Selective palladation of a large (32 ring atom) macrocyclic ligand at a bis(*N*-heterocyclic carbene) coordination pocket through transmetallation of the corresponding mercury(II) derivative.

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SUPPLEMENTARY INFORMATION

Table S1. Summary of crystallographic data for **2**, $[HgL^2][HgBr_4]$ and $[PdClL^2][PF_6]$. [a] R1= $\sum||Fo| - |Fc||/\sum|Fo|$; wR2 = $\{\sum[w(Fo^2 - Fc^2)^2]/\sum[w(Fo^2)^2]\}^{1/2}$

Compound	**2**	**$[HgL^2][HgBr_4]$**	**$[PdClL^2][PF_6]$**
Empirical formula	$C_{37}H_{31}N_{11}O_4$• $4(CH_4O)$•H_2O	$C_{44}H_{36}HgN_{12}O_4$• $HgBr_4$•$2(H_2O)$	$C_{44}H_{36}ClN_{12}O_4Pd$•$PF_6$• $4.8(C_4H_8O)$•$0.2(C_7H_8)$
Molecular weight (g mol^{-1})	839.91	1553.70	1410.02
Crystal system	Triclinic	Monoclinic	Triclinic
Space group	$P\bar{1}$	$P2_1/a$	$P\bar{1}$
a (Å)	11.353(5)	15.1125(12)	10.9057(8)
b (Å)	13.359(5)	22.6846(9)	17.4282(13)
c (Å)	14.031(5)	17.6153(7)	20.758(2)
α (°)	90.767(5)	90.00	109.393(6)
β (°)	93.754(5)	109.727(8)	102.088(6)
γ (°)	105.809(5)	90.00	102.117(4)
V ($Å^3$)	2042.0(14)	5684.5(6)	3468.1(5)
T (K)	90(2)	123(2)	133(2)
Z	2	4	2
ρ_{calc} (g cm^{-3})	1.366	1.815	1.350
F(000)	888	2944	1442
μ (mm^{-1})	0.099	13.277	0.406
Crystal size (mm)	0.28 x 0.16 x 0.16	0.40 x 0.20 x 0.01	0.51 x 0.48 x 0.39
θ (min, max, °)	1.306, 27.95	6.52, 72.10	1.30, 30.36
Reflections collected	48885	58453	86684
Independent reflections	9683 [R_{int} 0.0401]	10893 [R_{int} 0.0625]	20443 [R_{int} 0.0659]
Completeness	98.8%	97.2%	97.7%
T (max, min)	0.984, 0.981	0.876, 0.076	0.854, 0.813
Goodness of fit on F^2	1.027	1.107	1.057
R, wR_2 ($I > 2\sigma(I)$)[a]	0.0566, 0.1531	0.0435, 0.1150	0.0614, 0.1818
R, wR_2 (all data)	0.0756, 0.1677	0.0543, 0.1257	0.0971, 0.2142

Crystallographic data for **2**, $[HgL^2][HgBr_4]$ and $[PdClL^2][PF_6]$ in CIF format.

1. Compound **2.**

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_publ_contact_author_address
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Department of Chemistry
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New Zealand
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angles
 and torsion angles; correlations between s.u.'s in cell parameters
are only
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l.s. planes.
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New Zealand
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_publ_contact_author_email       'lj.wright@auckland.ac.nz'
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'Meyer, Kim.'
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New Zealand
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'Dalebrook, Andrew F.'
;
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The University of Auckland
Private Bag 92019
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'Wright, L. James'
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Department of Chemistry
The University of Auckland
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wR and
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 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2\s(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-
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P=(Fo^2^+2Fc^2^)/3'
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H9 H 0.2052 0.2300 -0.1550 0.083 Uiso 1 1 calc R . .
C10 C 0.3078(6) 0.2940(3) -0.1179(5) 0.069(2) Uani 1 1 d . . .
H10 H 0.2698 0.3260 -0.1451 0.083 Uiso 1 1 calc R . .
C11 C 0.3975(5) 0.3032(3) -0.0748(4) 0.0600(19) Uani 1 1 d . . .
H11 H 0.4238 0.3416 -0.0712 0.072 Uiso 1 1 calc R . .
C12 C 0.4519(5) 0.2565(3) -0.0354(4) 0.0496(16) Uani 1 1 d . . .
C13 C 0.5082(4) -0.0474(3) 0.1318(3) 0.0461(15) Uani 1 1 d . . .
C14 C 0.5335(5) -0.1055(2) 0.1547(4) 0.0500(16) Uani 1 1 d . . .
H14 H 0.4974 -0.1376 0.1257 0.060 Uiso 1 1 calc R . .
C15 C 0.6131(5) -0.1145(3) 0.2209(4) 0.0511(16) Uani 1 1 d . . .
H15 H 0.6321 -0.1536 0.2383 0.061 Uiso 1 1 calc R . .
C16 C 0.6662(4) -0.0670(2) 0.2628(4) 0.0466(15) Uani 1 1 d . . .
H16 H 0.7218 -0.0730 0.3077 0.056 Uiso 1 1 calc R . .
C17 C 0.6348(4) -0.0113(2) 0.2365(3) 0.0423(14) Uani 1 1 d . . .
C18 C 0.6098(5) 0.3030(3) 0.0093(4) 0.0593(19) Uani 1 1 d . . .
C19 C 0.7097(5) 0.2910(3) 0.0627(4) 0.0565(19) Uani 1 1 d . . .
H19A H 0.7442 0.2728 0.0299 0.068 Uiso 1 1 calc R . .
H19B H 0.7090 0.2622 0.1048 0.068 Uiso 1 1 calc R . .
C20 C 0.7620(5) 0.3456(3) 0.1033(4) 0.0549(17) Uani 1 1 d . A .
H20A H 0.8267 0.3347 0.1372 0.066 Uiso 1 1 calc R . .
H20B H 0.7662 0.3738 0.0617 0.066 Uiso 1 1 calc R . .
