Supporting Information

Table 1SI. Summary of Crystal and Refinement Data

empirical formula	$C_{26}H_{31}IN_2PdS$
fw	636.9
cryst syst; space group	monoclinic; $P2_1/n$ (No. 14)
a , Å	10.698(2)
b , Å	17.019(3)
c , Å	14.729(3)
β , deg	104.98(3)
V, Å^3	2591(1)
Z, ρ_{calcd}, g cm^{-3}	4; 1.633
λ, Å; μ, cm^{-1}	0.71073; 20.04
Θ range, deg	3.1 – 26.0
reflns collected	4318
reflns obsd ($I > 2\sigma(I)$)	4150
data / params ratio	4318 / 280
$R1$ [a] (obsd reflns)	0.0651
$wR2$ [b] (obsd reflns)	0.140
GOF [c] on F^2	1.448
largest peak, eÅ^{-3}	0.57

[a] $R1 = \Sigma \mid |F_o| - |F_c| \mid / \Sigma |F_o|$; [b] $wR2 = [\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w (F_o^2)^2]^{1/2}$;
[c] $GOF = [\Sigma w (|F_o^2| - |F_c^2|)^2] / (N_{obsd} - N_{params})]^{1/2}$.

Table 2SI. Selected Bond Distances (Å) and Angles (deg)

Pd-I	2.642(1)
Pd-S	2.306(3)
Pd-N(1)	2.231(8)
Pd-C(11)	2.005(9)

S-C(6)	1.80(1)
S-C(7)	1.83(1)
C(11)-N(2)	1.28(1)
I-Pd-N(1)	95.5(2)
I-Pd-C(11)	93.4(3)
S-Pd-N(1)	82.7(2)
S-Pd-C(11)	89.1(3)
N(1)-Pd-C(11)	167.2(4)
I-Pd-S	174.6(1)
Pd-S-C(6)	95.6(4)
Pd-S-C(7)	109.9(4)
S-C(6)-C(5)	115.8(8)
Pd-N(1)-C(1)	126.4(7)
Pd-N(1)-C(5)	114.9(7)
Pd-C(11)-N(2)	121.2(7)
Pd-C(11)-C(12)	121.5(7)

Table 3SI. Summary of Crystal and Refinement Data

	2
empirical formula	$C_{39}H_{44}Cl_5N_4Pd_2$
fw	958.8
cryst syst; space group	orthorhombic; *Pbcn* (No. 60)
a, Å	23.344(5)
b, Å	10.706(2)
c, Å	17.979(4)
β, deg	90.00
V, Å^3	4493(1)
Z, ρ_{calcd}, g cm^{-3}	4; 1.417
λ, Å; μ, cm^{-1}	0.71073; 11.27
Θ range, deg	2.1 – 25.0
reflns collected	3946
reflns obsd ($I > 2\sigma(I)$)	2881
data / params ratio	3946 / 244

*R*1 [a] (obsd reflns)	0.0478
*wR*2 [b] (obsd reflns)	0.120
GOF[c] on F^2	1.069
largest peak, eÅ^{-3}	0.95

[a] $R1 = \Sigma \mid |F_o| - |F_c| \mid / \Sigma |F_o|$; [b] $wR2 = [\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w (F_o^2)^2]^{1/2}$;

[c] $GOF = [\Sigma w (|F_o^2| - |F_c^2|)^2] / (N_{obsd} - N_{params})]^{1/2}$.

Table 4SI. Selected Bond Distances (Å) and Angles (deg)

Pd-Cl(1)	2.389(2)
Pd-N(1)	2.088(4)
Pd-C(1)	1.984(6)
Pd-C(11)	1.953(6)
C(1)-N(1A)	1.290(7)
C(11)-N(2)	1.152(7)
Cl(1)-Pd-N(1)	94.2(1)
Cl(1)-Pd-C(1)	175.3(2)
Cl(1)-Pd-C(11)	87.1(2)
N(1)-Pd-C(1)	88.7(2)
N(1)-Pd-C(11)	176.0(2)
C(1)-Pd-C(11)	90.3(2)
Pd-C(1)-C(2)	120.5(4)
Pd-C(11)-N(2)	175.0(5)
Pd-C(1)-N(1A)	118.3(4)
Pd-N(1)-C(1A)	120.2(4)
C(11)-N(2)-C(12)	173.9(6)

Figure 1SI. ^{1}HNMR spectra at 298 and 223 K in CD_2Cl_2 of the complex

[Pd(NS-Me)(C(Me)=N$C_6H_3Me_2$)Cl]

