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#1 Data block identification for start of deposition

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_data                    br06
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_compound_id                   14a
_data                    HERNAI
_compound_id                   14b


#------------------------------------------------------------
#2 Person making the deposition

_publ_contact_author  'M.C. Ramirez de Arellano'
_publ_contact_author_address
;       Departamento de Quimica Organica
      Facultad de Farmacia
        Universidad de Valencia
        46100 Valencia
        Spain
;
_publ_contact_author_email        mcra@uv.es
_ccdc_journal_depnumber

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#3 Publication details

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_publ_title
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'J. Vicente, J.A. Abad, F.S. Hernandez-Mata, B. Rink, P.G. Jones
 and M.C. Ramirez de Arellano'
_journal_name_full 'Organometallics'

#------------------------------------------------------------
#4

data_br04

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_chemical_name_systematic
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;
_chemical_name_common             ?
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 'C22 H25 Cl N2 O4 Pd'
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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
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 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Cl'  'Cl'   0.1484   0.1585
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Pd'  'Pd'  -0.9988   1.0072
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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 'x, y, z'
 '-x, -y, -z'

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_cell_length_b                    9.9373(6)
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_cell_angle_beta                  82.327(5)
_cell_angle_gamma                 62.438(3)
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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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 'calc w=1/[\s^2^(Fo^2^)+(0.0543P)^2^+1.9262P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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Cl Cl 0.29597(11) 1.19921(11) 0.10033(8) 0.0402(2) Uani 1 1 d . . .
N1 N -0.0381(3) 1.0062(3) 0.1959(2) 0.0219(5) Uani 1 1 d . . .
N2 N -0.0388(3) 1.2014(3) 0.0451(2) 0.0227(5) Uani 1 1 d . . .
O1 O 0.2479(4) 1.2897(3) 0.3866(3) 0.0580(9) Uani 1 1 d . . .
O2 O 0.0474(4) 1.2430(4) 0.4649(2) 0.0480(7) Uani 1 1 d . . .
O3 O 0.4864(3) 0.5124(3) 0.2831(2) 0.0399(6) Uani 1 1 d . . .
O4 O 0.7282(3) 0.5278(3) 0.2918(2) 0.0468(7) Uani 1 1 d . . .
C1 C 0.2663(4) 0.9813(4) 0.2684(2) 0.0225(6) Uani 1 1 d . . .
C2 C 0.2653(4) 1.0528(4) 0.3556(3) 0.0269(7) Uani 1 1 d . . .
C3 C 0.3630(4) 0.9673(4) 0.4317(3) 0.0301(7) Uani 1 1 d . . .
H3 H 0.3618 1.0164 0.4904 0.036 Uiso 1 1 calc R . .
C4 C 0.4616(4) 0.8129(4) 0.4238(2) 0.0291(7) Uani 1 1 d . . .
H4 H 0.5290 0.7569 0.4759 0.035 Uiso 1 1 calc R . .
C5 C 0.4617(4) 0.7399(4) 0.3387(2) 0.0244(7) Uani 1 1 d . . .
C6 C 0.3650(4) 0.8251(4) 0.2624(2) 0.0235(6) Uani 1 1 d . . .
H6 H 0.3662 0.7751 0.2042 0.028 Uiso 1 1 calc R . .
C7 C 0.1557(4) 1.2199(4) 0.3712(3) 0.0337(8) Uani 1 1 d . . .
H7 H 0.0916 1.2678 0.3117 0.040 Uiso 1 1 calc R . .
C8 C 0.1586(7) 1.4515(6) 0.3823(5) 0.0671(15) Uani 1 1 d . . .
H8A H 0.0764 1.4829 0.3341 0.101 Uiso 1 1 calc R . .
H8B H 0.2342 1.4945 0.3599 0.101 Uiso 1 1 calc R . .
H8C H 0.1038 1.4881 0.4501 0.101 Uiso 1 1 calc R . .
C9 C -0.0855(5) 1.2156(5) 0.4540(3) 0.0474(10) Uani 1 1 d . . .
H9A H -0.1441 1.2789 0.3975 0.071 Uiso 1 1 calc R . .
H9B H -0.1600 1.2405 0.5170 0.071 Uiso 1 1 calc R . .
