Table 1. Crystal data for $PdCl_2(NCPh)_2$.

Identification code	mn694
Empirical formula	$C_{14}H_{10}Cl_2N_2Pd$
Formula weight	383.54
Crystal size	0.36 x 0.26 x 0.06 mm
Crystal habit	plate
Crystal color	pale red
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 5.715(2) Å α = 116.05(2)°
	b = 8.277(2) Å β = 95.09(2)°
	c = 8.576(2) Å γ = 93.31(2)°
Volume	360.9(2) $Å^3$
Z	1
Density (calculated)	1.765 $Mg \cdot m^{-3}$
Absorption coefficient	1.641 mm^{-1}
F(000)	188
Absorption correction[1]	XABS2
Max. and min. transmission	0.93 and 0.69

1) XABS2: an empirical absorption correction program. Parkin,S.; Moezzi, B.; Hope, H. *J. Appl. Cryst.* **1995**, 28, 53-56.

Table 2. Data collection for $PdCl_2(NCPh)_2$.

Diffractometer	Siemens R3m/v
Temperature	130(2) K
Radiation source	normal-focus sealed tube
Wavelength	0.71073 Å (MoKα)
Monochromator	graphite
θ range for data collection	2.67 to 27.49°
Scan type	ω
Index ranges	$-1 \le h \le 8$, $-11 \le k \le 11$, $-12 \le \ell \le 12$
Reflections collected	2160
Independent reflections	1660 (R_{int} = 0.0289)
Standard reflections	2
Percent decay of standards	<0.3 %

Table 3. Solution and refinement of $PdCl_2(NCPh)_2$.

System for solution	SHELXTL 5 (Sheldrick, 1994)
Structure solution	direct
System for refinement	SHELXTL 5 (Sheldrick, 1994)
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	riding
Data / restraints / parameters	1660 / 0 / 88
Goodness-of-fit on F^2	1.056
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.0342P)^2 + 0.0918P$, where $P = (Fo^2 + 2Fc^2)/3$
R indices (all data)	R1 = 0.0284, wR2 = 0.0632
R indices calcd from obsd data	R1 = 0.0260, wR2 = 0.0620
Observed data (>2sigma(I))	1594
Largest diff. peak and hole	0.686 and -0.403 $eÅ^{-3}$

1) $R1 = \sum||Fo-Fc||/\sum|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{½}$

2) $Goodness\text{-}of\text{-}Fit = [\sum[w(Fo^2-Fc^2)^2]/(M-N)]^{½}$

where M is the number of reflections
and N is the number of parameters refined.

3) Refinement is based on F^2 for ALL reflections except for those with very negative F^2 or flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating R indices for observed data and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Table 4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for $PdCl_2(NCPh)_2$.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd	5000	0	15000	25(1)
Cl	3803(1)	2086(1)	14114(1)	36(1)
N	6559(4)	-1184(3)	12875(3)	31(1)
C(1)	7524(5)	-1863(3)	11679(3)	29(1)
C(2)	8782(4)	-2664(3)	10195(3)	25(1)
C(3)	7865(5)	-4309(3)	8769(3)	30(1)
C(4)	9147(5)	-5042(4)	7373(3)	33(1)
C(5)	11279(5)	-4157(4)	7376(3)	34(1)
C(6)	12164(5)	-2526(4)	8794(4)	33(1)
C(7)	10939(5)	-1764(3)	10218(3)	30(1)

Table 5. Bond lengths [Å] for $PdCl_2(NCPh)_2$.

Pd-N	1.974(2)	Pd-N#1	1.974(2)
Pd-Cl	2.2857(8)	Pd-Cl#1	2.2857(8)
N-C(1)	1.141(3)	C(1)-C(2)	1.433(3)
C(2)-C(7)	1.397(4)	C(2)-C(3)	1.402(4)
C(3)-C(4)	1.381(4)	C(4)-C(5)	1.384(4)
C(5)-C(6)	1.388(4)	C(6)-C(7)	1.380(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+3

Table 6. Bond angles [°] for $PdCl_2(NCPh)_2$.

N-Pd-N#1	180.000(1)	N-Pd-Cl	90.52(7)
N#1-Pd-Cl	89.48(7)	N-Pd-Cl#1	89.48(7)
N#1-Pd-Cl#1	90.52(7)	Cl-Pd-Cl#1	180.0
C(1)-N-Pd	177.9(2)	N-C(1)-C(2)	178.2(3)
C(7)-C(2)-C(3)	121.3(2)	C(7)-C(2)-C(1)	118.1(2)
C(3)-C(2)-C(1)	120.5(2)	C(4)-C(3)-C(2)	118.6(2)
C(3)-C(4)-C(5)	120.6(2)	C(4)-C(5)-C(6)	120.2(2)
C(7)-C(6)-C(5)	120.7(3)	C(6)-C(7)-C(2)	118.5(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+3

Table 7. Anisotropic displacement parameters [$Å^2$ x 10^3] for $PdCl_2(NCPh)_2$.