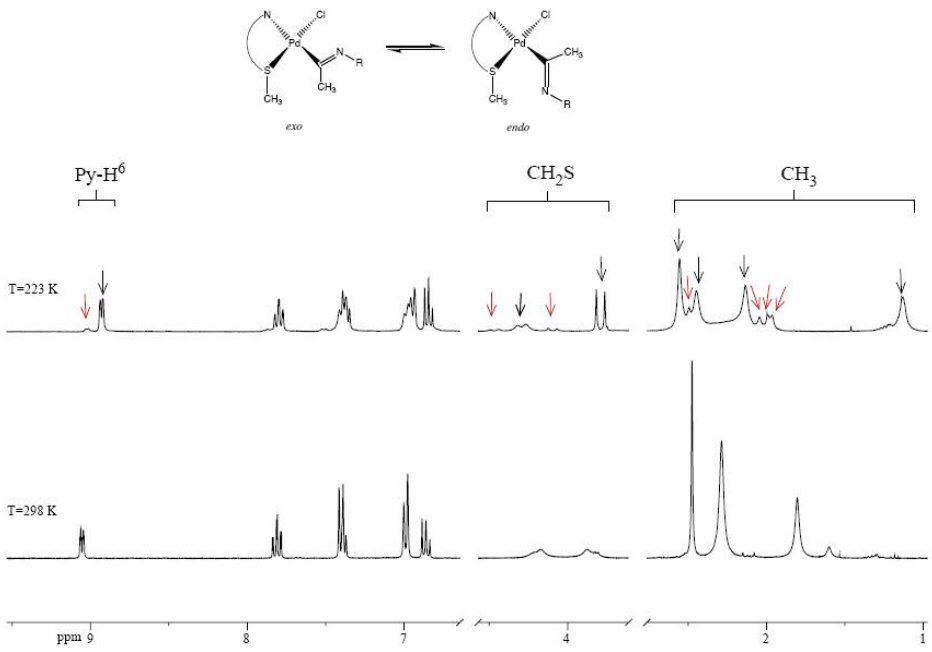
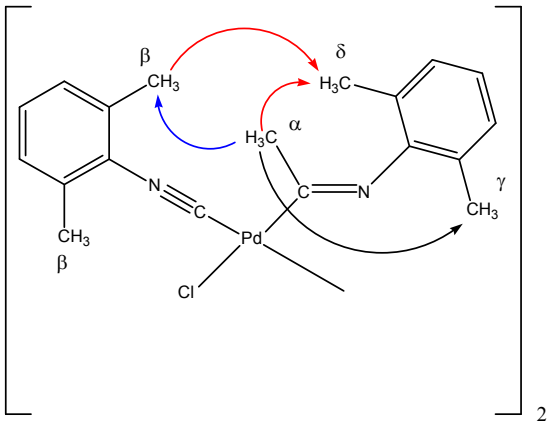
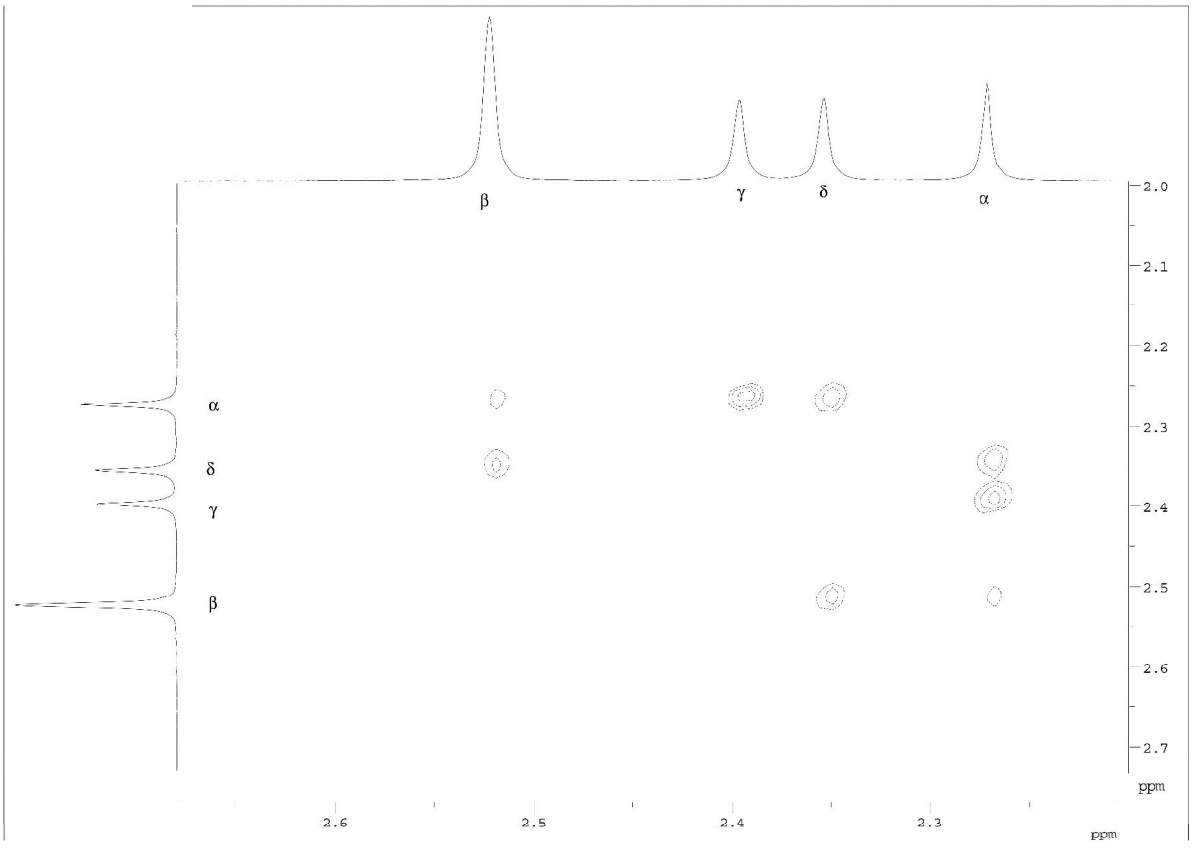