H9C H -0.0450 1.1083 0.4397 0.071 Uiso 1 1 calc R . .
C10 C 0.5655(4) 0.5704(4) 0.3334(3) 0.0318(8) Uani 1 1 d . . .
H10 H 0.5696 0.5282 0.4048 0.038 Uiso 1 1 calc R . .
C11 C 0.5593(6) 0.3504(5) 0.2873(3) 0.0475(10) Uani 1 1 d . . .
H11A H 0.6738 0.3087 0.2576 0.071 Uiso 1 1 calc R . .
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H11B H 0.4993 0.3166 0.2488 0.071 Uiso 1 1 calc R . .
H11C H 0.5549 0.3146 0.3584 0.071 Uiso 1 1 calc R . .
C12 C 0.7479(5) 0.5584(5) 0.1849(3) 0.0443(10) Uani 1 1 d . . .
H12A H 0.6957 0.5133 0.1490 0.066 Uiso 1 1 calc R . .
H12B H 0.8649 0.5145 0.1608 0.066 Uiso 1 1 calc R . .
H12C H 0.6966 0.6685 0.1716 0.066 Uiso 1 1 calc R . .
C21 C -0.1668(4) 1.0603(4) 0.1394(2) 0.0228(6) Uani 1 1 d . . .
C22 C -0.2889(4) 1.0165(4) 0.1593(3) 0.0308(7) Uani 1 1 d . . .
H22 H -0.3749 1.0526 0.1167 0.037 Uiso 1 1 calc R . .
C23 C -0.2861(4) 0.9202(4) 0.2414(3) 0.0347(8) Uani 1 1 d . . .
H23 H -0.3723 0.8929 0.2580 0.042 Uiso 1 1 calc R . .
C24 C -0.1549(4) 0.8643(4) 0.2990(3) 0.0325(8) Uani 1 1 d . . .
H24 H -0.1486 0.7961 0.3551 0.039 Uiso 1 1 calc R . .
C25 C -0.0346(4) 0.9083(4) 0.2742(2) 0.0274(7) Uani 1 1 d . . .
H25 H 0.0556 0.8683 0.3137 0.033 Uiso 1 1 calc R . .
C26 C -0.1701(4) 1.1748(4) 0.0580(2) 0.0234(6) Uani 1 1 d . . .
C27 C -0.3026(4) 1.2564(4) 0.0017(3) 0.0308(7) Uani 1 1 d . . .
H27 H -0.3943 1.2362 0.0108 0.037 Uiso 1 1 calc R . .
C28 C -0.2988(5) 1.3670(4) -0.0675(3) 0.0352(8) Uani 1 1 d . . .
H28 H -0.3893 1.4257 -0.1053 0.042 Uiso 1 1 calc R . .
C29 C -0.1619(5) 1.3917(4) -0.0815(3) 0.0346(8) Uani 1 1 d . . .
H29 H -0.1560 1.4660 -0.1298 0.042 Uiso 1 1 calc R . .
C30 C -0.0343(4) 1.3061(4) -0.0237(3) 0.0299(7) Uani 1 1 d . . .
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Cl 0.0271(4) 0.0399(5) 0.0594(6) 0.0192(4) -0.0141(4) -0.0211(4)
N1 0.0205(13) 0.0250(14) 0.0203(13) -0.0005(10) -0.0045(10) -0.0098(11)
N2 0.0205(13) 0.0207(13) 0.0219(13) -0.0004(10) -0.0025(10) -0.0052(11)
O1 0.0514(18) 0.0353(16) 0.093(3) -0.0133(16) -0.0180(17) -0.0199(14)
O2 0.0403(16) 0.0556(19) 0.0437(16) -0.0118(14) -0.0014(13) -0.0171(14)
O3 0.0398(15) 0.0281(13) 0.0511(17) -0.0002(12) -0.0088(12) -0.0139(12)
O4 0.0331(15) 0.0451(17) 0.0533(18) -0.0001(13) -0.0044(13) -0.0107(13)
C1 0.0179(14) 0.0240(16) 0.0267(16) 0.0022(12) -0.0060(12) -0.0102(13)
C2 0.0208(15) 0.0325(18) 0.0284(17) -0.0052(14) -0.0024(13) -0.0125(14)
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C4 0.0237(16) 0.043(2) 0.0198(16) 0.0046(14) -0.0062(13) -0.0141(15)
C5 0.0189(15) 0.0282(17) 0.0263(16) 0.0057(13) -0.0036(12) -0.0116(13)
C6 0.0223(15) 0.0258(16) 0.0230(15) -0.0003(12) -0.0056(12) -0.0106(13)
C7 0.0295(18) 0.0332(19) 0.0358(19) -0.0103(15) -0.0038(15) -0.0104(15)
C8 0.063(3) 0.041(3) 0.099(4) -0.017(3) 0.009(3) -0.028(2)
C9 0.035(2) 0.050(2) 0.050(2) 0.0031(19) -0.0053(18) -0.0148(19)
C10 0.0269(17) 0.0297(18) 0.0340(18) 0.0102(14) -0.0067(14) -0.0100(15)
C11 0.054(3) 0.031(2) 0.050(2) -0.0015(18) -0.002(2) -0.0147(19)
C12 0.042(2) 0.041(2) 0.043(2) -0.0042(17) 0.0124(18) -0.0169(18)
C21 0.0176(15) 0.0262(16) 0.0218(15) -0.0039(12) -0.0014(12) -0.0074(13)
C22 0.0209(16) 0.0349(19) 0.0367(19) -0.0033(15) -0.0051(14) -0.0120(14)
C23 0.0297(18) 0.038(2) 0.040(2) -0.0031(16) 0.0034(15) -0.0205(16)
C24 0.0358(19) 0.0342(19) 0.0296(18) 0.0023(14) 0.0014(15) -0.0195(16)
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C25 0.0298(17) 0.0289(17) 0.0236(16) 0.0036(13) -0.0050(13) -0.0136(14)
C26 0.0207(15) 0.0257(16) 0.0200(15) -0.0047(12) -0.0034(12) -0.0066(13)
C27 0.0267(17) 0.0332(18) 0.0287(17) -0.0020(14) -0.0117(14) -0.0082(15)
C28 0.037(2) 0.0300(18) 0.0294(18) -0.0013(14) -0.0173(15) -0.0036(15)
C29 0.044(2) 0.0290(18) 0.0238(17) 0.0046(14) -0.0088(15) -0.0098(16)
C30 0.0316(18) 0.0298(18) 0.0248(17) 0.0028(13) -0.0019(14) -0.0119(15)