C21 C 0.7654(4) 0.0464(2) 0.3294(3) 0.0409(14) Uani 1 1 d . . .
C22 C 0.7910(4) 0.1070(2) 0.3682(3) 0.0425(14) Uani 1 1 d . . .
H22A H 0.8136 0.1029 0.4277 0.051 Uiso 1 1 calc R . .
H22B H 0.7344 0.1324 0.3524 0.051 Uiso 1 1 calc R . .
C23 C 0.8676(4) 0.1361(2) 0.3419(3) 0.0407(14) Uani 1 1 d . . .
H23A H 0.9144 0.1061 0.3399 0.049 Uiso 1 1 calc R . .
H23B H 0.8392 0.1530 0.2872 0.049 Uiso 1 1 calc R . .
C24 C 0.7144(4) 0.3544(3) 0.2260(4) 0.0448(15) Uani 1 1 d . A .
C25 C 0.6531(11) 0.4202(6) 0.1253(8) 0.049(4) Uiso 0.510(15) 1 d PD
A 1
C26 C 0.6304(11) 0.4561(6) 0.0572(8) 0.056(4) Uiso 0.510(15) 1 d PD
A 1
H26 H 0.6490 0.4463 0.0123 0.067 Uiso 0.510(15) 1 calc PR A 1
C27 C 0.5808(10) 0.5056(6) 0.0580(8) 0.057(4) Uiso 0.510(15) 1 d PD
A 1
H27 H 0.5637 0.5304 0.0119 0.069 Uiso 0.510(15) 1 calc PR A 1
C28 C 0.5533(11) 0.5222(6) 0.1236(8) 0.062(4) Uiso 0.510(15) 1 d PD
A 1
H28 H 0.5180 0.5572 0.1213 0.074 Uiso 0.510(15) 1 calc PR A 1
C29 C 0.5791(10) 0.4860(6) 0.1931(8) 0.048(3) Uiso 0.510(15) 1 d PD
A 1
H29 H 0.5626 0.4963 0.2390 0.057 Uiso 0.510(15) 1 calc PR A 1
C30 C 0.6291(11) 0.4351(6) 0.1918(8) 0.045(4) Uiso 0.510(15) 1 d PD
A 1
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C25A C 0.6751(10) 0.4342(6) 0.1475(8) 0.044(4) Uiso 0.490(15) 1 d PD
A 2
C26A C 0.6691(10) 0.4748(5) 0.0854(8) 0.044(3) Uiso 0.490(15) 1 d PD
A 2
H26A H 0.6937 0.4673 0.0433 0.053 Uiso 0.490(15) 1 calc PR A 2
C27A C 0.6235(12) 0.5274(6) 0.0920(9) 0.063(5) Uiso 0.490(15) 1 d PD
A 2
H27A H 0.6123 0.5558 0.0501 0.075 Uiso 0.490(15) 1 calc PR A 2
C28A C 0.5934(12) 0.5401(6) 0.1576(8) 0.062(4) Uiso 0.490(15) 1 d PD
A 2
H28A H 0.5648 0.5771 0.1596 0.075 Uiso 0.490(15) 1 calc PR A 2
C29A C 0.6049(11) 0.4992(6) 0.2204(8) 0.050(4) Uiso 0.490(15) 1 d PD
A 2
H29A H 0.5844 0.5067 0.2649 0.060 Uiso 0.490(15) 1 calc PR A 2
C30A C 0.6476(10) 0.4482(6) 0.2120(8) 0.038(3) Uiso 0.490(15) 1 d P
A 2
C31 C 0.8983(4) 0.2417(2) 0.3915(3) 0.0374(13) Uani 1 1 d . A .
C32 C 0.9825(4) 0.1708(2) 0.4740(3) 0.0400(13) Uani 1 1 d D . .
C33 C 1.0245(4) 0.1185(2) 0.5059(4) 0.0486(16) Uani 1 1 d D . .
H33 H 1.0079 0.0821 0.4781 0.058 Uiso 1 1 calc R . .
C34 C 1.0933(4) 0.1225(3) 0.5822(4) 0.0581(18) Uani 1 1 d D . .
H34 H 1.1251 0.0877 0.6070 0.070 Uiso 1 1 calc R . .
C35 C 1.1168(5) 0.1761(3) 0.6232(4) 0.0589(18) Uani 1 1 d D . .
H35 H 1.1627 0.1766 0.6756 0.071 Uiso 1 1 calc R . .
C36 C 1.0742(4) 0.2292(3) 0.5886(3) 0.0427(14) Uani 1 1 d D . .
H36 H 1.0913 0.2660 0.6153 0.051 Uiso 1 1 calc R . .
C37 C 1.0057(4) 0.2248(2) 0.5131(3) 0.0359(12) Uani 1 1 d D . .
C38 C 0.6486(4) 0.3887(3) 0.3313(4) 0.0455(15) Uani 1 1 d . A .
H38A H 0.6223 0.3492 0.3343 0.055 Uiso 1 1 calc R . .
H38B H 0.6002 0.4182 0.3308 0.055 Uiso 1 1 calc R . .
C39 C 0.7337(4) 0.3981(3) 0.4058(4) 0.0459(15) Uani 1 1 d . . .
C40 C 0.7357(6) 0.4382(3) 0.4653(5) 0.074(2) Uani 1 1 d . . .
H40 H 0.6824 0.4621 0.4604 0.088 Uiso 1 1 calc R . .
C41 C 0.8170(6) 0.4433(4) 0.5326(5) 0.091(3) Uani 1 1 d . . .
H41 H 0.8218 0.4724 0.5726 0.109 Uiso 1 1 calc R . .
C42 C 0.8897(6) 0.4052(3) 0.5399(4) 0.070(2) Uani 1 1 d . . .
H42 H 0.9438 0.4053 0.5872 0.084 Uiso 1 1 calc R . .
C43 C 0.8838(5) 0.3663(2) 0.4773(4) 0.0465(15) Uani 1 1 d . . .
