Supporting Information

Intramolecular Pd-Mediated Processes of Amino-Tethered Aryl Halides and Ketones: Insight into the Ketone α-Arylation and Carbonyl-Addition Dichotomy. A New Class of Four-Membered Azapalladacycles

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Crystal data for azapalladacycle 46: $C_{36}H_{35}INOPPd$, crystal dimensions 0.10 x 0.10 x 0.20 mm, monoclinic, space group *Cc*, a = 9.619(8), b = 36.11(2), c = 10.078(18) Å, β = 112.07(10)°, V = 3244(7) Å^3, Z = 4, ρ_{calcd} = 1.560 Mg/m^3, Θ_{max} = 29.98°, $\lambda(Mo_{K\alpha})$ = 0.71069 Å, T = 298 K, 5149 collected reflections, 4933 unique reflections (R_{int} = 0.029). Lorentz and polarization corrections were applied, μ = 1.601 mm^{-1}, 370 parameters were refined, $R1$ = 0.039 (for 4933 observed reflections with $I > 2\sigma(I)$), $wR2$ = 0.0423 (on $|F|^2$), absolute structure parameter –0.05(3), max/min residual peaks in final difference map 0.736/-0.675 e. Å^{-3}, crystals were mounted in air on ENRAF-NONIUS CAD4 diffractometer with an image plate detector.

Crystal data for azapalladacycle 48: $C_{38}H_{37}Cl_2INOPPd$, crystal dimensions 0.10 x 0.10 x 0.20 mm, monoclinic, space group $P2_1/c$, a = 9.7190(10), b = 20.6330(10), c = 17.7930(10) Å, β = 90.542 (4)°, V = 3567.9(5) Å^3, Z = 4, ρ_{calcd} = 1.599 Mg/m^3, Θ_{max} = 28.86°, $\lambda(Mo_{K\alpha})$ = 0.71069 Å , T = 298 K, 17632 collected reflections, 6928 unique reflections (R_{int} = 0.032). Lorentz and polarization corrections were applied, μ = 1.611 mm^{-1}, 401 parameters were refined, $R1$ = 0.032 (for 6928 observed reflections with $I > 2\sigma(I)$), $wR2$ = 0.088 (on $|F|^2$), max/min residual peaks in final difference map 0.590/-0.741 e. Å^{-3}, Crystals were mounted in air on MAR345 diffractometer with an image plate detector.

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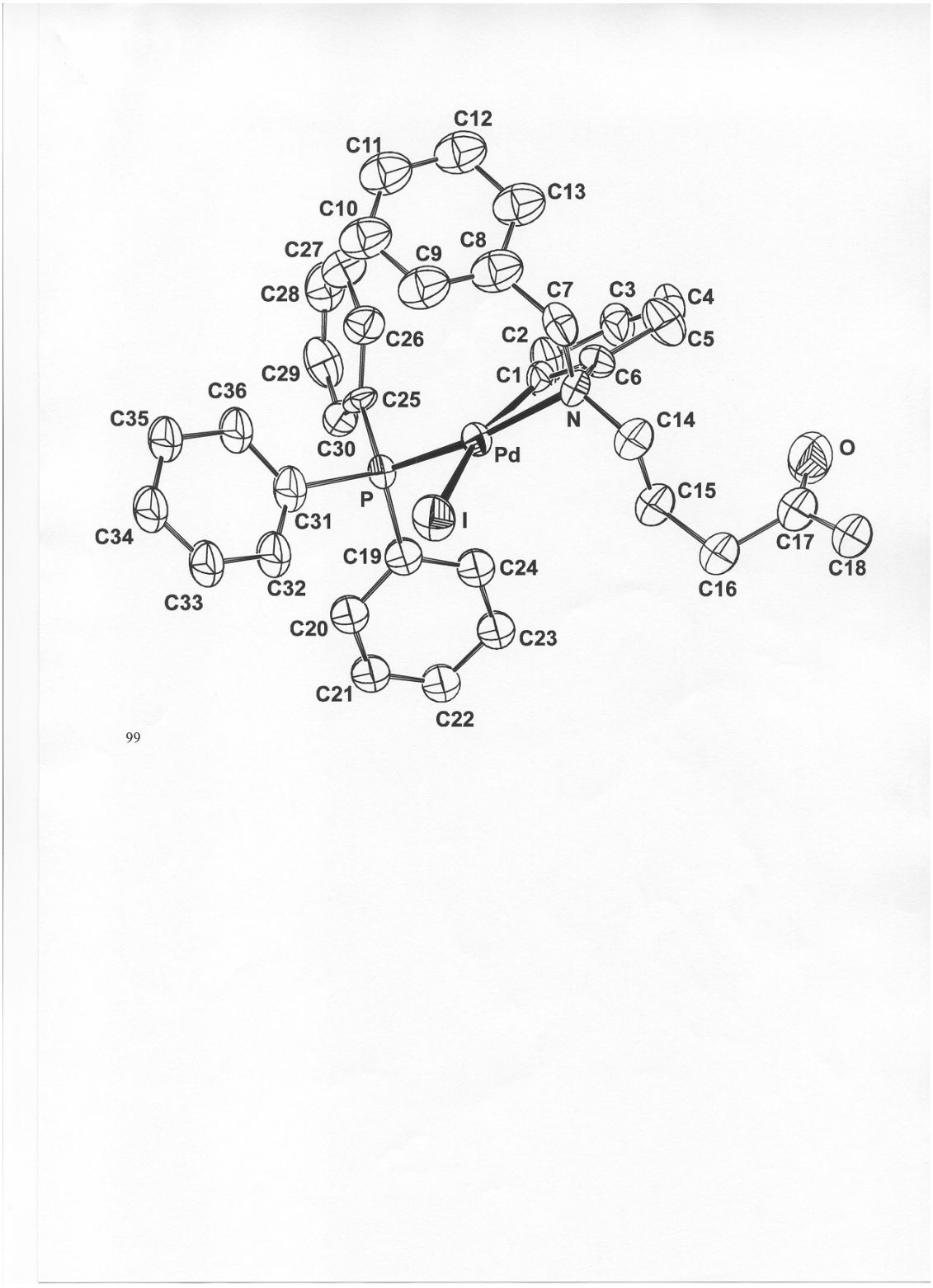
Both structures were solved by direct methods (SHELXL-97) and refined by full-matrix least-square techniques on F^2. Hydrogen atoms linked to carbon atoms were computed and refined with an isotropic temperature factor equal to 1.2 times the equivalent isotropic temperature factor of the atom to which they are linked and by using a riding model. Crystallographic data (excluding structure factors) for **46** and **48** have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no CCDC 178895 and CCDC 178896, respectively. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033: e-mail: deposit@ccdc.cam.ac.uk).

