

## Atomic coordinates in the geometry optimised model of (15)

Pt	0.0041	-0.0401	-0.0590
C	2.0911	0.0447	0.0290
C	2.9593	1.1298	0.0706
C	4.3360	0.9529	0.1217
C	4.8866	-0.3197	0.1336
C	4.0530	-1.4189	0.0942
C	2.6711	-1.2440	0.0405
C	1.7603	-2.3746	-0.0046
C	2.0902	-3.7241	-0.0132
C	1.0745	-4.6623	-0.0629
C	-0.2503	-4.2679	-0.1062
C	-0.5489	-2.9108	-0.0991
N	0.4632	-2.0286	-0.0477
C	-1.8648	-2.2964	-0.1488
C	-3.0293	-3.0588	-0.1927
C	-4.2606	-2.4381	-0.2371
C	-4.3237	-1.0527	-0.2397
C	-3.1640	-0.2903	-0.1972
C	-1.9078	-0.8849	-0.1477
C	-0.3661	1.7807	-0.0362
O	-0.5738	2.9122	-0.0078
H	2.5621	2.1512	0.0618
H	4.9946	1.8271	0.1527
H	5.9709	-0.4529	0.1729
H	4.4807	-2.4270	0.1034
H	3.1385	-4.0291	0.0164
H	1.3232	-5.7278	-0.0723
H	-1.0570	-5.0026	-0.1485
H	-2.9709	-4.1527	-0.1942
H	-5.1765	-3.0341	-0.2698
H	-5.2988	-0.5559	-0.2744
H	-3.2538	0.8020	-0.1994

## Atomic coordinates in the geometry optimised model of (9t)

Pt	-0.0378	0.0085	-0.0121
C	1.9873	-0.0222	-0.0659
C	2.8443	1.0645	-0.1365
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C	4.7540	-0.4070	0.0207
C	3.9127	-1.4977	0.0962
C	2.5310	-1.3084	0.0506
C	1.5802	-2.3939	0.0582
C	1.9203	-3.7303	0.2139
C	0.9440	-4.6993	0.1710
C	-0.3581	-4.3202	-0.0957
C	-0.6643	-2.9776	-0.2701
N	0.2821	-2.0294	-0.1231
C	-2.0099	-2.6119	-0.7075
C	-3.1242	-3.1777	-0.0985
C	-4.3955	-2.8726	-0.5508
C	-4.5612	-2.0237	-1.6339
C	-3.4530	-1.4783	-2.2632

C	-2.1816	-1.7603	-1.7980
C	-2.0155	0.1443	0.2720
O	-3.0955	0.3732	0.5594
Cl	-0.1027	2.3423	0.0479
H	2.4177	2.0702	-0.2148
H	4.8872	1.7339	-0.1647
H	5.8387	-0.5500	0.0493
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H	2.9694	-3.9891	0.3761
H	1.1979	-5.7543	0.3046
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H	-2.9854	-3.8462	0.7582
H	-5.2686	-3.3001	-0.0499
H	-5.5675	-1.7863	-1.9935
H	-3.5817	-0.8173	-3.1251
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## Atomic coordinates in the geometry optimised model of (9c)

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C	4.7447	-0.3812	-0.0064
C	3.8993	-1.4669	-0.1085
C	2.5200	-1.2902	-0.0454
C	1.5814	-2.3901	-0.0879
C	1.9309	-3.7038	-0.3569
C	0.9639	-4.6861	-0.3082
C	-0.3149	-4.3464	0.0816
C	-0.6279	-3.0191	0.3604
N	0.2966	-2.0555	0.1861
C	-1.9113	-2.7052	0.9751
C	-1.9683	-1.7863	2.0183
C	-3.1486	-1.5871	2.7060
C	-4.2873	-2.2905	2.3487
C	-4.2418	-3.1980	1.3013
C	-3.0573	-3.4116	0.6233
C	-0.2622	1.8719	-0.1154
O	-0.3893	3.0074	-0.1651
Cl	-2.4416	0.1895	-0.4515
H	2.4387	2.0885	0.3466
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H	5.8278	-0.5226	-0.0521
H	4.3173	-2.4717	-0.2283
H	2.9666	-3.9410	-0.6072
H	1.2169	-5.7275	-0.5285
H	-1.0837	-5.1066	0.2422
H	-1.0602	-1.2419	2.3008
H	-3.1816	-0.8711	3.5317
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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  $F^2 > 2\sigma(F^2)$  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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loop\_