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Pd	23(1)	25(1)	25(1)	11(1)	3(1)	2(1)
Cl	45(1)	31(1)	34(1)	16(1)	5(1)	8(1)
N	32(1)	30(1)	32(1)	14(1)	5(1)	5(1)
C(1)	28(1)	31(1)	33(1)	19(1)	0(1)	4(1)
C(2)	24(1)	29(1)	27(1)	15(1)	3(1)	8(1)
C(3)	29(1)	31(1)	34(1)	18(1)	0(1)	1(1)
C(4)	41(2)	29(1)	26(1)	11(1)	-3(1)	8(1)
C(5)	35(2)	44(2)	29(1)	20(1)	9(1)	15(1)
C(6)	24(1)	41(1)	40(1)	24(1)	5(1)	4(1)
C(7)	27(1)	30(1)	33(1)	16(1)	-2(1)	3(1)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $PdCl_2(NCPh)_2$.

	x	y	z	U(eq)
H(3)	6392(5)	-4907(3)	8764(3)	36
H(4)	8562(5)	-6164(4)	6403(3)	40
H(5)	12139(5)	-4667(4)	6403(3)	40
H(6)	13630(5)	-1929(4)	8785(4)	39
H(7)	11550(5)	-652(3)	11192(3)	36

STRUCTURE DETERMINATION SUMMARY FOR MN455

Crystal Data for *trans*-$PdBr_2(NCPh)_2$

Empirical Formula	$C_{14}H_{10}Br_2N_2Pd$
Color; Habit	Yellow/orange plates
Crystal Size (mm)	0.04 x 0.16 x 0.16
Crystal System	Monoclinic
Space Group	C2/c
Unit Cell Dimensions	a = 8.272(3) Å
	b = 20.529(9) Å
	c = 18.102(7) Å
	β = 97.43(2)°
Volume	3048(2) $Å^3$
Z	8
Formula Weight	472.5
Density(calc.)	2.059 Mg/m^3
Absorption Coefficient	6.447 mm^{-1}
F(000)	1792

Data Collection for *trans*-$PdBr_2(NCPh)_2$

Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	130
Monochromator	Highly oriented graphite crystal
2θ Range	0.0 to 50.0°
Scan Type	ω
Scan Speed	Constant; 6.00°/min. in ω
Scan Range (ω)	1.00°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 50.0% of total scan time
Standard Reflections	2 measured every 198 reflections
Index Ranges	$-9 \le h \le 9$, $0 \le k \le 24$ $0 \le \ell \le 21$
Reflections Collected	2965
Independent Reflections	2695 (R_{int} = 2.69%)
Observed Reflections	1471 ($F > 4.0\sigma(F)$)
Absorption Correction	XABS[1]
Range Transmission coefs	0.42 - 0.78

1) Program XABS provides an empirical correction based on F_o and F_c differences. Hope, H.; Moezzi, B. Chemistry Department, University of California, Davis.

Solution and Refinement for *trans*-$PdBr_2(NCPh)_2$

System Used	Siemens SHELXTL PLUS[1,2] (VMS)
Solution	Patterson Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o-F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0018F^2$
Number of Parameters Refined	94
Final R Indices[3] (obs. data)	R = 6.82 %, Rw = 6.82 %
Goodness-of-Fit[4]	1.17
Largest and Mean Δ/σ	0.001, 0.000
Data-to-Parameter Ratio	15.6:1
Largest Difference Peak	1.30 eÅ^{-3}
Largest Difference Hole	-1.06 eÅ^{-3}

1) G. M. Sheldrick, SHELXTL PLUS, *A Program For Crystal Structure Determination*, Version 4.2, 1990, Siemens Analytical X-ray Instruments, Madison, Wisconsin.

2) Scattering factors (neutral atoms) are from "International Tables for Crystallography'" Vol. C, D. Reidel Publishing Co. Boston, 1992.

3) $R = \sum||F_o|-|F_c||/\sum|F_o|$; $Rw = \sum||F_o|-|F_c||\sqrt{w}/\sum|F_o|\sqrt{w}$

4) Goodness-of-Fit = $[\sum(w\cdot||F_o|-|F_c||^2)/(M-N)]^{\frac{1}{2}}$ where M is the number of observed reflections and N is the number of parameters refined.

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$) for *trans*-$PdBr_2(NCPh)_2$

	x	y	z	U(eq)
Pd(1)	0	2344(1)	2500	26(1)
Br(1)	-2678(2)	2349(1)	1771(1)	37(1)
N(1)	0	3315(11)	2500	42(6)
N(2)	0	1397(10)	2500	33(5)
C(1)	0	3863(12)	2500	28(6)
C(2)	0	4527(12)	2500	27(6)
C(3)	-830(22)	4895(8)	3005(10)	31(4)
C(4)	-788(25)	5561(9)	3004(11)	40(5)
C(5)	0	5911(13)	2500	35(7)
C(6)	0	830(13)	2500	35(7)
C(7)	0	123(10)	2500	16(5)
C(8)	465(22)	-201(8)	1898(11)	30(4)
C(9)	499(25)	-873(9)	1913(12)	42(5)
C(10)	0	-1218(13)	2500	31(6)
Pd(2)	5000	0	5000	26(1)
Br(2)	2089(2)	120(1)	4931(1)	41(1)
N(3)	5289(18)	927(7)	5225(8)	31(4)
C(11)	5552(22)	1461(8)	5342(10)	28(4)
C(12)	5814(21)	2142(8)	5504(10)	26(4)
C(13)	7221(23)	2307(9)	6007(11)	37(5)
C(14)	7516(29)	2958(11)	6139(13)	58(6)
C(15)	6537(25)	3435(10)	5802(11)	44(5)
C(16)	5207(28)	3271(11)	5320(12)	52(6)
C(17)	4799(26)	2622(10)	5152(12)	46(5)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 2. Bond lengths (Å) for *trans*-$PdBr_2(NCPh)_2$