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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 N1 2.050(3) . ?
Pd N2 2.122(3) . ?
Pd Cl 2.2985(9) . ?
N1 C25 1.352(4) . ?
N1 C21 1.358(4) . ?
N2 C30 1.334(4) . ?
N2 C26 1.346(4) . ?
O1 C7 1.367(5) . ?
O1 C8 1.428(6) . ?
O2 C9 1.404(5) . ?
O2 C7 1.451(5) . ?
O3 C10 1.378(5) . ?
O3 C11 1.428(5) . ?
O4 C10 1.408(4) . ?
O4 C12 1.428(5) . ?
C1 C6 1.392(5) . ?
C1 C2 1.406(5) . ?
C2 C3 1.393(5) . ?
C2 C7 1.507(5) . ?
C3 C4 1.380(5) . ?
C4 C5 1.394(5) . ?
C5 C6 1.390(5) . ?
C5 C10 1.507(5) . ?
C21 C22 1.376(5) . ?
C21 C26 1.489(5) . ?
C22 C23 1.379(5) . ?
C23 C24 1.384(5) . ?
C24 C25 1.368(5) . ?
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C1 Pd N2 174.38(11) . . ?
N1 Pd N2 79.15(10) . . ?
C1 Pd Cl 90.05(9) . . ?
N1 Pd Cl 174.40(7) . . ?
N2 Pd Cl 95.29(8) . . ?
C25 N1 C21 117.6(3) . . ?
C25 N1 Pd 126.6(2) . . ?
C21 N1 Pd 115.7(2) . . ?
C30 N2 C26 119.6(3) . . ?
C30 N2 Pd 126.1(2) . . ?
C26 N2 Pd 113.6(2) . . ?
C7 O1 C8 113.0(4) . . ?
C9 O2 C7 112.2(3) . . ?
C10 O3 C11 113.6(3) . . ?
C10 O4 C12 114.8(3) . . ?
C6 C1 C2 118.0(3) . . ?
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C2 C1 Pd 123.5(2) . . ?
C3 C2 C1 119.7(3) . . ?
C3 C2 C7 118.6(3) . . ?
C1 C2 C7 121.7(3) . . ?
C4 C3 C2 121.5(3) . . ?
C3 C4 C5 119.5(3) . . ?
C6 C5 C4 119.1(3) . . ?
C6 C5 C10 122.3(3) . . ?
C4 C5 C10 118.6(3) . . ?
C5 C6 C1 122.3(3) . . ?
O1 C7 O2 104.0(3) . . ?
O1 C7 C2 109.7(3) . . ?
O2 C7 C2 110.5(3) . . ?
O3 C10 O4 113.6(3) . . ?
O3 C10 C5 108.3(3) . . ?
O4 C10 C5 113.2(3) . . ?
N1 C21 C22 121.8(3) . . ?
N1 C21 C26 115.5(3) . . ?
C22 C21 C26 122.6(3) . . ?
C21 C22 C23 119.8(3) . . ?
C22 C23 C24 118.5(3) . . ?
C25 C24 C23 119.2(3) . . ?
N1 C25 C24 122.9(3) . . ?
N2 C26 C27 121.0(3) . . ?
N2 C26 C21 115.6(3) . . ?
C27 C26 C21 123.3(3) . . ?
C28 C27 C26 119.1(3) . . ?
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N2 Pd N1 C25 -179.0(3) . . . . ?
Cl Pd N1 C25 -173.0(6) . . . . ?
C1 Pd N1 C21 176.5(2) . . . . ?
N2 Pd N1 C21 -1.8(2) . . . . ?
Cl Pd N1 C21 4.3(9) . . . . ?
C1 Pd N2 C30 157.4(11) . . . . ?
N1 Pd N2 C30 175.1(3) . . . . ?
Cl Pd N2 C30 -4.3(3) . . . . ?
C1 Pd N2 C26 -13.1(12) . . . . ?
N1 Pd N2 C26 4.6(2) . . . . ?
Cl Pd N2 C26 -174.8(2) . . . . ?
N1 Pd C1 C6 72.6(3) . . . . ?
N2 Pd C1 C6 90.1(12) . . . . ?
Cl Pd C1 C6 -108.1(2) . . . . ?
N1 Pd C1 C2 -104.7(3) . . . . ?
N2 Pd C1 C2 -87.2(12) . . . . ?
Cl Pd C1 C2 74.6(3) . . . . ?
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Pd C1 C2 C3 178.2(2) . . . . ?
C6 C1 C2 C7 -176.8(3) . . . . ?
Pd C1 C2 C7 0.5(5) . . . . ?
C1 C2 C3 C4 -0.1(5) . . . . ?
C7 C2 C3 C4 177.7(3) . . . . ?
C2 C3 C4 C5 -1.1(5) . . . . ?
C3 C4 C5 C6 1.5(5) . . . . ?
C3 C4 C5 C10 -177.8(3) . . . . ?
C4 C5 C6 C1 -0.7(5) . . . . ?
C10 C5 C6 C1 178.6(3) . . . . ?
C2 C1 C6 C5 -0.5(5) . . . . ?
Pd C1 C6 C5 -178.0(2) . . . . ?
C8 O1 C7 O2 -73.2(5) . . . . ?
C8 O1 C7 C2 168.6(4) . . . . ?
C9 O2 C7 O1 164.0(3) . . . . ?
C9 O2 C7 C2 -78.3(4) . . . . ?
C3 C2 C7 O1 57.8(5) . . . . ?
C1 C2 C7 O1 -124.5(4) . . . . ?
C3 C2 C7 O2 -56.3(4) . . . . ?
C1 C2 C7 O2 121.4(3) . . . . ?
C11 O3 C10 O4 62.8(4) . . . . ?
C11 O3 C10 C5 -170.5(3) . . . . ?
C12 O4 C10 O3 52.8(4) . . . . ?
C12 O4 C10 C5 -71.3(4) . . . . ?
C6 C5 C10 O3 -32.7(4) . . . . ?
C4 C5 C10 O3 146.6(3) . . . . ?
C6 C5 C10 O4 94.2(4) . . . . ?
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C4 C5 C10 O4 -86.5(4) . . . . ?
C25 N1 C21 C22 -0.9(5) . . . . ?
Pd N1 C21 C22 -178.4(2) . . . . ?
C25 N1 C21 C26 176.5(3) . . . . ?
Pd N1 C21 C26 -1.0(3) . . . . ?
N1 C21 C22 C23 2.9(5) . . . . ?
C26 C21 C22 C23 -174.3(3) . . . . ?
C21 C22 C23 C24 -3.0(5) . . . . ?
C22 C23 C24 C25 1.3(5) . . . . ?
C21 N1 C25 C24 -0.9(5) . . . . ?
Pd N1 C25 C24 176.3(3) . . . . ?
C23 C24 C25 N1 0.7(5) . . . . ?
C30 N2 C26 C27 -1.0(5) . . . . ?
Pd N2 C26 C27 170.3(2) . . . . ?
C30 N2 C26 C21 -177.7(3) . . . . ?
Pd N2 C26 C21 -6.5(3) . . . . ?
N1 C21 C26 N2 5.1(4) . . . . ?
C22 C21 C26 N2 -177.6(3) . . . . ?
N1 C21 C26 C27 -171.5(3) . . . . ?
C22 C21 C26 C27 5.8(5) . . . . ?
N2 C26 C27 C28 -0.6(5) . . . . ?
C21 C26 C27 C28 175.9(3) . . . . ?
C26 C27 C28 C29 1.7(5) . . . . ?
C27 C28 C29 C30 -1.3(5) . . . . ?
C26 N2 C30 C29 1.4(5) . . . . ?
Pd N2 C30 C29 -168.6(3) . . . . ?
C28 C29 C30 N2 -0.3(5) . . . . ?

