Supplementary Information

Table 1SI: Crystallographic Data for the Ttwo Complexes [Pd(η^3–C_3H_5)(IMes)(DIC)](ClO_4) (left) and [Pd(η^3–1,1-$Me_2C_3H_3$)(IMes)(PPh_3)] (ClO_4) (right)

Empirical formula	$C_{33}H_{38}N_3O_4ClPd$	$C_{44}H_{48}N_2O_4PClPd$
Formula weight	682.51	841.66
Wavelength (Å) / Temperature (K)	0.71073 / 150.0	0.71073 / 150.0
Crystal system	monoclinic	monoclinic
Crystal size	0.50 × 0.22 × 0.11	0.30 × 0.08 × 0.08
Space group	*P* $2_1/c$ (No. 14)	*P* $2_1/n$ (No. 14)
a (Å)	12.8436(1)	10.5270(2)
b (Å)	13.2013(1)	19.8437(4)
c (Å)	19.8990(2)	19.0977(4)
β (deg)	107.063(1)	89.893(2)
Volume ($Å^3$)	3225.4(1)	3989.4(1)
Z (molecules/unit cell)	4	4
Calculated density (Mg m^{-3})	1.406	1.401
Absorption coefficient, μ (cm^{-1})	6.98	6.17
F(000)	1408	1744
Total reflections	48218	52550
Independent (unique) reflections / R_{int}	7959 / 0.027	8271 / 0.080
Observed reflections [$I > 2\sigma(I)$]	6699	4843
Data / parameters / restraints	7959 / 395 / 0	8271 / 475 / 0
Goodness–of–fit [a] on F^2	1.080	0.802
Final *R* indices [$I > 2\sigma(I)$]	R_1 [b] = 0.0264; wR_2 [c] = 0.0750	R_1 [b] = 0.0338; wR_2 [c] = 0.0586
Largest difference peak and hole ($eÅ^{-3}$)	0.442 and –0.592	0.364 and –0.430

[a] Goodness–of–fit = $[\Sigma (w (F_o^2 - F_c^2)^2)] / (N_{obsevns} - N_{params})]^{1/2}$, based on all data;

[b] $R_1 = \Sigma (|F_o| - |F_c|) / \Sigma |F_o|$;

[c] $wR_2 = [\Sigma[w (F_o^2 - F_c^2)^2] / \Sigma[w (F_o^2)^2]]^{1/2}$.

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data_exp_63

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'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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 '-x, -y, -z'
 'x-1/2, -y-1/2, z-1/2'

