Novel heteroleptic *cis*-(C^N)$_2$Pd(II) chelates for the preparation of enantiopure planar chiral cyclopalladated 2-[tricarbonyl(η^6-phenyl)chromium]pyridine

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Electronic Supplementary Information

Experimental Section

All experiments were carried out under a dry atmosphere of argon and with dry and degassed solvents. The chloromercurated (η^6-arene)tricarbonylchromium complex **1a**[1], the di-μ-chloro-bis(*N,N*-dimethylbenzylamine-2*C,N*)dipalladium(II) **4a**[2] and [(+) and (-)]di-μ-chloro-bis[*(S)* and *(R)*-*N,N*-dimethyl-α-phenylethylamine-2*C,N*]dipalladium(II) **4b-c**[3] were synthesized following published procedures. Neutral silica gel (Si 60, 40-63 μm) for column chromatography was purchased from Merck. NMR spectra were acquired on a Bruker DRX 500 (^{13}C and ^{1}H nuclei) and a Bruker AV-300 (^{1}H nucleus) spectrometers at room temperature unless otherwise stated. Chemical shifts were reported in parts per million downfield of Me_4Si. IR spectra were measured on a Perkin-Elmer FT spectrometer. Elemental analyses (reported in percent mass) were performed at the "Institut de Chimie de Strasbourg". Absorption circular dichroism characterisations were performed with a JASCO J-715 spectropolarimeter (University of Geneva) with 1cm quartz cells.

***rac*-(*SP*$_d$-4-4)-{2'-[tricarbonyl(η^6-phenyl-*kC*$^{1'}$)chromium(0)]pyridine-*kN*}[*N,N*-dimethyl,1-(phenyl-*kC*$^{1'}$)-methylamine-*kN*]palladium(II), 5a.** A solution of **4a** (460 mg,

[1] A. Berger, A. de Cian, J.P. Djukic, J. Fischer and M. Pfeffer, *Organometallics* 2001, **20**, 3230-3240.
[2] A.C. Cope and E.C. Friedrich, *J. Am. Chem. Soc.* 1968, **90**, 909-913.

0.79 mmol) in dry acetone (20 mL) was added dropwise to a mixture of **1a** (830 mg, 1.58 mmol) and $[Me_4N]Cl$ (1.73 g, 15.8 mmol) in acetone (40 mL) at –20°C. The resulting mixture was vigorously stirred and slowly warmed to room temperature over 7 h. Then, the mixture was filtered over celite to remove $[Me_4N]_2[Hg_2Cl_6]$ and remaining $[Me_4N]Cl$. The filtrate was striped of solvents. The product was purified by low temperature (5°C) flash chromatography over silica gel. The starting chloromercurated compound **1a** was eluted with 20% acetone/hexane mixture. The orange-brown product **5a** (520 mg, 0.98 mmol, 62% yield) was eluted with 50% acetone/hexane mixture. Complex **5a:** Anal. Calcd for $C_{23}H_{20}N_2O_3CrPd$; C: 52.07, H: 3.77, N: 5.28. Found; C: 51.57, H: 3.69, N: 5.08. IR (CH_2Cl_2): ν(CO) 1951, 1875 cm^{-1}. ^1H NMR ($CDCl_3$): δ 8.41 (d, ^3J= 5.4 Hz, 1H, Py), 7.84 (t, ^3J= 7.6 Hz, 1H, Py), 7.64 (d, ^3J= 7.4 Hz, 1H, Ph), 7.58 (d, ^3J= 8.0 Hz, 1H, Py), 7.26 (t, ^3J= 4.2 Hz, 1H, Py), 7.12 (m, 1H, Ph), 7.04 (m, 2H, Ph), 5.99 (d, ^3J= 6.5 Hz, 1H, ArCr), 5.89 (d, ^3J= 6.4 Hz, 1H, ArCr), 5.62 (t, ^3J= 6.4 Hz, 1H, ArCr), 5.17 (t, ^3J= 6.4 Hz, 1H, ArCr), 4.35 (d, ^2J= 12.8 Hz, 1H, CH_2), 3.54 (d, ^2J= 12.8 Hz, 1H, CH_2), 2.86 (s, 3H, NMe_2), 2.57 (s, 3H, NMe_2). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 234.7 (CO), 162.7, 157.6, 147.8, 147.6, 138.5, 137.4, 130.0, 126.5, 123.8, 122.6, 122.1, 118.4, 109.1, 101.4, 97.7, 92.4, 88.4, 73.0, 50.1, 49.1.

Complex 5b. A solution of **4b** (860 mg, 1.48 mmol) in dry acetone (20 mL) was added dropwise to a mixture of **1a** (1.56 g, 2.96 mmol) and $[Me_4N]Cl$ (3.2 g, 29.6 mmol) in acetone (60 mL) at –20°C. The reaction medium was vigorously stirred and slowly warmed to room temperature over 7 h. The resulting mixture was filtered over celite and the solvent evaporated under reduced pressure. Low temperature (5°C) chromatography over silica gel using mixtures of 20% and 50% acetone/hexane afforded the unreacted chloromercurated compound **1a** and an orange fraction corresponding to a mixture of diastereoisomers endo-**5b** and exo-**5b** [*dr=1.3:1* (endo:exo), 1.14 g, 2.09 mmol, 70% conversion] respectively. Complexes **5b:** Anal. Calcd for $C_{24}H_{22}N_2O_3CrPd$; C: 52.89, H: 4.04, N: 5.14. Found; C: 52.96, H: 4.02, N: 5.04. IR (CH_2Cl_2): ν(CO) 1951, 1875 cm^{-1}.

(+)-(*pR,1S*)-*Λ*-(*SP*$_d$-4-4)-{2'-[tricarbonyl(η^6-phenyl-*kC*$^{1'}$)chromium(0)]pyridine-*kN*}[*N,N*-dimethyl,1-(phenyl-*kC*^{1})ethylamine-*kN*]palladium(II), (+)-*(pR,7S)-endo*-5b. The two diasteroisomers endo-**5b** and exo-**5b** (400 mg) were separated by low temperature (0°C) chromatography (column: 40 cm length x 3 cm diameter) over silica gel with dry $CHCl_3$.[4] The orange-red fraction corresponding to endo-**5b** (83 mg) was eluted first followed by a mixture of exo-**5b** and the products of decomposition identified as $[Cr(CO)_3PhPy]$ and **4b**. Complex endo-**5b:** $[\alpha]_D$ (CH_2Cl_2, 298K)= +788 (c= 0.04 g/100 mL). Anal. Calcd for $C_{24}H_{22}N_2O_3CrPd$; C: 52.89, H: 4.04, N: 5.14. Found; C: 52.82, H: 4.33, N: 4.89. IR (CH_2Cl_2): ν(CO) 1951, 1875 cm^{-1}. ^1H NMR ($CDCl_3$): δ 8.48 (d, ^3J= 5.1 Hz, 1H, Py), 7.83 (t, ^3J= 7.5 Hz, 1H, Py), 7.61 (d, ^3J= 7.4 Hz, 1H,

[3] (a) S. Otsuka, A. Nakamura, T. Kano and K. Tani, *J. Am. Chem. Soc.* 1971, **93**, 4301-4303. (b) K. Tani, L.D. Brown, J. Ahmed, J.A. Ibers, M. Yokota, A. Nakamura and S. Otsuka, *J. Am. Chem. Soc.* 1977, **99**, 7876-7886.

Ph), 7.58 (d, ^{3}J= 8.1 Hz, 1H, Py), 7.26 (t, ^{3}J= 6.0, 1H, Py), 7.09 (m, 1H, Ph), 7.03 (m, 2H, Ph), 5.95 (d, ^{3}J= 6.5 Hz, 2H, ArCr), 5.57 (t, ^{3}J= 6.2 Hz, 1H, ArCr), 5.24 (t, ^{3}J= 6.2 Hz, 1H, ArCr), 3.47 (q, ^{3}J= 7.0Hz, 1H, CH), 2.83 (s, 3H, NMe_2), 2.54 (s, 3H, NMe_2), 1.92 (d, ^{3}J= 6.4 Hz, 3H, CH_3). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$): δ 234.7 (CO), 162.7, 155.5, 154.1, 147.7, 138.2, 137.7, 130.4, 126.0, 123.6, 122.4, 121.4, 118.2, 109.2, 101.9, 96.6, 91.0, 89.4, 76.4, 50.9, 46.8, 23.7. Complex ***(pS,7S)-exo*-5b.** Unfortunately, exo-**5b** could not be purified because of its high sensitivity. The NMR spectroscopic data of exo-**5b** were deduced by difference between the NMR spectra of the mixture of endo and exo-**5b** and pure endo-**5b**. Complex exo-**5b:** ^{1}H NMR ($CDCl_3$): δ 8.45 (d, ^{3}J= 5.2 Hz, 1H, Py), 7.83 (t, ^{3}J= 7.2 Hz, 1H, Py), 7.66 (d, ^{3}J= 7.2 Hz, 1H, Ph), 7.58 (d, ^{3}J= 8.1 Hz, 1H, Py) 7.26 (t, 1H, Py), 7.14 (t, ^{3}J= 7.2 Hz, 1H, Ph), 7.06 (t, ^{3}J= 7.2 Hz, 1H, Ph), 6.93 (d, ^{3}J= 7.3 Hz, 1H, Ph), 5.97 (d, ^{3}J= 6.5 Hz, 1H, ArCr), 5.88 (d, ^{3}J= 6.3 Hz, 1H, ArCr), 5.60 (t, ^{3}J= 6.3 Hz, 1H, ArCr), 5.18 (t, ^{3}J= 6.2 Hz, 1H, ArCr), 4.26 (q, ^{3}J= 6.5 Hz, 1H, CH), 2.89 (s, 3H, NMe_2), 2.47 (s, 3H, NMe_2), 1.55 (d, ^{3}J= 6.5 Hz, 3H, CH_3). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$): δ 234.6 (CO),162.4, 158.5, 151.8, 147.5, 138.2, 137.1, 130.4, 126.4, 123.4, 122.5, 121.8, 118.3, 109.2, 101.7, 97.5, 92.3, 88.1, 72.4, 47.9, 42.9, 23.6.

Figure 1. *Left*: at mid-elution with chloroform a net separation of the two diastereomers endo-**5b** and exo-**5b** is already noticeable, the upper dark-orange polar band indicates the presence of 2-[tricarbonyl(η^6-phenyl)chromium]pyridine in the band containing exo-**5b** ; *Right*: diastereomer endo-**5b** reaches the lower end of the column.

[4] See figure 1.

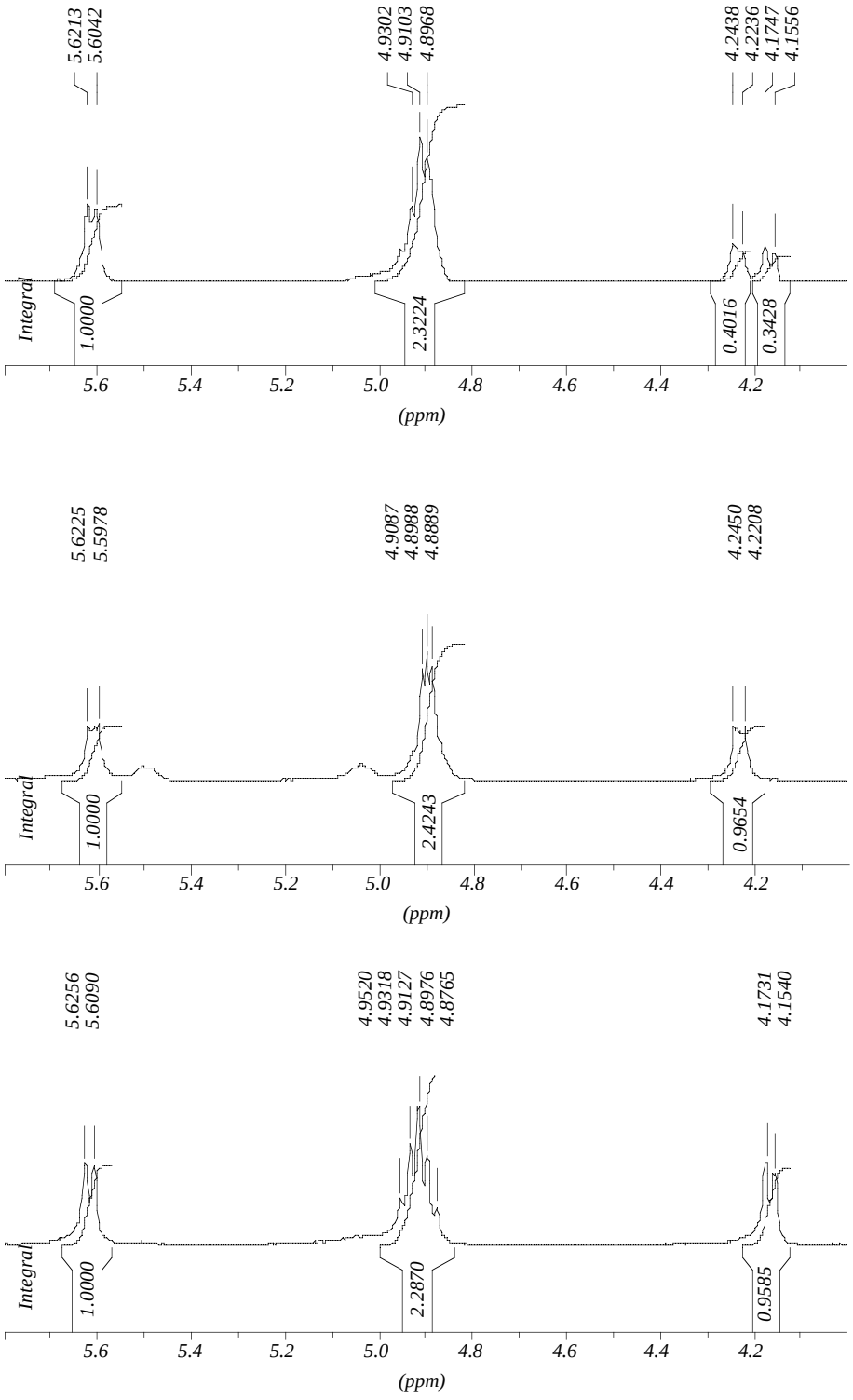
Complex 5c. The procedure for this reaction was similar to that described for **5b**. The conditions were slightly changed as follows: **4c** (550 mg, 0.95 mmol) solution in acetone (20 mL), mixture of **1a** (1.0 g, 1.90 mmol) and $[Me_4N]Cl$ (2.1 g, 19 mmol) in acetone (60 mL) at – 20°C; low temperature (5°C) chromatography over silica gel with mixture of 20% and 50% acetone/hexane afforded the two diastereoisomers endo-**5c** and exo-**5c** [*dr*=1.3:1 (endo:exo), 670 mg, 1.23 mmol, 65% conversion]. Complexes **5c:** Anal. Calcd for $C_{24}H_{22}N_2O_3CrPd$; C: 52.89, H: 4.04, N: 5.14. Found; C: 53.03, H: 3.81, N: 5.00. IR (CH_2Cl_2): ν(CO) 1951, 1875 cm^{-1}.