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Cl2 Cl -0.0046(4) 0.2831(2) 0.8742(10) 0.056(2) Uani 1 1 d . . .
Cl1 Cl -0.0338(3) 0.20214(18) 0.7113(10) 0.050(2) Uani 1 1 d . . .
O1 O 0.4410(9) 0.0702(5) 0.271(3) 0.052(5) Uani 1 1 d . . .
O2 O -0.4769(10) 0.4362(5) 1.152(3) 0.054(6) Uani 1 1 d . . .
N1 N 0.1280(9) 0.2121(5) 0.556(3) 0.029(5) Uiso 1 1 d . . .
N2 N -0.1708(10) 0.2794(6) 0.973(3) 0.042(6) Uiso 1 1 d . . .
C1 C 0.1363(14) 0.2783(8) 0.726(4) 0.053(8) Uiso 1 1 d U . .
C2 C 0.1327(15) 0.3166(7) 0.785(4) 0.051(7) Uani 1 1 d U . .
H2 H 0.0939 0.3288 0.8194 0.062 Uiso 1 1 d R . .
C3 C 0.1933(15) 0.3359(9) 0.794(4) 0.060(8) Uani 1 1 d U . .
H3A H 0.1934 0.3621 0.8320 0.072 Uiso 1 1 d R . .
C4 C 0.2524(16) 0.3197(10) 0.749(4) 0.066(9) Uani 1 1 d U . .

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H4A H 0.2916 0.3328 0.7712 0.079 Uiso 1 1 d R . . .  
C5 C 0.2496(13) 0.2843(9) 0.670(4) 0.061(9) Uani 1 1 d U . . .  
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C6 C 0.1933(13) 0.2642(8) 0.658(3) 0.047(7) Uani 1 1 d U . . .  
C7 C 0.1845(12) 0.2238(7) 0.578(3) 0.034(7) Uiso 1 1 d . . .  
C8 C 0.2376(12) 0.2034(6) 0.527(3) 0.033(7) Uiso 1 1 d . . .  
H8 H 0.2798 0.2131 0.5437 0.039 Uiso 1 1 d R . . .  
C9 C 0.2286(13) 0.1655(7) 0.447(4) 0.040(7) Uiso 1 1 d . . .  
C10 C 0.1685(11) 0.1543(6) 0.419(3) 0.026(6) Uiso 1 1 d . . .  
H10 H 0.1607 0.1299 0.3659 0.031 Uiso 1 1 d R . . .  
C11 C 0.1179(12) 0.1769(7) 0.466(3) 0.032(6) Uiso 1 1 d . . .  
C12 C 0.0508(14) 0.1662(6) 0.410(3) 0.040(8) Uani 1 1 d . . .  
C13 C 0.0139(15) 0.1909(8) 0.303(4) 0.055(9) Uiso 1 1 d . . .  
H13 H 0.0289 0.2159 0.2714 0.066 Uiso 1 1 d R . . .  
C14 C -0.0455(14) 0.1788(9) 0.239(4) 0.057(9) Uani 1 1 d . . .  
H14 H -0.0717 0.1955 0.1703 0.068 Uiso 1 1 d R . . .  
C15 C -0.0682(16) 0.1403(10) 0.282(5) 0.074(11) Uani 1 1 d . . .  
H15 H -0.1097 0.1315 0.2501 0.089 Uiso 1 1 d R . . .  
C16 C -0.0257(14) 0.1161(9) 0.375(5) 0.061(9) Uani 1 1 d . . .  
H16 H -0.0359 0.0894 0.3892 0.073 Uiso 1 1 d R . . .  
C17 C 0.0296(16) 0.1291(8) 0.437(4) 0.052(9) Uani 1 1 d . . .  
H17 H 0.0549 0.1121 0.5070 0.063 Uiso 1 1 d R . . .  
C18 C 0.2875(12) 0.1431(6) 0.397(3) 0.034(7) Uani 1 1 d . . .  