C44 C 0.9685(4) 0.3312(2) 0.4767(3) 0.0403(14) Uani 1 1 d . . .
H44A H 0.9918 0.3480 0.4352 0.048 Uiso 1 1 calc R . .
H44B H 1.0188 0.3363 0.5296 0.048 Uiso 1 1 calc R . .
N1 N 0.3006(4) 0.1337(2) -0.0775(3) 0.0497(13) Uani 1 1 d . . .
H1 H 0.3357 0.1122 -0.0369 0.060 Uiso 1 1 calc R . .
N2 N 0.2905(4) 0.0168(2) -0.0579(3) 0.0506(13) Uani 1 1 d . . .
N3 N 0.4308(3) -0.0316(2) 0.0656(3) 0.0482(13) Uani 1 1 d . . .
H3A H 0.4258 0.0056 0.0506 0.058 Uiso 1 1 calc R . .
N4 N 0.4184(4) 0.2027(2) -0.0363(3) 0.0456(13) Uani 1 1 d . . .
N5 N 0.5578(3) -0.00036(19) 0.1720(3) 0.0387(11) Uani 1 1 d . . .
N6 N 0.5484(4) 0.2605(2) 0.0098(3) 0.0514(14) Uani 1 1 d . . .
H6 H 0.5716 0.2309 0.0430 0.062 Uiso 1 1 calc R . .
N7 N 0.6780(3) 0.04062(19) 0.2769(3) 0.0442(12) Uani 1 1 d . . .
H7 H 0.6434 0.0728 0.2663 0.053 Uiso 1 1 calc R . .
N8 N 0.7140(4) 0.3737(2) 0.1535(3) 0.0523(14) Uani 1 1 d . . .
N9 N 0.6681(4) 0.3932(2) 0.2560(3) 0.0496(13) Uani 1 1 d . . .
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N10 N 0.9146(3) 0.18324(19) 0.3994(3) 0.0375(11) Uani 1 1 d . . .
N11 N 0.9524(3) 0.26697(19) 0.4608(3) 0.0392(11) Uani 1 1 d . . .
N12 N 0.8070(3) 0.36372(19) 0.4123(3) 0.0403(11) Uani 1 1 d . A .
O1 O 0.1626(3) 0.1308(2) -0.1883(3) 0.0643(13) Uani 1 1 d . . .
O2 O 0.3582(3) -0.12136(19) 0.0357(3) 0.0742(15) Uani 1 1 d . . .
O3 O 0.5891(4) 0.3494(3) -0.0298(4) 0.103(2) Uani 1 1 d . . .
O4 O 0.8227(3) 0.00671(16) 0.3484(3) 0.0546(11) Uani 1 1 d . . .
O5 O 0.4605(4) 0.0948(2) 0.0604(3) 0.0641(13) Uani 1 1 d D . .
O6 O 0.5179(3) 0.49661(19) 0.3704(3) 0.0591(12) Uani 1 1 d D . .
Br1 Br 0.43516(6) 0.29079(3) 0.18288(4) 0.0587(2) Uani 1 1 d . . .
Br2 Br 0.65879(5) 0.23938(3) 0.40548(4) 0.04621(17) Uani 1 1 d . . .
Br3 Br 0.65262(5) 0.17482(3) 0.18118(4) 0.04604(17) Uani 1 1 d . . .
Br4 Br 0.46318(5) 0.11260(3) 0.28323(4) 0.05409(19) Uani 1 1 d . . .
Hg1 Hg 0.800392(18) 0.290352(10) 0.301239(14) 0.04134(10) Uani 1 1 d
. . .
Hg2 Hg 0.54487(2) 0.210698(11) 0.262592(16) 0.05012(11) Uani 1 1 d .
. .
H5A H 0.476(5) 0.1292(15) 0.051(4) 0.075 Uiso 1 1 d D . .
H5B H 0.466(5) 0.101(3) 0.1084(18) 0.075 Uiso 1 1 d D . .
H6B H 0.523(5) 0.5334(10) 0.373(4) 0.075 Uiso 1 1 d D . .
H6A H 0.463(3) 0.500(3) 0.376(4) 0.075 Uiso 1 1 d D . .