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C30 H30 Cl  0.95 2.75 3.348(4) 121.4 .
C4 H4 O1  0.95 2.79 3.662(5) 153.2 2_676
C8 H8C O2  0.98 2.65 3.412(6) 135.0 2_586
C24 H24 O2  0.95 2.61 3.345(5) 134.3 2_576
C8 H8B O3  0.98 2.50 3.436(6) 160.1 1_565
C28 H28 O3  0.95 2.56 3.379(4) 144.9 2_575
C9 H9A O4  0.98 2.57 3.477(5) 153.8 1_465

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_cell_volume                      1456.3(2)
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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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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      SHELXL
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Cl Cl -0.29207(6) -0.33801(6) 0.73002(4) 0.03152(14) Uani 1 1 d . . .
P P -0.00810(5) -0.12373(5) 0.68698(3) 0.01806(12) Uani 1 1 d . . .
S1 S -0.08975(6) -0.23309(5) 0.94029(3) 0.02074(12) Uani 1 1 d . . .
S2 S 0.17383(6) -0.34132(6) 0.95812(5) 0.03657(16) Uani 1 1 d . . .
S3 S 0.31909(6) 0.39649(5) 0.90178(4) 0.02751(13) Uani 1 1 d . . .
S4 S 0.49458(8) 0.23641(6) 0.81678(5) 0.03987(16) Uani 1 1 d . . .
C1 C 0.1337(2) -0.04258(19) 0.89427(12) 0.0167(4) Uani 1 1 d DU . .
C2 C 0.1888(2) -0.0680(2) 0.97666(13) 0.0185(4) Uani 1 1 d DU . .
C3 C 0.3201(2) 0.0180(2) 1.03769(14) 0.0234(4) Uani 1 1 d DU . .
H3 H 0.3544 -0.0006 1.0928 0.028 Uiso 1 1 calc R . .
C4 C 0.4014(2) 0.1306(2) 1.01882(14) 0.0217(4) Uani 1 1 d DU . .
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H4 H 0.4924 0.1877 1.0600 0.026 Uiso 1 1 calc R . .
C5 C 0.3486(2) 0.1591(2) 0.93922(13) 0.0187(4) Uani 1 1 d DU . .
C6 C 0.2155(2) 0.0736(2) 0.87846(13) 0.0184(4) Uani 1 1 d DU . .
H6 H 0.1797 0.0954 0.8247 0.022 Uiso 1 1 calc R . .
C7 C 0.1075(2) -0.1925(2) 0.99720(13) 0.0222(4) Uani 1 1 d U . .
H7 H 0.1208 -0.1731 1.0630 0.027 Uiso 1 1 calc R . .
C8 C -0.1258(2) -0.4170(2) 0.91017(16) 0.0300(5) Uani 1 1 d U . .
H8A H -0.1351 -0.4514 0.9624 0.036 Uiso 1 1 calc R . .
H8B H -0.2201 -0.4605 0.8623 0.036 Uiso 1 1 calc R . .
C9 C 0.0028(3) -0.4509(2) 0.87846(16) 0.0323(5) Uani 1 1 d U . .
H9A H -0.0016 -0.4358 0.8190 0.039 Uiso 1 1 calc R . .
H9B H -0.0020 -0.5482 0.8736 0.039 Uiso 1 1 calc R . .
C10 C 0.4336(2) 0.2828(2) 0.91822(14) 0.0208(4) Uani 1 1 d U . .
H10 H 0.5235 0.3330 0.9695 0.025 Uiso 1 1 calc R . .
C11 C 0.4308(3) 0.4815(2) 0.84100(18) 0.0363(6) Uani 1 1 d U . .
H11A H 0.3795 0.5408 0.8134 0.044 Uiso 1 1 calc R . .
H11B H 0.5285 0.5392 0.8817 0.044 Uiso 1 1 calc R . .
C12 C 0.4527(3) 0.3717(3) 0.76993(16) 0.0397(6) Uani 1 1 d U . .
H12A H 0.5357 0.4115 0.7469 0.048 Uiso 1 1 calc R . .
H12B H 0.3610 0.3336 0.7197 0.048 Uiso 1 1 calc R . .
C21 C -0.1355(2) -0.2446(2) 0.58407(13) 0.0226(4) Uani 1 1 d DU . .
C22 C -0.1201(3) -0.3767(2) 0.56151(15) 0.0307(5) Uani 1 1 d DU . .
H22 H -0.0379 -0.3977 0.5951 0.037 Uiso 1 1 calc R . .
C23 C -0.2242(3) -0.4781(3) 0.49008(16) 0.0383(6) Uani 1 1 d DU . .
H23 H -0.2124 -0.5676 0.4743 0.046 Uiso 1 1 calc R . .
C24 C -0.3454(3) -0.4476(3) 0.44209(16) 0.0401(6) Uani 1 1 d DU . .
H24 H -0.4186 -0.5171 0.3946 0.048 Uiso 1 1 calc R . .
C25 C -0.3594(3) -0.3167(3) 0.46340(15) 0.0378(6) Uani 1 1 d DU . .
H25 H -0.4416 -0.2960 0.4296 0.045 Uiso 1 1 calc R . .
C26 C -0.2548(2) -0.2142(2) 0.53373(14) 0.0279(5) Uani 1 1 d DU . .
H26 H -0.2648 -0.1239 0.5473 0.033 Uiso 1 1 calc R . .
C31 C -0.0354(2) 0.0424(2) 0.68102(13) 0.0206(4) Uani 1 1 d DU . .
C32 C -0.1530(3) 0.0759(2) 0.71171(15) 0.0309(5) Uani 1 1 d DU . .
H32 H -0.2092 0.0159 0.7373 0.037 Uiso 1 1 calc R . .
C33 C -0.1881(3) 0.1960(3) 0.70518(18) 0.0400(6) Uani 1 1 d DU . .
H33 H -0.2694 0.2170 0.7252 0.048 Uiso 1 1 calc R . .
C34 C -0.1055(3) 0.2856(2) 0.66959(16) 0.0363(6) Uani 1 1 d DU . .
H34 H -0.1303 0.3675 0.6647 0.044 Uiso 1 1 calc R . .
C35 C 0.0133(3) 0.2552(2) 0.64122(16) 0.0353(5) Uani 1 1 d DU . .
H35 H 0.0714 0.3172 0.6177 0.042 Uiso 1 1 calc R . .
C36 C 0.0484(3) 0.1344(2) 0.64681(15) 0.0280(5) Uani 1 1 d DU . .
H36 H 0.1304 0.1145 0.6271 0.034 Uiso 1 1 calc R . .
C41 C 0.1730(2) -0.1323(2) 0.67021(13) 0.0220(4) Uani 1 1 d DU . .
C42 C 0.2085(3) -0.1141(2) 0.59201(15) 0.0292(5) Uani 1 1 d DU . .
H42 H 0.1402 -0.0924 0.5486 0.035 Uiso 1 1 calc R . .
C43 C 0.3440(3) -0.1280(3) 0.57825(16) 0.0372(6) Uani 1 1 d DU . .
H43 H 0.3693 -0.1132 0.5260 0.045 Uiso 1 1 calc R . .
C44 C 0.4420(3) -0.1632(3) 0.63990(16) 0.0362(6) Uani 1 1 d DU . .
H44 H 0.5343 -0.1725 0.6300 0.043 Uiso 1 1 calc R . .
C45 C 0.4061(2) -0.1850(2) 0.71594(16) 0.0324(5) Uani 1 1 d DU . .
H45 H 0.4727 -0.2112 0.7576 0.039 Uiso 1 1 calc R . .
C46 C 0.2723(2) -0.1685(2) 0.73155(14) 0.0253(5) Uani 1 1 d DU . .
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P 0.0163(2) 0.0208(3) 0.0151(2) 0.0052(2) 0.00409(19) 0.0012(2)
S1 0.0214(3) 0.0254(3) 0.0228(3) 0.0114(2) 0.0125(2) 0.0103(2)
S2 0.0220(3) 0.0202(3) 0.0685(4) 0.0161(3) 0.0070(3) 0.0091(2)
S3 0.0243(3) 0.0215(3) 0.0416(3) 0.0123(2) 0.0131(2) 0.0088(2)
S4 0.0510(4) 0.0331(3) 0.0459(4) 0.0097(3) 0.0363(3) 0.0119(3)
C1 0.0175(9) 0.0163(9) 0.0161(9) 0.0016(7) 0.0060(7) 0.0055(7)
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C3 0.0262(11) 0.0225(10) 0.0204(10) 0.0057(8) 0.0012(8) 0.0100(8)
C4 0.0182(10) 0.0197(10) 0.0231(10) 0.0016(8) 0.0009(8) 0.0062(8)
C5 0.0172(9) 0.0170(10) 0.0233(10) 0.0025(8) 0.0091(8) 0.0069(8)
C6 0.0195(10) 0.0206(10) 0.0154(9) 0.0039(8) 0.0052(8) 0.0068(8)
C7 0.0261(11) 0.0222(10) 0.0176(10) 0.0066(8) 0.0033(8) 0.0067(8)
C8 0.0260(11) 0.0236(11) 0.0380(13) 0.0160(10) 0.0020(9) 0.0012(9)
C9 0.0406(13) 0.0211(11) 0.0339(13) 0.0060(9) 0.0044(10) 0.0132(10)
C10 0.0179(10) 0.0203(10) 0.0231(10) 0.0029(8) 0.0072(8) 0.0046(8)
C11 0.0359(13) 0.0300(13) 0.0452(14) 0.0201(11) 0.0119(11) 0.0034(10)
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C23 0.0426(14) 0.0292(13) 0.0320(13) 0.0026(10) 0.0083(11) -0.0043(10)
C24 0.0321(13) 0.0458(15) 0.0239(12) -0.0036(10) 0.0047(10) -0.0100(11)
C25 0.0227(11) 0.0612(17) 0.0214(11) 0.0034(11) 0.0031(9) 0.0065(11)
C26 0.0245(11) 0.0393(13) 0.0182(10) 0.0050(9) 0.0074(8) 0.0071(9)
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C33 0.0444(15) 0.0393(14) 0.0452(15) 0.0129(12) 0.0194(12) 0.0213(12)
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C44 0.0233(11) 0.0401(14) 0.0392(13) -0.0022(11) 0.0147(10) 0.0041(10)
C45 0.0240(11) 0.0367(13) 0.0305(12) -0.0022(10) 0.0055(9) 0.0101(10)
C46 0.0229(11) 0.0281(11) 0.0212(10) 0.0004(9) 0.0065(8) 0.0057(9)