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(compiled Nov  6 2009,16:24:50)
Empirical absorption correction using spherical harmonics,
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. 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.
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O2 O 0.82936(19) 0.05023(11) 0.85385(11) 0.0419(6) Uani 1 1 d . . .
O3 O 0.9428(2) 0.01541(11) 0.75484(12) 0.0480(6) Uani 1 1 d . . .
O4 O 0.7250(2) 0.03922(12) 0.74607(12) 0.0525(7) Uani 1 1 d . . .
N1 N 0.1299(2) 0.19314(11) 1.02035(11) 0.0204(6) Uani 1 1 d . . .
N2 N 0.2477(2) 0.10933(11) 0.99115(12) 0.0215(6) Uani 1 1 d . . .
C1 C 0.2096(2) 0.17178(14) 0.96887(14) 0.0199(7) Uani 1 1 d . B .
C2 C 0.1200(3) 0.14538(15) 1.07319(15) 0.0273(7) Uani 1 1 d . B .
H2A H 0.0715 0.1489 1.1137 0.033 Uiso 1 1 calc R . .
C3 C 0.1931(3) 0.09368(15) 1.05487(15) 0.0263(7) Uani 1 1 d . B .
H3A H 0.2053 0.0542 1.0803 0.032 Uiso 1 1 calc R . .
C4 C 0.0549(3) 0.25396(14) 1.01999(14) 0.0194(7) Uani 1 1 d . B .
C5 C -0.0548(3) 0.25582(14) 0.97888(15) 0.0211(7) Uani 1 1 d . . .
C6 C -0.1264(3) 0.31488(15) 0.98023(15) 0.0247(7) Uani 1 1 d . B .
H6A H -0.2000 0.3172 0.9534 0.030 Uiso 1 1 calc R . .
C7 C -0.0916(3) 0.37030(15) 1.02023(16) 0.0275(8) Uani 1 1 d . . .
C8 C 0.0153(3) 0.36426(15) 1.06271(15) 0.0279(8) Uani 1 1 d . B .
H8A H 0.0380 0.4003 1.0912 0.034 Uiso 1 1 calc R . .
C9 C 0.0890(3) 0.30676(15) 1.06410(14) 0.0239(7) Uani 1 1 d . . .
C10 C -0.0993(3) 0.19630(14) 0.93698(16) 0.0329(8) Uani 1 1 d . B .
H10A H -0.1761 0.2078 0.9126 0.049 Uiso 1 1 calc R . .
H10B H -0.1152 0.1590 0.9678 0.049 Uiso 1 1 calc R . .
H10C H -0.0350 0.1840 0.9038 0.049 Uiso 1 1 calc R . .
C11 C -0.1690(3) 0.43419(15) 1.01828(17) 0.0386(9) Uani 1 1 d . B .
H11A H -0.2388 0.4287 0.9864 0.058 Uiso 1 1 calc R . .
H11B H -0.1165 0.4708 1.0029 0.058 Uiso 1 1 calc R . .
H11C H -0.2010 0.4437 1.0643 0.058 Uiso 1 1 calc R . .
C12 C 0.1994(3) 0.30049(15) 1.11383(14) 0.0331(8) Uani 1 1 d . B .
H12A H 0.2088 0.3416 1.1398 0.050 Uiso 1 1 calc R . .
H12B H 0.2756 0.2919 1.0878 0.050 Uiso 1 1 calc R . .
H12C H 0.1843 0.2639 1.1457 0.050 Uiso 1 1 calc R . .
C13 C 0.3249(3) 0.06242(14) 0.95248(14) 0.0205(7) Uani 1 1 d . B .
C14 C 0.2668(3) 0.00424(15) 0.92692(15) 0.0243(7) Uani 1 1 d . . .
C15 C 0.3412(3) -0.04065(15) 0.89010(15) 0.0271(7) Uani 1 1 d . B .
H15A H 0.3038 -0.0798 0.8729 0.033 Uiso 1 1 calc R . .
C16 C 0.4695(3) -0.02991(15) 0.87760(15) 0.0262(8) Uani 1 1 d . . .
C17 C 0.5221(3) 0.02866(15) 0.90294(15) 0.0259(7) Uani 1 1 d . B .
H17A H 0.6072 0.0374 0.8938 0.031 Uiso 1 1 calc R . .
C18 C 0.4532(3) 0.07516(14) 0.94155(14) 0.0228(7) Uani 1 1 d . . .
C19 C 0.1269(3) -0.00994(16) 0.93678(17) 0.0375(9) Uani 1 1 d . B .
H19A H 0.0892 0.0257 0.9636 0.056 Uiso 1 1 calc R . .
H19B H 0.1166 -0.0519 0.9612 0.056 Uiso 1 1 calc R . .
H19C H 0.0862 -0.0127 0.8919 0.056 Uiso 1 1 calc R . .
C20 C 0.5470(3) -0.08076(16) 0.83672(16) 0.0351(8) Uani 1 1 d . B .
H20A H 0.6334 -0.0655 0.8336 0.053 Uiso 1 1 calc R . .
H20B H 0.5122 -0.0855 0.7905 0.053 Uiso 1 1 calc R . .
H20C H 0.5447 -0.1235 0.8602 0.053 Uiso 1 1 calc R . .
C21 C 0.5176(3) 0.13662(14) 0.97062(16) 0.0296(8) Uani 1 1 d . B .
H21A H 0.6054 0.1365 0.9572 0.044 Uiso 1 1 calc R . .
H21B H 0.5113 0.1364 1.0208 0.044 Uiso 1 1 calc R . .