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C2 0.034(4) 0.063(4) 0.048(3) -0.004(3) 0.008(3) 0.011(3)
C3 0.033(4) 0.073(5) 0.051(3) -0.011(3) -0.001(3) 0.006(3)
C4 0.028(4) 0.073(5) 0.061(4) -0.013(4) -0.003(3) -0.010(3)
C5 0.036(4) 0.063(4) 0.071(4) -0.025(4) 0.005(3) -0.001(3)
C6 0.030(4) 0.057(4) 0.047(3) -0.007(3) 0.005(3) 0.003(3)
C7 0.031(4) 0.060(4) 0.052(3) -0.010(3) 0.004(3) -0.004(3)
C8 0.045(4) 0.051(4) 0.052(3) 0.009(3) 0.011(3) 0.011(3)
C9 0.042(5) 0.088(6) 0.066(4) 0.025(4) 0.002(4) 0.019(4)
C10 0.054(5) 0.056(4) 0.086(5) 0.030(4) 0.007(4) 0.010(4)
C11 0.043(5) 0.054(4) 0.073(4) 0.018(3) 0.007(4) 0.007(3)
C12 0.048(4) 0.049(4) 0.047(3) 0.009(3) 0.009(3) 0.003(3)
C13 0.036(4) 0.047(3) 0.049(3) 0.002(3) 0.006(3) 0.002(3)
C14 0.043(4) 0.031(3) 0.066(4) 0.000(3) 0.006(3) -0.002(3)
C15 0.045(4) 0.031(3) 0.068(4) 0.003(3) 0.008(3) -0.004(3)
C16 0.038(4) 0.038(3) 0.054(3) 0.006(3) 0.002(3) 0.002(3)
C17 0.037(4) 0.032(3) 0.051(3) 0.001(3) 0.006(3) -0.006(3)
C18 0.055(5) 0.060(4) 0.059(4) 0.019(4) 0.013(4) 0.001(4)
C19 0.050(5) 0.064(4) 0.051(4) 0.021(3) 0.011(3) 0.000(3)
C20 0.053(5) 0.052(4) 0.056(4) 0.007(3) 0.014(3) 0.006(3)
C21 0.037(4) 0.028(3) 0.049(3) 0.007(2) 0.004(3) 0.000(3)
C22 0.040(4) 0.030(3) 0.048(3) 0.004(2) 0.003(3) -0.001(3)
C23 0.036(4) 0.029(3) 0.049(3) -0.002(2) 0.003(3) -0.003(2)
C24 0.028(4) 0.044(3) 0.059(4) 0.012(3) 0.010(3) 0.004(3)
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C31 0.024(3) 0.031(3) 0.050(3) 0.002(2) 0.003(3) -0.002(2)
C32 0.024(3) 0.035(3) 0.054(3) 0.005(3) 0.004(3) -0.002(2)
C33 0.029(4) 0.034(3) 0.070(4) 0.009(3) 0.000(3) 0.006(3)
C34 0.039(4) 0.041(3) 0.074(4) 0.018(3) -0.007(3) 0.005(3)
C35 0.048(4) 0.052(4) 0.055(4) 0.013(3) -0.011(3) -0.001(3)
C36 0.033(4) 0.037(3) 0.054(3) 0.004(3) 0.009(3) -0.001(3)
C37 0.020(3) 0.040(3) 0.046(3) 0.006(3) 0.009(3) 0.004(2)
C38 0.027(4) 0.046(3) 0.066(4) 0.014(3) 0.020(3) 0.004(3)
C39 0.030(4) 0.045(3) 0.062(4) 0.004(3) 0.014(3) 0.005(3)
C40 0.066(6) 0.081(5) 0.076(5) -0.007(4) 0.028(4) 0.030(4)
C41 0.082(7) 0.102(6) 0.073(5) -0.027(5) 0.005(5) 0.050(5)
C42 0.071(6) 0.076(5) 0.053(4) -0.011(4) 0.006(4) 0.035(4)
C43 0.044(4) 0.038(3) 0.056(3) 0.001(3) 0.016(3) 0.001(3)
C44 0.030(3) 0.031(3) 0.053(3) -0.007(3) 0.005(3) -0.004(2)
N1 0.032(3) 0.059(3) 0.048(3) 0.012(3) 0.001(2) 0.005(3)
N2 0.046(3) 0.052(3) 0.049(3) -0.007(3) 0.009(3) 0.002(3)
N3 0.033(3) 0.038(3) 0.062(3) 0.004(2) 0.002(3) -0.001(2)
N4 0.034(3) 0.048(3) 0.049(3) 0.002(2) 0.006(3) 0.008(2)
N5 0.028(3) 0.034(2) 0.046(2) 0.002(2) 0.002(2) 0.000(2)
N6 0.050(4) 0.045(3) 0.049(3) 0.007(2) 0.003(3) 0.006(3)
N7 0.033(3) 0.028(2) 0.057(3) -0.004(2) -0.004(2) 0.001(2)
N8 0.049(4) 0.048(3) 0.058(3) 0.018(3) 0.015(3) 0.007(3)
N9 0.042(3) 0.037(3) 0.070(3) 0.022(3) 0.019(3) 0.010(2)
N10 0.028(3) 0.034(2) 0.046(2) 0.002(2) 0.006(2) -0.001(2)
N11 0.030(3) 0.032(2) 0.052(3) 0.000(2) 0.009(2) 0.000(2)
N12 0.035(3) 0.035(2) 0.051(3) 0.003(2) 0.013(2) 0.005(2)
O1 0.040(3) 0.085(3) 0.054(3) 0.007(2) -0.003(2) 0.015(2)
O2 0.060(3) 0.043(3) 0.090(3) -0.004(2) -0.013(3) -0.009(2)
O3 0.060(4) 0.109(4) 0.122(5) 0.077(4) 0.006(3) -0.006(3)
O4 0.034(3) 0.032(2) 0.082(3) 0.006(2) -0.002(2) 0.0009(18)
O5 0.069(3) 0.044(2) 0.058(3) 0.001(2) -0.007(3) -0.009(2)
O6 0.048(3) 0.039(2) 0.089(3) -0.002(2) 0.021(3) 0.009(2)
Br1 0.0524(5) 0.0534(4) 0.0614(4) 0.0015(3) 0.0075(4) 0.0200(3)
Br2 0.0380(4) 0.0421(3) 0.0547(3) 0.0008(3) 0.0106(3) 0.0021(3)
Br3 0.0404(4) 0.0427(3) 0.0508(3) 0.0089(3) 0.0098(3) 0.0075(3)
Br4 0.0496(5) 0.0462(4) 0.0671(4) -0.0003(3) 0.0205(4) 0.0008(3)
Hg1 0.03437(19) 0.03523(15) 0.04694(15) 0.00570(10) 0.00390(12)
0.00391(10)
Hg2 0.0397(2) 0.04588(17) 0.05963(18) 0.00191(11) 0.01003(15)
0.00642(11)

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;
 All s.u.'s (except the s.u. in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell s.u.'s
are taken
 into account individually in the estimation of s.u.'s in distances,
angles
 and torsion angles; correlations between s.u.'s in cell parameters
are only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
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 treatment of cell s.u.'s is used for estimating s.u.'s involving
l.s. planes.
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C4 C5 1.371(9) . ?
C5 C6 1.412(8) . ?
C6 N2 1.316(7) . ?
C6 C7 1.513(8) . ?
C7 O2 1.207(7) . ?
C7 N3 1.368(7) . ?
C8 N4 1.325(8) . ?
C8 C9 1.408(8) . ?
C8 N1 1.415(8) . ?
C9 C10 1.396(9) . ?
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C18 O3 1.240(7) . ?