Pd(1)-Br(1)	2.427 (2)	Pd(1)-N(1)	1.992 (23)
Pd(1)-N(2)	1.945 (21)	N(1)-C(1)	1.125 (33)
N(2)-C(6)	1.164 (33)	C(1)-C(2)	1.365 (34)
C(2)-C(3)	1.428 (23)	C(3)-C(4)	1.367 (25)
C(4)-C(5)	1.388 (25)	C(6)-C(7)	1.451 (33)
C(7)-C(8)	1.373 (21)	C(8)-C(9)	1.380 (25)
C(9)-C(10)	1.383 (25)	Pd(2)-Br(2)	2.407 (2)
Pd(2)-N(3)	1.955 (14)	N(3)-C(11)	1.132 (22)
C(11)-C(12)	1.440 (23)	C(12)-C(13)	1.422 (24)
C(12)-C(17)	1.394 (26)	C(13)-C(14)	1.375 (29)
C(14)-C(15)	1.363 (30)	C(15)-C(16)	1.355 (29)
C(16)-C(17)	1.399 (30)		

Table 3. Bond angles (°) for *trans*-$PdBr_2(NCPh)_2$

Br(1)-Pd(1)-N(1)	89.8(1)	Br(1)-Pd(1)-N(2)	90.2(1)
N(1)-Pd(1)-N(2)	180.0(1)	Br(1)-Pd(1)-Br(1')	179.5(1)
N(1)-Pd(1)-Br(1')	89.8(1)	N(2)-Pd(1)-Br(1')	90.2(1)
Pd(1)-N(1)-C(1)	180.0(1)	Pd(1)-N(2)-C(6)	180.0(1)
N(1)-C(1)-C(2)	180.0(1)	C(1)-C(2)-C(3)	121.9(11)
C(1)-C(2)-C(3')	121.9(11)	C(3)-C(2)-C(3')	116.2(21)
C(2)-C(3)-C(4)	120.8(18)	C(3)-C(4)-C(5)	122.2(20)
C(4)-C(5)-C(4')	117.7(25)	N(2)-C(6)-C(7)	180.0(1)
C(6)-C(7)-C(8)	119.0(10)	C(6)-C(7)-C(8')	119.0(10)
C(8)-C(7)-C(8')	122.1(21)	C(7)-C(8)-C(9)	118.4(18)
C(8)-C(9)-C(10)	121.3(20)	C(9)-C(10)-C(9')	118.5(24)
Br(2)-Pd(2)-N(3)	90.3(4)	Br(2)-Pd(2)-Br(A")	180.0(1)
N(3)-Pd(2)-Br(2")	89.7(4)	Br(2)-Pd(2)-N(3")	89.7(4)
N(3)-Pd(2)-N(3")	180.0(1)	Br(2")-Pd(2)-N(3")	90.3(4)
Pd(2)-N(3)-C(11)	175.6(15)	N(3)-C(11)-C(12)	177.3(21)
C(11)-C(12)-C(13)	116.8(15)	C(11)-C(12)-C(17)	121.8(16)
C(13)-C(12)-C(17)	121.3(16)	C(12)-C(13)-C(14)	117.0(17)
C(13)-C(14)-C(15)	122.6(20)	C(14)-C(15)-C(16)	119.8(20)
C(15)-C(16)-C(17)	121.9(20)	C(12)-C(17)-C(16)	117.4(18)

Symmetry code: ' = -x,y,0.5-z; " = 1-x,-y,1-z

Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$) for *trans*-$PdBr_2(NCPh)_2$

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pd(1)	35(1)	25(1)	18(1)	0	6(1)	0
Br(1)	38(1)	39(1)	32(1)	0(1)	1(1)	2(1)
Pd(2)	26(1)	27(1)	27(1)	-5(1)	6(1)	-3(1)
Br(2)	27(1)	40(1)	57(2)	3(1)	7(1)	3(1)

The anisotropic displacement factor exponent takes the form:
$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x 10^3$) for *trans*-$PdBr_2(NCPh)_2$

	x	y	z	U
H(3)	-1392	4667	3358	40
H(4)	-1339	5788	3362	40
H(5)	0	6378	2500	40
H(8)	763	28	1474	40
H(9)	875	-1102	1506	40
H(10)	0	-1685	2500	40
H(13)	7944	1981	6244	40
H(14)	8407	3080	6508	40
H(15)	6834	3882	5894	40
H(16)	4525	3608	5080	40
H(17)	3828	2516	4824	40

Table 1. Crystal data for Pd_6Cl_{12}•*p*-xylene•$PdCl_2(NCPh)_2$.

Identification code	mn688
Empirical formula	$C_{22}H_{20}Cl_{14}N_2Pd_7$
Formula weight	1553.50
Crystal size	0.12 x 0.12 x 0.04 mm
Crystal habit	wedge
Crystal color	dark red
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 16.550(5) Å α = 90° b = 15.489(4) Å β = 109.91(2)° c = 15.850(4) Å γ = 90°
Volume	3820(2) $Å^3$
Z	4
Density (calculated)	2.701 $Mg•m^{-3}$
Absorption coefficient	4.221 mm^{-1}
F(000)	2904
Absorption correction[1]	XABS2
Max. and min. transmission	0.873 and 0.638

1) XABS2: an empirical absorption correction program. Parkin,S.; Moezzi, B.; Hope, H. *J. Appl. Cryst.* **1995**, 28, 53-56.

Table 2. Data collection for Pd_6Cl_{12}•*p*-xylene•$PdCl_2(NCPh)_2$.

Diffractometer	Siemens R3m/v
Temperature	130(2) K
Radiation source	normal-focus sealed tube
Wavelength	0.71073 Å (MoKα)
Monochromator	graphite
θ range for data collection	1.86 to 27.50°
Scan type	ω
Index ranges	$-21 \le h \le 20$, $0 \le k \le 20$, $0 \le \ell \le 20$
Reflections collected	4682
Independent reflections	4385 (R_{int} = 0.0539)
Standard reflections	2
Percent decay of standards	< 1%

Table 3. Solution and refinement of Pd_6Cl_{12}•p-xylene•$PdCl_2(NCPh)_2$.