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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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P C31 1.827(2) . ?
P C21 1.829(2) . ?
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S4 C12 1.815(3) . ?
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C2 C3 1.391(3) . ?
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C21 P Pd 112.27(7) . . ?
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C2 C1 Pd 117.24(14) . . ?
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C3 C2 C7 119.26(18) . . ?
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C10 H10 S2  1.00 2.85 3.699(2) 142.7 2_657
C12 H12A Cl  0.99 2.86 3.707(2) 143.8 1_665

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 'S'  'S'   0.1246   0.1234
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 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x-1/2, -y-1/2, z-1/2'

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_cell_angle_beta                  100.062(3)
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    0.00   -1.00    0.00    0.1130
    0.00    0.00    1.00    0.1720
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_refine_special_details
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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
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S2 S 0.73371(4) 0.43242(3) 0.30807(4) 0.02468(11) Uani 1 1 d . . .
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C15 C 0.54679(17) 0.66241(10) 0.37623(14) 0.0218(4) Uani 1 1 d DU . .
H15 H 0.4846 0.6877 0.3886 0.026 Uiso 1 1 calc R . .
C16 C 0.53640(16) 0.59332(10) 0.36361(13) 0.0191(4) Uani 1 1 d DU . .
C20 C 0.22995(17) 0.59620(10) 0.22592(14) 0.0219(4) Uani 1 1 d U . .
C21 C 0.04710(17) 0.66190(10) 0.20023(14) 0.0233(4) Uani 1 1 d DU . .
C22 C -0.04658(17) 0.62170(11) 0.16959(14) 0.0263(4) Uani 1 1 d DU . .
C23 C -0.14974(19) 0.65407(13) 0.15077(16) 0.0349(5) Uani 1 1 d DU . .
H23 H -0.2156 0.6287 0.1295 0.042 Uiso 1 1 calc R . .
C24 C -0.1576(2) 0.72268(13) 0.16257(18) 0.0412(6) Uani 1 1 d DU . .
H24 H -0.2288 0.7439 0.1490 0.049 Uiso 1 1 calc R . .
C25 C -0.0635(2) 0.76082(12) 0.19380(17) 0.0393(6) Uani 1 1 d DU . .
H25 H -0.0708 0.8079 0.2019 0.047 Uiso 1 1 calc R . .
C26 C 0.0424(2) 0.73127(11) 0.21363(16) 0.0306(5) Uani 1 1 d DU . .
C27 C -0.0349(2) 0.54716(11) 0.15794(16) 0.0331(5) Uani 1 1 d U . .
H27A H -0.1074 0.5282 0.1291 0.040 Uiso 1 1 calc R . .
H27B H -0.0104 0.5264 0.2191 0.040 Uiso 1 1 calc R . .
H27C H 0.0206 0.5383 0.1180 0.040 Uiso 1 1 calc R . .
C28 C 0.1464(2) 0.77178(12) 0.2436(2) 0.0445(6) Uani 1 1 d U . .
H28A H 0.1879 0.7752 0.1919 0.053 Uiso 1 1 calc R . .
H28B H 0.1933 0.7498 0.2968 0.053 Uiso 1 1 calc R . .
H28C H 0.1260 0.8169 0.2620 0.053 Uiso 1 1 calc R . .
C31 C 0.26362(16) 0.54158(10) 0.42631(13) 0.0216(4) Uani 1 1 d DU . .
C32 C 0.23021(18) 0.47476(11) 0.40953(14) 0.0253(4) Uani 1 1 d DU . .
C33 C 0.11569(19) 0.46064(13) 0.39904(15) 0.0333(5) Uani 1 1 d DU . .
H33 H 0.0906 0.4157 0.3875 0.040 Uiso 1 1 calc R . .
C34 C 0.0384(2) 0.51043(14) 0.40509(16) 0.0386(6) Uani 1 1 d DU . .
H34 H -0.0392 0.5000 0.3946 0.046 Uiso 1 1 calc R . .
C35 C 0.07373(19) 0.57563(14) 0.42639(16) 0.0365(5) Uani 1 1 d DU . .
H35 H 0.0202 0.6095 0.4325 0.044 Uiso 1 1 calc R . .
C36 C 0.18698(18) 0.59210(11) 0.43899(14) 0.0272(4) Uani 1 1 d DU . .
C37 C 0.3119(2) 0.41898(11) 0.40326(16) 0.0320(5) Uani 1 1 d U . .
H37A H 0.3127 0.4086 0.3376 0.038 Uiso 1 1 calc R . .
H37B H 0.2894 0.3789 0.4345 0.038 Uiso 1 1 calc R . .
H37C H 0.3870 0.4330 0.4336 0.038 Uiso 1 1 calc R . .
C38 C 0.2265(2) 0.66228(12) 0.46313(18) 0.0380(6) Uani 1 1 d U . .
H38A H 0.1629 0.6902 0.4727 0.046 Uiso 1 1 calc R . .
H38B H 0.2600 0.6809 0.4121 0.046 Uiso 1 1 calc R . .
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N2 N 0.15180(14) 0.62985(8) 0.21654(12) 0.0227(4) Uani 1 1 d U . .
N3 N 0.37835(13) 0.56191(8) 0.43332(11) 0.0207(3) Uani 1 1 d U . .
C99 C -0.5645(2) 0.68807(13) 0.10028(19) 0.0441(6) Uani 1 1 d . . .
H99A H -0.6321 0.6593 0.0929 0.053 Uiso 1 1 calc R . .
H99B H -0.5347 0.6923 0.1678 0.053 Uiso 1 1 calc R . .
Cl1 Cl -0.60132(7) 0.76798(3) 0.05334(6) 0.0579(2) Uani 1 1 d . . .
Cl2 Cl -0.46258(7) 0.64980(4) 0.04398(7) 0.0653(2) Uani 1 1 d . . .