(−)-(*pS,1R*)-*Δ*-(*SP*$_d$-4-4)-{2'-[tricarbonyl(η^6-phenyl-*kC*$^{1'}$)chromium(0)]pyridine-*kN*}[*N,N*-dimethyl,1-(phenyl-*kC*^{1})ethylamine-*kN*]palladium(II), (−)-*(pS,7R)-endo*-5c. (74 mg) of endo-**5c** was obtained from a mixture of endo and exo-**5c** (300 mg) by the same procedure that was applied to **5b**. Complex endo-**5c:** $[\alpha]_D$ (CH_2Cl_2, 298K)= -813 (c= 0.04 g/100 mL). Anal. Calcd for $C_{24}H_{22}N_2O_3CrPd$; C: 52.89, H: 4.04, N: 5.14. Found; C: 52.59, H: 4.24, N: 4.86. IR (CH_2Cl_2): ν(CO) 1951, 1875 cm^{-1}. ^{1}H NMR ($CDCl_3$): δ 8.48 (d, ^3J= 5.0 Hz, 1H, Py), 7.83 (t, ^3J= 7.5 Hz, 1H, Py), 7.61 (d, ^3J= 7.4 Hz, 1H, Ph), 7.58 (d, ^3J= 8.1 Hz, 1H, Py), 7.26 (t, 1H, Py), 7.09 (m, 1H, Ph), 7.03 (m, 2H, Ph), 5.94 (d, ^3J= 6.3 Hz, 2H, ArCr), 5.57 (t, ^3J= 6.1 Hz, 1H, ArCr), 5.24 (t, ^3J= 6.2 Hz, 1H, ArCr), 3.47 (q, ^3J= 6.6 Hz, 1H, CH), 2.83 (s, 3H, NMe_2), 2.54 (s, 3H, NMe_2), 1.92 (d, ^3J= 6.5 Hz, 3H, CH_3). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 234.7 (CO), 162.7, 155.5, 154.1, 147.7, 138.2, 137.7, 130.4, 126.0, 123.6, 122.4, 121.4, 118.2, 109.2, 101.9, 96.6, 91.0, 89.4, 76.4, 50.9, 46.8, 23.7. Complex *(pR,7R)-exo*-**5c.** The NMR spectroscopic data of exo-**5c** were identical to those observed for complex exo-**5b** and were deduced by difference between the NMR spectra of the mixture of endo and exo-**5c** and pure endo-**5c** .

(+)-(*pR*)-(*SP*-4-4)-(chloro)(pyridine){2'-[tricarbonyl(η^6-phenyl-*kC*$^{1'}$)chromium(0)]pyridine-*kN*}palladium(II), (+)-*(pR)*-3. A mixture of endo-**5b** (80 mg, 0.15 mmol) and $HgCl_2$ (60 mg, 0.22 mmol) in dry acetone (20 mL) was stirred at room temperature for 14 h. Excess of pyridine was added dropwise and the resulting mixture was stirred for additional 15 min and then filtered through celite. The filtrate was striped of solvents. The product was purified by low temperature (0°C) flash chromatography over silica gel. The colorless [*(S)-N,N*-dimethyl-α-phenylethylamine-*2C*]chloromercurated by-product was eluted with 10% acetone/hexane mixture, followed by the orange product **(+)-*(pR)*-3** (50 mg, 0.098 mmol, 65% yield), which was eluted with 40% acetone/hexane mixture. Complex **(+)-*(pR)*-3:** $[\alpha]_D$ (CH_2Cl_2, 298K)= +751 (c= 0.04 g/100 mL). Anal. Calcd for $C_{19}H_{13}N_2O_3ClCrPd$; C: 44.62, H: 2.54, N: 5.48. Found; C: 44.45, H: 2.51, N: 5.38.

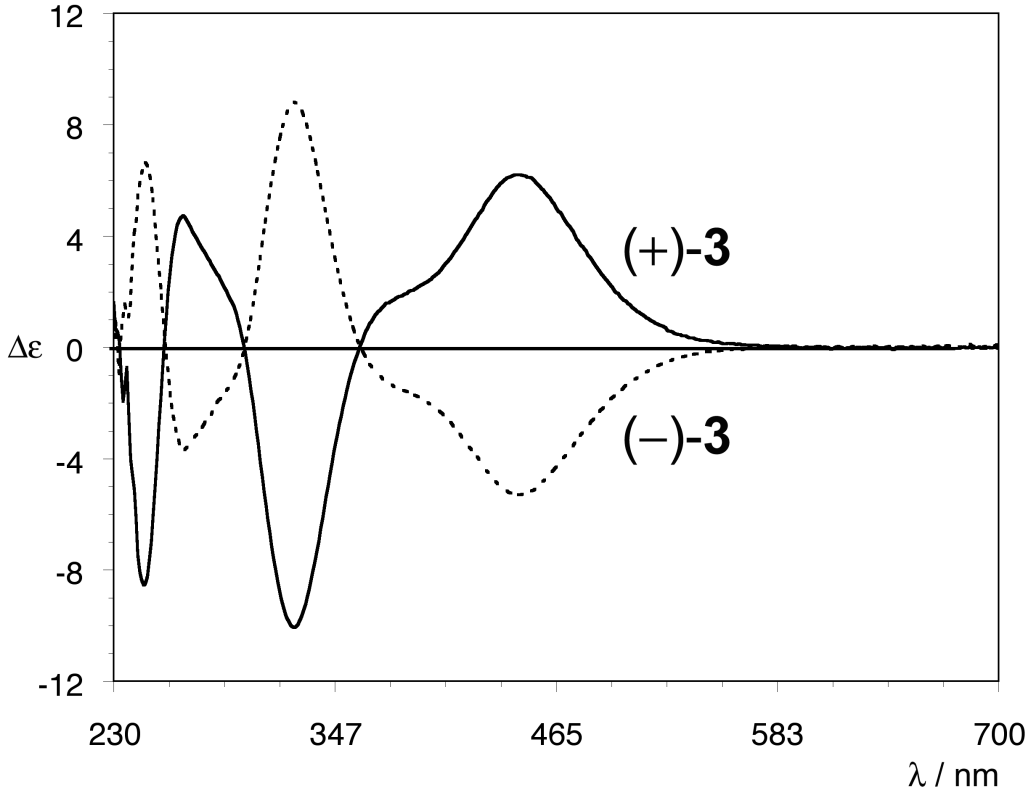
(−)-(*pS*)-(*SP*-4-4)-(chloro)(pyridine){2'-[tricarbonyl(η^6-phenyl-*kC*$^{1'}$)chromium(0)]pyridine-*kN*}palladium(II), (−)-*(pS)*-3. The procedure for this reaction was similar to that described above. Endo-**5c** (74 mg, 0.14 mmol) and $HgCl_2$ (55 mg, 0.20 mmol) in dry acetone (20 mL), room temperature, 14 h. Excess of pyridine was added. Low temperature (0°C) flash chromatography over silica gel afforded [*(R)-N,N*-dimethyl-α-phenylethylamine-2*C*]chloromercurated by-product with 10% acetone/hexane mixture, followed by the orange product (−)-***(pS)*-3** (50 mg, 0.098 mmol, 72% yield) which was eluted with 40% acetone/hexane mixture. Complex (−)-***(pS)*-3:** $[\alpha]_D$ (CH_2Cl_2, 298K)= -733 (c= 0.04 g/100 mL).

^{1}H NMR spectra of mixtures of 3 with [*n*-Bu$_4$N][TRISPHAT] in a 1:4 mixture of d_6.acetone and d_6.benzene of the resonance region typical of Cr-bound arene protons: upper spectrum, *rac*-3; middle, (−)-(p*S*)-3; lower, (+)-(p*R*)-3.



Circular Dichroism spectroscopy

Complexes (+)-3 (continuous curve) and (−)-3 (dashed curve) (c ~ 10^{-4}M, MeOH)



$\Delta\varepsilon$ in $dm^3.mol^{-1}.cm^{-1}$

Listing of crystallographic data related to :

(ORTEP diagrams are drawn at 30% probability level)

Complexes 5b

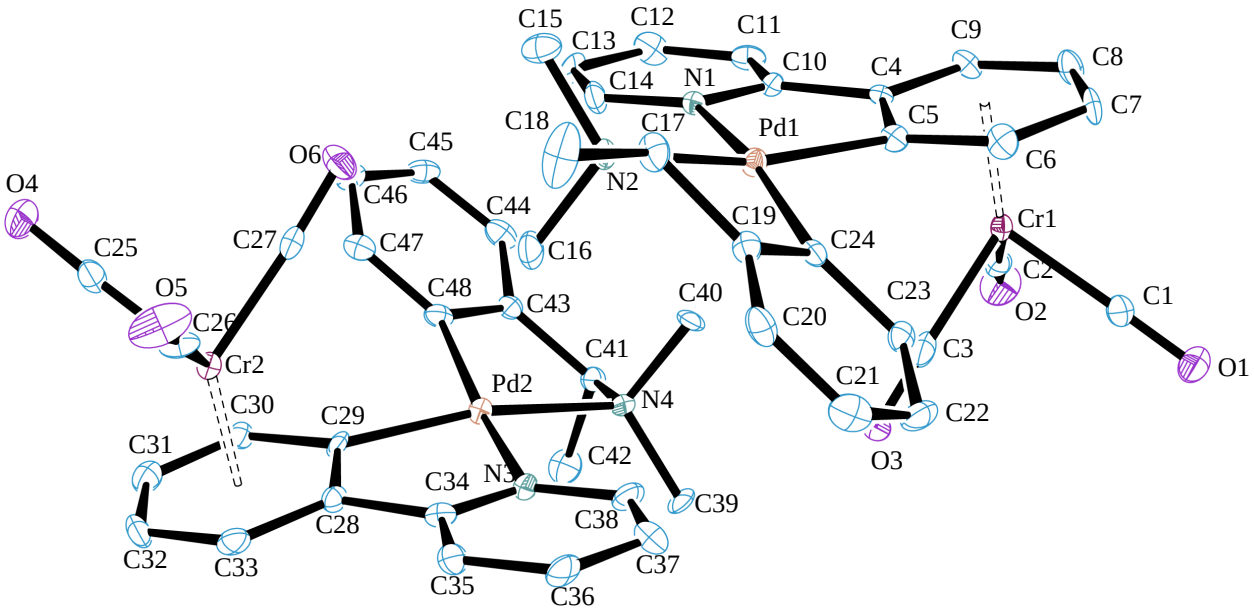

C15
C12
C11
C9
C13
C10
C4
C8
C14
N1
C7
C18
C17
Pd1
C5
O6
C45
C6
N2
O4
C46
C44
C19
Cr1
C25
C27
C47
C16
C24
C2
O5
C48
C43
C40
C23
C1
C26
C20
O2
C3
Cr2
C41
O1
Pd2
C21
C30
C29
N4
C22
C31
C42
O3
N3
C34
C39
C38
C28
C32
C33
C37
C35
C36

Table 1 : X-ray experimental data

Formula	: $C_{48}H_{44}Cr_2N_4O_6Pd_2$
Molecular weight	: 1089.70
Crystal system	: monoclinic
Space group	: $P\,2_1$
a(Å)	: 11.1217(3)
b(Å)	: 17.0324(4)
c(Å)	: 11.5570(3)
β(deg)	: 102.118(5)
$V(Å^3)$	: 2140.45(9)
Z	: 2
Color	: orange
Crystal dim(mm)	: 0.20*0.14*0.14
$Dcalc(gcm^{-3})$	: 1.69
F000	: 1096
$\mu(mm^{-1})$	: 1.377
Trans. min and max	: 0.9609/1.0000
Temperature(K)	: 173
Wavelength(Å)	: 0.71073
Radiation	: MoKα graphite monochromated
Diffractometer	: KappaCCD
Scan mode	: 'phi scans'
hkl limits	: -7,15/-20,23/-15,16
Theta limits(deg)	: 2.5/30.03
Number of data meas.	: 12332
Number of data with I > 3 σ(I)	: 4310
Number of variables	: 558
R	: 0.030
Rw	: 0.046
GOF	: 1.046
Largest peak in final difference ($eÅ^{-3}$)	: 0.424

Table of Positional Parameters and Their E.S.D.