System for solution	SHELXTL v. 5 (Sheldrick, 1994)
Structure solution	direct
System for refinement	SHELXTL v. 5 (Sheldrick, 1994)
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	riding
Data / restraints / parameters	4385 / 0 / 206
Goodness-of-fit on F^2	1.048
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.0477P)^2 + 5.9260P$, where $P = (Fo^2 + 2Fc^2)/3$
R indices (all data)	R1 = 0.0571, wR2 = 0.1051
R indices calcd from obsd data	R1 = 0.0418, wR2 = 0.0963
Observed data (>2sigma(I))	3491
Largest diff. peak and hole	0.818 and -0.895 eÅ^{-3}

1) $R1 = \sum||Fo-Fc||/\sum|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{½}$

2) $Goodness\text{-}of\text{-}Fit = [\sum[w(Fo^2-Fc^2)^2]/(M-N)]^{½}$

where M is the number of reflections
and N is the number of parameters refined.

3) Refinement is based on F^2 for ALL reflections except for those with very negative F^2 or flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating R indices for observed data and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Table 4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for Pd_6Cl_{12}•*p*-xylene•$PdCl_2(NCPh)_2$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	5239(1)	5085(1)	6540(1)	22(1)
Pd(2)	6079(1)	6039(1)	5183(1)	23(1)
Pd(3)	3948(1)	6097(1)	4748(1)	22(1)
Cl(1)	4178(1)	4057(1)	6335(1)	29(1)
Cl(2)	6246(1)	4003(1)	6761(1)	28(1)
Cl(3)	6297(1)	6113(1)	6702(1)	28(1)
Cl(4)	4208(1)	6151(1)	6278(1)	28(1)
Cl(5)	7093(1)	4952(1)	5424(1)	29(1)
Cl(6)	5031(1)	7093(1)	4911(1)	28(1)
Pd(4)	2500	7500	5000	30(1)
Cl(7)	2335(1)	7225(1)	6356(1)	40(1)
N(1)	3519(4)	8220(4)	5602(4)	36(1)
C(1)	4146(4)	8589(4)	5897(4)	31(2)
C(2)	4934(4)	9060(4)	6273(4)	31(2)
C(3)	4977(5)	9916(5)	6055(5)	42(2)
C(4)	5736(6)	10346(6)	6378(6)	56(2)
C(5)	6473(6)	9923(6)	6928(6)	55(2)
C(6)	6430(5)	9072(6)	7136(5)	44(2)
C(7)	5666(5)	8618(5)	6814(5)	39(2)
C(8)	6903(5)	8082(5)	5042(6)	41(2)
C(9)	7462(5)	7733(5)	5818(5)	38(2)
C(10)	8077(5)	7147(5)	5798(5)	38(2)
C(11)	8696(6)	6771(6)	6651(6)	57(2)

Table 5. Bond lengths [Å] for Pd_6Cl_{12}•p-xylene•$PdCl_2(NCPh)_2$.

Pd(1)-Cl(2)	2.305(2)	Pd(1)-Cl(4)	2.308(2)
Pd(1)-Cl(1)	2.310(2)	Pd(1)-Cl(3)	2.316(2)
Pd(2)-Cl(1)#1	2.301(2)	Pd(2)-Cl(6)	2.313(2)
Pd(2)-Cl(3)	2.313(2)	Pd(2)-Cl(5)	2.316(2)
Pd(3)-Cl(2)#1	2.308(2)	Pd(3)-Cl(6)	2.312(2)
Pd(3)-Cl(5)#1	2.316(2)	Pd(3)-Cl(4)	2.316(2)
Cl(1)-Pd(2)#1	2.301(2)	Cl(2)-Pd(3)#1	2.308(2)
Cl(5)-Pd(3)#1	2.316(2)	Pd(4)-N(1)	1.976(6)
Pd(4)-N(1)#2	1.976(6)	Pd(4)-Cl(7)#2	2.296(2)
Pd(4)-Cl(7)	2.296(2)	N(1)-C(1)	1.137(8)
C(1)-C(2)	1.433(9)	C(2)-C(3)	1.377(10)
C(2)-C(7)	1.402(10)	C(3)-C(4)	1.358(12)
C(4)-C(5)	1.398(13)	C(5)-C(6)	1.367(12)
C(6)-C(7)	1.383(10)	C(8)-C(9)	1.374(10)
C(8)-C(10)#3	1.389(11)	C(9)-C(10)	1.372(11)
C(10)-C(8)#3	1.389(11)	C(10)-C(11)	1.507(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x+1/2,-y+3/2,-z+1 #3 -x+3/2,-y+3/2,-z+1

Table 6. Bond angles [°] for Pd_6Cl_{12}•p-xylene•$PdCl_2(NCPh)_2$.