H21C H 0.4771 0.1763 0.9525 0.044 Uiso 1 1 calc R . .
C24 C 0.1658(3) 0.13296(15) 0.81821(15) 0.0350(8) Uani 1 1 d . B .
H24A H 0.1894 0.0880 0.8332 0.042 Uiso 1 1 calc R A 1
H24B H 0.0760 0.1376 0.8080 0.042 Uiso 1 1 calc R A 1
C27 C 0.2612(3) 0.38411(14) 0.85842(14) 0.0197(7) Uani 1 1 d . . .
C28 C 0.1355(3) 0.38474(14) 0.88129(15) 0.0254(7) Uani 1 1 d . B .
H28A H 0.1078 0.3522 0.9128 0.031 Uiso 1 1 calc R . .
C29 C 0.0518(3) 0.43308(16) 0.85769(15) 0.0306(8) Uani 1 1 d . . .
H29A H -0.0316 0.4331 0.8736 0.037 Uiso 1 1 calc R B .
C30 C 0.0910(3) 0.48139(16) 0.81071(16) 0.0330(8) Uani 1 1 d . B .
H30A H 0.0342 0.5137 0.7945 0.040 Uiso 1 1 calc R . .
C31 C 0.2150(3) 0.48138(15) 0.78792(16) 0.0323(8) Uani 1 1 d . . .
H31A H 0.2417 0.5142 0.7565 0.039 Uiso 1 1 calc R B .
C32 C 0.3003(3) 0.43328(14) 0.81104(14) 0.0250(7) Uani 1 1 d . B .
H32A H 0.3836 0.4337 0.7950 0.030 Uiso 1 1 calc R . .
C33 C 0.4103(3) 0.35005(14) 0.97886(14) 0.0211(7) Uani 1 1 d . . .
C34 C 0.3596(3) 0.40761(15) 1.00868(16) 0.0309(8) Uani 1 1 d . B .
H34A H 0.2939 0.4302 0.9861 0.037 Uiso 1 1 calc R . .
C35 C 0.4055(3) 0.43182(17) 1.07141(17) 0.0396(9) Uani 1 1 d . . .
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C36 C 0.5022(3) 0.39933(18) 1.10595(17) 0.0382(9) Uani 1 1 d . B .
H36A H 0.5325 0.4157 1.1484 0.046 Uiso 1 1 calc R . .
C37 C 0.5538(3) 0.34205(17) 1.07666(16) 0.0353(8) Uani 1 1 d . . .
H37A H 0.6198 0.3199 1.0994 0.042 Uiso 1 1 calc R B .
C38 C 0.5083(3) 0.31728(15) 1.01383(15) 0.0295(8) Uani 1 1 d . B .
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C39 C 0.5149(3) 0.31952(14) 0.84997(14) 0.0212(7) Uani 1 1 d . . .
C40 C 0.5858(3) 0.37836(15) 0.84471(15) 0.0272(8) Uani 1 1 d . B .
H40A H 0.5539 0.4183 0.8631 0.033 Uiso 1 1 calc R . .
C41 C 0.7033(3) 0.37811(18) 0.81243(16) 0.0369(9) Uani 1 1 d . . .
H41A H 0.7482 0.4181 0.8072 0.044 Uiso 1 1 calc R B .
C42 C 0.7539(3) 0.31846(19) 0.78799(16) 0.0381(9) Uani 1 1 d . B .
H42A H 0.8332 0.3185 0.7667 0.046 Uiso 1 1 calc R . .
C43 C 0.6882(3) 0.25893(18) 0.79479(15) 0.0350(9) Uani 1 1 d . . .
H43A H 0.7237 0.2186 0.7796 0.042 Uiso 1 1 calc R B .
C44 C 0.5675(3) 0.25991(15) 0.82479(14) 0.0269(7) Uani 1 1 d . B .
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C23 C 0.2518(4) 0.1660(2) 0.77099(19) 0.0261(12) Uiso 0.769(5) 1 d P B 1
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C25 C 0.1029(4) 0.2635(2) 0.7501(2) 0.0395(13) Uiso 0.769(5) 1 d P B 1
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H26C H 0.3460 0.3122 0.7228 0.054 Uiso 0.769(5) 1 calc PR B 1
C22A C 0.2721(13) 0.2172(8) 0.7541(6) 0.013(3) Uiso 0.231(5) 1 d P B 2
C23A C 0.1597(14) 0.1923(7) 0.7788(7) 0.030(4) Uiso 0.231(5) 1 d P B 2
H23B H 0.0783 0.2132 0.7666 0.036 Uiso 0.231(5) 1 calc PR B 2