Atom	x	y	z	Ueqv
CR1	0.5659(1)	0.10801(7)	0.45685(9)	0.0172(5)
PD1	0.86745(4)	0.2043	0.38139(4)	0.0193(2)
CR2	0.9203(1)	0.55008(7)	0.04263(9)	0.0179(5)
PD2	0.62165(4)	0.44670(3)	0.11565(4)	0.0201(2)
C1	0.5064(7)	0.1069(4)	0.5928(7)	0.030(4)
O1	0.4709(6)	0.1076(4)	0.6787(5)	0.047(3)
C2	0.4060(7)	0.1108(4)	0.3762(6)	0.024(3)
O2	0.3035(5)	0.1097(4)	0.3265(5)	0.042(3)
C3	0.5600(6)	0.2167(5)	0.4668(6)	0.028(3)
O3	0.5555(5)	0.2847(3)	0.4750(4)	0.029(3)
C4	0.6797(6)	0.0857(4)	0.3180(6)	0.018(3)
C5	0.7593(6)	0.1205(4)	0.4198(6)	0.017(3)
C6	0.7641(6)	0.0827(4)	0.5283(7)	0.024(3)
C7	0.6927(7)	0.0147(4)	0.5396(6)	0.024(3)
C8	0.6138(7)	-0.0167(4)	0.4378(6)	0.024(3)
C9	0.6071(6)	0.0198(4)	0.3286(6)	0.021(3)
C10	0.6810(6)	0.1217(4)	0.2013(6)	0.019(3)
C11	0.6016(7)	0.1017(4)	0.0949(6)	0.023(3)
C12	0.6108(8)	0.1367(5)	-0.0082(7)	0.030(4)
C13	0.6997(7)	0.1950(5)	-0.0046(5)	0.019(3)
C14	0.7745(7)	0.2136(4)	0.1031(6)	0.025(3)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
N1	0.7705(5)	0.1775(3)	0.2046(5)	0.018(3)
N2	1.0211(5)	0.2753(3)	0.3496(5)	0.019(3)
C15	1.0736(6)	0.2418(5)	0.2534(7)	0.028(4)
C16	0.9893(7)	0.3563(5)	0.3261(6)	0.030(4)
C17	1.1135(6)	0.2667(5)	0.4662(7)	0.025(3)
C18	1.2298(8)	0.3153(6)	0.4757(7)	0.043(5)
C19	1.0445(6)	0.2794(4)	0.5648(6)	0.021(3)
C20	1.0909(7)	0.3238(4)	0.6635(6)	0.026(4)
C21	1.0230(7)	0.3327(5)	0.7500(7)	0.029(4)
C22	0.9076(7)	0.2975(5)	0.7352(6)	0.028(4)
C23	0.8603(6)	0.2531(4)	0.6360(6)	0.019(3)
C24	0.9278(6)	0.2441(4)	0.5458(6)	0.016(3)
C25	0.9860(7)	0.5497(4)	-0.0924(6)	0.026(4)
O4	1.0261(6)	0.5475(4)	-0.1770(5)	0.044(3)
C26	1.0777(7)	0.5559(5)	0.1313(6)	0.030(4)
O5	1.1788(5)	0.5564(4)	0.1853(5)	0.043(3)
C27	0.9312(6)	0.4431(5)	0.0380(6)	0.023(3)
O6	0.9424(5)	0.3758(3)	0.0315(5)	0.036(3)
C28	0.8036(6)	0.5707(4)	0.1771(6)	0.018(3)
C29	0.7257(6)	0.5342(4)	0.0765(6)	0.019(3)
C30	0.7212(6)	0.5712(4)	-0.0340(6)	0.018(3)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C31	0.7867(7)	0.6394(5)	-0.0439(6)	0.028(4)
C32	0.8617(7)	0.6748(4)	0.0535(7)	0.026(3)
C33	0.8713(7)	0.6396(4)	0.1641(6)	0.026(3)
C34	0.8046(6)	0.5351(4)	0.2941(6)	0.020(3)
C35	0.8848(7)	0.5579(5)	0.3975(6)	0.026(3)
C36	0.8784(7)	0.5195(5)	0.5033(6)	0.024(4)
C37	0.7935(8)	0.4611(4)	0.5014(7)	0.034(4)
C38	0.7154(7)	0.4420(5)	0.3958(6)	0.027(3)
N3	0.7187(5)	0.4791(4)	0.2917(5)	0.021(3)
N4	0.4736(5)	0.3708(3)	0.1479(5)	0.022(3)
C39	0.4108(6)	0.4024(5)	0.2391(6)	0.026(3)
C40	0.5238(7)	0.2908(4)	0.1877(6)	0.021(3)
C41	0.3852(6)	0.3604(4)	0.0311(6)	0.021(3)
C42	0.2908(7)	0.4248(5)	0.0038(7)	0.033(4)
C43	0.4613(6)	0.3555(4)	-0.0613(6)	0.020(3)
C44	0.4246(7)	0.3073(5)	-0.1626(7)	0.028(4)
C45	0.4937(7)	0.3062(5)	-0.2493(6)	0.027(4)
C46	0.5973(6)	0.3513(5)	-0.2380(6)	0.024(3)
C47	0.6356(7)	0.3965(4)	-0.1359(7)	0.024(3)
C48	0.5680(6)	0.4011(4)	-0.0473(6)	0.021(3)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as one third of the trace of the orthogonalized Uij tensor.

Table of Positional Parameters

Atom	x	y	z	Ueqv	
H1	0.8170	0.1032	0.5971	0.0328	*
H2	0.6980	-0.0093	0.6147	0.0317	*
H3	0.5660	-0.0621	0.4439	0.0325	*
H4	0.5525	-0.0002	0.2605	0.0288	*

H5	0.5402	0.0629	0.0949	0.0311	*
H6	0.5583	0.1221	-0.0808	0.0408	*
H7	0.7086	0.2213	-0.0748	0.0349	*
H8	0.8326	0.2547	0.1050	0.0328	*
H9	1.0161	0.2471	0.1805	0.0374	*
H10	1.1472	0.2690	0.2491	0.0374	*
H11	1.0915	0.1878	0.2688	0.0374	*
H12	0.9316	0.3605	0.2531	0.0385	*
H13	0.9541	0.3767	0.3880	0.0385	*
H14	1.0612	0.3854	0.3218	0.0385	*
H15	1.1469	0.2152	0.4723	0.0341	*
H16	1.2824	0.3067	0.5507	0.0645	*
H17	1.2709	0.3003	0.4149	0.0645	*
H18	1.2088	0.3694	0.4674	0.0645	*
H19	1.1692	0.3481	0.6722	0.0356	*
H20	1.0547	0.3626	0.8190	0.0416	*
H21	0.8606	0.3041	0.7943	0.0375	*

Table of Positional Parameters (cont.)

Atom	x	y	z	Ueqv	
H22	0.7823	0.2285	0.6283	0.0254	*
H23	0.6720	0.5488	-0.1033	0.0235	*
H24	0.7801	0.6626	-0.1197	0.0359	*
H25	0.9053	0.7217	0.0450	0.0346	*
H26	0.9239	0.6620	0.2315	0.0337	*
H27	0.9427	0.5988	0.3966	0.0339	*
H28	0.9324	0.5338	0.5754	0.0363	*
H29	0.7884	0.4339	0.5721	0.0463	*
H30	0.6568	0.4014	0.3955	0.0346	*
H31	0.4687	0.4083	0.3117	0.0314	*
H32	0.3755	0.4519	0.2142	0.0314	*
H33	0.3479	0.3670	0.2498	0.0314	*
H34	0.5803	0.2954	0.2614	0.0309	*
H35	0.4582	0.2572	0.1962	0.0309	*
H36	0.5648	0.2695	0.1304	0.0309	*
H37	0.3383	0.3140	0.0333	0.0273	*
H38	0.2379	0.4150	-0.0707	0.0450	*
H39	0.2439	0.4264	0.0636	0.0450	*
H40	0.3311	0.4738	0.0012	0.0450	*
H41	0.3528	0.2758	-0.1710	0.0386	*
H42	0.4689	0.2740	-0.3172	0.0358	*

Table of Positional Parameters (cont.)

Atom	x	y	z	Ueqv	
H43	0.6429	0.3519	-0.2989	0.0312	*
H44	0.7103	0.4251	-0.1265	0.0325	*

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
CR1	.0185(5)	.0178(5)	.0155(5)	-.0036(5)	.0042(4)	.0015(4)
PD1	.0192(2)	.0198(2)	.0187(2)	-.0024(2)	.0044(2)	-.0003(2)
CR2	.0175(5)	.0194(5)	.0169(5)	-.0011(5)	.0048(4)	.0009(4)
PD2	.0211(2)	.0202(2)	.0190(2)	-.0005(2)	.0064(2)	.0008(2)
C1	.034(4)	.022(4)	.035(4)	-.003(3)	.016(3)	.003(3)
O1	.069(3)	.036(3)	.042(3)	-.006(3)	.034(2)	-.002(3)
C2	.030(3)	.026(4)	.017(3)	.007(3)	.009(3)	.002(3)
O2	.026(3)	.063(4)	.045(3)	.003(3)	.002(3)	.002(3)
C3	.025(3)	.039(4)	.021(3)	.006(3)	.010(3)	.012(3)
O3	.044(3)	.020(3)	.027(2)	.005(2)	.015(2)	.002(2)
C4	.024(3)	.011(3)	.020(3)	.001(3)	.008(2)	-.002(3)
C5	.011(3)	.020(3)	.024(3)	-.001(3)	.002(2)	-.000(3)
C6	.016(3)	.027(4)	.033(4)	-.008(3)	.004(3)	.000(3)
C7	.026(3)	.021(3)	.026(3)	-.005(3)	.006(3)	.013(3)
C8	.030(4)	.019(3)	.023(3)	-.010(3)	.000(3)	.002(3)
C9	.023(3)	.015(3)	.026(3)	-.001(3)	-.001(3)	.001(3)
C10	.022(3)	.018(3)	.017(3)	.003(3)	.008(2)	.002(3)
C11	.023(3)	.021(3)	.025(3)	-.002(3)	-.001(3)	-.012(3)
C12	.035(4)	.029(4)	.026(4)	.001(4)	-.004(3)	-.001(3)
C13	.037(3)	.041(4)	.004(2)	.009(4)	.007(2)	.007(3)
C14	.030(3)	.020(3)	.026(3)	-.000(3)	.008(3)	.010(3)
N1	.022(3)	.015(3)	.017(2)	.001(2)	.006(2)	.000(2)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
N2	.016(2)	.020(3)	.022(3)	-.001(2)	.006(2)	.005(2)
C15	.020(3)	.031(4)	.036(4)	.001(3)	.007(3)	-.009(3)
C16	.035(4)	.029(4)	.027(3)	.002(3)	.011(3)	.013(3)
C17	.015(3)	.029(4)	.034(4)	-.005(3)	.004(3)	.005(3)

C18	.038(4)	.082(7)	.025(4)	-.033(4)	-.000(3)	.002(5)
C19	.018(3)	.022(3)	.023(3)	.000(3)	.004(2)	.003(3)
C20	.032(4)	.020(3)	.028(4)	-.009(3)	.001(3)	.003(3)
C21	.036(4)	.032(4)	.021(3)	.003(4)	-.008(3)	-.005(3)
C22	.035(4)	.036(4)	.018(3)	.011(3)	.009(3)	-.002(3)
C23	.020(3)	.023(3)	.016(3)	.003(3)	.002(2)	.005(3)
C24	.015(3)	.013(3)	.023(3)	.000(3)	.004(2)	.003(3)
C25	.036(4)	.020(3)	.024(3)	-.004(3)	.005(3)	.002(3)
O4	.060(3)	.043(4)	.034(3)	-.004(3)	.025(2)	.001(3)
C26	.034(4)	.030(4)	.026(3)	.004(3)	.008(3)	-.012(3)
O5	.032(3)	.087(5)	.029(3)	.012(3)	-.009(3)	-.022(3)
C27	.021(3)	.032(4)	.018(3)	-.002(3)	.009(2)	.004(3)
O6	.054(3)	.021(3)	.040(3)	.005(3)	.013(3)	.008(2)
C28	.020(3)	.021(3)	.014(3)	.002(3)	.004(2)	.002(3)
C29	.017(3)	.024(3)	.017(3)	.001(3)	.011(2)	.001(3)
C30	.017(3)	.019(3)	.019(3)	.004(3)	.004(2)	.006(3)
C31	.027(3)	.033(4)	.023(3)	.004(3)	.008(3)	.004(3)
C32	.031(4)	.016(3)	.033(4)	-.003(3)	.008(3)	.007(3)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C33	.027(3)	.027(4)	.025(3)	-.005(3)	.009(3)	-.012(3)
C34	.017(3)	.021(3)	.022(3)	.001(3)	.003(2)	-.006(3)
C35	.034(4)	.022(3)	.022(3)	.005(3)	.007(3)	.005(3)
C36	.037(4)	.035(4)	.011(3)	.003(4)	.005(3)	-.004(3)
C37	.049(4)	.019(4)	.041(4)	.003(4)	.015(3)	.004(3)
C38	.033(3)	.029(4)	.022(3)	-.006(3)	.013(2)	-.011(3)
N3	.027(3)	.020(3)	.017(2)	.002(3)	.009(2)	.002(2)
N4	.028(3)	.017(3)	.021(3)	-.000(2)	.012(2)	-.003(2)
C39	.021(3)	.029(4)	.029(3)	-.002(3)	.019(2)	-.005(3)
C40	.041(4)	.011(3)	.020(3)	.009(3)	.007(3)	.002(3)
C41	.020(3)	.019(3)	.026(3)	-.002(3)	.008(3)	-.001(3)

C42	.022(3)	.043(5)	.038(4)	-.001(4)	.005(3)	.001(4)
C43	.020(3)	.018(3)	.020(3)	.005(3)	.003(2)	.004(3)
C44	.033(4)	.020(4)	.032(4)	-.002(3)	-.001(3)	-.002(3)
C45	.031(4)	.027(4)	.022(3)	.007(3)	.001(3)	-.008(3)
C46	.022(3)	.030(4)	.021(3)	.004(3)	.005(3)	-.002(3)
C47	.023(3)	.021(4)	.030(4)	.001(3)	.002(3)	-.003(3)
C48	.028(3)	.018(3)	.017(3)	.005(3)	.001(3)	-.002(3)