Comments: The four-membered palladacycle of **48** is planar (largest deviation to mean plane 0.004(4) Å in C-13). The dihedral angle between this ring and the adjacent phenyl ring is 1.4 (2)°. The electronic coupling due to the planarity of the Pd(C_6H_4)N moiety in **48** produces the shortening of Pd-C(Ar) bond length (1.989(3) Å, average value for the shortest Pd-C in CCDC data base 2.07(2) Å, [1] range 2.022-2.102 Å) and decreases the N-Pd-C bond angle (65.91(13)°, average value 67.8(7)°, range 66.33 – 70.76°). The steric hindrance produced by this geometric shortening produces the lengthening of Pd-N bond length (2.228(3) Å, average value 2.03(2) Å, range 2.006 – 2.084 Å), Pd-C-C bond angle (99.5(3)°, average value 89(2)°, range 86.5 – 92.6°) and N-C-C bond angle (109.6(3)°, average value 105.5(17), range 101.9 – 108.4°).

[1] F. H. Allen, O. Kennard, Chem. Design Automat. News **1993**, 8, 31-37.



Molecular structure of **46** (ORTEP view). Selected interatomic distances [Å] and angles [°]: Pd-N 2.160(8), Pd-C(1) 2.013(10), N-C(6) 1.476(3), C(1)-C(6) 1.360(15); N-Pd-C(1) 67.1(4), Pd-N-C(6) 87.0(5), Pd-C(1)-C(6) 96.5(7), N-C(6)-C(1) 109.0(9).

Crystallographic Tables of Azapalladacycle **46**

SOFC42a

Experimental. A prismatic crystal (0.1x0.1x0.2 mm) was selected and mounted on a Enraf-Nonius CAD4 four-circle diffractometer. Unit-cell parameters were determined from automatic centering of 25 reflections ($12 < \theta < 21°$) and refined by least-squares method. Intensities were collected with graphite monochromatized Mo Kα radiation, using $\omega/2\theta$ scan-technique. 4933 reflections were measured in the range $2.35 \leq \theta \leq 29.98$. 1947 reflections were assumed as observed applying the condition $I > 2\sigma(I)$. Three reflections were measured every two hours as orientation and intensity control, significant intensity decay was not observed. Lorentz-polarization but no absorption corrections were made.

The structure was solved by Direct methods, using SHELXS computer program (Sheldrick, G.M., (1997), A computer program for determination of crystal structure. Univer Göttingen, Germany) and refined by full-matrix least-squares method with SHELX97 computer program (Sheldrick, G.M., (1997), A computer program for determination of crystal structure. Univer Göttingen, Germany), using 4933 reflections, (very negative intensities were not assumed). The function minimized was $\Sigma\ w\ ||Fo|^2 - |Fc|^2|^2$, where $w = [\sigma^2(I)]^{-1}$, and $P = (|Fo|^2 + 2\ |Fc|^2)/3$, f, f' and f" were taken from International Tables of X-Ray Crystallography (International Tables of X-Ray Crystallography, (1974), Ed. Kynoch press, Vol. IV, pp 99-100 and 149). The chyrality of structure was define from the Flack coefficient, which it is equal to 0.05(3) for the given results (Flack, H.D., (1983), Acta Cryst., A39, 876-881). All H atoms were computed and refined,using a riding model, with an isotropic temperature factor equal to 1.2 time the equivalent temperature factor of the atom which are linked. The final R(on F) factor was 0.039, wR(on $|F|2$) = 0.042 and goodness of fit = 0.749 for all observed reflections. Number of refined parameters was 370. Max. shift/esd = 0.00, Mean shift/esd = 0.00. Max. and min. peaks in final difference synthesis was 0.736 and -0.675 $eÅ^{-3}$, respectively.

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Table 1. Crystal data and structure refinement for sofc42a.

Identification code	sofc42a
Empirical formula	C_{36} H_{35} I N O P Pd
Formula weight	761.92
Temperature	293(2) K
Wavelength	0.71069 Å
Crystal system, space group	Monoclinic, Cc
Unit cell dimensions	a = 9.619(8) Å α = 90 °. b = 36.11(2) Å β = 112.07(10) °. c = 10.078(18) Å γ = 90 deg.
Volume	3244(7) $Å^3$
Z, Calculated density	4, 1.560 Mg/m^3
Absorption coefficient	1.601 mm^{-1}
F(000)	1520
Crystal size	0.1 x 0.1 x 0.2 mm
Theta range for data collection	2.35 to 29.98 °.
Index ranges	-13<=h<=12, 0<=k<=50, -2<=l<=14
Reflections collected / unique	4933 / 4933 [R(int) = 0.0292]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4933 / 134 / 370
Goodness-of-fit on F^2	0.758
Final R indices [I>2σ(I)]	R1 = 0.0394, wR2 = 0.0423
R indices (all data)	R1 = 0.2056, wR2 = 0.0629
Absolute structure parameter	-0.05(3)
Largest diff. peak and hole	0.736 and -0.675 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for sofc42a.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd	6354(1)	3827(1)	8506(1)	33(1)
I	3648(1)	3962(1)	6475(1)	60(1)
P	6871(3)	3294(1)	7685(3)	33(1)
O	5526(9)	4467(3)	13513(9)	97(3)
N	6425(8)	4333(2)	9671(8)	37(2)
C(1)	8141(10)	3854(3)	10364(10)	38(3)
C(2)	9377(11)	3653(3)	11230(11)	43(3)
C(3)	10140(17)	3802(3)	12634(15)	54(3)
C(4)	9786(14)	4123(4)	13017(13)	62(4)
C(5)	8578(12)	4339(3)	12151(12)	62(4)
C(6)	7769(10)	4181(3)	10813(11)	44(3)
C(7)	6744(11)	4675(2)	9035(10)	48(3)
C(8)	7882(13)	4631(3)	8346(14)	68(2)
C(9)	7503(13)	4503(3)	7018(14)	68(2)
C(10)	8604(16)	4452(3)	6422(18)	68(2)
C(11)	10008(15)	4551(3)	7198(14)	68(2)
C(12)	10474(13)	4690(3)	8576(13)	69(2)
C(13)	9358(12)	4727(3)	9197(14)	69(2)
C(14)	5213(12)	4406(3)	10201(12)	57(2)
C(15)	4833(11)	4077(3)	10910(12)	58(2)
C(16)	3637(14)	4172(2)	11519(14)	59(2)
C(17)	4209(13)	4452(3)	12791(14)	60(2)
C(18)	3079(11)	4671(3)	13071(12)	61(2)
C(19)	6280(15)	2892(3)	8427(15)	62(2)
C(20)	5633(12)	2574(3)	7619(13)	63(2)
C(21)	5292(13)	2278(3)	8293(12)	64(2)
C(22)	5416(13)	2287(3)	9642(12)	64(2)
C(23)	5985(12)	2599(3)	10453(12)	64(2)
C(24)	6378(13)	2899(3)	9804(12)	63(2)
C(25)	8875(9)	3207(3)	8173(9)	33(2)
C(26)	9764(11)	3497(3)	8183(11)	49(3)
C(27)	11272(18)	3442(4)	8465(18)	76(4)
C(28)	11872(13)	3110(4)	8812(15)	69(4)
C(29)	11030(14)	2807(3)	8882(11)	57(3)
C(30)	9531(11)	2857(3)	8548(10)	44(3)
C(31)	6100(13)	3243(3)	5752(11)	57(1)
C(32)	4617(13)	3169(3)	4985(11)	58(1)
C(33)	4061(13)	3155(3)	3552(11)	59(1)
C(34)	4870(14)	3226(3)	2732(13)	58(1)
C(35)	6418(14)	3314(3)	3479(13)	58(1)
C(36)	6972(14)	3332(3)	4970(12)	57(1)

Table 3. Bond lengths [Å] and angles [°] for sofc42a.