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C18 C19 1.510(9) . ?
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C20 N8 1.465(8) . ?
C21 O4 1.215(6) . ?
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C22 C23 1.534(8) . ?
C23 N10 1.480(6) . ?
C24 N9 1.340(7) . ?
C24 N8 1.350(7) . ?
C24 Hg1 2.095(6) . ?
C25 N8 1.378(13) . ?
C25 C30 1.380(14) . ?
C25 C26 1.393(13) . ?
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C26 C27 1.352(13) . ?
C27 C28 1.404(13) . ?
C28 C29 1.415(13) . ?
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C30 N9 1.441(12) . ?
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C25A N8 1.482(13) . ?
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C28A C29A 1.408(14) . ?
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C31 N10 1.347(7) . ?
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C39 C40 1.379(9) . ?
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C41 C42 1.370(9) . ?
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C43 C44 1.511(8) . ?
C44 N11 1.488(6) . ?
N12 Hg1 2.545(5) . ?
Br1 Hg2 2.5396(7) . ?
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_publ_contact_author_address
;
Department of Chemistry
The University of Auckland
Private Bag 92019
Auckland
New Zealand
;

_publ_contact_author_email       'lj.wright@auckland.ac.nz'
_publ_contact_author_phone       '0064 9 3737599 Ext 88257'
_publ_contact_author_fax         '0064 9 3737422'
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'Meyer, Kim.'
;
Department of Chemistry
The University of Auckland
Private Bag 92019
Auckland
New Zealand
;

'Dalebrook, Andrew F.'
;
Department of Chemistry
The University of Auckland
Private Bag 92019
Auckland
New Zealand
;

'Wright, L. James'
;
Department of Chemistry
The University of Auckland
Private Bag 92019
Auckland
New Zealand
;



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expression of
 F^2^ > 2\s(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-
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 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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H3 H 1.2388 1.4238 1.2352 0.064 Uiso 1 1 calc R B .
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C8 C 1.1336(4) 1.1539(3) 1.0124(2) 0.0485(10) Uani 1 1 d . . .
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C12 C 1.0253(4) 1.0206(2) 0.9256(2) 0.0440(9) Uani 1 1 d . . .
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H23A H 0.6157 1.0216 0.5693 0.050 Uiso 1 1 calc R B .
H23B H 0.6318 1.0744 0.5199 0.050 Uiso 1 1 calc R . .
C24 C 0.5607(3) 0.76839(19) 0.60248(18) 0.0290(6) Uani 1 1 d . . .
C25 C 0.4833(3) 0.68991(19) 0.65974(17) 0.0294(6) Uani 1 1 d . . .
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C28 C 0.2431(4) 0.5750(2) 0.6268(2) 0.0450(9) Uani 1 1 d . B .
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C41 C 0.4968(4) 0.5972(2) 0.3435(2) 0.0421(8) Uani 1 1 d . B .
H41 H 0.4685 0.5455 0.3021 0.050 Uiso 1 1 calc R . .
C42 C 0.6194(3) 0.6549(2) 0.36211(19) 0.0360(7) Uani 1 1 d . . .
H42 H 0.6755 0.6441 0.3330 0.043 Uiso 1 1 calc R B .
C43 C 0.6592(3) 0.7282(2) 0.42340(19) 0.0320(7) Uani 1 1 d . B .
C44 C 0.7941(4) 0.7912(2) 0.4473(2) 0.0431(9) Uani 1 1 d . . .
H44A H 0.8492 0.7883 0.4904 0.052 Uiso 1 1 calc R B .
H44B H 0.8362 0.7757 0.4089 0.052 Uiso 1 1 calc R . .
N1 N 1.1177(4) 1.2329(2) 1.04558(18) 0.0555(10) Uani 1 1 d . B 1
H1 H 1.0507 1.2433 1.0217 0.067 Uiso 0.9554(12) 1 calc PR C 1
N3 N 0.8845(4) 1.3833(2) 0.96764(17) 0.0522(9) Uani 1 1 d . B 1
H3A H 0.9383 1.3520 0.9677 0.063 Uiso 0.9554(12) 1 calc PR C 1
Pd2 Pd 0.9630(5) 1.2921(3) 0.9890(3) 0.0274(18) Uani 0.0446(12) 1 d
P B 2
N2 N 1.0468(4) 1.3750(2) 1.07591(16) 0.0453(8) Uani 1 1 d . . .
N4 N 1.0225(4) 1.0983(2) 0.96291(17) 0.0456(8) Uani 1 1 d . B .
N5 N 0.8186(3) 1.3071(2) 0.84648(16) 0.0425(7) Uani 1 1 d . B .
N6 N 0.9035(3) 0.96869(19) 0.87601(17) 0.0432(7) Uani 1 1 d . B .
H6 H 0.8394 0.9921 0.8750 0.052 Uiso 1 1 calc R . .
N7 N 0.7729(3) 1.22291(19) 0.72933(15) 0.0380(7) Uani 1 1 d . B .
H7 H 0.8448 1.2107 0.7449 0.046 Uiso 1 1 calc R . .
N8 N 0.5899(3) 0.74997(17) 0.66018(14) 0.0291(5) Uani 1 1 d . B .
N9 N 0.4353(3) 0.72135(18) 0.56422(15) 0.0312(6) Uani 1 1 d . B .
N10 N 0.7388(4) 0.99304(19) 0.51202(16) 0.0451(8) Uani 1 1 d . A .
N11 N 0.7879(3) 0.87780(19) 0.46376(17) 0.0443(8) Uani 1 1 d . A .
N12 N 0.5807(3) 0.74500(17) 0.46485(15) 0.0283(5) Uani 1 1 d . . .
O1 O 1.2906(4) 1.2958(2) 1.14814(17) 0.0722(11) Uani 1 1 d . B .
O2 O 0.8396(4) 1.4957(3) 1.04189(19) 0.0819(12) Uani 1 1 d . B .