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
CR1	C1	1.83(1)	CR2	C33	2.22(1)
CR1	C2	1.83(1)	PD2	C29	2.00(1)
CR1	C3	1.86(1)	PD2	N3	2.165(9)
CR1	C4	2.28(1)	PD2	N4	2.186(8)
CR1	C5	2.290(9)	PD2	C48	2.01(1)
CR1	C6	2.23(1)	C1	O1	1.14(1)
CR1	C7	2.20(1)	C2	O2	1.16(1)
CR1	C8	2.21(1)	C3	O3	1.16(2)
CR1	C9	2.22(1)	C4	C5	1.44(1)
PD1	C5	1.98(1)	C4	C9	1.40(1)
PD1	N1	2.149(9)	C4	C10	1.48(1)
PD1	N2	2.187(8)	C5	C6	1.40(2)
PD1	C24	2.00(1)	C6	C7	1.43(1)
CR2	C25	1.86(1)	C7	C8	1.42(2)
CR2	C26	1.84(1)	C8	C9	1.40(2)
CR2	C27	1.83(1)	C10	C11	1.40(1)
CR2	C28	2.25(1)	C10	N1	1.37(1)
CR2	C29	2.295(9)	C11	C12	1.36(2)
CR2	C30	2.235(9)	C12	C13	1.39(2)
CR2	C31	2.21(1)	C13	C14	1.38(1)
CR2	C32	2.23(1)	C14	N1	1.33(1)

Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
N2	C15	1.47(1)	C31	C32	1.39(2)
N2	C16	1.44(2)	C32	C33	1.39(2)
N2	C17	1.52(1)	C34	C35	1.39(1)
C17	C18	1.52(1)	C34	N3	1.35(1)
C17	C19	1.52(1)	C35	C36	1.40(2)
C19	C20	1.38(2)	C36	C37	1.37(2)
C19	C24	1.40(1)	C37	C38	1.38(2)
C20	C21	1.38(2)	C38	N3	1.36(1)
C21	C22	1.39(2)	N4	C39	1.48(1)
C22	C23	1.38(2)	N4	C40	1.51(1)
C23	C24	1.41(1)	N4	C41	1.50(1)
C25	O4	1.16(1)	C41	C42	1.51(1)
C26	O5	1.17(1)	C41	C43	1.50(1)
C27	O6	1.16(2)	C43	C44	1.42(2)
C28	C29	1.44(1)	C43	C48	1.40(1)
C28	C33	1.42(2)	C44	C45	1.38(2)
C28	C34	1.48(1)	C45	C46	1.37(2)
C29	C30	1.42(1)	C46	C47	1.40(2)
C30	C31	1.39(2)	C47	C48	1.39(2)

Table of Bond Angles in Degrees

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C1	CR1	C2	87.1(5)	C4	CR1	C5	36.8(4)
C1	CR1	C3	86.2(5)	C4	CR1	C6	64.9(4)
C1	CR1	C4	163.7(5)	C4	CR1	C7	77.6(4)
C1	CR1	C5	133.2(4)	C4	CR1	C8	65.7(4)
C1	CR1	C6	100.8(5)	C4	CR1	C9	36.3(4)
C1	CR1	C7	86.2(5)	C5	CR1	C6	36.1(4)
C1	CR1	C8	102.3(5)	C5	CR1	C7	66.9(4)
C1	CR1	C9	136.7(5)	C5	CR1	C8	79.3(4)
C2	CR1	C3	87.9(5)	C5	CR1	C9	66.7(4)
C2	CR1	C4	105.7(4)	C6	CR1	C7	37.5(4)
C2	CR1	C5	139.0(4)	C6	CR1	C8	67.1(4)
C2	CR1	C6	167.3(5)	C6	CR1	C9	77.9(4)
C2	CR1	C7	134.9(4)	C7	CR1	C8	37.4(4)
C2	CR1	C8	101.7(4)	C7	CR1	C9	66.4(4)
C2	CR1	C9	89.6(4)	C8	CR1	C9	36.7(4)
C3	CR1	C4	104.0(4)	C5	PD1	N1	81.5(4)
C3	CR1	C5	88.0(4)	C5	PD1	N2	166.2(3)
C3	CR1	C6	102.4(4)	C5	PD1	C24	97.5(4)
C3	CR1	C7	136.0(4)	N1	PD1	N2	102.2(3)
C3	CR1	C8	167.4(4)	N1	PD1	C24	168.0(3)
C3	CR1	C9	136.8(5)	N2	PD1	C24	81.6(4)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C25	CR2	C26	88.4(5)	C28	CR2	C29	36.8(4)
C25	CR2	C27	86.1(5)	C28	CR2	C30	65.3(4)
C25	CR2	C28	165.0(5)	C28	CR2	C31	77.0(4)
C25	CR2	C29	134.0(4)	C28	CR2	C32	66.1(4)
C25	CR2	C30	101.5(4)	C28	CR2	C33	37.0(4)
C25	CR2	C31	88.2(5)	C29	CR2	C30	36.4(4)
C25	CR2	C32	102.8(5)	C29	CR2	C31	65.8(4)
C25	CR2	C33	136.6(5)	C29	CR2	C32	78.8(4)
C26	CR2	C27	90.5(5)	C29	CR2	C33	66.8(4)
C26	CR2	C28	103.1(5)	C30	CR2	C31	36.4(4)
C26	CR2	C29	137.2(5)	C30	CR2	C32	66.0(4)
C26	CR2	C30	164.1(5)	C30	CR2	C33	77.6(4)
C26	CR2	C31	133.3(5)	C31	CR2	C32	36.4(4)
C26	CR2	C32	99.9(5)	C31	CR2	C33	65.3(4)
C26	CR2	C33	86.7(4)	C32	CR2	C33	36.5(4)
C27	CR2	C28	103.2(4)	C29	PD2	N3	79.9(4)
C27	CR2	C29	87.6(4)	C29	PD2	N4	166.7(4)
C27	CR2	C30	102.4(4)	C29	PD2	C48	98.6(4)
C27	CR2	C31	135.6(4)	N3	PD2	N4	103.6(3)
C27	CR2	C32	166.4(4)	N3	PD2	C48	166.2(3)
C27	CR2	C33	137.0(5)	N4	PD2	C48	81.1(4)

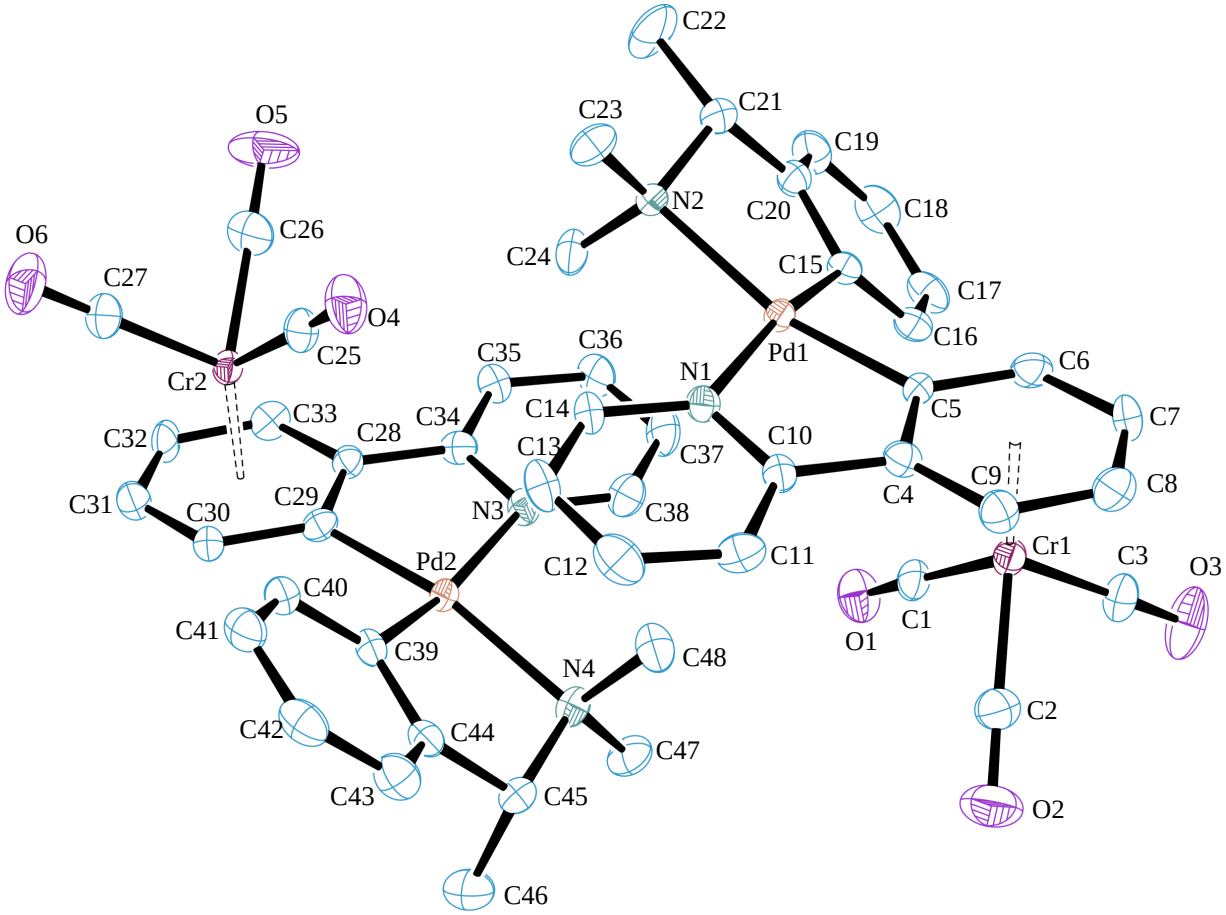
Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C5	C4	C9	121(1)	C18	C17	C19	115.2(9)
C5	C4	C10	116.8(9)	C17	C19	C20	122.7(9)
C9	C4	C10	121.7(9)	C17	C19	C24	114(1)
C4	C5	C6	116.3(9)	C20	C19	C24	122(1)
C5	C6	C7	122(1)	C19	C20	C21	119.6(9)
C6	C7	C8	119(1)	C20	C21	C22	119(1)
C7	C8	C9	119.3(9)	C21	C22	C23	121(1)
C4	C9	C8	120(1)	C22	C23	C24	120.1(9)
C4	C10	C11	125(1)	C19	C24	C23	117(1)
C4	C10	N1	113.9(9)	C29	C28	C33	120(1)
C11	C10	N1	121(1)	C29	C28	C34	116.7(9)
C10	C11	C12	121(1)	C33	C28	C34	122.3(9)
C11	C12	C13	118(1)	C28	C29	C30	116.0(9)
C12	C13	C14	118(1)	C29	C30	C31	121(1)
C13	C14	N1	124(1)	C30	C31	C32	122(1)
C10	N1	C14	116.9(9)	C31	C32	C33	118(1)
C15	N2	C16	110(1)	C28	C33	C32	120(1)
C15	N2	C17	109.3(8)	C28	C34	C35	123(1)
C16	N2	C17	110.7(9)	C28	C34	N3	113.8(9)
N2	C17	C18	114.7(8)	C35	C34	N3	122(1)
N2	C17	C19	107.3(7)	C34	C35	C36	118(1)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C35	C36	C37	119(1)	C42	C41	C43	111.4(8)
C36	C37	C38	119(1)	C41	C43	C44	120.8(9)
C37	C38	N3	122(1)	C41	C43	C48	118(1)
C34	N3	C38	117.4(9)	C44	C43	C48	120(1)
C39	N4	C40	108.1(9)	C43	C44	C45	119(1)
C39	N4	C41	111.3(7)	C44	C45	C46	120(1)
C40	N4	C41	107.3(8)	C45	C46	C47	119(1)
N4	C41	C42	113.5(8)	C46	C47	C48	122(1)
N4	C41	C43	106.5(7)	C43	C48	C47	117(1)

Complexes 5c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C26
O6
C24
C15
C27
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C25
Pd1
C6
C35
C36
N1
Cr2
C5
C7
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C34
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C11
C40
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C41
C39
O1
N4
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O2
C46

Table 1 : X-ray experimental data

Formula	: $C_{48}H_{44}Cr_2N_4O_6Pd_2$
Molecular weight	: 1089.70
Crystal system	: monoclinic
Space group	: $P\,2_1$
a(Å)	: 11.1267(2)
b(Å)	: 17.0317(3)
c(Å)	: 11.5572(2)
β(deg)	: 102.140(5)
$V(Å^3)$	: 2141.19(6)
Z	: 2
Color	: orange
Crystal dim(mm)	: 0.18*0.14*0.10
$Dcalc(gcm^{-3})$	: 1.69
F000	: 1096
$\mu(mm^{-1})$	: 1.376
Trans. min and max	: 0.9783/1.1570
Temperature(K)	: 173
Wavelength(Å)	: 0.71073
Radiation	: MoKα graphite monochromated
Diffractometer	: KappaCCD
Scan mode	: 'phi scans'
hkl limits	: -15,15/-23,20/-16,16
Theta limits(deg)	: 2.5/30.02
Number of data meas.	: 10295
Number of data with I > 3 σ(I)	: 5557
Number of variables	: 558
R	: 0.023
Rw	: 0.028
GOF	: 0.941
Largest peak in final difference ($eÅ^{-3}$)	: 0.372

Table of Positional Parameters and Their E.S.D.