Pd-C(1)	2.013(10)
Pd-N	2.161(8)
Pd-P	2.222(3)
Pd-C(6)	2.554(11)
Pd-I	2.684(4)
P-C(31)	1.815(11)
P-C(19)	1.820(11)
P-C(25)	1.829(9)
O-C(17)	1.202(12)
N-C(7)	1.476(11)
N-C(6)	1.476(12)
N-C(14)	1.477(12)
C(1)-C(6)	1.362(13)
C(1)-C(2)	1.385(12)
C(2)-C(3)	1.431(15)
C(3)-C(4)	1.308(15)
C(4)-C(5)	1.399(15)
C(5)-C(6)	1.399(13)
C(7)-C(8)	1.509(15)
C(8)-C(9)	1.331(16)
C(8)-C(13)	1.398(14)
C(9)-C(10)	1.412(17)
C(10)-C(11)	1.330(18)
C(11)-C(12)	1.383(16)
C(12)-C(13)	1.438(15)
C(14)-C(15)	1.499(12)
C(15)-C(16)	1.532(14)
C(16)-C(17)	1.564(15)
C(17)-C(18)	1.455(14)
C(19)-C(24)	1.356(16)
C(19)-C(20)	1.410(14)
C(20)-C(21)	1.369(13)
C(21)-C(22)	1.320(14)
C(22)-C(23)	1.380(13)
C(23)-C(24)	1.389(13)
C(25)-C(26)	1.351(12)
C(25)-C(30)	1.397(11)
C(26)-C(27)	1.384(17)
C(27)-C(28)	1.319(15)
C(28)-C(29)	1.379(15)
C(29)-C(30)	1.364(13)
C(31)-C(32)	1.369(14)
C(31)-C(36)	1.387(14)
C(32)-C(33)	1.340(14)
C(33)-C(34)	1.355(14)
C(34)-C(35)	1.429(16)
C(35)-C(36)	1.395(15)
C(1)-Pd-N	67.2(4)
C(1)-Pd-P	99.0(3)
N-Pd-P	165.7(2)
C(1)-Pd-C(6)	32.0(4)
N-Pd-C(6)	35.3(3)
P-Pd-C(6)	131.0(3)
C(1)-Pd-I	160.9(3)
N-Pd-I	94.8(2)
P-Pd-I	99.34(10)
C(6)-Pd-I	129.4(3)
C(31)-P-C(19)	107.2(5)
C(31)-P-C(25)	103.6(5)

C(19)-P-C(25)	102.2(5)
C(31)-P-Pd	115.4(4)
C(19)-P-Pd	113.0(4)
C(25)-P-Pd	114.2(3)
C(7)-N-C(6)	112.7(8)
C(7)-N-C(14)	109.2(8)
C(6)-N-C(14)	111.3(8)
C(7)-N-Pd	116.2(6)
C(6)-N-Pd	87.1(6)
C(14)-N-Pd	118.6(6)
C(6)-C(1)-C(2)	121.0(9)
C(6)-C(1)-Pd	96.4(7)
C(2)-C(1)-Pd	142.3(9)
C(1)-C(2)-C(3)	115.3(10)
C(4)-C(3)-C(2)	122.0(12)
C(3)-C(4)-C(5)	123.9(12)
C(4)-C(5)-C(6)	113.9(11)
C(1)-C(6)-C(5)	123.6(10)
C(1)-C(6)-N	109.0(9)
C(5)-C(6)-N	127.4(10)
C(1)-C(6)-Pd	51.6(5)
C(5)-C(6)-Pd	173.9(9)
N-C(6)-Pd	57.7(5)
N-C(7)-C(8)	114.7(8)
C(9)-C(8)-C(13)	122.3(13)
C(9)-C(8)-C(7)	121.8(11)
C(13)-C(8)-C(7)	115.9(12)
C(8)-C(9)-C(10)	120.5(13)
C(11)-C(10)-C(9)	118.2(14)
C(10)-C(11)-C(12)	124.2(13)
C(11)-C(12)-C(13)	117.2(12)
C(8)-C(13)-C(12)	117.5(12)
N-C(14)-C(15)	113.4(8)
C(14)-C(15)-C(16)	111.7(8)
C(15)-C(16)-C(17)	112.7(10)
O-C(17)-C(18)	123.6(12)
O-C(17)-C(16)	119.4(11)
C(18)-C(17)-C(16)	116.9(11)
C(24)-C(19)-C(20)	116.9(11)
C(24)-C(19)-P	119.5(9)
C(20)-C(19)-P	123.5(10)
C(21)-C(20)-C(19)	119.0(12)
C(22)-C(21)-C(20)	123.1(12)
C(21)-C(22)-C(23)	119.6(11)
C(22)-C(23)-C(24)	118.3(11)
C(19)-C(24)-C(23)	122.8(11)
C(26)-C(25)-C(30)	118.6(9)
C(26)-C(25)-P	117.9(8)
C(30)-C(25)-P	123.5(7)
C(25)-C(26)-C(27)	120.0(10)
C(28)-C(27)-C(26)	120.4(13)
C(27)-C(28)-C(29)	121.9(13)
C(30)-C(29)-C(28)	117.8(10)
C(29)-C(30)-C(25)	121.1(10)
C(32)-C(31)-C(36)	116.7(11)
C(32)-C(31)-P	123.0(9)
C(36)-C(31)-P	119.7(9)
C(33)-C(32)-C(31)	121.7(12)
C(32)-C(33)-C(34)	124.2(12)
C(33)-C(34)-C(35)	116.4(12)
C(36)-C(35)-C(34)	118.5(12)
C(31)-C(36)-C(35)	122.3(12)

Table 4. Hydrogen bond lengths [Å] and angles [°] for sofc42a.

C(2)-H(2)	0.9300
C(3)-H(3)	0.9300
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(7)-H(7)	0.9700
C(7)-H(7A)	0.9700
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-H(13)	0.9300
C(14)-H(14)	0.9700
C(14)-H(14A)	0.9700
C(15)-H(15)	0.9700
C(15)-H(15A)	0.9700
C(16)-H(16)	0.9700
C(16)-H(16A)	0.9700
C(18)-H(18)	0.9600
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(20)-H(20)	0.9300
C(21)-H(21)	0.9300
C(22)-H(22)	0.9300
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(26)-H(26)	0.9300
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300
C(29)-H(29)	0.9300
C(30)-H(30)	0.9300
C(32)-H(32)	0.9300
C(33)-H(33)	0.9300
C(34)-H(34)	0.9300
C(35)-H(35)	0.9300
C(36)-H(36)	0.9300

