.4(2)	C9	-C8	-H8	120.00
C1	-N2	-C4	124.3(2)	C2	-C13	-H13	122.00
C3	-N2	-C4	125.4(2)	C14	-C13	-H13	122.00
C9	-N3	-C10	124.8(2)	C13	-C14	-H14	119.00
C9	-N3	-C12	125.3(3)	C15	-C14	-H14	119.00
C10	-N3	-C12	109.9(3)	C14	-C15	-H15	119.00
C10	-N4	-C11	110.6(3)	C16	-C15	-H15	119.00
C10	-N4	-C22	125.2(3)	C3	-C16	-H16	122.00
C11	-N4	-C22	124.1(2)	C15	-C16	-H16	122.00
Pd1	-C1	-N1	128.9(2)	C11	-C17	-H17	122.00
Pd1	-C1	-N2	124.20(19)	C18	-C17	-H17	122.00
N1	-C1	-N2	106.7(2)	C17	-C18	-H18	119.00
N1	-C2	-C3	106.8(2)	C19	-C18	-H18	119.00
N1	-C2	-C13	131.6(3)	C18	-C19	-H19	119.00
C3	-C2	-C13	121.7(3)	C20	-C19	-H19	119.00
N2	-C3	-C2	105.4(2)	C12	-C20	-H20	122.00
N2	-C3	-C16	132.6(2)	C19	-C20	-H20	122.00
C2	-C3	-C16	122.0(3)	N1	-C21	-H21A	109.00
N2	-C4	-C5	119.8(3)	N1	-C21	-H21B	109.00
N2	-C4	-C9	120.6(3)	N1	-C21	-H21C	109.00
C5	-C4	-C9	119.6(3)	H21A	-C21	-H21B	110.00
C4	-C5	-C6	120.1(3)	H21A	-C21	-H21C	109.00
C5	-C6	-C7	120.1(3)	H21B	-C21	-H21C	110.00
C6	-C7	-C8	120.2(3)	N4	-C22	-H22A	110.00
C7	-C8	-C9	120.3(3)	N4	-C22	-H22B	109.00
N3	-C9	-C4	120.7(2)	N4	-C22	-H22C	109.00
N3	-C9	-C8	119.6(3)	H22A	-C22	-H22B	109.00
C4	-C9	-C8	119.7(3)	H22A	-C22	-H22C	109.00
Pd1	-C10	-N3	124.1(2)	H22B	-C22	-H22C	109.00
Pd1	-C10	-N4	128.6(2)	N5	-C24	-C23	179.7(4)
N3	-C10	-N4	107.2(3)	C24	-C23	-H23A	109.00
N4	-C11	-C12	106.6(3)	C24	-C23	-H23B	109.00
N4	-C11	-C17	131.3(3)	C24	-C23	-H23C	110.00
C12	-C11	-C17	122.2(3)	H23A	-C23	-H23B	109.00
N3	-C12	-C11	105.8(3)	H23A	-C23	-H23C	109.00
N3	-C12	-C20	132.7(3)	H23B	-C23	-H23C	109.00
C11	-C12	-C20	121.4(3)	N6	-C26	-C25	179.0(5)

C2	-C13	-C14	116.6(3)	C26	-C25	-H25A	109.00
C13	-C14	-C15	121.5(3)	C26	-C25	-H25B	109.00
C14	-C15	-C16	121.7(3)	C26	-C25	-H25C	109.00
C3	-C16	-C15	116.5(3)	H25A	-C25	-H25B	109.00
C11	-C17	-C18	116.2(3)	H25A	-C25	-H25C	110.00
C17	-C18	-C19	122.4(3)	H25B	-C25	-H25C	109.00

Figure F2 – Ortep drawing with 50% ellipsoids for: **Compound 8b**



Compound 11a

Table S7 - Crystal Data and Details of the Structure Determination for: **Compound 11a**

Crystal Data			
Formula	2(C26 H21 Br4 N4 Pd), 3(C H2 Cl2)		
Formula Weight			1885.71
Crystal System			Orthorhombic
Space group		Pbcn	(No. 60)
a, b, c [Angstrom]	21.297(2)	18.653(5)	15.986(4)
V [Ang**3]			6351(2)
Z			4
D(calc) [g/cm**3]			1.972
Mu(MoKa) [/mm]			5.896
F(000)			3632
Crystal Size [mm]		0.15 x	0.20 x 0.20