Cl(2)-Pd(1)-Cl(4)	178.31(6)	Cl(2)-Pd(1)-Cl(1)	89.76(6)
Cl(4)-Pd(1)-Cl(1)	89.31(6)	Cl(2)-Pd(1)-Cl(3)	90.17(6)
Cl(4)-Pd(1)-Cl(3)	90.72(6)	Cl(1)-Pd(1)-Cl(3)	178.34(6)
Cl(1)#1-Pd(2)-Cl(6)	89.49(6)	Cl(1)#1-Pd(2)-Cl(3)	178.25(6)
Cl(6)-Pd(2)-Cl(3)	90.04(6)	Cl(1)#1-Pd(2)-Cl(5)	89.50(6)
Cl(6)-Pd(2)-Cl(5)	178.09(6)	Cl(3)-Pd(2)-Cl(5)	90.93(6)
Cl(2)#1-Pd(3)-Cl(6)	89.41(6)	Cl(2)#1-Pd(3)-Cl(5)#1	89.76(6)
Cl(6)-Pd(3)-Cl(5)#1	177.27(6)	Cl(2)#1-Pd(3)-Cl(4)	176.91(6)
Cl(6)-Pd(3)-Cl(4)	89.87(6)	Cl(5)#1-Pd(3)-Cl(4)	90.83(6)
Pd(2)#1-Cl(1)-Pd(1)	93.01(6)	Pd(1)-Cl(2)-Pd(3)#1	93.02(5)
Pd(2)-Cl(3)-Pd(1)	90.35(5)	Pd(1)-Cl(4)-Pd(3)	91.45(6)
Pd(3)#1-Cl(5)-Pd(2)	91.25(6)	Pd(3)-Cl(6)-Pd(2)	93.03(6)
N(1)-Pd(4)-N(1)#2	180.000(2)	N(1)-Pd(4)-Cl(7)#2	89.6(2)
N(1)#2-Pd(4)-Cl(7)#2	90.4(2)	N(1)-Pd(4)-Cl(7)	90.4(2)
N(1)#2-Pd(4)-Cl(7)	89.6(2)	Cl(7)#2-Pd(4)-Cl(7)	179.997(1)
C(1)-N(1)-Pd(4)	172.9(6)	N(1)-C(1)-C(2)	179.5(7)
C(3)-C(2)-C(7)	121.0(7)	C(3)-C(2)-C(1)	120.2(6)
C(7)-C(2)-C(1)	118.7(6)	C(4)-C(3)-C(2)	119.8(8)
C(3)-C(4)-C(5)	120.3(8)	C(6)-C(5)-C(4)	119.7(8)
C(5)-C(6)-C(7)	121.2(8)	C(6)-C(7)-C(2)	118.0(7)
C(9)-C(8)-C(10)#3	121.9(7)	C(8)-C(9)-C(10)	121.3(7)
C(9)-C(10)-C(8)#3	116.8(7)	C(9)-C(10)-C(11)	121.2(8)
C(8)#3-C(10)-C(11)	122.0(8)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x+1/2,-y+3/2,-z+1 #3 -x+3/2,-y+3/2,-z+1

Table 7. Anisotropic displacement parameters [$Å^2 \times 10^3$] for Pd_6Cl_{12}•p-xylene•$PdCl_2(NCPh)_2$.

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Pd(1)	25(1)	24(1)	18(1)	0(1)	8(1)	3(1)
Pd(2)	22(1)	23(1)	23(1)	-1(1)	9(1)	-2(1)
Pd(3)	22(1)	22(1)	23(1)	0(1)	8(1)	4(1)
Cl(1)	33(1)	32(1)	26(1)	2(1)	15(1)	-2(1)
Cl(2)	29(1)	32(1)	21(1)	4(1)	6(1)	7(1)
Cl(3)	29(1)	29(1)	23(1)	-5(1)	6(1)	-2(1)
Cl(4)	32(1)	30(1)	24(1)	-1(1)	13(1)	9(1)
Cl(5)	21(1)	31(1)	35(1)	0(1)	10(1)	1(1)
Cl(6)	31(1)	20(1)	34(1)	1(1)	11(1)	2(1)
Pd(4)	21(1)	23(1)	39(1)	-2(1)	3(1)	3(1)
Cl(7)	36(1)	39(1)	43(1)	3(1)	10(1)	6(1)
N(1)	26(3)	32(3)	45(3)	-8(3)	6(3)	0(3)
C(1)	32(4)	31(4)	32(3)	2(3)	12(3)	0(3)
C(2)	25(3)	33(4)	33(4)	-8(3)	8(3)	-4(3)
C(3)	47(4)	31(4)	39(4)	2(3)	4(3)	-1(3)
C(4)	77(7)	35(5)	52(5)	-12(4)	16(5)	-16(5)
C(5)	40(4)	73(7)	49(5)	-24(5)	12(4)	-16(4)
C(6)	27(4)	56(5)	43(4)	-17(4)	5(3)	-2(3)
C(7)	37(4)	41(4)	40(4)	-4(3)	16(3)	5(3)
C(8)	29(4)	32(4)	65(5)	-2(4)	20(4)	-5(3)
C(9)	40(4)	34(4)	45(4)	0(3)	22(3)	-13(3)
C(10)	39(4)	29(4)	46(4)	5(3)	15(3)	-7(3)
C(11)	67(6)	43(5)	56(5)	17(4)	16(5)	2(4)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Pd_6Cl_{12}•p-xylene•$PdCl_2(NCPh)_2$.

	x	y	z	U(eq)
H(3)	4477(5)	10205(5)	5680(5)	50
H(4)	5766(6)	10936(6)	6229(6)	68
H(5)	7003(6)	10226(6)	7157(6)	66
H(6)	6933(5)	8786(6)	7509(5)	52
H(7)	5638(5)	8025(5)	6955(5)	46
H(8)	6491(5)	8493(5)	5080(6)	49
H(9)	7423(5)	7901(5)	6379(5)	46
H(11A)	9274(9)	6996(32)	6748(23)	85
H(11B)	8700(31)	6141(6)	6600(17)	85
H(11C)	8516(24)	6932(34)	7158(8)	85

Table 1. Crystal data for Pd_6Cl_{12}•0.5stilbene•2benzene.