Figure 2SI: NOESY spectrum for the complex $[Pd(CNR^2)(C(=NR^2)Me)Cl]_2$ ($R^2 = C_6H_3Me_2$) in $CDCl_3$ at R.T.





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Pd N1 2.231(8) . ?
Pd S 2.306(3) . ?
S C6 1.797(12) . ?
S C7 1.831(10) . ?
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C1 C2 1.398(15) . ?
C2 C3 1.373(18) . ?
C3 C4 1.356(16) . ?
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C5 C6 1.490(14) . ?
C7 C8 1.506(15) . ?
C7 C9 1.523(16) . ?
C7 C10 1.526(18) . ?
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C12 C17 1.386(14) . ?
C12 C13 1.400(12) . ?
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C14 C15 1.377(16) . ?
C15 C16 1.378(15) . ?
C15 C18 1.529(15) . ?
C16 C17 1.399(15) . ?
C19 C24 1.405(14) . ?
C19 C20 1.413(15) . ?
C20 C21 1.384(17) . ?
C20 C25 1.490(17) . ?
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C1 N1 Pd 126.4(7) . . ?
C5 N1 Pd 114.9(7) . . ?
C11 N2 C19 124.8(8) . . ?
N1 C1 C2 122.1(11) . . ?
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N1 C5 C4 121.6(10) . . ?
N1 C5 C6 117.8(9) . . ?
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C5 C6 S 115.8(8) . . ?
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N2 C11 Pd 121.2(7) . . ?
C12 C11 Pd 121.5(7) . . ?
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C17 C12 C11 122.5(8) . . ?
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C12 C17 C16 121.0(10) . . ?
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C24 C19 C20 119.9(10) . . ?
C21 C20 C19 117.9(11) . . ?
C21 C20 C25 122.0(12) . . ?
C19 C20 C25 120.1(11) . . ?
C22 C21 C20 122.0(12) . . ?
C23 C22 C21 120.1(13) . . ?
C22 C23 C24 121.0(13) . . ?
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CIF file for dimer