C19 C 0.3464(12) 0.1569(7) 0.377(3) 0.035(6) Uiso 1 1 d . . .  
H19 H 0.3517 0.1839 0.3936 0.041 Uiso 1 1 d R . . .  
C20 C 0.4022(13) 0.1348(7) 0.332(3) 0.044(7) Uiso 1 1 d . . .  
H20 H 0.4426 0.1469 0.3147 0.053 Uiso 1 1 d R . . .  
C21 C 0.3937(13) 0.0946(6) 0.315(4) 0.037(7) Uani 1 1 d . . .  
C22 C 0.3327(16) 0.0795(9) 0.329(4) 0.061(9) Uani 1 1 d . . .  
H22 H 0.3269 0.0526 0.3085 0.073 Uiso 1 1 d R . . .  
C23 C 0.2806(15) 0.1023(8) 0.366(4) 0.053(8) Uani 1 1 d . . .  
H23 H 0.2397 0.0905 0.3761 0.063 Uiso 1 1 d R . . .  
C24 C 0.5058(13) 0.0840(8) 0.279(4) 0.046(8) Uani 1 1 d . . .  
H24A H 0.5129 0.0978 0.3922 0.055 Uiso 1 1 d R . . .  
H24B H 0.5134 0.1025 0.1808 0.055 Uiso 1 1 d R . . .  
C25 C 0.5501(15) 0.0523(9) 0.264(4) 0.065(10) Uani 1 1 d . . .  
H25A H 0.5410 0.0380 0.1531 0.079 Uiso 1 1 d R . . .  
H25B H 0.5427 0.0344 0.3643 0.079 Uiso 1 1 d R . . .  
C26 C 0.6220(13) 0.0649(8) 0.266(4) 0.057(9) Uani 1 1 d . . .  
H26A H 0.6304 0.0809 0.1600 0.068 Uiso 1 1 d R . . .  
H26B H 0.6302 0.0812 0.3720 0.068 Uiso 1 1 d R . . .  
C27 C 0.6688(12) 0.0308(7) 0.268(4) 0.053(9) Uani 1 1 d . . .  
H27A H 0.6589 0.0141 0.3709 0.064 Uiso 1 1 d R . . .  
H27B H 0.6619 0.0151 0.1593 0.064 Uiso 1 1 d R . . .  
C28 C 0.7378(15) 0.0427(8) 0.277(4) 0.059(10) Uani 1 1 d . . .  
H28A H 0.7440 0.0602 0.3792 0.071 Uiso 1 1 d R . . .  
H28B H 0.7489 0.0572 0.1681 0.071 Uiso 1 1 d R . . .  
C29 C 0.7845(15) 0.0077(9) 0.297(4) 0.069(10) Uani 1 1 d . . .  
H29A H 0.7728 -0.0067 0.4058 0.082 Uiso 1 1 d R . . .  
H29B H 0.7774 -0.0099 0.1953 0.082 Uiso 1 1 d R . . .  
C30 C 0.8525(15) 0.0171(11) 0.302(5) 0.079(11) Uani 1 1 d . . .  
H30A H 0.8595 0.0362 0.3979 0.095 Uiso 1 1 d R . . .  
H30B H 0.8653 0.0296 0.1890 0.095 Uiso 1 1 d R . . .  
C31 C 0.8962(18) -0.0179(12) 0.336(6) 0.122(16) Uani 1 1 d . . .  
H31A H 0.9408 -0.0092 0.3425 0.183 Uiso 1 1 d R . . .  
H31B H 0.8914 -0.0363 0.2381 0.183 Uiso 1 1 d R . . .  
H31C H 0.8841 -0.0304 0.4474 0.183 Uiso 1 1 d R . . .  
C36 C -0.1808(12) 0.2126(7) 0.826(3) 0.037(7) Uiso 1 1 d . . .  
C37 C -0.1828(15) 0.1749(8) 0.750(4) 0.048(8) Uiso 1 1 d . . .  
H37 H -0.1437 0.1626 0.7184 0.058 Uiso 1 1 d R . . .