C(1)-C(2)-H(2)	122.4
C(3)-C(2)-H(2)	122.4
C(4)-C(3)-H(3)	119.0
C(2)-C(3)-H(3)	119.0
C(3)-C(4)-H(4)	118.1
C(5)-C(4)-H(4)	118.1
C(4)-C(5)-H(5)	123.0
C(6)-C(5)-H(5)	123.0
N-C(7)-H(7)	108.6
C(8)-C(7)-H(7)	108.6
N-C(7)-H(7A)	108.6
C(8)-C(7)-H(7A)	108.6
H(7)-C(7)-H(7A)	107.6
C(8)-C(9)-H(9)	119.8
C(10)-C(9)-H(9)	119.8
C(11)-C(10)-H(10)	120.9
C(9)-C(10)-H(10)	120.9
C(10)-C(11)-H(11)	117.9
C(12)-C(11)-H(11)	117.9
C(11)-C(12)-H(12)	121.4
C(13)-C(12)-H(12)	121.4
C(8)-C(13)-H(13)	121.2
C(12)-C(13)-H(13)	121.2
N-C(14)-H(14)	108.9

C(15)-C(14)-H(14)	108.9
N-C(14)-H(14A)	108.9
C(15)-C(14)-H(14A)	108.9
H(14)-C(14)-H(14A)	107.7
C(14)-C(15)-H(15)	109.3
C(16)-C(15)-H(15)	109.3
C(14)-C(15)-H(15A)	109.3
C(16)-C(15)-H(15A)	109.3
H(15)-C(15)-H(15A)	107.9
C(15)-C(16)-H(16)	109.0
C(17)-C(16)-H(16)	109.0
C(15)-C(16)-H(16A)	109.0
C(17)-C(16)-H(16A)	109.0
H(16)-C(16)-H(16A)	107.8
C(17)-C(18)-H(18)	109.5
C(17)-C(18)-H(18A)	109.5
H(18)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(21)-C(20)-H(20)	120.5
C(19)-C(20)-H(20)	120.5
C(22)-C(21)-H(21)	118.5
C(20)-C(21)-H(21)	118.5
C(21)-C(22)-H(22)	120.2
C(23)-C(22)-H(22)	120.2
C(22)-C(23)-H(23)	120.8
C(24)-C(23)-H(23)	120.8
C(19)-C(24)-H(24)	118.6
C(23)-C(24)-H(24)	118.6
C(25)-C(26)-H(26)	120.0
C(27)-C(26)-H(26)	120.0
C(28)-C(27)-H(27)	119.8
C(26)-C(27)-H(27)	119.8
C(27)-C(28)-H(28)	119.1
C(29)-C(28)-H(28)	119.1
C(30)-C(29)-H(29)	121.1
C(28)-C(29)-H(29)	121.1
C(29)-C(30)-H(30)	119.5
C(25)-C(30)-H(30)	119.5
C(33)-C(32)-H(32)	119.2
C(31)-C(32)-H(32)	119.2
C(32)-C(33)-H(33)	117.9
C(34)-C(33)-H(33)	117.9
C(33)-C(34)-H(34)	121.8
C(35)-C(34)-H(34)	121.8
C(36)-C(35)-H(35)	120.7
C(34)-C(35)-H(35)	120.7
C(31)-C(36)-H(36)	118.9
C(35)-C(36)-H(36)	118.9

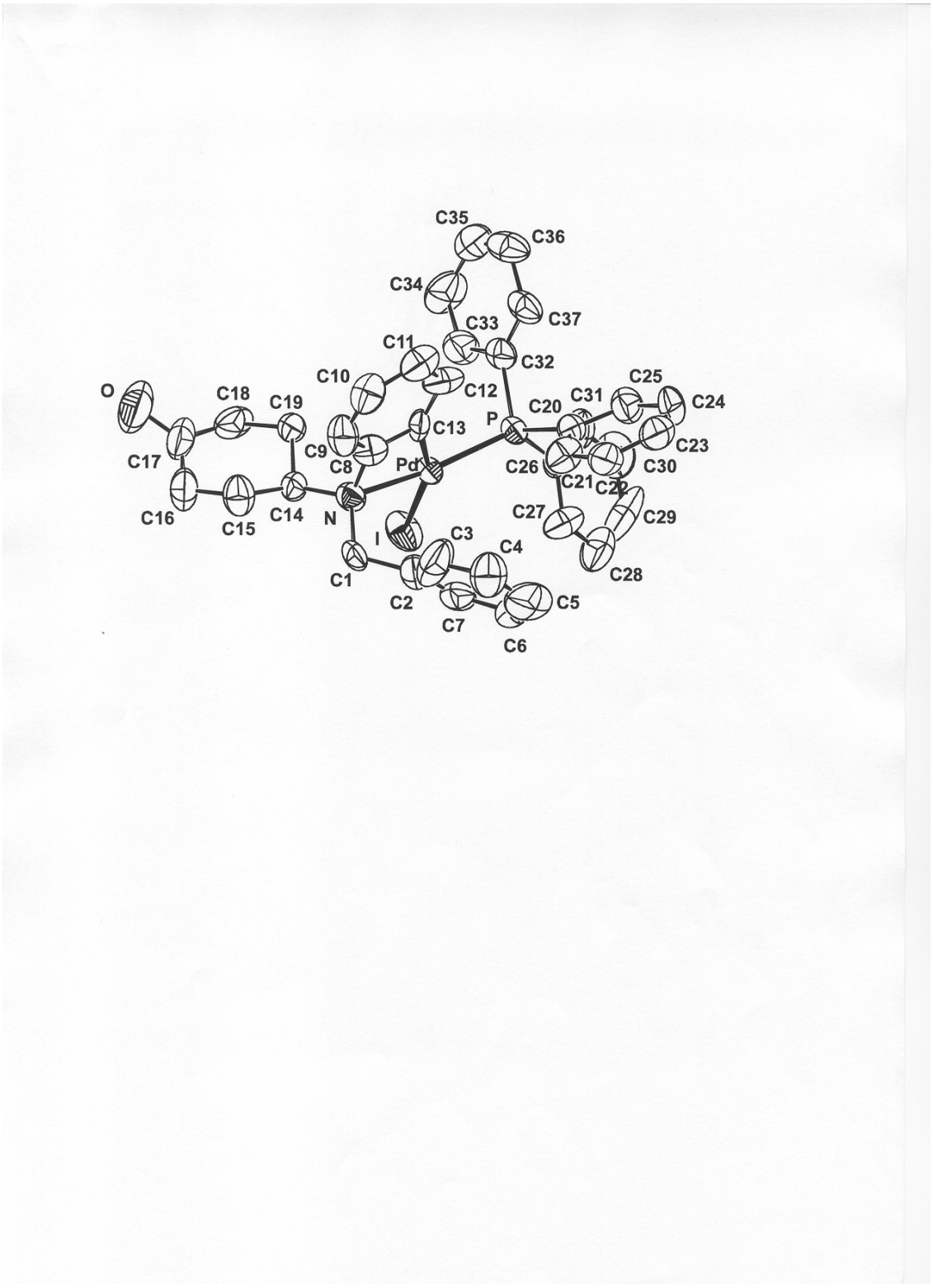
Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters ($Å^2$ x 10^3) for sofc42a. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pd	35(1)	34(1)	28(1)	-2(1)	9(1)	0(1)
I	39(1)	81(1)	49(1)	-4(1)	4(1)	7(1)
P	38(2)	37(2)	26(2)	-5(1)	12(1)	-3(1)
O	65(6)	157(9)	73(7)	-31(6)	31(6)	-17(6)
N	41(5)	44(6)	33(5)	0(4)	22(5)	2(4)
C(1)	28(5)	47(7)	40(7)	-16(6)	15(5)	4(6)
C(2)	52(7)	33(6)	39(7)	-5(6)	12(6)	15(6)
C(3)	86(9)	42(10)	38(8)	-2(7)	28(7)	-12(8)
C(4)	60(9)	81(10)	49(9)	-32(8)	25(7)	-16(8)
C(5)	53(8)	70(9)	44(8)	-10(6)	-5(7)	0(7)
C(6)	24(6)	64(8)	37(7)	-12(6)	4(5)	-10(6)
C(7)	66(8)	36(6)	37(7)	-4(5)	12(6)	0(5)
C(8)	59(4)	73(3)	71(4)	19(3)	23(3)	-2(3)
C(9)	59(4)	73(3)	71(4)	18(3)	24(3)	-1(3)
C(10)	59(4)	73(3)	71(4)	19(3)	24(3)	-2(3)
C(11)	60(4)	73(3)	72(4)	19(3)	24(3)	-1(3)
C(12)	60(4)	74(3)	72(4)	19(3)	23(3)	-2(3)
C(13)	60(4)	73(3)	72(4)	19(3)	23(3)	-2(3)
C(14)	56(4)	65(4)	62(4)	-5(3)	34(3)	-1(3)
C(15)	56(4)	65(4)	62(4)	-5(3)	34(3)	-1(3)
C(16)	57(4)	66(4)	63(4)	-6(3)	34(3)	-1(3)
C(17)	58(4)	67(4)	64(4)	-7(3)	34(3)	-1(3)
C(18)	59(4)	67(4)	65(4)	-8(3)	33(3)	-1(3)
C(19)	85(3)	59(4)	55(3)	-13(3)	40(3)	-30(3)
C(20)	86(4)	60(4)	55(3)	-13(3)	39(3)	-30(3)
C(21)	87(4)	60(4)	56(3)	-12(3)	39(3)	-31(3)
C(22)	87(3)	60(4)	56(3)	-12(3)	39(3)	-30(3)
C(23)	86(4)	60(4)	55(3)	-13(3)	39(3)	-30(3)
C(24)	86(4)	60(4)	55(3)	-13(3)	39(3)	-30(3)
C(25)	17(5)	57(7)	22(6)	8(5)	5(4)	-9(5)
C(26)	32(7)	65(8)	47(7)	2(6)	11(5)	2(6)
C(27)	62(9)	98(11)	85(11)	-25(13)	45(8)	-26(11)
C(28)	34(7)	111(13)	61(10)	-23(9)	16(7)	11(8)
C(29)	67(9)	52(8)	40(8)	-4(6)	5(7)	11(7)
C(30)	31(6)	65(8)	32(7)	-3(6)	9(5)	-4(6)
C(31)	71(4)	68(3)	32(3)	-7(3)	19(3)	-6(3)
C(32)	71(4)	68(3)	33(3)	-6(3)	19(3)	-6(3)
C(33)	72(4)	68(3)	34(3)	-7(3)	18(3)	-6(3)
C(34)	72(4)	68(3)	33(3)	-6(3)	18(3)	-6(3)
C(35)	71(4)	69(3)	33(3)	-6(3)	19(3)	-6(3)
C(36)	71(4)	68(3)	32(3)	-7(3)	19(3)	-6(3)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for sofc42a.