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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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Pd Pd 0.451257(17) 0.14999(4) 0.18407(2) 0.03432(17) Uani 1 1 d . . .
Cl1 Cl 0.37179(7) 0.28710(17) 0.20257(9) 0.0599(4) Uani 1 1 d . . .
N1 N 0.43848(19) 0.0536(4) 0.2836(2) 0.0358(10) Uani 1 1 d . . .
C1 C 0.5212(2) 0.0485(5) 0.1674(3) 0.0374(12) Uani 1 1 d . . .
C2 C 0.5279(3) -0.0272(7) 0.0976(3) 0.0533(16) Uani 1 1 d . . .
H2A H 0.5640 -0.0701 0.0986 0.080 Uiso 1 1 calc R . .
H2B H 0.5265 0.0272 0.0551 0.080 Uiso 1 1 calc R . .
H2C H 0.4973 -0.0870 0.0944 0.080 Uiso 1 1 calc R . .
C3 C 0.3827(2) -0.0036(6) 0.2967(3) 0.0436(13) Uani 1 1 d . . .
C4 C 0.3698(3) -0.1164(6) 0.2627(3) 0.0564(17) Uani 1 1 d . . .
C5 C 0.3157(4) -0.1678(9) 0.2740(5) 0.088(3) Uani 1 1 d . . .
H5A H 0.3062 -0.2438 0.2522 0.105 Uiso 1 1 calc R . .
C6 C 0.2758(4) -0.1055(12) 0.3183(5) 0.101(3) Uani 1 1 d . . .
H6A H 0.2394 -0.1391 0.3248 0.122 Uiso 1 1 calc R . .
C7 C 0.2899(4) 0.0037(10) 0.3517(5) 0.086(3) Uani 1 1 d . . .
H7A H 0.2629 0.0434 0.3815 0.103 Uiso 1 1 calc R . .
C8 C 0.3437(3) 0.0582(7) 0.3426(3) 0.0567(17) Uani 1 1 d . . .
C9 C 0.4133(4) -0.1841(8) 0.2148(5) 0.079(2) Uani 1 1 d . . .
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H9A H 0.4480 -0.1363 0.2126 0.119 Uiso 1 1 calc R . .
H9B H 0.3982 -0.1943 0.1655 0.119 Uiso 1 1 calc R . .
H9C H 0.4212 -0.2647 0.2359 0.119 Uiso 1 1 calc R . .
N2 N 0.4629(2) 0.2777(5) 0.0299(2) 0.0460(12) Uani 1 1 d . . .
C10 C 0.3578(3) 0.1751(8) 0.3816(4) 0.071(2) Uani 1 1 d . . .
H10A H 0.3254 0.2020 0.4102 0.106 Uiso 1 1 calc R . .
H10B H 0.3675 0.2383 0.3459 0.106 Uiso 1 1 calc R . .
H10C H 0.3898 0.1613 0.4141 0.106 Uiso 1 1 calc R . .
C11 C 0.4613(2) 0.2297(6) 0.0872(3) 0.0448(14) Uani 1 1 d . . .
C12 C 0.4606(3) 0.3457(5) -0.0370(3) 0.0431(14) Uani 1 1 d . . .
C13 C 0.4062(3) 0.3718(6) -0.0665(3) 0.0546(17) Uani 1 1 d . . .
C14 C 0.4060(4) 0.4450(7) -0.1312(3) 0.068(2) Uani 1 1 d . . .
H14A H 0.3713 0.4650 -0.1537 0.081 Uiso 1 1 calc R . .
C15 C 0.4561(4) 0.4877(7) -0.1619(4) 0.068(2) Uani 1 1 d . . .
H15A H 0.4548 0.5378 -0.2041 0.082 Uiso 1 1 calc R . .
C16 C 0.5078(4) 0.4580(6) -0.1315(3) 0.0637(19) Uani 1 1 d . . .
H16A H 0.5410 0.4877 -0.1540 0.076 Uiso 1 1 calc R . .
C17 C 0.5125(3) 0.3845(5) -0.0680(3) 0.0480(15) Uani 1 1 d . . .
C18 C 0.3525(4) 0.3269(8) -0.0305(5) 0.083(2) Uani 1 1 d . . .
H18A H 0.3619 0.2784 0.0127 0.125 Uiso 1 1 calc R . .
H18B H 0.3314 0.2761 -0.0649 0.125 Uiso 1 1 calc R . .
H18C H 0.3296 0.3973 -0.0161 0.125 Uiso 1 1 calc R . .
C19 C 0.5688(3) 0.3513(7) -0.0351(4) 0.0596(17) Uani 1 1 d . . .
H19A H 0.5630 0.3003 0.0082 0.089 Uiso 1 1 calc R . .
H19B H 0.5888 0.4261 -0.0213 0.089 Uiso 1 1 calc R . .
H19C H 0.5911 0.3059 -0.0710 0.089 Uiso 1 1 calc R . .
Cl2 Cl 0.32404(14) 0.0085(3) 0.06509(18) 0.1227(10) Uani 1 1 d . . .
Cl3 Cl 0.23321(14) 0.1840(4) 0.0394(3) 0.191(2) Uani 1 1 d . . .
Cl4 Cl 0.21816(14) 0.0045(4) 0.15137(18) 0.1316(11) Uani 1 1 d . . .
C20 C 0.2686(4) 0.0984(9) 0.1067(6) 0.095(3) Uani 1 1 d . . .
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Cl1 0.0547(9) 0.0693(11) 0.0557(9) 0.0046(8) 0.0007(7) 0.0179(8)
N1 0.043(3) 0.040(2) 0.024(2) -0.0004(19) -0.0002(18) 0.001(2)