C38 C -0.2382(19) 0.1557(10) 0.727(4) 0.079(11) Uani 1 1 d . . . .  
H38 H -0.2371 0.1290 0.6968 0.095 Uiso 1 1 d R . . . .  
C39 C -0.2964(17) 0.1739(8) 0.744(5) 0.081(13) Uani 1 1 d . . . .  
H39 H -0.3353 0.1610 0.7156 0.097 Uiso 1 1 d R . . . .  
C40 C -0.2971(12) 0.2145(8) 0.808(4) 0.050(8) Uani 1 1 d . . . .  
H40 H -0.3359 0.2284 0.8234 0.061 Uiso 1 1 d R . . . .  
C41 C -0.2411(11) 0.2307(6) 0.847(3) 0.030(6) Uiso 1 1 d . . . .  
C42 C -0.2296(12) 0.2703(6) 0.922(3) 0.033(7) Uiso 1 1 d . . . .  
C43 C -0.2827(13) 0.2933(8) 0.945(4) 0.056(9) Uani 1 1 d . . . .  
H43 H -0.3240 0.2854 0.9069 0.067 Uiso 1 1 d R . . . .  
C44 C -0.2724(13) 0.3303(7) 1.035(3) 0.037(7) Uani 1 1 d . . . .  
C45 C -0.2104(14) 0.3379(7) 1.096(4) 0.044(8) Uani 1 1 d . . . .  
H45 H -0.2028 0.3612 1.1594 0.053 Uiso 1 1 d R . . . .  
C46 C -0.1589(12) 0.3124(6) 1.064(3) 0.029(6) Uani 1 1 d . . . .  
C47 C -0.0967(13) 0.3190(7) 1.149(4) 0.042(7) Uiso 1 1 d . . . .  
C48 C -0.0707(12) 0.2927(7) 1.258(3) 0.033(6) Uiso 1 1 d . . . .  
H48 H -0.0924 0.2688 1.2756 0.040 Uiso 1 1 d R . . . .  
C49 C -0.0124(17) 0.2997(9) 1.343(4) 0.070(10) Uani 1 1 d . . . .  
H49 H 0.0079 0.2795 1.4082 0.084 Uiso 1 1 d R . . . .  
C50 C 0.0151(16) 0.3343(9) 1.332(5) 0.067(10) Uiso 1 1 d . . . .  
H50 H 0.0521 0.3399 1.4002 0.080 Uiso 1 1 d R . . . .  
C51 C -0.0105(14) 0.3630(9) 1.224(4) 0.060(10) Uani 1 1 d . . . .  
H51 H 0.0117 0.3866 1.2050 0.072 Uiso 1 1 d R . . . .  
C52 C -0.0685(13) 0.3559(8) 1.137(4) 0.048(8) Uani 1 1 d . . . .  
H52 H -0.0893 0.3762 1.0746 0.057 Uiso 1 1 d R . . . .  
C53 C -0.3281(11) 0.3574(7) 1.071(3) 0.032(7) Uani 1 1 d . . . .  
C54 C -0.3157(17) 0.3971(9) 1.100(4) 0.066(10) Uani 1 1 d . . . .  
H54 H -0.2736 0.4076 1.0979 0.079 Uiso 1 1 calc R . . . .  
C55 C -0.3704(14) 0.4202(8) 1.133(5) 0.061(10) Uani 1 1 d . . . .  
H55 H -0.3629 0.4463 1.1670 0.074 Uiso 1 1 calc R . . . .  
C56 C -0.4279(14) 0.4098(7) 1.122(4) 0.040(7) Uani 1 1 d . . . .  
C57 C -0.4423(13) 0.3707(6) 1.086(3) 0.039(7) Uiso 1 1 d . . . .  
H57 H -0.4852 0.3617 1.0781 0.047 Uiso 1 1 calc R . . . .  
C58 C -0.3888(14) 0.3454(8) 1.062(4) 0.049(8) Uiso 1 1 d . . . .  
H58 H -0.3968 0.3188 1.0380 0.059 Uiso 1 1 calc R . . . .  
C59 C -0.5407(13) 0.4220(7) 1.153(4) 0.040(7) Uani 1 1 d . . . .  
H59A H -0.5458 0.4023 1.2479 0.048 Uiso 1 1 d R . . . .  
H59B H -0.5508 0.4096 1.0385 0.048 Uiso 1 1 d R . . . .  
C60 C -0.5866(15) 0.4564(8) 1.185(4) 0.067(11) Uani 1 1 d . . . .  
H60A H -0.5749 0.4693 1.2976 0.080 Uiso 1 1 d R . . . .  
H60B H -0.5820 0.4756 1.0884 0.080 Uiso 1 1 d R . . . .  
C61 C -0.6544(15) 0.4434(7) 1.199(4) 0.055(9) Uani 1 1 d . . . .  
H61A H -0.6603 0.4271 1.3062 0.066 Uiso 1 1 d R . . . .  
H61B H -0.6642 0.4272 1.0945 0.066 Uiso 1 1 d R . . . .  
C62 C -0.7014(15) 0.4772(9) 1.206(4) 0.061(9) Uani 1 1 d . . . .  
H62A H -0.6884 0.4939 1.3064 0.073 Uiso 1 1 d R . . . .  
H62B H -0.6953 0.4925 1.0965 0.073 Uiso 1 1 d R . . . .  
C63 C -0.7698(14) 0.4700(8) 1.224(4) 0.055(9) Uani 1 1 d . . . .  
H63A H -0.7768 0.4565 1.3378 0.066 Uiso 1 1 d R . . . .  
H63B H -0.7828 0.4521 1.1281 0.066 Uiso 1 1 d R . . . .  
C64 C -0.8139(14) 0.5056(7) 1.217(4) 0.042(7) Uani 1 1 d . . . .  
H64A H -0.8035 0.5226 1.3189 0.051 Uiso 1 1 d R . . . .  
H64B H -0.8051 0.5203 1.1076 0.051 Uiso 1 1 d R . . . .  
C65 C -0.8832(16) 0.4958(10) 1.223(5) 0.082(12) Uani 1 1 d . . . .  
H65A H -0.8928 0.4806 1.3315 0.098 Uiso 1 1 d R . . . .  
H65B H -0.8950 0.4799 1.1191 0.098 Uiso 1 1 d R . . . .  
C66 C -0.9248(16) 0.5357(10) 1.224(5) 0.103(14) Uani 1 1 d . . . .  
H66A H -0.9705 0.5293 1.2295 0.155 Uiso 1 1 d R . . . .  
H66B H -0.9159 0.5504 1.1160 0.155 Uiso 1 1 d R . . . .  
H66C H -0.9132 0.5513 1.3278 0.155 Uiso 1 1 d R . . . .