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S2 0.0199(2) 0.0248(2) 0.0287(3) 0.0004(2) 0.0023(2) 0.00453(19)
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S4 0.0623(4) 0.0266(3) 0.0222(3) -0.0045(2) 0.0036(3) 0.0014(3)
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C4 0.0298(11) 0.0233(10) 0.0252(11) -0.0022(8) 0.0018(9) -0.0073(8)
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C13 0.0225(10) 0.0279(10) 0.0253(11) -0.0009(8) 0.0049(8) -0.0088(8)
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C15 0.0237(10) 0.0213(9) 0.0202(10) -0.0013(8) 0.0037(8) -0.0012(8)
C16 0.0195(9) 0.0217(9) 0.0156(9) -0.0013(7) 0.0020(7) -0.0020(7)
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C23 0.0250(11) 0.0506(14) 0.0283(12) 0.0085(10) 0.0022(9) 0.0053(10)
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C33 0.0317(12) 0.0461(13) 0.0212(11) 0.0036(10) 0.0023(9) -0.0159(10)
C34 0.0233(11) 0.0664(17) 0.0257(12) 0.0101(11) 0.0036(9) -0.0085(11)
C35 0.0253(11) 0.0599(16) 0.0259(12) 0.0118(11) 0.0089(9) 0.0100(11)
C36 0.0269(11) 0.0358(12) 0.0202(10) 0.0038(9) 0.0080(8) 0.0042(9)
C37 0.0434(13) 0.0247(11) 0.0298(12) 0.0003(9) 0.0115(10) -0.0073(9)
C38 0.0461(15) 0.0341(13) 0.0357(13) -0.0017(10) 0.0127(11) 0.0109(11)
N2 0.0237(9) 0.0226(8) 0.0218(9) 0.0021(7) 0.0038(7) 0.0030(7)
N3 0.0185(8) 0.0222(8) 0.0211(8) -0.0006(7) 0.0031(6) -0.0009(6)
C99 0.0555(17) 0.0338(13) 0.0410(15) 0.0054(11) 0.0028(12) 0.0026(12)
Cl1 0.0621(5) 0.0366(3) 0.0641(5) 0.0045(3) -0.0192(4) 0.0077(3)
Cl2 0.0479(4) 0.0576(5) 0.0886(6) -0.0151(4) 0.0066(4) 0.0079(4)

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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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S1 C1 1.8318(19) . ?
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C4 C14 1.512(3) . ?
C5 C6 1.505(4) . ?
C10 N3 1.262(2) . ?
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C21 C22 1.397(3) . ?
C21 N2 1.403(2) . ?
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C23 C24 1.381(4) . ?
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C26 C28 1.496(3) . ?
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C31 C36 1.403(3) . ?
C31 N3 1.435(2) . ?
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C32 C37 1.501(3) . ?
C33 C34 1.377(4) . ?
C34 C35 1.384(4) . ?
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C20 Pd S1 176.35(6) . . ?
C10 Pd S1 87.34(5) . . ?
C20 Pd I 91.27(6) . . ?
C10 Pd I 175.79(5) . . ?
S1 Pd I 89.408(13) . . ?
C2 S1 C1 92.03(10) . . ?
C2 S1 Pd 109.93(7) . . ?
C1 S1 Pd 110.71(6) . . ?
C1 S2 C3 97.60(9) . . ?
C5 S3 C4 97.34(12) . . ?
C6 S4 C4 98.34(11) . . ?
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C14 C4 S3 112.72(14) . . ?
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C6 C5 S3 107.95(19) . . ?
C5 C6 S4 108.06(18) . . ?
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N3 C10 Pd 127.51(14) . . ?
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C12 C11 C16 118.59(18) . . ?
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C13 C14 C15 118.63(18) . . ?
C13 C14 C4 120.45(18) . . ?
C15 C14 C4 120.91(19) . . ?
C16 C15 C14 120.95(19) . . ?
C15 C16 C11 120.27(18) . . ?
C15 C16 C10 117.22(17) . . ?
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N2 C20 Pd 174.30(18) . . ?
C26 C21 C22 124.1(2) . . ?
C26 C21 N2 118.90(19) . . ?
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C31 C36 C38 120.44(19) . . ?
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Cl1 C99 Cl2 111.07(15) . . ?

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_computing_publication_material   SHELXL-97

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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.

 Slow convergence of the methyl group at C27 may indicate rotational disorder.
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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Pd Pd 0.464170(10) 0.772420(10) 0.446758(9) 0.01356(4) Uani 1 1 d . . .
I I 0.425970(9) 0.647857(9) 0.363563(9) 0.02050(4) Uani 1 1 d . . .
S1 S 0.51669(3) 0.82698(3) 0.35164(3) 0.01536(12) Uani 1 1 d . . .
S2 S 0.63688(4) 0.91280(3) 0.31229(3) 0.01991(14) Uani 1 1 d . . .
C1 C 0.58241(12) 0.86275(12) 0.51661(12) 0.0128(5) Uani 1 1 d U . .
C2 C 0.61927(13) 0.84283(13) 0.58446(12) 0.0161(5) Uani 1 1 d U . .
C3 C 0.69487(14) 0.83635(13) 0.59376(13) 0.0178(5) Uani 1 1 d U . .
C4 C 0.73456(13) 0.84982(13) 0.53598(13) 0.0179(5) Uani 1 1 d U . .
C5 C 0.69870(13) 0.87000(13) 0.46853(13) 0.0165(5) Uani 1 1 d U . .
H5 H 0.7258 0.8792 0.4290 0.020 Uiso 1 1 calc R . .
C6 C 0.62362(13) 0.87648(12) 0.45942(12) 0.0149(5) Uani 1 1 d U . .
C7 C 0.57886(16) 0.75903(15) 0.67158(15) 0.0295(6) Uani 1 1 d U . .
H7A H 0.5519 0.7247 0.6365 0.035 Uiso 1 1 calc R . .
H7B H 0.5553 0.7601 0.7162 0.035 Uiso 1 1 calc R . .
H7C H 0.6291 0.7408 0.6825 0.035 Uiso 1 1 calc R . .
C8 C 0.76472(16) 0.87908(15) 0.69963(14) 0.0288(6) Uani 1 1 d U . .
H8A H 0.7979 0.9042 0.6696 0.035 Uiso 1 1 calc R . .
H8B H 0.7924 0.8606 0.7444 0.035 Uiso 1 1 calc R . .
H8C H 0.7278 0.9156 0.7115 0.035 Uiso 1 1 calc R . .
C9 C 0.85261(14) 0.85971(16) 0.49457(15) 0.0292(6) Uani 1 1 d U . .
H9A H 0.8394 0.8254 0.4536 0.035 Uiso 1 1 calc R . .
H9B H 0.9041 0.8526 0.5127 0.035 Uiso 1 1 calc R . .
H9C H 0.8445 0.9127 0.4788 0.035 Uiso 1 1 calc R . .
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O1 O 0.57934(10) 0.83409(9) 0.64185(9) 0.0223(4) Uani 1 1 d U . .

O2 O 0.72974(9) 0.81596(9) 0.66071(9) 0.0221(4) Uani 1 1 d U . .