C25A C 0.3752(12) 0.1682(7) 0.7360(7) 0.039(4) Uiso 0.231(5) 1 d P B 2
H25D H 0.3871 0.1676 0.6862 0.058 Uiso 0.231(5) 1 calc PR B 2
H25E H 0.3518 0.1240 0.7518 0.058 Uiso 0.231(5) 1 calc PR B 2
H25F H 0.4529 0.1817 0.7584 0.058 Uiso 0.231(5) 1 calc PR B 2
C26A C 0.2722(14) 0.2815(7) 0.7108(6) 0.026(3) Uiso 0.231(5) 1 d P B 2
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O3 0.0460(15) 0.0292(13) 0.0690(17) -0.0101(12) 0.0172(12) 0.0128(12)
O4 0.0408(16) 0.0582(17) 0.0586(16) -0.0044(13) -0.0163(13) -0.0140(13)
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C39 0.0261(17) 0.0198(17) 0.0176(16) -0.0003(13) 0.0001(13) 0.0008(14)
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C42 0.0243(19) 0.058(3) 0.032(2) 0.0123(19) 0.0080(15) 0.0063(19)
C43 0.038(2) 0.045(2) 0.0224(18) 0.0020(16) 0.0058(16) 0.0207(19)
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are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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Cl O3 1.434(2) . ?
Cl O2 1.435(2) . ?
Cl O1 1.438(2) . ?
P C39 1.826(3) . ?
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(compiled Nov 6 2009,16:24:50)