Atom	x	y	z	Ueqv
PD1	0.63257(2)	0.5538	0.61860(2)	0.01598(9)
CR1	0.93412(4)	0.64951(2)	0.54315(4)	0.0195(2)
C1	0.9389(3)	0.5428(2)	0.5340(3)	0.024(1)
O1	0.9447(2)	0.4755(1)	0.5253(2)	0.034(1)
C2	1.0950(3)	0.6497(2)	0.6249(3)	0.030(2)
O2	1.1965(2)	0.6497(2)	0.6744(2)	0.043(1)
C3	0.9925(3)	0.6521(2)	0.4062(3)	0.029(1)
O3	1.0301(2)	0.6517(1)	0.3199(2)	0.048(1)
C4	0.8201(2)	0.6733(2)	0.6808(3)	0.020(1)
C5	0.7406(2)	0.6394(1)	0.5809(3)	0.017(1)
C6	0.7359(3)	0.6770(2)	0.4713(3)	0.022(1)
C7	0.8068(3)	0.7440(2)	0.4609(3)	0.027(1)
C8	0.8854(3)	0.7759(2)	0.5614(3)	0.025(1)
C9	0.8929(3)	0.7400(2)	0.6711(3)	0.023(1)
C10	0.8192(2)	0.6380(1)	0.7980(3)	0.018(1)
C11	0.8997(3)	0.6577(2)	0.9036(3)	0.023(1)
C12	0.8902(3)	0.6214(2)	1.0084(3)	0.029(2)
C13	0.8002(3)	0.5644(2)	1.0042(3)	0.027(1)
C14	0.7249(3)	0.5466(2)	0.8973(3)	0.026(1)
N1	0.7302(2)	0.5827(1)	0.7953(2)	0.019(1)
C15	0.5727(2)	0.5153(1)	0.4534(3)	0.018(1)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C16	0.6399(3)	0.5054(2)	0.3650(3)	0.021(1)
C17	0.5923(3)	0.4621(2)	0.2635(3)	0.026(1)
C18	0.4793(3)	0.4266(2)	0.2491(3)	0.031(2)
C19	0.4110(3)	0.4354(2)	0.3345(3)	0.029(2)
C20	0.4561(3)	0.4801(2)	0.4358(3)	0.022(1)
C21	0.3866(3)	0.4931(2)	0.5334(3)	0.024(1)
C22	0.2699(3)	0.4449(3)	0.5235(3)	0.045(2)
N2	0.4784(2)	0.4844(1)	0.6498(2)	0.019(1)
C23	0.4261(3)	0.5170(2)	0.7467(3)	0.028(1)
C24	0.5119(3)	0.4010(2)	0.6750(3)	0.027(1)
PD2	0.87817(2)	0.31142(1)	0.88417(2)	0.01695(9)
CR2	0.57978(4)	0.20748(3)	0.95723(4)	0.0189(2)
C25	0.5665(3)	0.3154(2)	0.9612(3)	0.026(1)
O4	0.5562(2)	0.3838(1)	0.9684(2)	0.036(1)
C26	0.4224(3)	0.2053(2)	0.8700(3)	0.029(2)
O5	0.3227(2)	0.2034(2)	0.8154(2)	0.046(2)
C27	0.5139(3)	0.2093(2)	1.0916(3)	0.026(1)
O6	0.4743(2)	0.2120(1)	1.1750(2)	0.047(1)
C28	0.6971(3)	0.1891(1)	0.8221(3)	0.020(1)
C29	0.7739(2)	0.2257(2)	0.9235(3)	0.020(1)
C30	0.7791(3)	0.1881(2)	1.0338(3)	0.021(1)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C31	0.7115(3)	0.1186(2)	1.0435(3)	0.026(1)
C32	0.6379(3)	0.0846(2)	0.9460(3)	0.025(1)
C33	0.6283(3)	0.1198(2)	0.8354(3)	0.024(1)
C34	0.6960(3)	0.2243(2)	0.7054(3)	0.020(1)
C35	0.6169(3)	0.2022(2)	0.6018(3)	0.023(1)
C36	0.6220(3)	0.2389(2)	0.4963(3)	0.025(1)
C37	0.7077(3)	0.2979(2)	0.4987(3)	0.031(2)
C38	0.7837(3)	0.3178(2)	0.6043(3)	0.027(1)
N3	0.7816(2)	0.2814(1)	0.7077(2)	0.021(1)
C39	0.9316(2)	0.3581(1)	1.0459(3)	0.018(1)
C40	0.8652(3)	0.3621(2)	1.1360(3)	0.024(1)
C41	0.9016(3)	0.4083(2)	1.2365(3)	0.026(1)
C42	1.0070(3)	0.4533(2)	1.2487(3)	0.026(1)
C43	1.0755(3)	0.4515(2)	1.1608(3)	0.027(1)
C44	1.0390(3)	0.4033(2)	1.0619(3)	0.020(1)
C45	1.1142(3)	0.3997(2)	0.9692(3)	0.022(1)
C46	1.2107(3)	0.3340(2)	0.9968(3)	0.034(2)
N4	1.0255(2)	0.3889(1)	0.8508(2)	0.020(1)
C47	1.0889(3)	0.3575(2)	0.7611(3)	0.030(2)
C48	0.9752(3)	0.4674(2)	0.8132(3)	0.029(2)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as one third of the trace of the orthogonalized Uij tensor.

Table of Positional Parameters

Atom	x	y	z	Ueqv	
H1	0.6833	0.6564	0.4024	0.0299	*
H2	0.8015	0.7680	0.3857	0.0354	*
H3	0.9329	0.8213	0.5546	0.0346	*
H4	0.9470	0.7603	0.7392	0.0300	*

H5	0.9613	0.6963	0.9037	0.0303	*
H6	0.9437	0.6350	1.0810	0.0395	*
H7	0.7909	0.5381	1.0743	0.0374	*
H8	0.6654	0.5064	0.8955	0.0336	*
H9	0.7191	0.5284	0.3743	0.0290	*
H10	0.6385	0.4570	0.2035	0.0362	*
H11	0.4484	0.3961	0.1805	0.0430	*
H12	0.3328	0.4109	0.3247	0.0396	*
H13	0.3533	0.5447	0.5271	0.0324	*
H14	0.2325	0.4567	0.5881	0.0698	*
H15	0.2145	0.4571	0.4513	0.0698	*
H16	0.2897	0.3906	0.5248	0.0698	*
H17	0.4839	0.5114	0.8195	0.0350	*
H18	0.4079	0.5710	0.7321	0.0350	*
H19	0.3529	0.4895	0.7509	0.0350	*
H20	0.5694	0.3973	0.7483	0.0349	*
H21	0.4403	0.3718	0.6793	0.0349	*

Table of Positional Parameters (cont.)

Atom	x	y	z	Ueqv	
H22	0.5476	0.3805	0.6136	0.0349	*
H23	0.8292	0.2099	1.1031	0.0280	*
H24	0.7174	0.0950	1.1190	0.0338	*
H25	0.5940	0.0377	0.9538	0.0330	*
H26	0.5755	0.0976	0.7681	0.0316	*
H27	0.5587	0.1616	0.6031	0.0307	*
H28	0.5684	0.2240	0.4245	0.0359	*
H29	0.7141	0.3244	0.4279	0.0410	*
H30	0.8407	0.3594	0.6047	0.0343	*
H31	0.7922	0.3320	1.1282	0.0315	*
H32	0.8544	0.4090	1.2961	0.0344	*
H33	1.0327	0.4853	1.3168	0.0363	*
H34	1.1470	0.4831	1.1682	0.0360	*
H35	1.1597	0.4467	0.9670	0.0284	*
H36	1.2576	0.3326	0.9370	0.0447	*
H37	1.2636	0.3438	1.0713	0.0447	*
H38	1.1705	0.2850	0.9992	0.0447	*
H39	1.0315	0.3513	0.6882	0.0384	*
H40	1.1517	0.3930	0.7507	0.0384	*
H41	1.1244	0.3081	0.7865	0.0384	*
H42	0.9191	0.4632	0.7392	0.0379	*

Table of Positional Parameters (cont.)

Atom	x	y	z	Ueqv	
H43	0.9339	0.4877	0.8707	0.0379	*
H44	1.0405	0.5016	0.8056	0.0379	*

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
PD1	.01548(9)	.01806(8)	.0146(1)	-.00225(7)	.00366(8)	-.00020(8)
CR1	.0200(2)	.0206(2)	.0179(2)	-.0029(2)	.0049(2)	.0013(2)
C1	.026(1)	.027(1)	.020(2)	-.002(1)	.008(1)	.004(1)
O1	.048(1)	.0262(9)	.031(1)	.004(1)	.012(1)	.000(1)
C2	.025(1)	.036(1)	.029(2)	.000(1)	.006(1)	.002(2)
O2	.027(1)	.079(2)	.036(1)	.006(1)	-.000(1)	.005(2)
C3	.034(2)	.024(1)	.029(2)	-.007(1)	.010(1)	.003(1)
O3	.078(2)	.047(1)	.031(1)	-.018(1)	.034(1)	-.004(1)
C4	.019(1)	.019(1)	.021(2)	.001(1)	.003(1)	.000(1)
C5	.014(1)	.020(1)	.018(1)	-.002(1)	.003(1)	.004(1)
C6	.017(1)	.029(1)	.022(2)	-.003(1)	.000(1)	-.001(1)
C7	.031(2)	.021(1)	.030(2)	.001(1)	.007(1)	.013(1)
C8	.025(1)	.019(1)	.034(2)	-.009(1)	.002(1)	-.002(1)
C9	.025(1)	.021(1)	.022(2)	-.002(1)	.003(1)	.000(1)
C10	.021(1)	.016(1)	.017(1)	.004(1)	.007(1)	.001(1)
C11	.020(1)	.027(1)	.022(2)	-.004(1)	.003(1)	-.009(1)
C12	.036(2)	.030(1)	.021(2)	.003(1)	-.002(1)	-.004(1)
C13	.038(2)	.030(1)	.017(2)	.002(1)	.004(1)	.007(1)
C14	.025(1)	.030(1)	.022(2)	-.000(1)	.005(1)	.013(1)
N1	.019(1)	.0215(9)	.015(1)	.0007(9)	.0045(9)	.001(1)
C15	.018(1)	.018(1)	.019(1)	.002(1)	.003(1)	.000(1)
C16	.020(1)	.025(1)	.020(2)	.001(1)	-.001(1)	-.000(1)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C17	.035(2)	.030(1)	.017(1)	.010(1)	.002(1)	-.002(1)
C18	.042(2)	.029(1)	.024(2)	-.002(1)	-.004(2)	-.006(1)
C19	.030(2)	.029(1)	.027(2)	-.009(1)	-.006(1)	.003(1)
C20	.021(1)	.026(1)	.019(2)	-.002(1)	.002(1)	.003(1)

C21	.019(1)	.031(1)	.025(2)	-.001(1)	.004(1)	.005(1)
C22	.027(2)	.095(3)	.035(2)	-.035(2)	-.002(2)	.010(2)
N2	.016(1)	.0201(9)	.023(1)	.0010(9)	.0062(9)	.005(1)
C23	.025(1)	.030(1)	.030(2)	-.002(1)	.014(1)	-.007(1)
C24	.035(2)	.021(1)	.027(2)	.001(1)	.015(1)	.005(1)
PD2	.01715(9)	.01856(8)	.0153(1)	-.00031(7)	.00573(8)	.00125(8)
CR2	.0199(2)	.0216(2)	.0156(2)	-.0012(2)	.0050(2)	.0016(2)
C25	.031(1)	.034(1)	.017(2)	.001(1)	.008(1)	.003(1)
O4	.055(1)	.0236(9)	.036(1)	.004(1)	.015(1)	.006(1)
C26	.036(2)	.044(2)	.016(2)	.007(1)	.004(1)	-.009(1)
O5	.026(1)	.091(2)	.039(2)	.013(1)	-.009(1)	-.023(2)
C27	.032(1)	.022(1)	.024(2)	-.002(1)	.008(1)	.001(1)
O6	.061(1)	.044(1)	.038(1)	.007(1)	.031(1)	.007(1)
C28	.020(1)	.021(1)	.019(1)	.003(1)	.007(1)	.002(1)
C29	.018(1)	.021(1)	.020(1)	.001(1)	.008(1)	-.003(1)
C30	.020(1)	.024(1)	.020(2)	-.001(1)	.004(1)	.006(1)
C31	.027(1)	.028(1)	.023(2)	.004(1)	.006(1)	.006(1)
C32	.032(2)	.018(1)	.028(2)	-.001(1)	.010(1)	.010(1)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C33	.027(1)	.020(1)	.028(2)	-.002(1)	.008(1)	-.005(1)
C34	.020(1)	.025(1)	.017(1)	.001(1)	.004(1)	-.005(1)
C35	.029(2)	.022(1)	.020(2)	.001(1)	.004(1)	.001(1)
C36	.035(2)	.035(1)	.012(1)	.001(1)	.004(1)	-.005(1)
C37	.045(2)	.034(1)	.019(2)	.002(1)	.015(1)	.002(1)
C38	.031(1)	.026(1)	.024(2)	-.003(1)	.011(1)	-.004(1)
N3	.025(1)	.023(1)	.016(1)	.002(1)	.007(1)	-.000(1)
C39	.022(1)	.019(1)	.015(1)	.002(1)	.003(1)	.003(1)
C40	.022(1)	.031(1)	.020(2)	.003(1)	.005(1)	.006(1)
C41	.028(1)	.035(1)	.017(1)	.007(1)	.006(1)	.000(1)
C42	.033(2)	.031(1)	.018(2)	.009(1)	-.000(1)	-.005(1)

C43	.031(2)	.026(1)	.024(2)	-.002(1)	-.000(1)	-.003(1)
C44	.021(1)	.022(1)	.018(1)	.003(1)	.001(1)	.003(1)
C45	.019(1)	.022(1)	.024(2)	-.003(1)	.006(1)	.000(1)
C46	.026(2)	.039(2)	.038(2)	.004(1)	.005(1)	-.001(2)
N4	.024(1)	.0171(9)	.020(1)	-.0015(9)	.0100(9)	-.003(1)
C47	.025(1)	.037(1)	.029(2)	.001(1)	.014(1)	-.005(1)
C48	.038(2)	.026(1)	.025(2)	.005(1)	.009(1)	.004(1)