Data Collection			
Temperature (K)			198
Radiation [Angstrom]		MoKα	0.71073
Theta Min-Max [Deg]			4.8, 26.4
Dataset		-26: 26 ; -23: 23 ; -19: 20	
Tot., Uniq. Data, R(int)		148489,	6472, 0.074
Observed data [I > 2.0 sigma(I)]			4896

Refinement			
Nref, Npar			6472, 357
R, wR2, S		0.0321,	0.0537, 1.09
w = 1/[\s^2^(Fo^2^)+(0.0056P)^2^+16.6044P] where P=(Fo^2^+2Fc^2^)/			
Max. and Av. Shift/Error			0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]			-0.72, 0.69

Table S8 - Bond Distances (Angstrom) for: **Compound 11a**

Pd1	-Br1	2.4817(8)	C17	-C18	1.383(8)
Pd1	-Br2	2.4842(8)	C18	-C19	1.380(7)
Pd1	-C1	1.961(3)	C20	-C21	1.510(5)
Pd1	-C10	1.975(3)	C21	-C26	1.373(5)
Br3	-C6	1.891(4)	C21	-C22	1.377(6)
Br4	-C7	1.883(4)	C22	-C23	1.374(8)
Cl1	-C27	1.748(10)	C23	-C24	1.380(10)
Cl2	-C27	1.738(8)	C24	-C25	1.353(11)
Cl3	-C28	1.737(5)	C25	-C26	1.389(8)
N1	-C2	1.390(4)	C2	-H2	0.9500
N1	-C1	1.341(4)	C3	-H3	0.9500
N1	-C13	1.477(4)	C5	-H5	0.9500
N2	-C3	1.398(4)	C8	-H8	0.9500
N2	-C4	1.426(4)	C11	-H11	0.9500
N2	-C1	1.361(4)	C12	-H12	0.9500
N3	-C12	1.393(5)	C13	-H13B	0.9900
N3	-C10	1.364(4)	C13	-H13A	0.9900
N3	-C9	1.423(5)	C15	-H15	0.9500
N4	-C20	1.478(4)	C16	-H16	0.9500
N4	-C11	1.382(5)	C17	-H17B	0.9900
N4	-C10	1.345(5)	C17	-H17A	0.9900
C2	-C3	1.335(5)	C18	-H18	0.9500
C4	-C9	1.401(5)	C19	-H19	0.9500
C4	-C5	1.383(5)	C20	-H20B	0.9900
C5	-C6	1.381(5)	C20	-H20A	0.9900
C6	-C7	1.375(5)	C22	-H22	0.9500
C7	-C8	1.385(5)	C23	-H23	0.9500
C8	-C9	1.386(5)	C24	-H24	0.9500
C11	-C12	1.336(5)	C25	-H25	0.9500
C13	-C14	1.508(5)	C26	-H26	0.9500
C14	-C19	1.391(6)	C27	-H27A	0.9900
C14	-C15	1.377(6)	C27	-H27B	0.9900
C15	-C16	1.373(8)	C28	-H28A	0.9900
C16	-C17	1.369(9)	C28	-H28B	0.9900

Table S9 - Bond Angles (Degrees) for: **Compound 11a**

Br1	-Pd1	-Br2	92.12(2)	C22	-C23	-C24	119.5(5)
Br1	-Pd1	-C1	90.59(10)	C23	-C24	-C25	120.4(6)
Br1	-Pd1	-C10	174.07(10)	C24	-C25	-C26	120.0(6)
Br2	-Pd1	-C1	176.39(9)	C21	-C26	-C25	120.3(5)
Br2	-Pd1	-C10	91.73(9)	N1	-C2	-H2	126.00
C1	-Pd1	-C10	85.39(13)	C3	-C2	-H2	126.00
C1	-N1	-C2	111.1(3)	N2	-C3	-H3	127.00
C1	-N1	-C13	125.1(3)	C2	-C3	-H3	127.00
C2	-N1	-C13	123.6(3)	C4	-C5	-H5	120.00
C1	-N2	-C3	110.6(3)	C6	-C5	-H5	120.00
C1	-N2	-C4	124.4(3)	C7	-C8	-H8	120.00
C3	-N2	-C4	124.5(3)	C9	-C8	-H8	120.00
C9	-N3	-C10	124.7(3)	N4	-C11	-H11	126.00
C9	-N3	-C12	124.0(3)	C12	-C11	-H11	126.00
C10	-N3	-C12	110.8(3)	N3	-C12	-H12	127.00
C10	-N4	-C11	110.9(3)	C11	-C12	-H12	127.00
C10	-N4	-C20	125.1(3)	N1	-C13	-H13A	109.00
C11	-N4	-C20	123.9(3)	N1	-C13	-H13B	109.00
Pd1	-C1	-N1	130.6(2)	C14	-C13	-H13A	109.00
Pd1	-C1	-N2	124.6(2)	C14	-C13	-H13B	109.00
N1	-C1	-N2	104.7(3)	H13A	-C13	-H13B	108.00