	x	y	z	U(eq)
H(2)	9688	3437	10921	52
H(3)	10912	3665	13294	65
H(4)	10372	4213	13918	74
H(5)	8335	4566	12438	75
H(7)	7103	4862	9778	58
H(7A)	5814	4765	8320	58
H(9)	6506	4447	6479	81
H(10)	8354	4352	5511	82
H(11)	10722	4525	6788	82
H(12)	11468	4757	9080	83
H(13)	9608	4811	10131	83
H(14)	4321	4483	9403	69
H(14A)	5513	4609	10879	69
H(15)	5733	3991	11678	69
H(15A)	4471	3878	10219	69
H(16)	3322	3945	11845	71
H(16A)	2768	4276	10763	71
H(18)	3560	4833	13868	73
H(18A)	2403	4510	13290	73
H(18B)	2529	4816	12240	73
H(20)	5440	2565	6644	76
H(21)	4958	2061	7776	77
H(22)	5122	2084	10043	76
H(23)	6101	2609	11412	76
H(24)	6724	3113	10336	76
H(26)	9362	3735	8001	59
H(27)	11866	3640	8409	92
H(28)	12891	3079	9016	83
H(29)	11470	2575	9148	69
H(30)	8936	2656	8569	52
H(32)	3980	3128	5472	69
H(33)	3056	3092	3090	70
H(34)	4440	3218	1738	70
H(35)	7043	3358	2981	69
H(36)	7960	3406	5457	69



Molecular structure of **48** (ORTEP view). Selected interatomic distances [Å] and angles [°]:Pd-N 2.228(3), Pd-C(13) 1.989(3), N-C(8) 1.487(5), C(8)-C(13) 1.330(5); N-Pd-C(13) 65.91(13), Pd-N-C(8) 85.0(2), Pd-C(13)-C(8) 99.5(3), N-C(8)-C(13) 109.6(3).

SOFM66b

Experimental. A prismatic crystal (0.1x0.1x0.2 mm) was selected and mounted on a MAR345 diffractometer with image plate detector. Unit-cell parameters were determined from automatic centering of 25 reflections ($3 < \theta < 31°$) and refined by least-squares method. Intensities were collected with graphite monochromatized Mo Kα radiation. 17632 reflections were measured in the range $1.97 \leq \theta \leq 28.86$. 6928 of which were non-equivalent by symmetry (Rint(on I) = 0.031). 4320 reflections were assumed as observed applying the condition $I > 2\sigma(I)$. Lorentz-polarization but no absorption corrections were made.

The structure was solved by Direct methods, using SHELXS computer program (Sheldrick, G.M., (1997), A computer program for determination of crystal structure. Univer Göttingen, Germany) and refined by full-matrix least-squares method with SHELX97 computer program (Sheldrick, G.M., (1997), A computer program for determination of crystal structure. Univer Göttingen, Germany), using 6928 reflections, (very negative intensities were not assumed). The function minimized was $\Sigma\ w\ ||Fo|^2 - |Fc|^2|^2$, where $w = [\sigma^2(I) + (0.0761\ P)^2]^{-1}$, and $P = (|Fo|^2 + 2\ |Fc|^2)/3$, f, f' and f" were taken from International Tables of X-Ray Crystallography (International Tables of X-Ray Crystallography, (1974), Ed. Kynoch press, Vol. IV, pp 99-100 and 149). All H atoms were computed and refined, using a riding model, with an isotropic temperature factorequal to 1.2 time the equivalent temperature factor of the atom which are linked. The final R(on F) factor was 0.031, wR(on $|F|^2$) = 0.088 and goodness of fit = 0.907 for all observed reflections. Number of refined parameters was 401. Max. shift/esd = 0.00, Mean shift/esd = 0.00. Max. and min. peaks in final difference synthesis was 0.590 and -0.741 $eÅ^{-3}$, respectively.