O3 O 0.80862(9) 0.84295(10) 0.55090(9) 0.0249(4) Uani 1 1 d U . .

C10 C 0.58313(13) 0.89974(13) 0.38629(12) 0.0156(5) Uani 1 1 d U . .

H10 H 0.5562 0.9482 0.3931 0.019 Uiso 1 1 calc R . .

C11 C 0.58814(14) 0.76467(13) 0.32747(13) 0.0192(5) Uani 1 1 d U . .

H11A H 0.6149 0.7422 0.3716 0.023 Uiso 1 1 calc R . .

H11B H 0.5669 0.7227 0.2963 0.023 Uiso 1 1 calc R . .

C12 C 0.64001(13) 0.81190(13) 0.28692(13) 0.0185(5) Uani 1 1 d U . .

H12A H 0.6262 0.8066 0.2341 0.022 Uiso 1 1 calc R . .

H12B H 0.6903 0.7925 0.2984 0.022 Uiso 1 1 calc R . .

N2 N 0.39853(11) 0.69248(11) 0.57358(11) 0.0181(4) Uani 1 1 d U . .

C20 C 0.41950(13) 0.72820(13) 0.52815(13) 0.0178(5) Uani 1 1 d U . .

C21 C 0.38373(13) 0.64171(13) 0.62854(12) 0.0164(5) Uani 1 1 d U . .

C22 C 0.32710(14) 0.65780(14) 0.66948(13) 0.0208(5) Uani 1 1 d U . .

C23 C 0.31720(15) 0.60675(14) 0.72495(14) 0.0248(6) Uani 1 1 d U . .

H23 H 0.2796 0.6158 0.7546 0.030 Uiso 1 1 calc R . .

C24 C 0.36130(16) 0.54304(15) 0.73759(14) 0.0272(6) Uani 1 1 d U . .

H24 H 0.3546 0.5098 0.7766 0.033 Uiso 1 1 calc R . .

C25 C 0.41480(15) 0.52768(15) 0.69386(15) 0.0277(6) Uani 1 1 d U . .

H25 H 0.4433 0.4827 0.7021 0.033 Uiso 1 1 calc R . .

C26 C 0.42806(14) 0.57652(14) 0.63793(14) 0.0221(6) Uani 1 1 d U . .

C27 C 0.27627(16) 0.72447(15) 0.65253(15) 0.0299(6) Uani 1 1 d U . .

H27A H 0.2285 0.7057 0.6316 0.045 Uiso 1 1 calc R . .

H27B H 0.2963 0.7584 0.6179 0.045 Uiso 1 1 calc R . .

H27C H 0.2710 0.7526 0.6971 0.045 Uiso 1 1 calc R . .

C28 C 0.48618(16) 0.56092(16) 0.59022(16) 0.0337(7) Uani 1 1 d U . .

H28A H 0.4659 0.5665 0.5394 0.040 Uiso 1 1 calc R . .

H28B H 0.5045 0.5088 0.5986 0.040 Uiso 1 1 calc R . .

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H28C H 0.5263 0.5972 0.6013 0.040 Uiso 1 1 calc R . .
N3 N 0.46556(11) 0.91700(10) 0.53160(10) 0.0153(4) Uani 1 1 d U . .
C30 C 0.50110(13) 0.86457(12) 0.50646(12) 0.0141(5) Uani 1 1 d U . .
C31 C 0.38812(13) 0.92024(12) 0.52683(13) 0.0158(5) Uani 1 1 d U . .
C32 C 0.34581(13) 0.94149(13) 0.46202(13) 0.0175(5) Uani 1 1 d U . .
C33 C 0.27094(14) 0.94842(13) 0.46286(14) 0.0213(5) Uani 1 1 d U . .
H33 H 0.2415 0.9627 0.4197 0.026 Uiso 1 1 calc R . .
C34 C 0.23834(14) 0.93504(14) 0.52486(15) 0.0251(6) Uani 1 1 d U . .
H34 H 0.1869 0.9389 0.5238 0.030 Uiso 1 1 calc R . .
C35 C 0.28102(14) 0.91587(13) 0.58881(15) 0.0231(6) Uani 1 1 d U . .
H35 H 0.2586 0.9073 0.6316 0.028 Uiso 1 1 calc R . .
C36 C 0.35641(14) 0.90911(13) 0.59074(13) 0.0187(5) Uani 1 1 d U . .
C37 C 0.37943(14) 0.95778(14) 0.39358(13) 0.0219(6) Uani 1 1 d U . .
H37A H 0.3893 0.9096 0.3699 0.026 Uiso 1 1 calc R . .
H37B H 0.4251 0.9858 0.4054 0.026 Uiso 1 1 calc R . .
H37C H 0.3457 0.9885 0.3609 0.026 Uiso 1 1 calc R . .
C38 C 0.40372(14) 0.88899(15) 0.66026(13) 0.0237(6) Uani 1 1 d U . .
H38A H 0.3750 0.8936 0.7012 0.028 Uiso 1 1 calc R . .
H38B H 0.4454 0.9239 0.6672 0.028 Uiso 1 1 calc R . .
H38C H 0.4213 0.8365 0.6573 0.028 Uiso 1 1 calc R . .

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I 0.02453(9) 0.01683(8) 0.01961(8) -0.00292(7) 0.00030(6) -0.00351(7)

S1 0.0153(3) 0.0179(3) 0.0126(3) -0.0007(2) 0.0004(2) -0.0008(2)

S2 0.0244(4) 0.0202(3) 0.0160(3) 0.0017(2) 0.0064(3) -0.0027(3)

C1 0.0138(12) 0.0099(11) 0.0149(11) -0.0013(9) 0.0020(9) -0.0021(9)

C2 0.0225(13) 0.0130(12) 0.0131(11) 0.0000(9) 0.0029(9) 0.0009(10)

C3 0.0186(13) 0.0159(12) 0.0178(12) 0.0005(9) -0.0032(10) 0.0016(10)

C4 0.0147(12) 0.0153(11) 0.0230(13) -0.0017(10) -0.0011(10) 0.0005(10)

C5 0.0168(13) 0.0183(12) 0.0147(12) -0.0014(9) 0.0030(9) -0.0008(10)

C6 0.0192(13) 0.0119(11) 0.0130(11) -0.0018(9) -0.0008(9) -0.0012(9)

C7 0.0314(17) 0.0315(16) 0.0264(15) 0.0052(12) 0.0066(12) -0.0023(13)

C8 0.0303(16) 0.0333(15) 0.0206(14) -0.0001(11) -0.0068(12) -0.0010(12)

C9 0.0154(14) 0.0375(16) 0.0352(16) 0.0021(13) 0.0046(11) 0.0019(12)

O1 0.0253(10) 0.0273(10) 0.0149(9) 0.0042(7) 0.0047(7) 0.0050(8)

O2 0.0223(10) 0.0235(9) 0.0185(9) 0.0040(7) -0.0069(7) -0.0004(8)

O3 0.0128(9) 0.0347(11) 0.0266(10) 0.0052(8) -0.0006(7) 0.0032(8)