C1 0.049(3) 0.038(3) 0.025(3) 0.003(2) 0.002(2) -0.008(3)
C2 0.063(4) 0.067(4) 0.030(3) -0.011(3) -0.003(3) 0.006(3)
C3 0.042(3) 0.060(4) 0.029(3) 0.005(3) -0.002(2) -0.003(3)
C4 0.064(4) 0.064(4) 0.040(3) 0.005(3) -0.005(3) -0.023(3)
C5 0.095(6) 0.097(7) 0.070(5) 0.015(5) -0.020(5) -0.049(5)
C6 0.060(5) 0.152(10) 0.091(7) 0.023(7) 0.005(5) -0.041(6)
C7 0.063(5) 0.124(8) 0.071(5) 0.016(6) 0.009(4) -0.009(5)
C8 0.043(3) 0.086(5) 0.042(3) 0.016(3) 0.005(3) -0.002(3)
C9 0.101(6) 0.069(5) 0.068(5) -0.016(4) 0.006(5) -0.026(5)
N2 0.062(3) 0.052(3) 0.025(2) 0.007(2) -0.003(2) 0.001(2)
C10 0.070(5) 0.096(6) 0.046(4) -0.010(4) 0.015(3) 0.023(4)
C11 0.045(3) 0.049(3) 0.040(3) -0.003(3) -0.004(2) -0.003(3)
C12 0.065(4) 0.039(3) 0.025(3) 0.007(2) -0.002(2) 0.001(3)
C13 0.078(5) 0.052(4) 0.035(3) 0.000(3) -0.006(3) 0.008(3)
C14 0.094(6) 0.075(5) 0.034(3) 0.003(3) -0.019(4) 0.021(4)
C15 0.119(7) 0.057(4) 0.028(3) 0.010(3) 0.005(4) 0.014(4)
C16 0.104(6) 0.052(4) 0.035(3) 0.006(3) 0.020(4) -0.001(4)
C17 0.070(4) 0.045(3) 0.029(3) -0.004(3) 0.008(3) 0.000(3)
C18 0.067(5) 0.104(7) 0.079(5) 0.016(5) -0.006(4) 0.000(5)
C19 0.067(4) 0.072(5) 0.040(3) -0.002(3) 0.002(3) -0.002(4)
Cl2 0.117(2) 0.120(2) 0.131(2) -0.004(2) 0.0091(18) 0.0055(18)
Cl3 0.091(2) 0.218(4) 0.265(5) 0.147(4) 0.020(3) 0.012(2)
Cl4 0.129(2) 0.159(3) 0.106(2) 0.038(2) 0.0166(18) -0.025(2)
C20 0.093(7) 0.092(6) 0.099(7) -0.014(6) 0.007(5) -0.006(5)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
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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
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 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 1.984(6) . ?
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Pd Cl1 2.3888(17) . ?
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N1 C3 1.459(7) . ?
C1 N1 1.290(7) 3_655 ?
C1 C2 1.502(7) . ?
C3 C4 1.387(9) . ?
C3 C8 1.395(9) . ?
C4 C5 1.392(11) . ?
C4 C9 1.515(11) . ?
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N2 C12 1.406(7) . ?
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C13 C18 1.491(10) . ?
C14 C15 1.371(11) . ?
C15 C16 1.362(11) . ?
C16 C17 1.391(8) . ?
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Cl3 C20 1.729(11) . ?
Cl4 C20 1.744(10) . ?

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C11 Pd N1 176.0(2) . . ?
C1 Pd N1 88.68(19) . . ?

C11 Pd Cl1 87.06(18) . . ?
C1 Pd Cl1 175.27(16) . . ?
N1 Pd Cl1 94.21(13) . . ?
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C5 C4 C9 120.1(7) . . ?
C4 C5 C6 120.0(8) . . ?
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N2 C11 Pd 175.0(5) . . ?
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C13 C12 N2 117.4(5) . . ?
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C15 C16 C17 122.1(7) . . ?
C16 C17 C12 115.3(6) . . ?
C16 C17 C19 122.2(6) . . ?
C12 C17 C19 122.5(5) . . ?
Cl3 C20 Cl4 107.8(5) . . ?
Cl3 C20 Cl2 109.9(6) . . ?
Cl4 C20 Cl2 111.9(6) . . ?

_diffrn_measured_fraction_theta_max    0.998
_diffrn_reflns_theta_full              24.98
_diffrn_measured_fraction_theta_full   0.998
_refine_diff_density_max    0.954
_refine_diff_density_min   -1.005
_refine_diff_density_rms    0.117
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