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Table 1. Crystal data and structure refinement for sofm66b.

Identification code	sofm66b
Empirical formula	$(C_{37}\ H_{35}\ I\ N\ O\ P\ Pd)\ (Cl_2\ CH_2)$
Formula weight	858.86
Temperature	293(2) K
Wavelength	0.71069 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 9.7190(10) Å α = 90 °. b = 20.6330(10) Å β = 90.54 °. c = 17.7930(10) Å γ = 90 °.
Volume	3567.9(5) $Å^3$
Z, Calculated density	4, 1.599 Mg/m^3
Absorption coefficient	1.611 mm^{-1}
F(000)	1712
Crystal size	0.1 x 0.1 x 0.1 mm
Theta range for data collection	1.97 to 28.86 °.
Index ranges	-11<=h<=10, 0<=k<=28, 0<=l<=23
Reflections collected / unique	17632 / 6928 [R(int) = 0.0319]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6928 / 6 / 401
Goodness-of-fit on F^2	0.906
Final R indices [$I>2\sigma(I)$]	R1 = 0.0319, wR2 = 0.0880
R indices (all data)	R1 = 0.0766, wR2 = 0.1156
Largest diff. peak and hole	0.590 and -0.741 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for sofm66b.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd	2325(1)	3513(1)	2981(1)	40(1)
I	2368(1)	2588(1)	1928(1)	73(1)
P	2373(1)	4390(1)	2252(1)	41(1)
O	-2476(5)	1474(2)	4449(3)	124(2)
N	2288(3)	2864(2)	3981(2)	48(1)
C(1)	3639(4)	2596(2)	4205(3)	65(1)
C(2)	4816(5)	3048(2)	4065(3)	59(1)
C(3)	5315(6)	3452(4)	4602(4)	109(2)
C(4)	6344(6)	3881(3)	4536(3)	86(2)
C(5)	6980(6)	3901(3)	3813(5)	112(2)
C(6)	6556(5)	3524(3)	3267(4)	88(2)
C(7)	5461(5)	3112(2)	3353(3)	76(2)
C(8)	1981(4)	3464(2)	4409(2)	54(1)
C(9)	1811(5)	3511(2)	5188(2)	66(1)
C(10)	1587(5)	4095(3)	5466(2)	67(1)
C(11)	1491(4)	4662(2)	5010(3)	68(1)
C(12)	1667(4)	4564(2)	4236(3)	67(1)
C(13)	1945(4)	3967(2)	3942(2)	43(1)
C(14)	1192(4)	2370(2)	3967(2)	46(1)
C(15)	994(5)	1981(2)	4675(2)	67(1)
C(16)	-31(6)	1465(2)	4590(3)	76(1)
C(17)	-1315(6)	1649(2)	4223(3)	81(2)
C(18)	-1228(5)	2086(2)	3619(3)	75(1)
C(19)	-176(4)	2637(2)	3688(3)	63(1)
C(20)	3482(4)	5061(2)	2601(2)	43(1)
C(21)	4290(4)	4992(2)	3198(2)	64(1)
C(22)	5190(5)	5446(2)	3450(3)	74(1)
C(23)	5239(5)	6008(2)	3093(4)	82(2)
C(24)	4468(6)	6127(2)	2408(4)	82(2)
C(25)	3598(5)	5623(2)	2158(3)	64(1)
C(26)	2965(4)	4329(2)	1289(2)	48(1)
C(27)	4186(5)	3987(3)	1162(3)	72(1)
C(28)	4763(6)	3961(3)	481(3)	90(2)
C(29)	4098(7)	4261(4)	-110(4)	124(3)
C(30)	2881(7)	4582(3)	-7(3)	93(2)
C(31)	2317(5)	4603(2)	702(2)	68(1)
C(32)	634(4)	4717(2)	2175(2)	51(1)
C(33)	-355(5)	4267(3)	1827(3)	73(1)
C(34)	-1715(6)	4436(4)	1750(3)	95(2)
C(35)	-2063(5)	5097(3)	2014(3)	77(2)
C(36)	-1175(5)	5512(3)	2371(2)	73(1)
C(37)	271(5)	5310(2)	2406(2)	63(1)
Cl(1)	8388(11)	1615(5)	1344(6)	289(5)
Cl(1')	8511(6)	1554(3)	1153(4)	98(2)
Cl(2')	6501(7)	2559(3)	1360(4)	146(4)
Cl(2)	7508(14)	2995(6)	1333(7)	372(6)
C(38)	7940(14)	2308(6)	793(11)	277(8)

Table 3. Bond lengths [Å] and angles [°] for sofm66b.

Pd-C(13)	1.989(4)
Pd-P	2.2263(9)
Pd-N	2.228(3)
Pd-C(8)	2.569(4)
Pd-I	2.6742(4)
P-C(26)	1.818(3)
P-C(32)	1.825(4)
P-C(20)	1.858(4)
O-C(17)	1.255(6)
N-C(14)	1.474(5)
N-C(1)	1.476(5)
N-C(8)	1.487(5)
C(1)-C(2)	1.498(6)
C(2)-C(3)	1.355(9)
C(2)-C(7)	1.425(7)
C(3)-C(4)	1.341(8)
C(4)-C(5)	1.433(9)
C(5)-C(6)	1.308(8)
C(6)-C(7)	1.372(7)
C(8)-C(13)	1.330(5)
C(8)-C(9)	1.401(5)
C(9)-C(10)	1.321(6)
C(10)-C(11)	1.426(7)
C(11)-C(12)	1.404(6)
C(12)-C(13)	1.366(6)
C(14)-C(15)	1.508(5)
C(14)-C(19)	1.518(6)
C(15)-C(16)	1.465(6)
C(16)-C(17)	1.453(8)
C(17)-C(18)	1.405(8)
C(18)-C(19)	1.533(6)
C(20)-C(21)	1.322(6)
C(20)-C(25)	1.408(5)
C(21)-C(22)	1.355(6)
C(22)-C(23)	1.325(7)
C(23)-C(24)	1.445(8)
C(24)-C(25)	1.410(7)
C(26)-C(31)	1.340(6)
C(26)-C(27)	1.401(6)
C(27)-C(28)	1.341(7)
C(28)-C(29)	1.376(10)
C(29)-C(30)	1.369(9)
C(30)-C(31)	1.380(7)
C(32)-C(37)	1.338(6)
C(32)-C(33)	1.469(6)
C(33)-C(34)	1.372(7)
C(34)-C(35)	1.484(8)
C(35)-C(36)	1.367(7)
C(36)-C(37)	1.467(7)
Cl(1)-C(38)	1.784(14)
Cl(1')-C(38)	1.769(14)
Cl(2')-Cl(2)	1.330(13)
Cl(2')-C(38)	1.808(13)
Cl(2)-C(38)	1.766(13)
C(13)-Pd-P	97.07(10)
C(13)-Pd-N	65.91(13)