N1	-C2	-C3	107.2(3)	C14	-C15	-H15	120.00
N2	-C3	-C2	106.4(3)	C16	-C15	-H15	120.00
N2	-C4	-C5	118.4(3)	C15	-C16	-H16	120.00
N2	-C4	-C9	122.1(3)	C17	-C16	-H16	120.00
C5	-C4	-C9	119.6(3)	C16	-C17	-H17A	107.00
C4	-C5	-C6	120.3(3)	C16	-C17	-H17B	107.00
Br3	-C6	-C5	117.8(3)	C18	-C17	-H17A	107.00
Br3	-C6	-C7	121.5(3)	C18	-C17	-H17B	107.00
C5	-C6	-C7	120.5(3)	H17A	-C17	-H17B	107.00
Br4	-C7	-C6	122.4(3)	C17	-C18	-H18	120.00
Br4	-C7	-C8	117.9(3)	C19	-C18	-H18	120.00
C6	-C7	-C8	119.6(3)	C14	-C19	-H19	120.00
C7	-C8	-C9	120.7(3)	C18	-C19	-H19	120.00
N3	-C9	-C4	123.0(3)	N4	-C20	-H20A	109.00
N3	-C9	-C8	117.9(3)	N4	-C20	-H20B	109.00
C4	-C9	-C8	119.2(3)	C21	-C20	-H20A	109.00
Pd1	-C10	-N3	123.8(3)	C21	-C20	-H20B	109.00
Pd1	-C10	-N4	131.7(2)	H20A	-C20	-H20B	108.00
N3	-C10	-N4	104.5(3)	C21	-C22	-H22	120.00
N4	-C11	-C12	107.7(3)	C23	-C22	-H22	120.00
N3	-C12	-C11	106.0(3)	C22	-C23	-H23	120.00
N1	-C13	-C14	113.0(3)	C24	-C23	-H23	120.00
C13	-C14	-C15	120.9(3)	C23	-C24	-H24	120.00
C13	-C14	-C19	120.2(3)	C25	-C24	-H24	120.00
C15	-C14	-C19	118.9(4)	C24	-C25	-H25	120.00
C14	-C15	-C16	120.9(5)	C26	-C25	-H25	120.00
C15	-C16	-C17	119.9(5)	C21	-C26	-H26	120.00
C16	-C17	-C18	120.4(5)	C25	-C26	-H26	120.00
C17	-C18	-C19	119.5(5)	Cl1	-C27	-Cl2	111.6(4)
C14	-C19	-C18	120.3(4)	Cl1	-C27	-H27A	109.00
N4	-C20	-C21	111.7(3)	Cl1	-C27	-H27B	109.00
C20	-C21	-C22	121.2(4)	Cl2	-C27	-H27A	109.00
C20	-C21	-C26	119.9(3)	Cl2	-C27	-H27B	109.00
C22	-C21	-C26	119.0(4)	H27A	-C27	-H27B	108.00
C21	-C22	-C23	120.8(5)	Cl3	-C28	-Cl3_a	110.7(4)
Cl3	-C28	-H28A	110.00	Cl3_a	-C28	-H28A	110.00
Cl3	-C28	-H28B	110.00	Cl3_a	-C28	-H28B	110.00
H28A	-C28	-H28B	108.00				

Figure F3 – Ortep drawing with 50% ellipsoids for: **Compound 11a**