Identification code	mn756
Empirical formula	$C_{19}H_{18}Cl_{12}Pd_6$
Formula weight	1310.13
Crystal size	0.14 x 0.12 x 0.10 mm
Crystal habit	parallelepiped
Crystal color	dark red
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 11.383(2) Å α = 78.050(14)°
	b = 12.155(2) Å β = 67.70(2)°
	c = 12.803(2) Å γ = 80.16(2)°
Volume	1595.0(5) $Å^3$
Z	2
Density (calculated)	2.728 $Mg•m^3$
Absorption coefficient	4.329 mm^{-1}
F(000)	1224
Absorption correction[1]	XABS2
Max. and min. transmission	0.696 and 0.567

1) XABS2: an empirical absorption correction program. Parkin,S.; Moezzi, B.; Hope, H. *J. Appl. Cryst.* **1995**, 28, 53-56.

Table 2. Data collection for Pd_6Cl_{12}•0.5stilbene•2benzene.

Diffractometer	Siemens R3m/V
Temperature	130(2) K
Radiation source	normal-focus sealed tube
Wavelength	0.71073 Å (MoKα)
Monochromator	graphite
θ range for data collection	1.72 to 27.50°
Scan type	ω
Index ranges	$-13 \le h \le 14$, $-15 \le k \le 15$, $0 \le \ell \le 16$
Reflections collected	7330
Independent reflections	7330 (R_{int} = 0.0000)
Standard reflections	2
Percent decay of standards	<0.1

Table 3. Solution and refinement of Pd_6Cl_{12}•0.5stilbene•2benzen

System for solution	SHELXTL 5 (Sheldrick, 1994)
Structure solution	direct
System for refinement	SHELXTL 5 (Sheldrick, 1994)
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	riding
Data / restraints / parameters	7324 / 0 / 310
Goodness-of-fit on F^2	1.057
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.0416P)^2 + 17.0981P$, where $P = (Fo^2 + 2Fc^2)/3$
R indices (all data)	R1 = 0.0723, wR2 = 0.1295
R indices calcd from obsd data	R1 = 0.0474, wR2 = 0.1102
Observed data (>2sigma(I))	5328
Largest diff. peak and hole	2.444 and -1.051 eÅ^{-3}

1) $R1 = \sum||Fo-Fc||/\sum|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{½}$

2) $\text{Goodness-of-Fit} = [\sum[w(Fo^2-Fc^2)^2]/(M-N)]^{½}$

where M is the number of reflections
and N is the number of parameters refined.

3) Refinement is based on F^2 for ALL reflections except for those with very negative F^2 or flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating R indices for observed data and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Table 4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for Pd_6Cl_{12}•0.5stilbene•2benzene.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	4768(1)	4288(1)	4033(1)	20(1)
Pd(2)	5544(1)	4345(1)	1246(1)	22(1)
Pd(3)	5796(1)	1560(1)	1638(1)	21(1)
Pd(4)	5026(1)	1500(1)	4407(1)	22(1)
Pd(5)	3108(1)	2984(1)	3120(1)	20(1)
Pd(6)	7459(1)	2879(1)	2551(1)	22(1)
Cl(1)	4528(2)	2858(2)	5577(2)	28(1)
Cl(2)	5040(2)	5671(2)	2449(2)	29(1)
Cl(3)	6041(2)	2977(2)	86(2)	29(1)
Cl(4)	5542(2)	168(2)	3211(2)	30(1)
Cl(5)	2642(2)	4339(2)	4291(2)	27(1)
Cl(6)	3411(2)	4382(2)	1542(2)	27(1)
Cl(7)	3652(2)	1642(2)	1945(2)	27(1)
Cl(8)	2892(2)	1569(2)	4678(2)	27(1)
Cl(9)	6903(2)	4223(2)	3745(2)	29(1)
Cl(10)	7671(2)	4294(2)	990(2)	31(1)
Cl(11)	7926(2)	1532(2)	1386(2)	31(1)
Cl(12)	7164(2)	1469(2)	4113(2)	30(1)
C(1)	487(7)	2677(5)	2390(6)	42(3)
C(2)	146(6)	2707(5)	3549(5)	38(2)
C(3)	-145(6)	3740(6)	3943(4)	41(3)
C(4)	-95(6)	4742(4)	3179(6)	37(2)
C(5)	246(6)	4712(5)	2020(5)	36(2)
C(6)	537(6)	3680(6)	1626(4)	41(3)
C(7)	7525(10)	-320(8)	-286(8)	33(2)
C(8)	8671(10)	-727(9)	-183(9)	36(2)
C(9)	8775(11)	-1667(10)	627(9)	42(3)
C(10)	7694(11)	-2165(10)	1337(9)	45(3)
C(11)	6526(9)	-1701(9)	1257(9)	36(2)
C(12)	6424(9)	-801(8)	426(8)	28(2)
C(13)	5137(10)	-417(8)	391(8)	32(2)
C(14)	11917(8)	-2461(6)	2786(7)	69(5)
C(15)	10762(9)	-2223(6)	2609(7)	63(4)
C(16)	9972(6)	-1249(7)	2926(6)	46(3)
C(17)	10338(7)	-513(5)	3419(6)	46(3)
C(18)	11493(8)	-751(7)	3595(6)	55(3)
C(19)	12283(6)	-1725(8)	3278(7)	63(4)

Table 5. Bond lengths [Å] for Pd_6Cl_{12}•0.5stilbene•2benzene.