P-Pd-N	162.61(9)
C(13)-Pd-C(8)	30.70(13)
P-Pd-C(8)	127.71(10)
N-Pd-C(8)	35.21(12)
C(13)-Pd-I	160.56(9)
P-Pd-I	99.90(3)
N-Pd-I	97.48(8)
C(8)-Pd-I	131.89(10)
C(26)-P-C(32)	104.83(17)
C(26)-P-C(20)	100.35(17)
C(32)-P-C(20)	106.45(18)
C(26)-P-Pd	120.08(13)
C(32)-P-Pd	108.66(12)
C(20)-P-Pd	115.24(12)
C(14)-N-C(1)	112.8(3)
C(14)-N-C(8)	115.8(3)
C(1)-N-C(8)	110.8(3)
C(14)-N-Pd	114.8(2)
C(1)-N-Pd	114.9(2)
C(8)-N-Pd	85.0(2)
N-C(1)-C(2)	113.6(3)
C(3)-C(2)-C(7)	114.4(5)
C(3)-C(2)-C(1)	122.3(5)
C(7)-C(2)-C(1)	123.3(4)
C(4)-C(3)-C(2)	127.4(6)
C(3)-C(4)-C(5)	115.2(6)
C(6)-C(5)-C(4)	120.9(6)
C(5)-C(6)-C(7)	121.7(7)
C(6)-C(7)-C(2)	120.3(6)
C(13)-C(8)-C(9)	124.1(4)
C(13)-C(8)-N	109.5(3)
C(9)-C(8)-N	126.3(4)
C(13)-C(8)-Pd	49.8(2)
C(9)-C(8)-Pd	173.7(3)
N-C(8)-Pd	59.76(18)
C(10)-C(9)-C(8)	117.1(4)
C(9)-C(10)-C(11)	123.0(4)
C(12)-C(11)-C(10)	115.7(4)
C(13)-C(12)-C(11)	122.1(5)
C(8)-C(13)-C(12)	118.0(4)
C(8)-C(13)-Pd	99.5(3)
C(12)-C(13)-Pd	142.5(3)
N-C(14)-C(15)	116.8(3)
N-C(14)-C(19)	112.7(3)
C(15)-C(14)-C(19)	110.3(3)
C(16)-C(15)-C(14)	113.0(4)
C(17)-C(16)-C(15)	115.9(4)
O-C(17)-C(18)	119.4(6)
O-C(17)-C(16)	123.5(6)
C(18)-C(17)-C(16)	116.9(4)
C(17)-C(18)-C(19)	117.3(5)
C(14)-C(19)-C(18)	109.8(4)
C(21)-C(20)-C(25)	119.3(4)
C(21)-C(20)-P	121.8(3)
C(25)-C(20)-P	118.4(3)
C(20)-C(21)-C(22)	124.7(5)
C(23)-C(22)-C(21)	118.1(5)
C(22)-C(23)-C(24)	122.3(4)
C(25)-C(24)-C(23)	116.4(4)
C(20)-C(25)-C(24)	118.8(5)
C(31)-C(26)-C(27)	118.7(4)

C(31)-C(26)-P	123.7(3)
C(27)-C(26)-P	117.6(3)
C(28)-C(27)-C(26)	121.8(5)
C(27)-C(28)-C(29)	118.3(6)
C(30)-C(29)-C(28)	121.1(6)
C(29)-C(30)-C(31)	119.3(6)
C(26)-C(31)-C(30)	120.7(5)
C(37)-C(32)-C(33)	122.3(4)
C(37)-C(32)-P	124.2(4)
C(33)-C(32)-P	113.5(3)
C(34)-C(33)-C(32)	120.5(5)
C(33)-C(34)-C(35)	115.1(5)
C(36)-C(35)-C(34)	125.3(5)
C(35)-C(36)-C(37)	116.2(5)
C(32)-C(37)-C(36)	120.1(5)
Cl(2)-Cl(2')-C(38)	66.5(5)
Cl(2')-Cl(2)-C(38)	69.8(7)
Cl(2)-C(38)-Cl(1')	125.8(12)
Cl(2)-C(38)-Cl(1)	113.7(12)
Cl(1')-C(38)-Cl(1)	12.4(5)
Cl(2)-C(38)-Cl(2')	43.7(5)
Cl(1')-C(38)-Cl(2')	107.0(9)
Cl(1)-C(38)-Cl(2')	96.3(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Hydrogen bond lengths [Å] and angles [°] for sofm66b.

C(1)-H(1)	0.9700
C(1)-H(1A)	0.9700
C(3)-H(3)	0.9300
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(14)-H(14)	0.9800
C(15)-H(15)	0.9700
C(15)-H(15A)	0.9700
C(16)-H(16)	0.9700
C(16)-H(16A)	0.9700
C(18)-H(18)	0.9700
C(18)-H(18A)	0.9700
C(19)-H(19)	0.9700
C(19)-H(19A)	0.9700
C(21)-H(21)	0.9300
C(22)-H(22)	0.9300
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(25)-H(25)	0.9300
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300
C(29)-H(29)	0.9300
C(30)-H(30)	0.9300
C(31)-H(31)	0.9300
C(33)-H(33)	0.9300
C(34)-H(34)	0.9300
C(35)-H(35)	0.9300
C(36)-H(36)	0.9300
C(37)-H(37)	0.9300

N-C(1)-H(1)	108.8
C(2)-C(1)-H(1)	108.8
N-C(1)-H(1A)	108.8
C(2)-C(1)-H(1A)	108.8
H(1)-C(1)-H(1A)	107.7
C(4)-C(3)-H(3)	116.3
C(2)-C(3)-H(3)	116.3
C(3)-C(4)-H(4)	122.4
C(5)-C(4)-H(4)	122.4
C(6)-C(5)-H(5)	119.5
C(4)-C(5)-H(5)	119.5
C(5)-C(6)-H(6)	119.2
C(7)-C(6)-H(6)	119.2
C(6)-C(7)-H(7)	119.9
C(2)-C(7)-H(7)	119.9
C(10)-C(9)-H(9)	121.5
C(8)-C(9)-H(9)	121.5
C(9)-C(10)-H(10)	118.5
C(11)-C(10)-H(10)	118.5
C(12)-C(11)-H(11)	122.2
C(10)-C(11)-H(11)	122.2