O3 O 0.9487(3) 0.8458(2) 0.8234(2) 0.0744(11) Uani 1 1 d . B .
O4 O 0.6069(3) 1.18888(19) 0.62776(14) 0.0496(7) Uani 1 1 d . B .
F1 F 0.0616(2) 0.58071(14) 0.41425(13) 0.0461(5) Uani 1 1 d . . .
F2 F 0.0815(2) 0.72079(13) 0.45403(12) 0.0478(5) Uani 1 1 d . . .
F3 F -0.0518(2) 0.70150(16) 0.34695(14) 0.0515(6) Uani 1 1 d . . .
F4 F -0.1198(2) 0.62446(14) 0.40840(12) 0.0439(5) Uani 1 1 d . . .
F5 F -0.0726(2) 0.55983(16) 0.30763(12) 0.0548(6) Uani 1 1 d . . .
F6 F 0.1298(2) 0.65782(14) 0.35338(13) 0.0478(5) Uani 1 1 d . . .
P P 0.00418(8) 0.64048(5) 0.38026(5) 0.03071(18) Uani 1 1 d . . .
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Cl Cl 0.73621(12) 0.95860(5) 0.67240(5) 0.0493(3) Uani 1 1 d . . .
Pd1 Pd 0.65133(2) 0.846321(15) 0.561661(14) 0.03132(9) Uani 1 1 d .
B .
O5 O 0.7540(3) 0.57671(19) 0.63713(15) 0.0522(7) Uani 1 1 d D . .
C45 C 0.8893(5) 0.6158(3) 0.6457(3) 0.0603(12) Uani 1 1 d D . .
H45A H 0.9445 0.5821 0.6598 0.072 Uiso 1 1 calc R . .
H45B H 0.9214 0.6743 0.6834 0.072 Uiso 1 1 calc R . .
C46 C 0.8963(5) 0.6183(4) 0.5751(3) 0.0690(14) Uani 1 1 d D . .
H46A H 0.9166 0.5677 0.5457 0.083 Uiso 1 1 calc R . .
H46B H 0.9632 0.6707 0.5816 0.083 Uiso 1 1 calc R . .
C47 C 0.7577(5) 0.6181(3) 0.5413(3) 0.0615(13) Uani 1 1 d D . .
H47A H 0.7486 0.6762 0.5584 0.074 Uiso 1 1 calc R . .
H47B H 0.7335 0.5941 0.4884 0.074 Uiso 1 1 calc R . .
C48 C 0.6761(4) 0.5610(3) 0.5677(2) 0.0505(10) Uani 1 1 d D . .
H48A H 0.5931 0.5749 0.5696 0.061 Uiso 1 1 calc R . .
H48B H 0.6545 0.5003 0.5356 0.061 Uiso 1 1 calc R . .
O6 O 0.4695(9) 0.5005(6) 0.9043(5) 0.118(4) Uiso 0.592(10) 1 d PD D
1
C49 C 0.5624(11) 0.5783(7) 0.9581(6) 0.096(4) Uiso 0.592(10) 1 d PD
D 1
C50 C 0.4946(12) 0.6463(8) 0.9672(7) 0.099(4) Uiso 0.592(10) 1 d PD
D 1
C51 C 0.3982(15) 0.6178(9) 0.8907(7) 0.110(5) Uiso 0.592(10) 1 d PD
D 1
C52 C 0.379(2) 0.5192(11) 0.8545(10) 0.152(7) Uiso 0.592(10) 1 d PD
D 1
O6A O 0.4266(12) 0.5020(8) 0.8274(7) 0.099(4) Uiso 0.408(10) 1 d PD
D 2
C49A C 0.3146(18) 0.5048(15) 0.8552(12) 0.119(8) Uiso 0.408(10) 1 d
PD D 2
C50A C 0.336(4) 0.600(2) 0.892(3) 0.48(6) Uiso 0.408(10) 1 d PD D 2
C51A C 0.485(4) 0.630(3) 0.936(2) 0.37(4) Uiso 0.408(10) 1 d PD D 2
C52A C 0.5395(18) 0.5650(15) 0.8861(12) 0.136(9) Uiso 0.408(10) 1 d
PD D 2
O7 O 0.2230(14) 0.7873(9) 0.7812(7) 0.199(6) Uiso 0.623(4) 1 d PD E
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C53 C 0.1698(13) 0.7310(8) 0.8138(7) 0.121(4) Uiso 0.623(4) 1 d PD E
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C54 C 0.2190(12) 0.7745(8) 0.8902(7) 0.111(4) Uiso 0.623(4) 1 d PD E
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C55 C 0.3482(12) 0.8409(8) 0.9012(7) 0.111(4) Uiso 0.623(4) 1 d PD E
1
C56 C 0.3655(15) 0.8267(12) 0.8309(8) 0.164(7) Uiso 0.623(4) 1 d PD
E 1
O8 O 0.4051(14) 0.9343(8) 0.6187(7) 0.045(4) Uiso 0.182(6) 1 d PD F
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C57 C 0.381(3) 0.9067(11) 0.6747(10) 0.057(7) Uiso 0.182(6) 1 d PD F
2
C58 C 0.364(2) 0.9778(11) 0.7329(10) 0.044(5) Uiso 0.182(6) 1 d PD F
2
C59 C 0.3939(18) 1.0552(9) 0.7116(9) 0.035(4) Uiso 0.182(6) 1 d PD F
2
C60 C 0.4583(17) 1.0265(9) 0.6517(9) 0.035(4) Uiso 0.182(6) 1 d PD F
2
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C57B C 0.4500 1.0502 0.6914 0.075(8) Uiso 0.195(6) 1 d P G 3
C58B C 0.3548 0.9002 0.6835 0.071(9) Uiso 0.195(6) 1 d P G 3
C59B C 0.3671 0.9886 0.7096 0.059(6) Uiso 0.195(6) 1 d P G 3
C60B C 0.2891 1.0134 0.7530 0.054(6) Uiso 0.195(6) 1 d P G 3
C61B C 0.2020 0.9574 0.7690 0.059(6) Uiso 0.195(6) 1 d P G 3
C62B C 0.1903 0.8707 0.7451 0.069(7) Uiso 0.195(6) 1 d P G 3