Pd(1)-Cl(9)	2.306(2)	Pd(1)-Cl(2)	2.307(2)
Pd(1)-Cl(5)	2.307(2)	Pd(1)-Cl(1)	2.310(2)
Pd(2)-Cl(6)	2.304(2)	Pd(2)-Cl(10)	2.309(2)
Pd(2)-Cl(2)	2.311(2)	Pd(2)-Cl(3)	2.314(2)
Pd(3)-Cl(4)	2.305(2)	Pd(3)-Cl(3)	2.307(2)
Pd(3)-Cl(7)	2.308(2)	Pd(3)-Cl(11)	2.316(2)
Pd(4)-Cl(8)	2.308(2)	Pd(4)-Cl(4)	2.309(2)
Pd(4)-Cl(12)	2.312(2)	Pd(4)-Cl(1)	2.313(2)
Pd(5)-Cl(7)	2.296(2)	Pd(5)-Cl(6)	2.310(2)
Pd(5)-Cl(8)	2.313(2)	Pd(5)-Cl(5)	2.315(2)
Pd(6)-Cl(11)	2.303(2)	Pd(6)-Cl(12)	2.306(2)
Pd(6)-Cl(9)	2.313(2)	Pd(6)-Cl(10)	2.316(2)
C(1)-C(2)	1.39	C(1)-C(6)	1.39
C(2)-C(3)	1.39	C(3)-C(4)	1.39
C(4)-C(5)	1.39	C(5)-C(6)	1.39
C(7)-C(8)	1.359(14)	C(7)-C(12)	1.380(13)
C(8)-C(9)	1.397(14)	C(9)-C(10)	1.37(2)
C(10)-C(11)	1.38(2)	C(11)-C(12)	1.382(13)
C(12)-C(13)	1.474(14)	C(13)-C(13)#1	1.36(2)
C(14)-C(15)	1.39	C(14)-C(19)	1.39
C(15)-C(16)	1.39	C(16)-C(17)	1.39
C(17)-C(18)	1.39	C(18)-C(19)	1.39

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z

Table 6. Bond angles [°] for Pd_6Cl_{12}•0.5stilbene•2benzene.

Cl(9)-Pd(1)-Cl(2)	89.44(9)	Cl(9)-Pd(1)-Cl(5)	178.93(8)
Cl(2)-Pd(1)-Cl(5)	90.19(9)	Cl(9)-Pd(1)-Cl(1)	90.12(9)
Cl(2)-Pd(1)-Cl(1)	178.03(8)	Cl(5)-Pd(1)-Cl(1)	90.21(9)
Cl(6)-Pd(2)-Cl(10)	178.77(8)	Cl(6)-Pd(2)-Cl(2)	89.84(8)
Cl(10)-Pd(2)-Cl(2)	89.59(9)	Cl(6)-Pd(2)-Cl(3)	90.11(9)
Cl(10)-Pd(2)-Cl(3)	90.43(9)	Cl(2)-Pd(2)-Cl(3)	178.35(8)
Cl(4)-Pd(3)-Cl(3)	178.94(8)	Cl(4)-Pd(3)-Cl(7)	89.73(9)
Cl(3)-Pd(3)-Cl(7)	90.23(9)	Cl(4)-Pd(3)-Cl(11)	90.04(9)
Cl(3)-Pd(3)-Cl(11)	89.95(9)	Cl(7)-Pd(3)-Cl(11)	177.50(8)
Cl(8)-Pd(4)-Cl(4)	90.74(9)	Cl(8)-Pd(4)-Cl(12)	178.77(8)
Cl(4)-Pd(4)-Cl(12)	89.66(9)	Cl(8)-Pd(4)-Cl(1)	89.66(8)
Cl(4)-Pd(4)-Cl(1)	178.95(8)	Cl(12)-Pd(4)-Cl(1)	89.93(9)
Cl(7)-Pd(5)-Cl(6)	89.52(8)	Cl(7)-Pd(5)-Cl(8)	89.88(8)
Cl(6)-Pd(5)-Cl(8)	177.71(8)	Cl(7)-Pd(5)-Cl(5)	177.81(8)
Cl(6)-Pd(5)-Cl(5)	90.31(8)	Cl(8)-Pd(5)-Cl(5)	90.21(8)
Cl(11)-Pd(6)-Cl(12)	89.68(9)	Cl(11)-Pd(6)-Cl(9)	177.64(8)
Cl(12)-Pd(6)-Cl(9)	89.78(9)	Cl(11)-Pd(6)-Cl(10)	90.15(9)
Cl(12)-Pd(6)-Cl(10)	177.70(8)	Cl(9)-Pd(6)-Cl(10)	90.29(9)
Pd(1)-Cl(1)-Pd(4)	91.14(8)	Pd(1)-Cl(2)-Pd(2)	92.04(8)
Pd(3)-Cl(3)-Pd(2)	91.05(8)	Pd(3)-Cl(4)-Pd(4)	91.38(8)
Pd(1)-Cl(5)-Pd(5)	91.25(8)	Pd(2)-Cl(6)-Pd(5)	92.20(8)
Pd(5)-Cl(7)-Pd(3)	92.74(8)	Pd(4)-Cl(8)-Pd(5)	91.14(8)
Pd(1)-Cl(9)-Pd(6)	92.12(8)	Pd(2)-Cl(10)-Pd(6)	91.24(8)
Pd(6)-Cl(11)-Pd(3)	91.88(8)	Pd(6)-Cl(12)-Pd(4)	92.21(8)
C(2)-C(1)-C(6)	120.0	C(3)-C(2)-C(1)	120.0
C(2)-C(3)-C(4)	120.0	C(3)-C(4)-C(5)	120.0
C(6)-C(5)-C(4)	120.0	C(5)-C(6)-C(1)	120.0
C(8)-C(7)-C(12)	121.2(9)	C(7)-C(8)-C(9)	120.9(10)
C(10)-C(9)-C(8)	118.9(10)	C(9)-C(10)-C(11)	119.2(10)
C(10)-C(11)-C(12)	122.0(9)	C(7)-C(12)-C(11)	117.7(9)
C(7)-C(12)-C(13)	125.3(9)	C(11)-C(12)-C(13)	117.0(9)
C(13)#1-C(13)-C(12)	125.2(12)	C(15)-C(14)-C(19)	120.0
C(16)-C(15)-C(14)	120.0	C(15)-C(16)-C(17)	120.0
C(16)-C(17)-C(18)	120.0	C(19)-C(18)-C(17)	120.0
C(18)-C(19)-C(14)	120.0		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z