loop\_  
\_atom\_site\_aniso\_label  
\_atom\_site\_aniso\_U\_11  
\_atom\_site\_aniso\_U\_22  
\_atom\_site\_aniso\_U\_33  
\_atom\_site\_aniso\_U\_23  
\_atom\_site\_aniso\_U\_13  
\_atom\_site\_aniso\_U\_12  
Pt1 0.0575(7) 0.0388(6) 0.0278(6) -0.0051(5) -0.0011(5) 0.0126(6)  
Pt2 0.0608(8) 0.0374(6) 0.0293(6) -0.0028(5) 0.0037(5) 0.0132(6)  
Cl2 0.070(6) 0.051(4) 0.047(5) -0.018(4) 0.008(4) 0.008(4)  
Cl1 0.052(5) 0.043(4) 0.054(5) -0.017(4) 0.020(4) 0.015(3)  
O1 0.030(12) 0.054(11) 0.072(15) -0.017(10) 0.016(12) 0.007(10)  
O2 0.052(15) 0.060(12) 0.051(14) -0.024(12) 0.009(11) 0.001(11)  
C2 0.064(15) 0.040(15) 0.051(19) -0.007(14) -0.018(16) 0.017(11)  
C3 0.079(17) 0.060(18) 0.040(19) -0.022(16) 0.021(18) -0.001(12)  
C4 0.065(16) 0.08(2) 0.05(2) -0.009(17) 0.015(18) -0.002(14)  
C5 0.036(15) 0.077(19) 0.07(2) -0.004(17) -0.005(17) 0.036(12)  
C6 0.063(17) 0.066(17) 0.014(14) -0.009(13) 0.002(13) 0.020(11)  
C12 0.07(2) 0.021(14) 0.025(16) -0.003(11) 0.014(15) 0.019(14)  
C14 0.05(2) 0.06(2) 0.06(2) -0.028(16) -0.005(18) 0.035(16)  
C15 0.05(2) 0.10(3) 0.08(3) -0.06(2) -0.02(2) 0.01(2)  
C16 0.03(2) 0.06(2) 0.09(3) -0.01(2) 0.030(19) -0.003(17)  
C17 0.09(3) 0.041(19) 0.030(17) 0.013(14) 0.016(17) -0.004(17)  
C18 0.046(19) 0.027(14) 0.028(17) 0.004(12) 0.008(14) -0.014(13)  
C21 0.030(17) 0.033(14) 0.048(19) -0.004(13) -0.001(16) 0.010(14)  
C22 0.07(3) 0.053(19) 0.06(2) 0.000(18) -0.01(2) -0.012(18)  
C23 0.05(2) 0.051(18) 0.05(2) 0.001(16) -0.004(17) -0.019(16)  
C24 0.04(2) 0.053(18) 0.043(18) -0.019(15) 0.006(17) 0.016(15)  
C25 0.08(3) 0.07(2) 0.05(2) -0.018(17) 0.02(2) -0.008(19)  
C26 0.05(2) 0.055(19) 0.07(2) 0.007(17) -0.024(17) 0.003(16)  
C27 0.022(18) 0.054(18) 0.08(2) -0.009(16) 0.017(16) -0.005(14)  
C28 0.10(3) 0.038(16) 0.04(2) -0.019(14) -0.023(19) 0.016(17)  
C29 0.06(3) 0.10(3) 0.05(2) -0.01(2) 0.026(19) 0.02(2)  
C30 0.03(2) 0.14(3) 0.06(3) -0.01(2) 0.01(2) 0.00(2)  
C31 0.07(3) 0.16(4) 0.14(5) -0.02(3) -0.03(3) -0.02(3)  
C38 0.11(3) 0.07(2) 0.05(2) -0.021(19) 0.02(2) 0.00(2)  
C39 0.08(3) 0.035(18) 0.13(4) -0.04(2) -0.01(2) 0.005(17)  
C40 0.035(18) 0.09(2) 0.031(18) 0.012(17) -0.014(14) 0.003(15)  
C43 0.024(18) 0.08(2) 0.07(2) 0.045(19) 0.011(16) 0.005(16)  
C44 0.04(2) 0.043(17) 0.026(17) -0.001(13) 0.002(14) -0.016(14)  
C45 0.06(2) 0.036(16) 0.040(19) -0.009(14) -0.009(16) 0.022(15)  
C46 0.036(17) 0.030(14) 0.022(14) -0.007(12) 0.001(12) 0.022(12)  
C49 0.11(3) 0.07(2) 0.04(2) -0.022(18) -0.02(2) 0.034(19)  
C51 0.04(2) 0.062(19) 0.08(2) -0.031(18) -0.029(19) 0.026(16)  
C52 0.035(18) 0.071(19) 0.037(18) -0.006(15) 0.016(16) 0.027(15)  
C53 0.014(15) 0.060(18) 0.024(15) 0.022(13) 0.009(12) 0.008(13)  
C54 0.08(3) 0.07(2) 0.05(2) -0.022(17) 0.014(19) -0.03(2)  
C55 0.02(2) 0.048(18) 0.11(3) -0.01(2) -0.03(2) 0.011(15)  
C56 0.04(2) 0.033(15) 0.044(18) -0.008(13) -0.002(15) 0.005(14)  
C59 0.05(2) 0.041(15) 0.030(17) 0.009(14) 0.000(15) 0.015(13)  
C60 0.09(3) 0.047(17) 0.07(2) -0.023(17) -0.06(2) 0.009(16)  
C61 0.06(2) 0.048(17) 0.05(2) 0.005(16) -0.022(19) 0.014(16)  
C62 0.07(3) 0.08(2) 0.032(18) 0.007(18) -0.002(17) -0.015(19)  
C63 0.05(2) 0.07(2) 0.05(2) -0.003(16) -0.011(17) -0.017(17)  
C64 0.05(2) 0.050(17) 0.023(16) 0.002(14) 0.002(16) 0.001(15)  
C65 0.05(2) 0.13(3) 0.06(3) 0.03(2) -0.01(2) 0.02(2)  
C66 0.07(3) 0.12(3) 0.12(4) 0.01(3) 0.02(3) 0.05(2)