C63B C 0.2702 0.8454 0.7018 0.101(11) Uiso 0.195(6) 1 d P G 3
O9 O 0.6777 1.0423 0.8665 0.067(2) Uiso 0.591(12) 1 d PD H 1
C61 C 0.6306 1.0793 0.8147 0.228(12) Uiso 0.591(12) 1 d PD H 1
C62 C 0.5326 1.1207 0.8391 0.153(7) Uiso 0.591(12) 1 d PD H 1
C63 C 0.5885 1.1509 0.9229 0.188(9) Uiso 0.591(12) 1 d PD H 1
C64 C 0.6322 1.0652 0.9334 0.289(18) Uiso 0.591(12) 1 d PD H 1
O9A O 0.7089(13) 1.0498(7) 0.8887(8) 0.094(4) Uiso 0.409(12) 1 d PD
H 2
C61A C 0.575(2) 1.0241(15) 0.890(2) 0.236(18) Uiso 0.409(12) 1 d PD
H 2
C62A C 0.546(2) 1.1067(15) 0.9259(14) 0.148(9) Uiso 0.409(12) 1 d PD
H 2
C63A C 0.6347(19) 1.1735(10) 0.9061(11) 0.109(7) Uiso 0.409(12) 1 d
PD H 2
C64A C 0.7211(14) 1.1238(9) 0.8688(8) 0.081(5) Uiso 0.409(12) 1 d PD
H 2
O10 O 1.0289(3) 1.2004(2) 0.77425(19) 0.0657(9) Uiso 1 1 d D I 1
C65 C 1.0495(7) 1.1539(4) 0.8209(4) 0.0895(18) Uiso 1 1 d D I 1
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I 1
C67 C 1.2518(11) 1.2511(9) 0.8375(8) 0.111(5) Uiso 0.594(19) 1 d PD
I 1
C68 C 1.1313(7) 1.2785(4) 0.8031(4) 0.096(2) Uiso 1 1 d D I 1
C66A C 1.194(2) 1.2175(16) 0.8767(13) 0.107(7) Uiso 0.406(19) 1 d P
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I 2

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C3 0.068(3) 0.050(2) 0.0251(18) 0.0061(17) -0.0010(18) 0.011(2)
C4 0.067(3) 0.060(3) 0.027(2) -0.0048(19) 0.0048(19) 0.015(2)
C5 0.067(3) 0.056(3) 0.039(2) -0.004(2) 0.009(2) 0.025(2)
C6 0.056(2) 0.053(2) 0.0272(18) 0.0051(17) 0.0071(16) 0.019(2)
C7 0.071(3) 0.055(3) 0.031(2) 0.0052(18) 0.0121(19) 0.031(2)
C8 0.067(3) 0.0354(19) 0.0293(19) 0.0093(16) -0.0040(17) 0.0121(18)
C9 0.065(3) 0.046(2) 0.039(2) 0.0095(19) -0.0115(19) 0.007(2)
C10 0.064(3) 0.053(3) 0.056(3) 0.011(2) -0.011(2) 0.020(2)
C11 0.058(3) 0.042(2) 0.054(3) 0.006(2) -0.006(2) 0.015(2)
C12 0.059(2) 0.0308(17) 0.0295(18) 0.0077(15) -0.0042(16) 0.0126(17)
```

C13 0.071(3) 0.053(2) 0.0308(19) 0.0155(18) 0.0131(18) 0.037(2)
C14 0.080(3) 0.076(3) 0.036(2) 0.014(2) 0.013(2) 0.052(3)
C15 0.075(3) 0.077(3) 0.047(3) 0.024(2) 0.017(2) 0.052(3)
C16 0.069(3) 0.065(3) 0.033(2) 0.019(2) 0.0101(19) 0.038(2)
C17 0.059(2) 0.0380(19) 0.0286(17) 0.0132(15) 0.0107(16) 0.0238(17)
C18 0.052(2) 0.0336(18) 0.037(2) 0.0053(16) -0.0037(16) 0.0156(17)
C19 0.0438(18) 0.0283(16) 0.0320(18) 0.0067(14) 0.0020(14)
0.0128(14)
C20 0.0332(15) 0.0278(15) 0.0303(17) 0.0050(13) 0.0013(13)
0.0108(13)
C21 0.055(2) 0.0262(15) 0.0281(17) 0.0125(14) 0.0078(15) 0.0107(15)
C22 0.052(2) 0.0252(15) 0.0287(17) 0.0092(13) 0.0110(15) 0.0052(14)
C23 0.064(2) 0.0261(16) 0.0299(18) 0.0097(14) 0.0122(16) 0.0077(16)
C24 0.0291(14) 0.0247(14) 0.0341(17) 0.0138(13) 0.0089(12)
0.0074(12)
C25 0.0352(15) 0.0214(13) 0.0295(16) 0.0092(12) 0.0097(13)
0.0057(12)
C26 0.052(2) 0.0330(17) 0.0275(17) 0.0126(14) 0.0103(15) 0.0103(15)
C27 0.064(2) 0.0353(19) 0.046(2) 0.0230(18) 0.0233(19) 0.0065(18)
C28 0.051(2) 0.0319(17) 0.046(2) 0.0138(17) 0.0187(18) -0.0018(16)
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C31 0.0483(19) 0.0251(15) 0.0334(18) 0.0074(14) 0.0168(15)
0.0009(14)
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C33 0.067(9) 0.033(4) 0.039(5) 0.012(3) 0.015(6) -0.003(5)
C34 0.087(12) 0.057(6) 0.051(6) 0.023(5) 0.022(8) -0.017(7)
C35 0.071(10) 0.058(6) 0.053(6) 0.014(5) 0.037(7) -0.006(7)
C36 0.057(8) 0.042(6) 0.038(6) 0.004(4) 0.022(6) 0.001(5)
C37 0.051(6) 0.032(5) 0.040(5) 0.021(4) 0.018(4) 0.005(4)
C32A 0.034(9) 0.017(5) 0.021(7) 0.012(4) 0.010(7) 0.005(6)
C33A 0.034(8) 0.022(5) 0.029(6) 0.011(4) 0.003(5) 0.004(5)
C34A 0.036(8) 0.038(7) 0.021(6) 0.012(5) 0.000(5) -0.015(6)
C35A 0.022(6) 0.044(7) 0.028(6) 0.010(5) 0.009(5) 0.007(5)