Table 7. Anisotropic displacement parameters [$Å^2$ x 10^3] for Pd_6Cl_{12}•0.5stilbene•2benzene.

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Pd(1)	19(1)	20(1)	24(1)	-8(1)	-7(1)	0(1)
Pd(2)	23(1)	19(1)	21(1)	3(1)	-8(1)	-5(1)
Pd(3)	26(1)	18(1)	18(1)	-5(1)	-7(1)	-2(1)
Pd(4)	27(1)	20(1)	17(1)	1(1)	-9(1)	-2(1)
Pd(5)	17(1)	22(1)	21(1)	-3(1)	-8(1)	-4(1)
Pd(6)	16(1)	27(1)	25(1)	-7(1)	-7(1)	0(1)
Cl(1)	35(1)	32(1)	18(1)	-7(1)	-8(1)	-2(1)
Cl(2)	34(1)	15(1)	38(1)	-2(1)	-13(1)	-3(1)
Cl(3)	38(1)	31(1)	16(1)	-1(1)	-8(1)	-7(1)
Cl(4)	45(1)	15(1)	29(1)	-1(1)	-14(1)	-1(1)
Cl(5)	18(1)	30(1)	34(1)	-14(1)	-7(1)	3(1)
Cl(6)	26(1)	29(1)	30(1)	3(1)	-16(1)	-2(1)
Cl(7)	30(1)	29(1)	27(1)	-8(1)	-12(1)	-9(1)
Cl(8)	25(1)	31(1)	23(1)	2(1)	-5(1)	-13(1)
Cl(9)	21(1)	36(1)	36(1)	-16(1)	-12(1)	-4(1)
Cl(10)	21(1)	36(1)	30(1)	0(1)	-3(1)	-10(1)
Cl(11)	23(1)	36(1)	31(1)	-16(1)	-4(1)	5(1)
Cl(12)	29(1)	32(1)	31(1)	-2(1)	-19(1)	5(1)
C(1)	29(5)	48(6)	50(7)	-17(5)	-13(5)	5(5)
C(2)	25(5)	39(6)	58(7)	-9(5)	-23(5)	-4(4)
C(3)	15(4)	75(8)	32(5)	-4(5)	-10(4)	-8(5)
C(4)	18(4)	42(6)	46(6)	-12(5)	-2(4)	-7(4)
C(5)	17(4)	43(6)	40(6)	7(5)	-7(4)	-7(4)
C(6)	23(5)	58(7)	40(6)	-15(5)	-4(4)	-2(5)
C(7)	42(6)	26(5)	28(5)	-3(4)	-9(4)	-5(4)
C(8)	36(6)	39(6)	33(5)	-6(4)	-9(4)	-6(4)
C(9)	33(6)	50(7)	37(6)	-3(5)	-12(5)	1(5)
C(10)	52(7)	42(6)	32(5)	-1(5)	-10(5)	3(5)
C(11)	25(5)	36(5)	39(6)	1(4)	-2(4)	-11(4)
C(12)	34(5)	25(4)	25(4)	-13(4)	-8(4)	-2(4)
C(13)	35(5)	32(5)	25(5)	-9(4)	-4(4)	-6(4)
C(14)	92(11)	58(8)	52(8)	-21(6)	-37(8)	48(8)
C(15)	115(13)	38(7)	38(7)	-2(5)	-27(7)	-21(7)
C(16)	36(6)	58(7)	40(6)	11(5)	-15(5)	-12(5)
C(17)	56(7)	34(6)	33(6)	-5(5)	-4(5)	2(5)
C(18)	70(9)	70(9)	33(6)	2(6)	-22(6)	-31(7)
C(19)	31(6)	109(12)	32(6)	11(7)	-7(5)	-3(7)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Pd_6Cl_{12}•0.5stilbene•2benzene.

	x	y	z	U(eq)
H(1)	686(7)	1972(5)	2121(6)	51
H(2)	112(9)	2022(5)	4071(7)	46
H(3)	-378(9)	3760(8)	4735(4)	49
H(4)	-293(9)	5447(5)	3448(8)	44
H(5)	281(9)	5397(6)	1498(7)	43
H(6)	770(9)	3659(8)	835(4)	50
H(7)	7480(10)	308(8)	-857(8)	40
H(8)	9411(10)	-367(9)	-669(9)	44
H(9)	9581(11)	-1957(10)	686(9)	50
H(10)	7746(11)	-2821(10)	1876(9)	54
H(11)	5772(9)	-2010(9)	1790(9)	44
H(13)	4444(10)	-783(8)	963(8)	38
H(14)	12457(8)	-3127(6)	2569(7)	83
H(15)	10512(13)	-2726(8)	2273(9)	75
H(16)	9183(7)	-1086(10)	2805(10)	56
H(17)	9799(10)	153(7)	3635(9)	55
H(18)	11743(12)	-248(9)	3932(9)	66
H(19)	13073(7)	-1888(12)	3399(10)	75