C10 0.0162(13) 0.0169(12) 0.0136(11) 0.0002(9) 0.0021(9) -0.0010(10)

C11 0.0222(14) 0.0172(12) 0.0185(12) -0.0036(10) 0.0028(10) 0.0013(10)

C12 0.0164(13) 0.0225(13) 0.0166(12) -0.0016(10) 0.0023(10) 0.0023(10)

N2 0.0191(11) 0.0182(11) 0.0174(11) -0.0028(8) 0.0038(8) -0.0003(9)

C20 0.0178(13) 0.0162(12) 0.0192(12) -0.0068(10) 0.0010(10) 0.0001(10)

C21 0.0190(13) 0.0139(11) 0.0164(12) 0.0023(9) 0.0022(9) -0.0046(10)

C22 0.0245(14) 0.0185(13) 0.0196(13) -0.0023(10) 0.0038(10) -0.0041(10)

C23 0.0305(16) 0.0235(14) 0.0219(14) -0.0027(11) 0.0097(11) -0.0078(12)

C24 0.0349(17) 0.0236(14) 0.0226(14) 0.0060(11) 0.0006(12) -0.0078(12)

C25 0.0312(16) 0.0177(13) 0.0333(16) 0.0062(11) 0.0001(12) -0.0013(11)

C26 0.0200(14) 0.0223(13) 0.0239(14) 0.0006(10) 0.0018(11) -0.0003(10)

C27 0.0306(16) 0.0242(14) 0.0377(16) 0.0025(12) 0.0160(13) 0.0042(12)

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C28 0.0333(17) 0.0267(15) 0.0434(18) 0.0031(13) 0.0148(14) 0.0107(13)
N3 0.0168(11) 0.0144(10) 0.0144(10) 0.0006(8) 0.0008(8) -0.0008(8)
C30 0.0190(13) 0.0125(11) 0.0106(11) 0.0015(9) 0.0010(9) -0.0014(9)
C31 0.0175(13) 0.0103(11) 0.0194(12) -0.0018(9) 0.0017(10) -0.0005(9)
C32 0.0192(13) 0.0118(11) 0.0209(12) -0.0041(10) -0.0002(10) -0.0001(10)
C33 0.0193(13) 0.0171(12) 0.0257(14) -0.0026(10) -0.0043(11) -0.0004(10)
C34 0.0147(13) 0.0189(13) 0.0418(17) -0.0035(12) 0.0036(12) 0.0005(10)
C35 0.0238(14) 0.0185(13) 0.0294(15) 0.0002(11) 0.0128(11) 0.0028(11)
C36 0.0218(14) 0.0131(11) 0.0217(13) -0.0021(10) 0.0038(10) 0.0000(10)
C37 0.0249(14) 0.0204(13) 0.0201(13) -0.0007(10) 0.0013(11) 0.0057(11)
C38 0.0252(15) 0.0248(14) 0.0217(13) 0.0009(11) 0.0060(11) 0.0027(11)

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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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S1 C11 1.810(3) . ?

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S2 C12 1.833(2) . ?

C1 C6 1.399(3) . ?

C1 C2 1.407(3) . ?

C1 C30 1.492(3) . ?

C2 O1 1.374(3) . ?

C2 C3 1.392(3) . ?

C3 O2 1.381(3) . ?

C3 C4 1.389(3) . ?

C4 O3 1.369(3) . ?

C4 C5 1.395(3) . ?

C5 C6 1.382(3) . ?

C6 C10 1.530(3) . ?

C7 O1 1.428(3) . ?

C8 O2 1.434(3) . ?

C9 O3 1.429(3) . ?

C11 C12 1.529(3) . ?

N2 C20 1.154(3) . ?

N2 C21 1.406(3) . ?

C21 C22 1.392(3) . ?

C21 C26 1.405(3) . ?

C22 C23 1.394(3) . ?

C22 C27 1.510(4) . ?

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C23 C24 1.386(4) . ?
C24 C25 1.377(4) . ?
C25 C26 1.391(4) . ?
C26 C28 1.495(4) . ?
N3 C30 1.251(3) . ?
N3 C31 1.424(3) . ?
C31 C36 1.398(3) . ?
C31 C32 1.409(3) . ?
C32 C33 1.390(3) . ?
C32 C37 1.507(3) . ?
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C20 Pd C30 92.12(9) . . ?
C20 Pd S1 178.88(7) . . ?
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C30 Pd I 175.29(7) . . ?
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S1 Pd I 90.059(16) . . ?

C11 S1 C10 91.69(11) . . ?

C11 S1 Pd 108.77(8) . . ?

C10 S1 Pd 109.90(8) . . ?

C10 S2 C12 96.34(11) . . ?

C6 C1 C2 118.4(2) . . ?

C6 C1 C30 121.9(2) . . ?

C2 C1 C30 119.6(2) . . ?

O1 C2 C3 121.0(2) . . ?

O1 C2 C1 118.5(2) . . ?

C3 C2 C1 120.4(2) . . ?

O2 C3 C4 120.6(2) . . ?

O2 C3 C2 119.3(2) . . ?

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O3 C4 C3 115.6(2) . . ?

O3 C4 C5 124.3(2) . . ?

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C6 C5 C4 119.8(2) . . ?

C5 C6 C1 121.3(2) . . ?

C5 C6 C10 120.8(2) . . ?

C1 C6 C10 118.0(2) . . ?

C2 O1 C7 115.56(19) . . ?

C3 O2 C8 113.04(18) . . ?

C4 O3 C9 118.22(19) . . ?

C6 C10 S2 117.19(17) . . ?

C6 C10 S1 111.44(16) . . ?

S2 C10 S1 103.01(11) . . ?

C12 C11 S1 108.19(16) . . ?

C11 C12 S2 110.81(17) . . ?

C20 N2 C21 170.3(2) . . ?

N2 C20 Pd 169.9(2) . . ?

C22 C21 C26 124.1(2) . . ?

C22 C21 N2 119.4(2) . . ?

C26 C21 N2 116.5(2) . . ?

C21 C22 C23 116.5(2) . . ?

C21 C22 C27 122.1(2) . . ?

C23 C22 C27 121.3(2) . . ?

C24 C23 C22 121.2(3) . . ?

C25 C24 C23 120.3(2) . . ?

C24 C25 C26 121.5(3) . . ?

C25 C26 C21 116.3(2) . . ?

C25 C26 C28 122.1(2) . . ?

C21 C26 C28 121.6(2) . . ?

C30 N3 C31 124.9(2) . . ?

N3 C30 C1 122.2(2) . . ?

N3 C30 Pd 129.09(18) . . ?

C1 C30 Pd 108.74(15) . . ?

C36 C31 C32 121.3(2) . . ?

C36 C31 N3 117.3(2) . . ?

C32 C31 N3 121.2(2) . . ?

C33 C32 C31 117.9(2) . . ?

C33 C32 C37 120.0(2) . . ?

C31 C32 C37 122.1(2) . . ?

C34 C33 C32 121.6(2) . . ?

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C34 C35 C36 120.6(3) . . ?

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