C36A 0.030(7) 0.032(7) 0.034(7) 0.014(5) 0.009(6) 0.005(5)
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0.0063(13)
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0.0033(15)
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0.0067(15)
C42 0.0358(16) 0.0287(16) 0.0356(18) 0.0075(14) 0.0026(14)
0.0110(14)
C43 0.0307(15) 0.0263(15) 0.0363(18) 0.0110(14) 0.0058(13)
0.0097(12)
C44 0.0354(17) 0.0346(18) 0.048(2) 0.0042(16) 0.0170(16) 0.0032(15)
N1 0.078(2) 0.0333(16) 0.0306(17) 0.0018(14) -0.0131(16) 0.0158(17)
N3 0.071(2) 0.059(2) 0.0253(16) 0.0071(15) 0.0059(15) 0.0414(19)
Pd2 0.039(3) 0.019(3) 0.018(3) 0.0053(19) 0.000(2) 0.008(2)
N2 0.060(2) 0.0410(17) 0.0242(15) 0.0070(13) 0.0027(14) 0.0141(15)

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N4 0.063(2) 0.0297(15) 0.0289(15) 0.0070(13) -0.0075(14) 0.0122(15)
N5 0.0574(19) 0.0449(18) 0.0287(15) 0.0132(14) 0.0090(14) 0.0283(16)
N6 0.0487(17) 0.0295(15) 0.0378(17) 0.0052(13) -0.0022(14)
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N8 0.0313(13) 0.0235(12) 0.0280(13) 0.0083(11) 0.0058(11) 0.0053(10)
N9 0.0277(12) 0.0334(14) 0.0345(15) 0.0199(12) 0.0060(11) 0.0054(11)
N10 0.073(2) 0.0251(14) 0.0294(15) 0.0060(12) 0.0219(15) -0.0006(14)
N11 0.0500(17) 0.0298(15) 0.0400(17) 0.0037(13) 0.0218(14) -
0.0058(13)
N12 0.0289(12) 0.0254(12) 0.0332(14) 0.0170(11) 0.0047(11)
0.0088(10)
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O2 0.099(3) 0.087(3) 0.051(2) 0.0022(19) 0.0075(19) 0.065(2)
O3 0.0623(19) 0.0473(18) 0.072(2) -0.0119(16) -0.0201(17) 0.0311(16)
O4 0.0657(18) 0.0485(16) 0.0308(14) 0.0146(13) 0.0036(13) 0.0222(14)
F1 0.0399(11) 0.0364(11) 0.0616(15) 0.0250(11) 0.0042(10) 0.0125(9)
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F3 0.0602(14) 0.0598(15) 0.0614(15) 0.0436(13) 0.0272(12) 0.0308(12)
F4 0.0383(10) 0.0494(13) 0.0552(14) 0.0296(11) 0.0214(10) 0.0140(10)
F5 0.0561(14) 0.0460(13) 0.0364(12) 0.0029(11) -0.0008(10)
0.0005(11)
F6 0.0451(12) 0.0398(12) 0.0613(15) 0.0157(11) 0.0295(11) 0.0119(10)
P 0.0292(4) 0.0262(4) 0.0352(5) 0.0122(4) 0.0083(3) 0.0064(3)
Cl 0.0843(7) 0.0242(4) 0.0376(5) 0.0124(4) 0.0302(5) 0.0009(4)
Pd1 0.03515(14) 0.02430(13) 0.03436(15) 0.01261(11) 0.01257(10)
0.00488(10)
O5 0.0632(18) 0.0471(16) 0.0382(15) 0.0166(13) 0.0094(13) 0.0072(14)
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C46 0.076(3) 0.065(3) 0.079(4) 0.033(3) 0.039(3) 0.025(3)
C47 0.097(4) 0.066(3) 0.054(3) 0.037(2) 0.039(3) 0.049(3)
C48 0.060(2) 0.052(2) 0.036(2) 0.0108(19) 0.0132(18) 0.022(2)

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 All s.u.'s (except the s.u. in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell s.u.'s
are taken
 into account individually in the estimation of s.u.'s in distances,
angles
 and torsion angles; correlations between s.u.'s in cell parameters
are only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving
l.s. planes.
;

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C1 N1 1.355(5) . ?
C1 C2 1.501(6) . ?
C2 N2 1.350(5) . ?
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C3 C4 1.380(7) . ?
C4 C5 1.369(7) . ?
C5 C6 1.387(6) . ?
C6 N2 1.326(6) . ?
C6 C7 1.499(6) . ?
C6 Pd2 2.637(7) . ?
C7 O2 1.217(5) . ?
C7 N3 1.340(5) . ?
C8 N4 1.337(5) . ?
C8 C9 1.385(7) . ?
C8 N1 1.387(5) . ?
C9 C10 1.368(7) . ?
C10 C11 1.372(6) . ?
C11 C12 1.388(6) . ?
C12 N4 1.329(5) . ?
C12 N6 1.395(5) . ?
C13 N5 1.335(5) . ?
C13 C14 1.381(6) . ?
C13 N3 1.411(5) . ?
C14 C15 1.396(6) . ?
C15 C16 1.381(6) . ?
C16 C17 1.388(6) . ?
C17 N5 1.326(5) . ?
C17 N7 1.386(5) . ?
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