\_geom\_special\_details

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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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loop\_

\_geom\_bond\_atom\_site\_label\_1

\_geom\_bond\_atom\_site\_label\_2

\_geom\_bond\_distance

\_geom\_bond\_site\_symmetry\_2

\_geom\_bond\_publ\_flag

Pt1 C1 1.98(3) . ?  
Pt1 N1 2.078(18) . ?  
Pt1 C12 2.339(7) . ?  
Pt1 C11 2.460(7) . ?  
Pt2 C36 1.96(2) . ?  
Pt2 N2 2.07(2) . ?  
Pt2 C11 2.312(6) . ?  
Pt2 C12 2.468(8) . ?  
O1 C21 1.34(3) . ?  
O1 C24 1.44(3) . ?  
O2 C56 1.39(3) . ?  
O2 C59 1.42(3) . ?  
N1 C7 1.26(3) . ?  
N1 C11 1.41(3) . ?  
N2 C42 1.32(3) . ?  
N2 C46 1.35(3) . ?  
C1 C6 1.38(3) . ?  
C1 C2 1.40(3) . ?  
C2 C3 1.43(4) . ?  
C3 C4 1.40(4) . ?  
C4 C5 1.36(4) . ?  
C5 C6 1.37(4) . ?  
C6 C7 1.53(3) . ?  
C7 C8 1.37(3) . ?  
C8 C9 1.45(3) . ?  
C9 C10 1.33(3) . ?  
C9 C18 1.50(3) . ?  
C10 C11 1.36(3) . ?  
C11 C12 1.51(4) . ?  
C12 C17 1.37(3) . ?  
C12 C13 1.40(4) . ?  
C13 C14 1.40(4) . ?  
C14 C15 1.45(4) . ?  
C15 C16 1.40(4) . ?  
C16 C17 1.33(4) . ?  
C18 C19 1.33(3) . ?  
C18 C23 1.44(3) . ?  
C19 C20 1.43(3) . ?  
C20 C21 1.40(3) . ?  
C21 C22 1.38(4) . ?  
C22 C23 1.37(4) . ?  
C24 C25 1.44(4) . ?  
C25 C26 1.57(4) . ?