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Empirical absorption correction using spherical harmonics,
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omega____ theta____ kappa____ phi______ frames
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness 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 threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. 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.
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N2 N 0.38940(12) 0.81342(11) 0.53735(7) 0.0222(3) Uani 1 1 d . . .
N3 N 0.10118(13) 0.66293(12) 0.50970(8) 0.0268(3) Uani 1 1 d . . .
C1 C 0.36059(14) 0.76272(12) 0.47554(9) 0.0208(3) Uani 1 1 d . . .
C2 C 0.49867(14) 0.79850(15) 0.57332(10) 0.0268(4) Uani 1 1 d . . .
H2A H 0.5366 0.8258 0.6167 0.032 Uiso 1 1 calc R . .
C3 C 0.53862(15) 0.73713(14) 0.53328(10) 0.0267(4) Uani 1 1 d . . .
H3A H 0.6098 0.7136 0.5436 0.032 Uiso 1 1 calc R . .
C4 C 0.46167(14) 0.65112(13) 0.41620(9) 0.0233(3) Uani 1 1 d . . .
C5 C 0.52799(15) 0.68195(14) 0.37533(10) 0.0267(4) Uani 1 1 d . . .
C6 C 0.53073(16) 0.62114(15) 0.31883(10) 0.0317(4) Uani 1 1 d . . .
H6A H 0.5742 0.6402 0.2909 0.038 Uiso 1 1 calc R . .
C7 C 0.46994(16) 0.53229(16) 0.30301(10) 0.0335(4) Uani 1 1 d . . .
C8 C 0.40806(16) 0.50297(15) 0.34599(11) 0.0331(4) Uani 1 1 d . . .
H8A H 0.3684 0.4430 0.3360 0.040 Uiso 1 1 calc R . .
C9 C 0.40308(14) 0.56031(14) 0.40386(10) 0.0269(4) Uani 1 1 d . . .
C10 C 0.59543(18) 0.77697(16) 0.39111(12) 0.0357(5) Uani 1 1 d . . .
H10A H 0.6345 0.7850 0.3571 0.054 Uiso 1 1 calc R . .
H10B H 0.6462 0.7722 0.4373 0.054 Uiso 1 1 calc R . .
H10C H 0.5486 0.8343 0.3891 0.054 Uiso 1 1 calc R . .
C11 C 0.4713(2) 0.46970(19) 0.23999(12) 0.0467(6) Uani 1 1 d . . .
H11A H 0.5181 0.5011 0.2163 0.070 Uiso 1 1 calc R . .
H11B H 0.3988 0.4651 0.2084 0.070 Uiso 1 1 calc R . .
H11C H 0.4978 0.4030 0.2550 0.070 Uiso 1 1 calc R . .
C12 C 0.33990(17) 0.52292(15) 0.45162(12) 0.0348(4) Uani 1 1 d . . .
H12A H 0.3058 0.4596 0.4343 0.052 Uiso 1 1 calc R . .
H12B H 0.2851 0.5717 0.4529 0.052 Uiso 1 1 calc R . .
H12C H 0.3884 0.5136 0.4981 0.052 Uiso 1 1 calc R . .
C13 C 0.31388(14) 0.86792(13) 0.56542(9) 0.0228(3) Uani 1 1 d . . .
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C14 C 0.28281(15) 0.82340(14) 0.62011(9) 0.0266(4) Uani 1 1 d . . .
C15 C 0.20854(17) 0.87580(17) 0.64581(10) 0.0350(5) Uani 1 1 d . . .
H15A H 0.1863 0.8475 0.6821 0.042 Uiso 1 1 calc R . .
C16 C 0.16682(18) 0.96895(16) 0.61888(11) 0.0377(5) Uani 1 1 d . . .
C17 C 0.20059(17) 1.01003(15) 0.56467(11) 0.0351(4) Uani 1 1 d . . .
H17A H 0.1727 1.0725 0.5463 0.042 Uiso 1 1 calc R . .
C18 C 0.27458(15) 0.96147(14) 0.53661(10) 0.0270(4) Uani 1 1 d . . .
C19 C 0.32728(19) 0.72262(16) 0.65133(11) 0.0363(5) Uani 1 1 d . . .
H19A H 0.2961 0.7052 0.6881 0.054 Uiso 1 1 calc R . .
H19B H 0.4050 0.7270 0.6703 0.054 Uiso 1 1 calc R . .
H19C H 0.3091 0.6715 0.6154 0.054 Uiso 1 1 calc R . .
C20 C 0.0868(2) 1.0254(2) 0.64804(16) 0.0623(8) Uani 1 1 d . . .
H20A H 0.0674 1.0883 0.6234 0.093 Uiso 1 1 calc R . .
H20B H 0.1197 1.0386 0.6971 0.093 Uiso 1 1 calc R . .
H20C H 0.0226 0.9849 0.6421 0.093 Uiso 1 1 calc R . .
C21 C 0.30934(19) 1.00895(15) 0.47786(11) 0.0360(5) Uani 1 1 d . . .
H21A H 0.3604 0.9653 0.4653 0.054 Uiso 1 1 calc R . .
H21B H 0.3431 1.0732 0.4930 0.054 Uiso 1 1 calc R . .
H21C H 0.2467 1.0187 0.4378 0.054 Uiso 1 1 calc R . .
C22 C 0.07799(18) 0.76211(17) 0.30389(11) 0.0337(4) Uani 1 1 d . . .
H22A H 0.0866(19) 0.694(2) 0.2867(12) 0.042(6) Uiso 1 1 d . . .
H22B H 0.001(2) 0.7801(19) 0.3002(13) 0.043(7) Uiso 1 1 d . . .
C23 C 0.15265(16) 0.83762(16) 0.30261(9) 0.0325(4) Uani 1 1 d . . .
H23A H 0.1305 0.9088 0.3012 0.039 Uiso 1 1 calc R . .
C24 C 0.26293(17) 0.81357(18) 0.31693(10) 0.0325(4) Uani 1 1 d . . .
H24A H 0.286(2) 0.7505(19) 0.3050(16) 0.049(8) Uiso 1 1 d . . .
H24B H 0.3147(19) 0.8684(18) 0.3222(12) 0.041(6) Uiso 1 1 d . . .
C25 C 0.13570(14) 0.70013(14) 0.46862(10) 0.0260(4) Uani 1 1 d . . .
C26 C 0.05765(14) 0.61992(14) 0.56013(9) 0.0248(4) Uani 1 1 d . . .
C27 C 0.09623(15) 0.52565(14) 0.58845(9) 0.0270(4) Uani 1 1 d . . .
C28 C 0.04900(17) 0.48468(16) 0.63692(10) 0.0330(4) Uani 1 1 d . . .
H28A H 0.0717 0.4215 0.6565 0.040 Uiso 1 1 calc R . .
C29 C -0.03067(18) 0.53610(17) 0.65632(10) 0.0368(5) Uani 1 1 d . . .
H29A H -0.0611 0.5072 0.6888 0.044 Uiso 1 1 calc R . .
C30 C -0.06624(17) 0.63029(16) 0.62820(11) 0.0351(4) Uani 1 1 d . . .
H30A H -0.1192 0.6645 0.6427 0.042 Uiso 1 1 calc R . .
C31 C -0.02338(16) 0.67400(15) 0.57853(10) 0.0292(4) Uani 1 1 d . . .
C32 C 0.18524(17) 0.47087(16) 0.56868(12) 0.0365(5) Uani 1 1 d . . .
H32A H 0.1998 0.4076 0.5935 0.055 Uiso 1 1 calc R . .
H32B H 0.2500 0.5116 0.5809 0.055 Uiso 1 1 calc R . .
H32C H 0.1629 0.4583 0.5190 0.055 Uiso 1 1 calc R . .
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H33A H -0.1196 0.7989 0.5640 0.061 Uiso 1 1 calc R . .
H33B H -0.0943 0.7643 0.4950 0.061 Uiso 1 1 calc R . .
H33C H -0.0052 0.8209 0.5540 0.061 Uiso 1 1 calc R . .
Cl Cl 0.22756(4) 0.33560(4) 0.78973(3) 0.03656(12) Uani 1 1 d . . .
O1 O 0.20528(15) 0.28997(15) 0.72150(9) 0.0554(4) Uani 1 1 d . . .
O2 O 0.12898(13) 0.37775(15) 0.79747(9) 0.0498(4) Uani 1 1 d . . .
O4 O 0.26850(15) 0.26025(15) 0.84275(11) 0.0696(7) Uani 1 1 d . . .
O3 O 0.30814(13) 0.41321(14) 0.79694(9) 0.0528(4) Uani 1 1 d . . .