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
PD1	C5	1.994(4)	CR2	C29	2.295(4)
PD1	N1	2.158(4)	CR2	C30	2.233(4)
PD1	C15	1.995(4)	CR2	C31	2.196(4)
PD1	N2	2.176(3)	CR2	C32	2.203(4)
CR1	C1	1.822(4)	CR2	C33	2.196(4)
CR1	C2	1.840(4)	PD1	C5	1.994(4)
CR1	C3	1.834(5)	PD1	C15	1.995(4)
CR1	C4	2.270(4)	CR1	C1	1.822(4)
CR1	C5	2.292(4)	CR1	C2	1.840(4)
CR1	C6	2.237(4)	CR1	C3	1.834(5)
CR1	C7	2.222(4)	C1	O1	1.155(5)
CR1	C8	2.240(4)	C2	O2	1.153(5)
CR1	C9	2.248(4)	C3	O3	1.160(5)
PD2	C29	1.977(4)	C4	C5	1.421(6)
PD2	N3	2.157(4)	C4	C9	1.413(5)
PD2	C39	2.003(4)	C4	C10	1.484(6)
PD2	N4	2.200(3)	C5	C6	1.411(6)
CR2	C25	1.845(5)	C6	C7	1.408(6)
CR2	C26	1.828(4)	C7	C8	1.408(6)
CR2	C27	1.851(5)	C8	C9	1.394(6)
CR2	C28	2.258(4)	C10	C11	1.395(6)

Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C10	N1	1.363(5)	C26	O5	1.156(5)
C11	C12	1.383(7)	C27	O6	1.142(5)
C12	C13	1.388(6)	C28	C29	1.439(6)
C13	C14	1.373(6)	C28	C33	1.431(5)
C14	N1	1.342(5)	C28	C34	1.473(6)
C15	C16	1.398(6)	C29	C30	1.418(6)
C15	C20	1.405(5)	C30	C31	1.420(6)
C16	C17	1.392(6)	C31	C32	1.374(6)
C17	C18	1.373(6)	C32	C33	1.396(6)
C18	C19	1.374(7)	C34	C35	1.380(6)
C19	C20	1.399(6)	C34	N3	1.358(5)
C20	C21	1.513(6)	C35	C36	1.382(6)
C21	C22	1.520(5)	C36	C37	1.382(6)
C21	N2	1.515(6)	C37	C38	1.373(6)
N2	C23	1.474(6)	C38	N3	1.352(6)
N2	C24	1.481(5)	C39	C40	1.399(6)
PD2	C29	1.977(4)	C39	C44	1.401(5)
CR2	C25	1.845(5)	C40	C41	1.391(6)
CR2	C26	1.828(4)	C41	C42	1.383(6)
CR2	C27	1.851(5)	C42	C43	1.392(6)
C25	O4	1.175(6)	C43	C44	1.397(6)

Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C44	C45	1.492(6)	N4	C47	1.471(6)
C45	C46	1.538(5)	N4	C48	1.479(5)
C45	N4	1.521(6)			

Table of Bond Angles in Degrees

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C5	PD1	N1	80.4(2)	C3	CR1	C4	162.2(2)
C5	PD1	C15	97.3(2)	C3	CR1	C5	133.1(2)
C5	PD1	N2	165.0(1)	C3	CR1	C6	100.1(2)
N1	PD1	C15	168.6(1)	C3	CR1	C7	85.6(2)
N1	PD1	N2	103.0(1)	C3	CR1	C8	101.2(2)
C15	PD1	N2	82.2(2)	C3	CR1	C9	135.2(2)
C1	CR1	C2	89.7(2)	C4	CR1	C5	36.3(1)
C1	CR1	C3	87.4(2)	C4	CR1	C6	64.5(2)
C1	CR1	C4	104.3(2)	C4	CR1	C7	76.7(2)
C1	CR1	C5	88.6(2)	C4	CR1	C8	65.2(2)
C1	CR1	C6	103.0(2)	C4	CR1	C9	36.4(1)
C1	CR1	C7	136.2(2)	C5	CR1	C6	36.3(2)
C1	CR1	C8	167.0(2)	C5	CR1	C7	66.2(1)
C1	CR1	C9	137.3(2)	C5	CR1	C8	78.4(1)
C2	CR1	C3	87.7(2)	C5	CR1	C9	66.2(1)
C2	CR1	C4	105.5(2)	C6	CR1	C7	36.8(1)
C2	CR1	C5	138.9(2)	C6	CR1	C8	66.1(2)
C2	CR1	C6	165.3(2)	C6	CR1	C9	77.3(2)
C2	CR1	C7	133.1(2)	C7	CR1	C8	36.8(2)
C2	CR1	C8	100.3(2)	C7	CR1	C9	65.5(2)
C2	CR1	C9	88.4(2)	C8	CR1	C9	36.2(2)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C29	PD2	N3	80.9(2)	C27	CR2	C28	166.1(2)
C29	PD2	C39	98.7(2)	C27	CR2	C29	133.9(2)
C29	PD2	N4	168.0(1)	C27	CR2	C30	101.9(2)
N3	PD2	C39	165.3(1)	C27	CR2	C31	88.6(2)
N3	PD2	N4	102.6(1)	C27	CR2	C32	103.8(2)
C39	PD2	N4	80.8(1)	C27	CR2	C33	138.0(2)
C25	CR2	C26	87.8(2)	C28	CR2	C29	36.8(1)
C25	CR2	C27	85.1(2)	C28	CR2	C30	65.4(2)
C25	CR2	C28	102.5(2)	C28	CR2	C31	77.9(2)
C25	CR2	C29	87.3(2)	C28	CR2	C32	66.9(1)
C25	CR2	C30	102.4(2)	C28	CR2	C33	37.5(1)
C25	CR2	C31	136.4(2)	C29	CR2	C30	36.5(2)
C25	CR2	C32	166.9(2)	C29	CR2	C31	66.9(1)
C25	CR2	C33	136.5(2)	C29	CR2	C32	79.6(1)
C26	CR2	C27	87.7(2)	C29	CR2	C33	67.4(1)
C26	CR2	C28	104.0(2)	C30	CR2	C31	37.4(2)
C26	CR2	C29	137.4(2)	C30	CR2	C32	66.6(2)
C26	CR2	C30	166.4(2)	C30	CR2	C33	78.2(2)
C26	CR2	C31	135.0(2)	C31	CR2	C32	36.4(2)
C26	CR2	C32	101.9(2)	C31	CR2	C33	65.9(2)
C26	CR2	C33	88.2(2)	C32	CR2	C33	37.0(2)

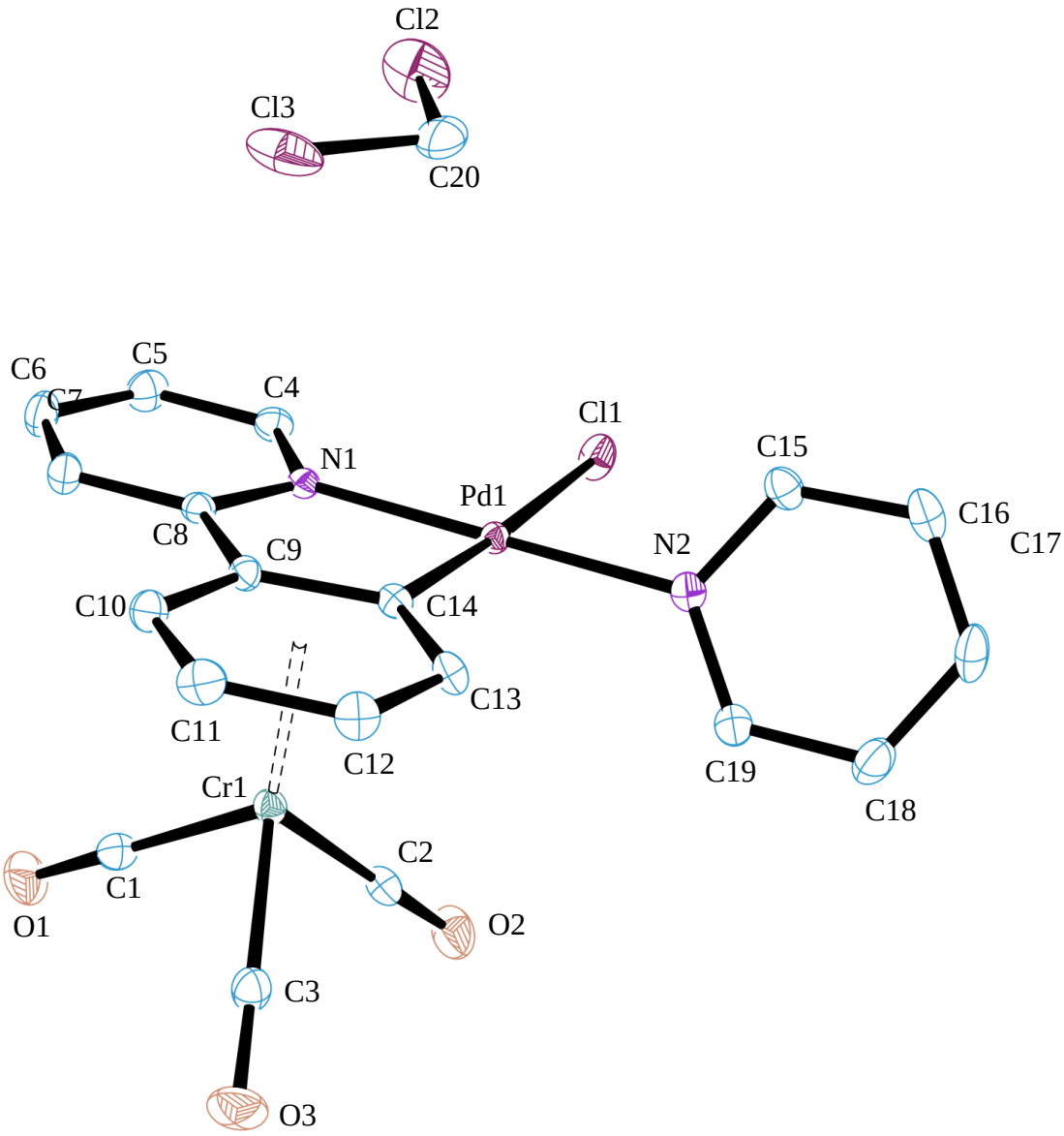
Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C5	PD1	C15	97.3(2)	C11	C12	C13	118.0(4)
C1	CR1	C2	89.7(2)	C12	C13	C14	119.0(4)
C1	CR1	C3	87.4(2)	C13	C14	N1	124.0(4)
C2	CR1	C3	87.7(2)	C10	N1	C14	117.5(4)
CR1	C1	O1	177.5(4)	PD1	C15	C16	128.1(3)
CR1	C2	O2	178.9(4)	PD1	C15	C20	113.0(3)
CR1	C3	O3	178.2(4)	C16	C15	C20	117.5(4)
C5	C4	C9	122.1(4)	C15	C16	C17	120.8(4)
C5	C4	C10	117.0(3)	C16	C17	C18	120.8(5)
C9	C4	C10	120.8(4)	C17	C18	C19	119.7(4)
PD1	C5	C4	114.9(3)	C18	C19	C20	120.3(4)
PD1	C5	C6	128.1(3)	C15	C20	C19	120.8(4)
C4	C5	C6	116.4(3)	C15	C20	C21	115.5(4)
C5	C6	C7	121.9(4)	C19	C20	C21	123.7(4)
C6	C7	C8	120.3(4)	C20	C21	C22	115.3(4)
C7	C8	C9	119.3(3)	C20	C21	N2	107.0(3)
C4	C9	C8	119.9(4)	C22	C21	N2	114.8(4)
C4	C10	C11	125.1(3)	C21	N2	C23	109.7(3)
C4	C10	N1	113.8(3)	C21	N2	C24	111.3(3)
C11	C10	N1	121.1(4)	C23	N2	C24	109.6(4)
C10	C11	C12	120.4(4)	C25	CR2	C26	87.8(2)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C25	CR2	C27	85.1(2)	C35	C36	C37	117.9(4)
C26	CR2	C27	87.7(2)	C36	C37	C38	119.4(5)
CR2	C25	O4	177.0(5)	C37	C38	N3	123.4(4)
CR2	C26	O5	179.5(5)	C34	N3	C38	117.0(4)
CR2	C27	O6	178.5(4)	C40	C39	C44	116.4(4)
C29	C28	C33	120.6(4)	C39	C40	C41	122.9(4)
C29	C28	C34	117.3(3)	C40	C41	C42	119.3(4)
C33	C28	C34	122.2(4)	C41	C42	C43	119.7(4)
PD2	C29	C28	114.2(3)	C42	C43	C44	120.1(4)
PD2	C29	C30	128.7(3)	C39	C44	C43	121.5(4)
C28	C29	C30	116.2(3)	C39	C44	C45	118.3(4)
C29	C30	C31	121.7(4)	C43	C44	C45	120.1(4)
C30	C31	C32	121.4(4)	C44	C45	C46	110.7(3)
C31	C32	C33	119.1(4)	C44	C45	N4	107.1(3)
C28	C33	C32	120.9(4)	C46	C45	N4	113.0(3)
C28	C34	C35	124.3(4)	C45	N4	C47	111.2(3)
C28	C34	N3	113.8(3)	C45	N4	C48	106.7(3)
C35	C34	N3	121.9(4)	C47	N4	C48	109.2(4)
C34	C35	C36	120.3(4)				

Complex (p*S*)-3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C6
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C7
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N1
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Pd1
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C9
C10
C14
C13
C11
C12
Cr1
C19
C18
C2
C1
O1
O2
C3
O3

Table 1 : X-ray experimental data

Formula	: $C_{20}H_{15}Cl_3CrN_2O_3Pd$: $C_{19}H_{13}ClCrN_2O_3Pd \cdot CH_2Cl_2$
Molecular weight	: 596.11
Crystal system	: orthorhombic
Space group	: $P\ 2_1\ 2_1\ 2_1$
a(Å)	: 18.0316(3)
b(Å)	: 18.0653(3)
c(Å)	: 6.6008(1)
$V(Å^3)$	: 2150.19(6)
Z	: 4
Color	: orange
Crystal dim(mm)	: 0.20*0.08*0.03
$Dcalc(gcm^{-3})$	: 1.84
F000	: 1176
$\mu(mm^{-1})$	: 1.739
Trans. min and max	: 0.9449/1.0000
Temperature(K)	: 173
Wavelength(Å)	: 0.71073
Radiation	: MoKα graphite monochromated
Diffractometer	: KappaCCD
Scan mode	: 'phi scans'
hkl limits	: -25,25/-25,25/-9,9
Theta limits(deg)	: 2.5/30.03
Number of data meas.	: 6317
Number of data with I > 3 σ(I)	: 5347
Number of variables	: 271
R	: 0.030
Rw	: 0.036
GOF	: 1.037
Largest peak in final difference ($eÅ^{-3}$)	: 0.893

Table of Positional Parameters and Their E.S.D.