C(13)-C(12)-H(12)	119.0
C(11)-C(12)-H(12)	119.0
N-C(14)-H(14)	105.3
C(15)-C(14)-H(14)	105.3
C(19)-C(14)-H(14)	105.3
C(16)-C(15)-H(15)	109.0
C(14)-C(15)-H(15)	109.0
C(16)-C(15)-H(15A)	109.0
C(14)-C(15)-H(15A)	109.0
H(15)-C(15)-H(15A)	107.8
C(17)-C(16)-H(16)	108.3
C(15)-C(16)-H(16)	108.3
C(17)-C(16)-H(16A)	108.3
C(15)-C(16)-H(16A)	108.3
H(16)-C(16)-H(16A)	107.4
C(17)-C(18)-H(18)	108.0
C(19)-C(18)-H(18)	108.0
C(17)-C(18)-H(18A)	108.0
C(19)-C(18)-H(18A)	108.0
H(18)-C(18)-H(18A)	107.2
C(14)-C(19)-H(19)	109.7
C(18)-C(19)-H(19)	109.7
C(14)-C(19)-H(19A)	109.7
C(18)-C(19)-H(19A)	109.7
H(19)-C(19)-H(19A)	108.2
C(20)-C(21)-H(21)	117.7
C(22)-C(21)-H(21)	117.7
C(23)-C(22)-H(22)	120.9
C(21)-C(22)-H(22)	120.9
C(22)-C(23)-H(23)	118.9
C(24)-C(23)-H(23)	118.9
C(25)-C(24)-H(24)	121.8
C(23)-C(24)-H(24)	121.8
C(20)-C(25)-H(25)	120.6
C(24)-C(25)-H(25)	120.6
C(28)-C(27)-H(27)	119.1
C(26)-C(27)-H(27)	119.1
C(27)-C(28)-H(28)	120.8
C(29)-C(28)-H(28)	120.8
C(30)-C(29)-H(29)	119.5
C(28)-C(29)-H(29)	119.5
C(29)-C(30)-H(30)	120.4
C(31)-C(30)-H(30)	120.4
C(26)-C(31)-H(31)	119.7
C(30)-C(31)-H(31)	119.7
C(34)-C(33)-H(33)	119.8
C(32)-C(33)-H(33)	119.8
C(33)-C(34)-H(34)	122.5
C(35)-C(34)-H(34)	122.5
C(36)-C(35)-H(35)	117.3
C(34)-C(35)-H(35)	117.3
C(35)-C(36)-H(36)	121.9
C(37)-C(36)-H(36)	121.9
C(32)-C(37)-H(37)	119.9
C(36)-C(37)-H(37)	119.9

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters ($Å^2$ x 10^3) for sofm66b. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pd	48(1)	33(1)	38(1)	1(1)	1(1)	2(1)
I	115(1)	47(1)	58(1)	-13(1)	5(1)	1(1)
P	48(1)	34(1)	42(1)	4(1)	0(1)	2(1)
O	98(3)	139(4)	135(4)	37(3)	33(3)	-34(3)
N	48(2)	44(2)	51(2)	6(1)	-5(1)	4(1)
C(1)	47(3)	43(2)	105(4)	40(2)	-5(2)	3(2)
C(2)	50(3)	59(3)	68(3)	17(2)	-17(2)	-7(2)
C(3)	53(4)	162(7)	112(5)	53(5)	-4(3)	-24(4)
C(4)	87(4)	84(4)	87(4)	-3(3)	-8(3)	-23(3)
C(5)	52(4)	92(5)	193(8)	-24(5)	-31(4)	-6(3)
C(6)	51(4)	66(3)	146(6)	8(3)	21(3)	2(3)
C(7)	43(3)	60(3)	125(5)	15(3)	-9(3)	11(2)
C(8)	47(3)	63(3)	50(2)	-7(2)	-10(2)	1(2)
C(9)	82(4)	72(3)	43(2)	16(2)	-5(2)	-13(2)
C(10)	76(4)	84(3)	41(2)	-11(2)	11(2)	-14(2)
C(11)	54(3)	79(3)	70(3)	-33(2)	3(2)	-12(2)
C(12)	43(3)	76(3)	80(3)	-26(2)	1(2)	13(2)
C(13)	41(2)	46(2)	42(2)	15(2)	4(1)	-13(2)
C(14)	36(2)	43(2)	59(2)	8(2)	-2(2)	-6(2)
C(15)	75(3)	68(3)	57(2)	11(2)	-8(2)	-15(2)
C(16)	76(4)	70(3)	82(3)	23(3)	7(3)	-23(3)
C(17)	84(4)	60(3)	100(4)	-14(3)	43(3)	-30(3)
C(18)	39(3)	74(3)	112(4)	-17(3)	-3(2)	-5(2)
C(19)	34(3)	43(2)	111(4)	12(2)	-2(2)	-6(2)
C(20)	45(2)	38(2)	46(2)	-7(2)	-1(2)	-3(2)
C(21)	56(3)	73(3)	63(2)	-19(2)	-6(2)	-12(2)
C(22)	45(3)	55(3)	122(4)	-6(3)	-10(3)	-9(2)
C(23)	60(4)	48(3)	138(5)	-29(3)	21(3)	-14(2)
C(24)	88(4)	37(2)	121(5)	9(2)	25(3)	-13(2)
C(25)	75(3)	52(2)	67(3)	0(2)	8(2)	-4(2)
C(26)	54(3)	43(2)	46(2)	0(2)	13(2)	-10(2)
C(27)	46(3)	90(4)	80(3)	-22(3)	9(2)	3(2)
C(28)	85(4)	104(5)	83(4)	0(4)	31(3)	-21(3)
C(29)	96(5)	160(7)	119(5)	-62(5)	66(4)	-76(5)
C(30)	128(5)	93(4)	58(3)	-3(3)	10(3)	-7(4)
C(31)	71(3)	78(3)	55(2)	24(2)	1(2)	-13(2)
C(32)	64(3)	55(2)	34(2)	13(2)	2(2)	10(2)
C(33)	56(4)	65(3)	97(4)	4(3)	-15(2)	0(2)
C(34)	50(4)	133(6)	100(4)	9(4)	-20(3)	-12(3)
C(35)	61(4)	109(5)	62(3)	25(3)	1(2)	9(3)
C(36)	94(4)	73(3)	52(2)	-5(2)	6(2)	34(3)
C(37)	90(4)	53(2)	47(2)	12(2)	6(2)	18(2)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for sofm66b.

	x	y	z	U(eq)
H(1)	3794	2197	3931	78
H(1A)	3621	2490	4736	78
H(3)	4897	3430	5069	131
H(4)	6624	4147	4931	103
H(5)	7703	4187	3731	135
H(6)	7010	3535	2809	105
H(7)	5137	2873	2944	91
H(9)	1855	3148	5497	79
H(10)	1487	4139	5983	81
H(11)	1323	5069	5212	81
H(12)	1592	4917	3913	80
H(14)	1473	2055	3586	55
H(15)	1867	1790	4823	80
H(15A)	710	2271	5075	80
H(16)	378	1115	4305	91
H(16A)	-241	1297	5085	91
H(18)	-2129	2278	3542	90
H(18A)	-1016	1839	3170	90
H(19)	-57	2842	3203	75
H(19A)	-509	2961	4037	75
H(21)	4236	4605	3463	77
H(22)	5758	5364	3863	89
H(23)	5788	6337	3289	98
H(24)	4542	6516	2147	98
H(25)	3111	5661	1708	77
H(27)	4608	3771	1561	86
H(28)	5591	3745	409	108
H(29)	4481	4246	-586	149
H(30)	2440	4784	-410	111
H(31)	1478	4811	773	82
H(33)	-57	3865	1658	87
H(34)	-2369	4156	1547	113
H(35)	-2958	5241	1931	93
H(36)	-1472	5900	2579	88
H(37)	937	5594	2589	76