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C32 0.0352(11) 0.0320(11) 0.0424(12) 0.0025(9) 0.0113(9) 0.0055(8)
C33 0.0375(12) 0.0368(12) 0.0469(13) 0.0061(10) 0.0113(10) 0.0108(9)
Cl 0.0259(2) 0.0456(3) 0.0338(3) 0.0113(2) 0.00171(19) -0.00385(19)
O1 0.0515(10) 0.0581(11) 0.0516(11) -0.0102(9) 0.0073(8) 0.0087(9)
O2 0.0359(8) 0.0737(12) 0.0406(9) 0.0029(8) 0.0123(7) 0.0023(8)
O4 0.0336(9) 0.0838(15) 0.0735(15) 0.0513(11) -0.0121(9) -0.0139(9)
O3 0.0457(9) 0.0547(10) 0.0570(11) 0.0102(9) 0.0136(8) -0.0172(8)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Pd C1 2.0463(19) . ?
Pd C24 2.133(2) . ?
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Pd C22 2.190(2) . ?
N1 C1 1.359(2) . ?
N1 C3 1.396(2) . ?
N1 C4 1.443(2) . ?
N2 C1 1.353(2) . ?
N2 C2 1.390(2) . ?
N2 C13 1.445(2) . ?
N3 C25 1.148(2) . ?
N3 C26 1.404(2) . ?
C2 C3 1.340(3) . ?
C4 C9 1.398(3) . ?
C4 C5 1.400(3) . ?
C5 C6 1.390(3) . ?
C5 C10 1.504(3) . ?
C6 C7 1.393(3) . ?
C7 C8 1.383(3) . ?
C7 C11 1.506(3) . ?
C8 C9 1.395(3) . ?
C9 C12 1.502(3) . ?
C13 C18 1.392(2) . ?
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C14 C15 1.392(3) . ?
C14 C19 1.508(3) . ?
C15 C16 1.385(3) . ?
C16 C17 1.386(3) . ?
C16 C20 1.516(3) . ?
C17 C18 1.392(3) . ?
C18 C21 1.505(3) . ?
C22 C23 1.389(3) . ?
C23 C24 1.397(3) . ?
C26 C27 1.396(3) . ?
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C26 C31 1.397(3) . ?
C27 C28 1.391(3) . ?
C27 C32 1.500(3) . ?
C28 C29 1.374(3) . ?
C29 C30 1.385(3) . ?
C30 C31 1.390(3) . ?
C31 C33 1.497(3) . ?
Cl O2 1.4320(17) . ?
Cl O4 1.4329(17) . ?
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C1 Pd C23 129.88(8) . . ?
C24 Pd C23 37.92(8) . . ?
C25 Pd C22 101.46(8) . . ?
C1 Pd C22 163.17(8) . . ?
C24 Pd C22 67.74(8) . . ?
C23 Pd C22 37.17(8) . . ?
C1 N1 C3 110.45(15) . . ?
C1 N1 C4 124.51(15) . . ?
C3 N1 C4 125.04(15) . . ?
C1 N2 C2 111.32(15) . . ?
C1 N2 C13 124.20(15) . . ?
C2 N2 C13 124.22(14) . . ?
C25 N3 C26 178.46(19) . . ?
N2 C1 N1 104.59(15) . . ?
N2 C1 Pd 126.73(13) . . ?
N1 C1 Pd 128.68(13) . . ?
C3 C2 N2 106.53(16) . . ?
C2 C3 N1 107.11(16) . . ?
C9 C4 C5 122.36(17) . . ?
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C6 C5 C4 117.78(18) . . ?
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C4 C5 C10 122.18(17) . . ?
C5 C6 C7 121.56(19) . . ?
C8 C7 C6 118.80(18) . . ?
C8 C7 C11 120.7(2) . . ?