Atom	x	y	z	Ueqv
PD	0.59166(1)	0.85213(1)	0.44461(3)	0.01584(7)
CR	0.40251(2)	0.88822(2)	0.69528(7)	0.0181(2)
CL1	0.71882(4)	0.81290(4)	0.4400(1)	0.0263(3)
C1	0.3776(2)	0.8084(2)	0.8571(5)	0.028(1)
O1	0.3630(1)	0.7583(1)	0.9587(4)	0.040(1)
C2	0.4806(2)	0.9068(2)	0.8671(5)	0.025(1)
O2	0.5302(1)	0.9187(1)	0.9740(4)	0.039(1)
C3	0.3433(2)	0.9460(2)	0.8562(5)	0.026(1)
O3	0.3055(1)	0.9818(1)	0.9587(4)	0.041(1)
N1	0.5485(1)	0.7486(1)	0.4489(4)	0.018(1)
C4	0.5881(2)	0.6848(1)	0.4502(4)	0.023(1)
C5	0.5546(2)	0.6163(2)	0.4505(5)	0.029(1)
C6	0.4780(2)	0.6127(2)	0.4466(5)	0.031(1)
C7	0.4372(2)	0.6767(2)	0.4450(5)	0.026(1)
C8	0.4729(1)	0.7443(1)	0.4447(4)	0.018(1)
C9	0.4371(1)	0.8168(1)	0.4378(4)	0.018(1)
C10	0.3590(2)	0.8266(2)	0.4299(5)	0.025(1)
C11	0.3285(2)	0.8974(2)	0.4269(5)	0.027(1)
C12	0.3754(2)	0.9599(2)	0.4342(5)	0.026(1)
C13	0.4526(1)	0.9506(1)	0.4392(5)	0.023(1)
C14	0.4856(1)	0.8794(1)	0.4397(4)	0.018(1)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
N2	0.6283(1)	0.9584(1)	0.4288(4)	0.020(1)
C15	0.6667(2)	0.9791(2)	0.2627(5)	0.025(1)
C16	0.6989(2)	1.0484(2)	0.2450(5)	0.030(2)
C17	0.6927(2)	1.0976(2)	0.4007(6)	0.030(2)
C18	0.6550(2)	1.0771(2)	0.5740(6)	0.033(2)
C19	0.6234(2)	1.0072(2)	0.5817(5)	0.029(1)
C20	0.6308(2)	0.7378(2)	-0.0540(6)	0.043(2)
CL2	0.69022(6)	0.66115(7)	-0.0585(2)	0.0616(6)
CL3	0.53767(5)	0.71108(7)	-0.0485(2)	0.0498(5)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as one third of the trace of the orthogonalized Uij tensor.

Table of Positional Parameters

Atom	x	y	z	Ueqv	
H1	0.6407	0.6875	0.4509	0.0305	*
H2	0.5836	0.5724	0.4533	0.0383	*
H3	0.4537	0.5660	0.4451	0.0408	*
H4	0.3846	0.6746	0.4440	0.0337	*
H5	0.3274	0.7845	0.4267	0.0325	*
H6	0.2762	0.9037	0.4200	0.0368	*
H7	0.3547	1.0083	0.4357	0.0340	*
H8	0.4836	0.9932	0.4422	0.0301	*
H9	0.6718	0.9449	0.1542	0.0323	*
H10	0.7251	1.0615	0.1255	0.0407	*
H11	0.7141	1.1455	0.3901	0.0445	*
H12	0.6507	1.1101	0.6854	0.0440	*
H13	0.5972	0.9932	0.7005	0.0374	*
H14	0.6393	0.7668	-0.1717	0.0620	*
H15	0.6413	0.7664	0.0633	0.0620	*

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
PD	.01417(8)	.01597(8)	.01757(7)	-.00053(8)	.00061(9)	-.00050(8)
CR	.0155(2)	.0175(2)	.0219(2)	.0007(2)	.0017(2)	.0003(2)
CL1	.0167(3)	.0246(3)	.0443(4)	.0016(3)	-.0032(4)	-.0042(4)
C1	.027(1)	.028(1)	.028(1)	-.001(1)	.004(1)	-.007(1)
O1	.051(1)	.030(1)	.043(1)	-.008(1)	.011(1)	.011(1)
C2	.025(1)	.028(1)	.023(1)	-.003(1)	.006(1)	.003(1)
O2	.034(1)	.060(1)	.030(1)	-.017(1)	-.006(1)	.005(1)
C3	.023(1)	.022(1)	.034(2)	.000(1)	.002(1)	-.001(1)
O3	.038(1)	.041(1)	.045(1)	.014(1)	.013(1)	-.009(1)
N1	.021(1)	.017(1)	.0158(9)	-.0013(9)	.002(1)	-.000(1)
C4	.024(1)	.023(1)	.023(1)	.004(1)	.002(1)	-.001(1)
C5	.037(2)	.020(1)	.032(1)	.003(1)	-.001(2)	.001(2)
C6	.036(2)	.023(1)	.035(1)	-.010(1)	-.001(2)	.001(2)
C7	.025(1)	.025(1)	.028(1)	-.006(1)	-.000(1)	.000(1)
C8	.019(1)	.022(1)	.015(1)	-.000(1)	.000(1)	-.001(1)
C9	.017(1)	.021(1)	.017(1)	-.002(1)	-.001(1)	.001(1)
C10	.020(1)	.029(1)	.026(1)	-.003(1)	-.001(1)	-.002(1)
C11	.019(1)	.035(1)	.031(1)	.007(1)	-.004(1)	-.003(1)
C12	.024(1)	.023(1)	.031(1)	.006(1)	-.003(1)	.004(1)
C13	.021(1)	.024(1)	.024(1)	-.002(1)	.004(1)	.006(1)
C14	.016(1)	.021(1)	.016(1)	.001(1)	-.001(1)	.002(1)
N2	.017(1)	.019(1)	.025(1)	.0023(9)	.000(1)	.002(1)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C15	.021(1)	.025(1)	.029(1)	.003(1)	.004(1)	.004(1)
C16	.024(1)	.028(2)	.042(2)	-.000(1)	.007(1)	.012(1)
C17	.027(2)	.017(1)	.058(2)	-.003(1)	.002(2)	.005(1)
C18	.036(2)	.023(1)	.042(2)	-.002(1)	.000(2)	-.007(2)

C19	.029(1)	.026(1)	.031(2)	-.004(1)	.005(1)	-.001(1)
C20	.073(2)	.046(2)	.023(1)	-.014(2)	-.006(2)	-.000(2)
CL2	.0383(5)	.0852(7)	.0717(6)	.0196(5)	.0032(5)	.0026(7)
CL3	.0429(5)	.1057(8)	.0273(4)	.0235(5)	.0007(4)	.0021(6)

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
PD	CL1	2.4001(7)	C5	C6	1.384(5)
PD	N1	2.026(2)	C6	C7	1.371(5)
PD	C14	1.975(3)	C7	C8	1.380(4)
PD	N2	2.034(2)	C8	C9	1.462(4)
CR	C1	1.850(4)	C9	C10	1.419(4)
CR	C2	1.839(3)	C9	C14	1.430(4)
CR	C3	1.833(3)	C10	C11	1.394(4)
CR	C9	2.223(3)	C11	C12	1.412(4)
CR	C10	2.219(3)	C12	C13	1.402(4)
CR	C11	2.224(3)	C13	C14	1.417(4)
CR	C12	2.211(4)	N2	C15	1.349(4)
CR	C13	2.224(3)	N2	C19	1.343(4)
CR	C14	2.262(3)	C15	C16	1.386(5)
C1	O1	1.157(4)	C16	C17	1.363(5)
C2	O2	1.160(4)	C17	C18	1.382(5)
C3	O3	1.157(4)	C18	C19	1.385(5)
N1	C4	1.355(4)	C20	CL2	1.750(4)
N1	C8	1.365(3)	C20	CL3	1.748(5)
C4	C5	1.376(4)			

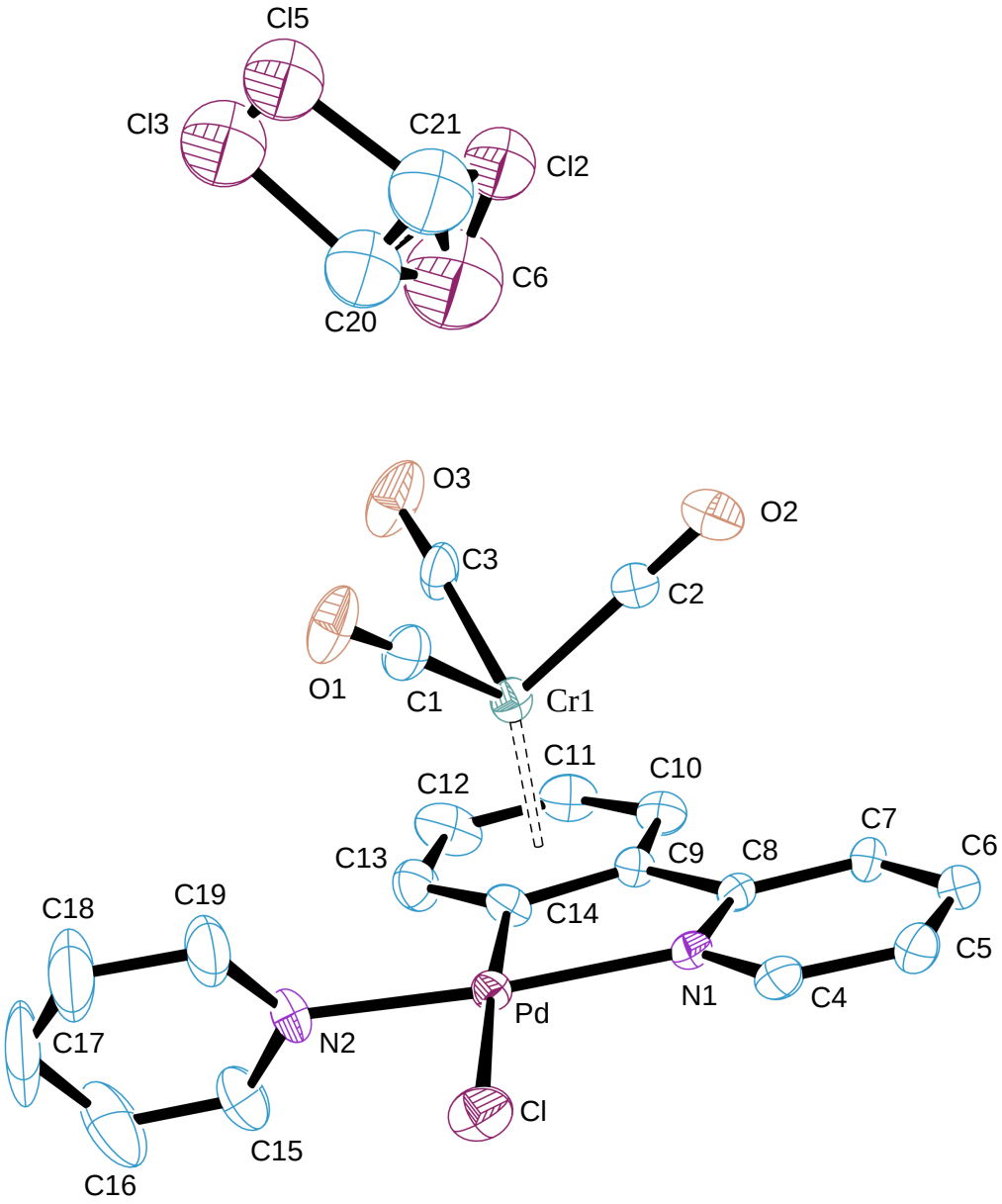
Table of Bond Angles in Degrees

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
CL1	PD	N1	95.43(7)	C3	CR	C9	159.5(1)
CL1	PD	C14	176.83(9)	C3	CR	C10	122.5(1)
CL1	PD	N2	88.16(7)	C3	CR	C11	94.0(1)
N1	PD	C14	81.9(1)	C3	CR	C12	89.4(1)
N1	PD	N2	175.8(1)	C3	CR	C13	112.9(1)
C14	PD	N2	94.5(1)	C3	CR	C14	149.1(1)
C1	CR	C2	88.4(1)	C9	CR	C10	37.3(1)
C1	CR	C3	88.2(1)	C9	CR	C11	66.6(1)
C1	CR	C9	93.3(1)	C9	CR	C12	78.8(1)
C1	CR	C10	88.8(1)	C9	CR	C13	66.4(1)
C1	CR	C11	111.9(1)	C9	CR	C14	37.2(1)
C1	CR	C12	148.6(1)	C10	CR	C11	36.6(1)
C1	CR	C13	158.9(1)	C10	CR	C12	66.5(1)
C1	CR	C14	122.5(1)	C10	CR	C13	78.3(1)
C2	CR	C3	89.1(1)	C10	CR	C14	67.1(1)
C2	CR	C9	111.3(1)	C11	CR	C12	37.1(1)
C2	CR	C10	148.1(1)	C11	CR	C13	66.5(1)
C2	CR	C11	159.5(1)	C11	CR	C14	79.0(1)
C2	CR	C12	122.9(1)	C12	CR	C13	36.9(1)
C2	CR	C13	93.7(1)	C12	CR	C14	66.8(1)
C2	CR	C14	88.0(1)	C13	CR	C14	36.8(1)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C4	N1	C8	118.5(2)	C10	C11	C12	119.8(3)
N1	C4	C5	122.2(3)	C11	C12	C13	120.0(3)
C4	C5	C6	118.7(3)	C12	C13	C14	121.7(3)
C5	C6	C7	119.7(3)	C9	C14	C13	117.4(2)
C6	C7	C8	119.8(3)	C15	N2	C19	117.6(3)
N1	C8	C7	121.1(3)	N2	C15	C16	122.2(3)
N1	C8	C9	113.1(2)	C15	C16	C17	119.4(3)
C7	C8	C9	125.9(3)	C16	C17	C18	119.3(3)
C8	C9	C10	123.4(3)	C17	C18	C19	118.5(3)
C8	C9	C14	116.0(2)	N2	C19	C18	122.9(3)
C10	C9	C14	120.6(3)	CL2	C20	CL3	111.7(2)
C9	C10	C11	120.4(3)				