C26 C27 1.53(3) . ?  
 C27 C28 1.50(4) . ?  
 C28 C29 1.56(4) . ?  
 C29 C30 1.46(4) . ?  
 C30 C31 1.54(5) . ?  
 C36 C41 1.42(3) . ?  
 C36 C37 1.42(3) . ?  
 C37 C38 1.34(4) . ?  
 C38 C39 1.37(4) . ?  
 C39 C40 1.48(4) . ?  
 C40 C41 1.33(3) . ?  
 C41 C42 1.50(3) . ?  
 C42 C43 1.38(3) . ?  
 C43 C44 1.46(4) . ?  
 C44 C45 1.40(4) . ?  
 C44 C53 1.52(3) . ?  
 C45 C46 1.41(3) . ?  
 C46 C47 1.46(3) . ?  
 C47 C48 1.34(3) . ?  
 C47 C52 1.41(3) . ?  
 C48 C49 1.40(4) . ?  
 C49 C50 1.33(4) . ?  
 C50 C51 1.38(4) . ?  
 C51 C52 1.40(4) . ?  
 C53 C58 1.34(3) . ?  
 C53 C54 1.42(3) . ?  
 C54 C55 1.42(4) . ?  
 C55 C56 1.26(3) . ?  
 C56 C57 1.41(3) . ?  
 C57 C58 1.43(3) . ?  
 C59 C60 1.55(3) . ?  
 C60 C61 1.49(4) . ?  
 C61 C62 1.53(4) . ?  
 C62 C63 1.46(4) . ?  
 C63 C64 1.54(4) . ?  
 C64 C65 1.49(4) . ?  
 C65 C66 1.63(4) . ?

loop\_

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 \_geom\_angle\_site\_symmetry\_3  
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C1 Pt1 N1 80.7(10) . . ?  
 C1 Pt1 C12 93.5(9) . . ?  
 N1 Pt1 C12 173.5(6) . . ?  
 C1 Pt1 C11 171.0(9) . . ?  
 N1 Pt1 C11 104.4(5) . . ?  
 C12 Pt1 C11 80.9(2) . . ?  
 C36 Pt2 N2 78.9(9) . . ?  
 C36 Pt2 C11 97.0(7) . . ?  
 N2 Pt2 C11 174.8(7) . . ?  
 C36 Pt2 C12 175.4(8) . . ?  
 N2 Pt2 C12 102.6(6) . . ?  
 C11 Pt2 C12 81.2(2) . . ?  
 Pt1 C12 Pt2 98.2(2) . . ?  
 Pt2 C11 Pt1 99.1(2) . . ?

C21 O1 C24 118(2) . . . ?  
C56 O2 C59 118(2) . . . ?  
C7 N1 C11 119(2) . . . ?  
C7 N1 Pt1 113.2(17) . . . ?  
C11 N1 Pt1 127.3(15) . . . ?  
C42 N2 C46 121(2) . . . ?  
C42 N2 Pt2 111.9(16) . . . ?  
C46 N2 Pt2 126.1(17) . . . ?  
C6 C1 C2 120(3) . . . ?  
C6 C1 Pt1 116(2) . . . ?  
C2 C1 Pt1 124(2) . . . ?  
C1 C2 C3 114(3) . . . ?  
C4 C3 C2 126(3) . . . ?  
C5 C4 C3 115(3) . . . ?  
C4 C5 C6 122(3) . . . ?  
C5 C6 C1 122(3) . . . ?  
C5 C6 C7 126(2) . . . ?  
C1 C6 C7 111(3) . . . ?  
N1 C7 C8 124(2) . . . ?  
N1 C7 C6 117(2) . . . ?  
C8 C7 C6 119(2) . . . ?  
C7 C8 C9 118(2) . . . ?  
C10 C9 C8 117(2) . . . ?  
C10 C9 C18 126(2) . . . ?  
C8 C9 C18 117(2) . . . ?  
C9 C10 C11 122(2) . . . ?  
C10 C11 N1 120(2) . . . ?  
C10 C11 C12 120(2) . . . ?  
N1 C11 C12 119(2) . . . ?  
C17 C12 C13 118(3) . . . ?  
C17 C12 C11 119(3) . . . ?  
C13 C12 C11 121(2) . . . ?  
C14 C13 C12 120(3) . . . ?  
C13 C14 C15 119(3) . . . ?  
C16 C15 C14 117(3) . . . ?  
C17 C16 C15 122(3) . . . ?  
C16 C17 C12 123(3) . . . ?  
C19 C18 C23 115(2) . . . ?  
C19 C18 C9 127(2) . . . ?  
C23 C18 C9 118(2) . . . ?  
C18 C19 C20 126(2) . . . ?  
C21 C20 C19 116(2) . . . ?  
O1 C21 C22 117(2) . . . ?  
O1 C21 C20 124(2) . . . ?  
C22 C21 C20 119(3) . . . ?  
C23 C22 C21 122(3) . . . ?  
C22 C23 C18 121(3) . . . ?  
O1 C24 C25 110(2) . . . ?  
C24 C25 C26 114(3) . . . ?  
C27 C26 C25 114(2) . . . ?  
C28 C27 C26 114(2) . . . ?  
C27 C28 C29 113(2) . . . ?  
C30 C29 C28 116(3) . . . ?  
C29 C30 C31 114(3) . . . ?  
C41 C36 C37 115(2) . . . ?  
C41 C36 Pt2 119.0(17) . . . ?  
C37 C36 Pt2 125(2) . . . ?  
C38 C37 C36 122(3) . . . ?  
C37 C38 C39 122(3) . . . ?  
C38 C39 C40 118(3) . . . ?