C6 C7 C11 120.5(2) . . ?
C7 C8 C9 122.18(19) . . ?
C8 C9 C4 117.22(18) . . ?
C8 C9 C12 120.52(18) . . ?
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C18 C13 N2 119.07(15) . . ?
C14 C13 N2 118.04(16) . . ?
C15 C14 C13 117.48(17) . . ?
C15 C14 C19 120.31(17) . . ?
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C17 C16 C20 120.5(2) . . ?
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C17 C18 C13 116.82(17) . . ?
C17 C18 C21 120.85(17) . . ?
C13 C18 C21 122.33(16) . . ?
C23 C22 Pd 70.44(11) . . ?
C22 C23 C24 119.8(2) . . ?
C22 C23 Pd 72.39(12) . . ?
C24 C23 Pd 69.80(11) . . ?
C23 C24 Pd 72.28(11) . . ?
N3 C25 Pd 174.45(16) . . ?
C27 C26 C31 123.61(17) . . ?
C27 C26 N3 118.72(16) . . ?
C31 C26 N3 117.67(16) . . ?
C28 C27 C26 116.83(17) . . ?
C28 C27 C32 121.04(18) . . ?
C26 C27 C32 122.12(17) . . ?
C29 C28 C27 121.00(19) . . ?
C28 C29 C30 120.97(18) . . ?
C29 C30 C31 120.50(19) . . ?
C30 C31 C26 117.08(18) . . ?
C30 C31 C33 121.47(18) . . ?
C26 C31 C33 121.43(18) . . ?
O2 Cl O4 109.61(12) . . ?
O2 Cl O3 110.29(11) . . ?
O4 Cl O3 108.92(11) . . ?
O2 Cl O1 109.12(11) . . ?
O4 Cl O1 109.47(13) . . ?
O3 Cl O1 109.40(12) . . ?

_diffrn_measured_fraction_theta_max 0.927
_diffrn_reflns_theta_full 29.01
_diffrn_measured_fraction_theta_full 0.927
_refine_diff_density_max 0.442
_refine_diff_density_min -0.592
_refine_diff_density_rms 0.065

Table 1 SI Close (< 2.500 Å) Nonbonding Contacts for the Complexes

[Pd(η^3–C_3H_5)(IMes)(DIC)](ClO_4) (top) and [Pd(η^3–$C_3H_3Me_2$)(IMes)(PPh_3)] (ClO_4) (bottom)

Donor Atom	Acceptor Atom	Parent Atom[a]	Symmetry	D–A Distance (Å)	D–A–P Angle (°)[b]
O(4)	H(30A)	C(30)	*–x,–1/2+y,3/2–z*	2.384	169.4
O(4)	H(3A)	C(3)	*1–x,–1/2+y,3/2–z*	2.421	116.4
O(3)	H(2A)	C(2)	*1–x,–1/2+y,3/2–z*	2.500	155.7
O(1)	H(24B)	C(24)	*1+x,y,z*	2.335	165.0
O(2)	H(3A)	C(3)	*1–x,–y,2–z*	2.451	163.6
O(1)	H(43A)	C(43)	*x,y,z*	2.417	161.8
O(2)	H(17A)	C(17)	*x,y,z*	2.473	171.5

[a] Parent atom of close contact acceptor.

[b] Donor–acceptor–parent angle.