Complex (p*R*)-3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C7
C6
C13
C9
C8
C18
C19
C14
C5
N1
C4
Pd
C17
N2
Cl
C15
C16

Table 1 : X-ray experimental data

Formula	: $C_{20}H_{15}Cl_3CrN_2O_3Pd$: $C_{19}H_{13}ClCrN_2O_3Pd \cdot CH_2Cl_2$
Molecular weight	: 596.11
Crystal system	: monoclinic
Space group	: $P\,2_1$
a(Å)	: 6.4747(2)
b(Å)	: 12.4324(3)
c(Å)	: 14.0935(5)
β(deg)	: 96.103(5)
$V(Å^3)$	: 1128.04(6)
Z	: 2
Color	: orange
Crystal dim(mm)	: 0.20*0.16*0.10
$Dcalc(gcm^{-3})$	: 1.75
F000	: 588
$\mu(mm^{-1})$	: 1.658
Trans. min and max	: 0.9592/1.0000
Temperature(K)	: 173
Wavelength(Å)	: 0.71073
Radiation	: MoKα graphite monochromated
Diffractometer	: KappaCCD
Scan mode	: 'phi scans'
hkl limits	: -9,9/-17,17/-19,19
Theta limits(deg)	: 2.5/30.04
Number of data meas.	: 6353
Number of data with I > 3 σ(I)	: 2879
Number of variables	: 255
R	: 0.040
Rw	: 0.057
GOF	: 1.129
Largest peak in final difference ($eÅ^{-3}$)	: 1.137

Table of Positional Parameters and Their E.S.D.

Atom	x	y	z	Ueqv
PD	0.14400(5)	0.2750	0.17214(2)	0.0297(1)
CR	-0.1062(1)	0.55527(9)	0.18650(7)	0.0348(4)
CL1	0.4170(3)	0.1457(1)	0.1815(1)	0.0511(8)
C1	0.108(1)	0.5397(6)	0.2834(5)	0.048(3)
O1	0.2317(8)	0.5280(5)	0.3463(3)	0.061(3)
C2	0.0569(9)	0.6520(5)	0.1269(5)	0.037(3)
O2	0.1638(7)	0.7091(5)	0.0907(4)	0.057(3)
C3	-0.203(1)	0.6686(6)	0.2552(4)	0.051(3)
O3	-0.270(1)	0.7353(5)	0.2978(4)	0.083(3)
N1	0.2021(7)	0.3381(4)	0.0442(3)	0.030(2)
C4	0.3596(9)	0.3118(5)	-0.0047(4)	0.039(3)
C5	0.391(1)	0.3567(6)	-0.0911(5)	0.045(3)
C6	0.250(1)	0.4338(5)	-0.1289(5)	0.046(3)
C7	0.083(1)	0.4636(5)	-0.0798(4)	0.037(3)
C8	0.0628(8)	0.4133(4)	0.0075(4)	0.029(2)
C9	-0.1010(9)	0.4373(5)	0.0699(4)	0.032(2)
C10	-0.2639(9)	0.5126(6)	0.0446(4)	0.039(3)
C11	-0.420(1)	0.5299(6)	0.1046(6)	0.050(4)
C12	-0.406(1)	0.4743(6)	0.1914(7)	0.057(4)
C13	-0.246(1)	0.3971(6)	0.2163(5)	0.049(3)
C14	-0.0883(8)	0.3778(5)	0.1566(4)	0.036(3)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv	
N2	0.0808(9)	0.2241(5)	0.3033(4)	0.047(3)	
C15	-0.093(1)	0.1675(7)	0.3140(6)	0.062(4)	
C16	-0.116(1)	0.124(1)	0.4001(8)	0.101(6)	
C17	0.000(4)	0.152(2)	0.4791(7)	0.13(1)	
C18	0.185(2)	0.203(1)	0.4647(6)	0.100(7)	
C19	0.213(2)	0.2443(9)	0.3775(6)	0.075(5)	
C20	0.2721(7)	0.8249(5)	0.3865(4)	0.109(8)	*
CL2	0.3045	0.9372	0.3093	0.095(2)	*
CL3	0.3398	0.8882	0.5087	0.132(3)	*
C21	0.373(1)	0.8832(6)	0.3566(4)	0.13(1)	*
CL5	0.4280	0.9354	0.4804	0.115(2)	*
Cl4	0.1703	0.8563	0.3159	0.188(4)	*

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as one third of the trace of the orthogonalized Uij tensor. Starred atoms were refined isotropically.

Table of Positional Parameters

Atom	x	y	z	Ueqv	
H1	0.4554	0.2591	0.0215	0.0508	*
H2	0.5058	0.3358	-0.1238	0.0586	*
H3	0.2673	0.4663	-0.1886	0.0607	*
H4	-0.0137	0.5165	-0.1048	0.0517	*
H5	-0.2666	0.5515	-0.0135	0.0529	*
H6	-0.5317	0.5778	0.0869	0.0675	*
H7	-0.5056	0.4882	0.2349	0.0809	*
H8	-0.2453	0.3580	0.2742	0.0628	*
H9	-0.1979	0.1586	0.2620	0.0798	*
H10	-0.2198	0.0707	0.4040	0.1336	*
H11	-0.0400	0.1380	0.5409	0.2368	*
H12	0.2925	0.2085	0.5158	0.1505	*
H13	0.3302	0.2886	0.3707	0.1102	*

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
PD	.0333(1)	.0270(1)	.0290(1)	.0008(2)	.0014(1)	.0011(2)
CR	.0314(4)	.0366(4)	.0368(4)	.0063(3)	.0100(3)	-.0009(4)
CL1	.0530(8)	.0437(8)	.0576(9)	.0177(6)	-.0092(7)	-.0044(7)
C1	.047(3)	.054(4)	.043(3)	.011(3)	.013(2)	-.006(3)
O1	.068(3)	.098(4)	.035(2)	.037(3)	-.004(2)	-.006(3)
C2	.033(3)	.037(3)	.042(3)	.004(2)	.002(2)	-.001(2)
O2	.053(3)	.046(2)	.075(3)	-.006(2)	-.001(2)	.008(3)
C3	.079(4)	.052(4)	.032(3)	.020(3)	.019(3)	.002(3)
O3	.117(4)	.092(3)	.054(3)	.067(3)	.003(3)	-.015(3)
N1	.033(2)	.029(2)	.027(2)	-.004(2)	.001(2)	-.005(2)
C4	.045(3)	.032(3)	.040(3)	.002(2)	.009(2)	-.007(2)
C5	.054(3)	.046(3)	.038(3)	-.004(3)	.016(2)	-.007(3)
C6	.068(4)	.038(3)	.037(3)	-.013(3)	.017(3)	-.004(3)
C7	.060(3)	.037(3)	.023(2)	-.004(3)	.005(2)	.000(2)
C8	.033(2)	.027(2)	.027(2)	.001(2)	.004(2)	-.003(2)
C9	.035(2)	.031(2)	.031(2)	-.002(2)	.003(2)	.000(2)
C10	.030(2)	.042(3)	.049(3)	-.003(2)	-.004(2)	-.002(3)
C11	.039(3)	.045(3)	.072(5)	.006(3)	.005(3)	-.005(3)
C12	.033(2)	.051(4)	.109(5)	.002(3)	.035(3)	-.001(4)
C13	.048(3)	.050(4)	.050(3)	.000(3)	.020(3)	.003(3)
C14	.034(2)	.030(2)	.045(3)	-.001(2)	.008(2)	.004(2)
N2	.066(3)	.043(3)	.036(2)	-.001(3)	.006(2)	.015(2)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C15	.057(3)	.066(4)	.065(4)	-.007(4)	.021(3)	.021(4)
C16	.079(5)	.119(6)	.111(7)	-.037(4)	.013(4)	.058(5)
C17	.30(2)	.21(1)	.037(5)	-.08(1)	.014(8)	.047(6)
C18	.139(9)	.16(1)	.045(4)	-.055(8)	.003(5)	.031(6)

C19	.117(7)	.095(6)	.039(4)	-.040(5)	-.010(4)	.022(4)

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
PD	CL1	2.382(2)	C7	C8	1.399(9)
PD	N1	2.039(5)	C8	C9	1.478(8)
PD	C14	1.969(6)	C9	C10	1.427(9)
PD	N2	2.036(6)	C9	C14	1.424(9)
CR	C1	1.851(8)	C10	C11	1.40(1)
CR	C2	1.859(7)	C11	C12	1.40(1)
CR	C3	1.856(8)	C12	C13	1.43(1)
CR	C9	2.206(6)	C13	C14	1.409(9)
CR	C10	2.211(7)	N2	C15	1.35(1)
CR	C11	2.250(8)	N2	C19	1.30(1)
CR	C12	2.195(8)	C15	C16	1.35(1)
CR	C13	2.223(8)	C16	C17	1.32(2)
CR	C14	2.251(7)	C17	C18	1.39(3)
C1	O1	1.139(9)	C18	C19	1.36(1)
C2	O2	1.148(9)	C20	CL2	1.796(7)
C3	O3	1.14(1)	C20	CL3	1.901(6)
N1	C4	1.330(8)	C20	C21	1.089(9)
N1	C8	1.362(8)	C20	Cl4	1.199(6)
C4	C5	1.37(1)	CL2	C21	1.013(8)
C5	C6	1.39(1)	CL2	Cl4	1.3386
C6	C7	1.39(1)	C21	CL5	1.860(8)

Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C21	Cl4	1.414(8)			

Table of Bond Angles in Degrees

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
CL1	PD	N1	95.9(2)	C3	CR	C9	157.9(3)
CL1	PD	C14	176.4(2)	C3	CR	C10	120.3(3)
CL1	PD	N2	87.7(2)	C3	CR	C11	92.2(4)
N1	PD	C14	82.1(2)	C3	CR	C12	89.0(4)
N1	PD	N2	175.4(3)	C3	CR	C13	114.0(3)
C14	PD	N2	94.5(3)	C3	CR	C14	150.3(3)
C1	CR	C2	89.0(3)	C9	CR	C10	37.7(2)
C1	CR	C3	87.9(3)	C9	CR	C11	67.0(3)
C1	CR	C9	114.2(3)	C9	CR	C12	78.6(3)
C1	CR	C10	151.7(3)	C9	CR	C13	65.9(3)
C1	CR	C11	158.3(3)	C9	CR	C14	37.2(2)
C1	CR	C12	121.7(4)	C10	CR	C11	36.6(3)
C1	CR	C13	93.2(3)	C10	CR	C12	66.0(3)
C1	CR	C14	89.2(3)	C10	CR	C13	78.5(3)
C2	CR	C3	89.1(3)	C10	CR	C14	67.9(3)
C2	CR	C9	92.2(3)	C11	CR	C12	36.7(4)
C2	CR	C10	88.7(3)	C11	CR	C13	67.0(3)
C2	CR	C11	112.6(3)	C11	CR	C14	80.1(3)
C2	CR	C12	149.1(4)	C12	CR	C13	37.8(3)
C2	CR	C13	156.9(3)	C12	CR	C14	67.7(3)
C2	CR	C14	120.4(3)	C13	CR	C14	36.7(2)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C4	N1	C8	119.0(5)	C17	C18	C19	120(1)
N1	C4	C5	123.7(7)	N2	C19	C18	120(1)
C4	C5	C6	117.7(6)	CL2	C20	CL3	101.3(3)
C5	C6	C7	120.4(7)	CL2	C20	C21	30.1(4)
C6	C7	C8	118.0(7)	CL2	C20	Cl4	48.2(2)
N1	C8	C7	121.3(6)	CL3	C20	C21	89.2(6)
N1	C8	C9	113.7(5)	CL3	C20	Cl4	132.1(5)
C7	C8	C9	125.0(6)	C21	C20	Cl4	76.1(6)
C8	C9	C10	122.9(6)	C20	CL2	C21	32.6(5)
C8	C9	C14	115.2(5)	C20	CL2	Cl4	41.9(2)
C10	C9	C14	121.9(6)	C21	CL2	Cl4	72.4(5)
C9	C10	C11	120.8(6)	C20	C21	CL2	117.3(8)
C10	C11	C12	117.9(7)	C20	C21	CL5	86.1(6)
C11	C12	C13	121.5(7)	C20	C21	Cl4	55.5(5)
C12	C13	C14	121.4(7)	CL2	C21	CL5	114.4(7)
C9	C14	C13	116.4(6)	CL2	C21	Cl4	64.5(4)
C15	N2	C19	119.8(8)	CL5	C21	Cl4	122.8(5)
N2	C15	C16	118(1)	C20	Cl4	CL2	89.9(3)
C15	C16	C17	123(1)	C20	Cl4	C21	48.4(4)
C16	C17	C18	114(1)	CL2	Cl4	C21	43.1(3)