C41 C40 C39 118(3) . . . ?  
 C40 C41 C36 125(2) . . . ?  
 C40 C41 C42 128(2) . . . ?  
 C36 C41 C42 108(2) . . . ?  
 N2 C42 C43 125(2) . . . ?  
 N2 C42 C41 118(2) . . . ?  
 C43 C42 C41 116(2) . . . ?  
 C42 C43 C44 116(3) . . . ?  
 C45 C44 C43 117(2) . . . ?  
 C45 C44 C53 122(2) . . . ?  
 C43 C44 C53 121(2) . . . ?  
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 N2 C46 C45 118(2) . . . ?  
 N2 C46 C47 121(2) . . . ?  
 C45 C46 C47 120(2) . . . ?  
 C48 C47 C52 119(3) . . . ?  
 C48 C47 C46 122(2) . . . ?  
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 C47 C48 C49 121(3) . . . ?  
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 C49 C50 C51 121(3) . . . ?  
 C50 C51 C52 119(3) . . . ?  
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 C58 C53 C54 119(3) . . . ?  
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 C53 C54 C55 115(3) . . . ?  
 C56 C55 C54 127(3) . . . ?  
 C55 C56 O2 120(2) . . . ?  
 C55 C56 C57 119(3) . . . ?  
 O2 C56 C57 120(3) . . . ?  
 C56 C57 C58 116(3) . . . ?  
 C53 C58 C57 123(3) . . . ?  
 O2 C59 C60 109(2) . . . ?  
 C61 C60 C59 112(2) . . . ?  
 C60 C61 C62 112(2) . . . ?  
 C63 C62 C61 120(3) . . . ?  
 C62 C63 C64 117(2) . . . ?  
 C65 C64 C63 114(2) . . . ?  
 C64 C65 C66 109(3) . . . ?

loop\_

\_geom\_torsion\_atom\_site\_label\_1  
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 \_geom\_torsion\_atom\_site\_label\_3  
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 C1 Pt1 C12 Pt2 -178.8(9) . . . . . ?  
 N1 Pt1 C12 Pt2 -150(5) . . . . . ?  
 C11 Pt1 C12 Pt2 -5.9(3) . . . . . ?  
 C36 Pt2 C12 Pt1 -61(9) . . . . . ?  
 N2 Pt2 C12 Pt1 -170.1(6) . . . . . ?  
 C11 Pt2 C12 Pt1 6.2(3) . . . . . ?  
 C36 Pt2 C11 Pt1 169.8(8) . . . . . ?  
 N2 Pt2 C11 Pt1 131(6) . . . . . ?

Cl2 Pt2 C11 Pt1 -5.9(3) . . . . ?  
 C1 Pt1 C11 Pt2 58(5) . . . . ?  
 N1 Pt1 C11 Pt2 -177.6(6) . . . . ?  
 Cl2 Pt1 C11 Pt2 6.3(3) . . . . ?  
 C1 Pt1 N1 C7 11.6(19) . . . . ?  
 Cl2 Pt1 N1 C7 -17(6) . . . . ?  
 C11 Pt1 N1 C7 -161.0(17) . . . . ?  
 C1 Pt1 N1 C11 -178(2) . . . . ?  
 Cl2 Pt1 N1 C11 153(4) . . . . ?  
 C11 Pt1 N1 C11 9(2) . . . . ?  
 C36 Pt2 N2 C42 -18.5(18) . . . . ?  
 C11 Pt2 N2 C42 21(8) . . . . ?  
 Cl2 Pt2 N2 C42 157.1(16) . . . . ?  
 C36 Pt2 N2 C46 172(2) . . . . ?  
 C11 Pt2 N2 C46 -148(6) . . . . ?  
 Cl2 Pt2 N2 C46 -12(2) . . . . ?  
 N1 Pt1 C1 C6 -5(2) . . . . ?  
 Cl2 Pt1 C1 C6 172(2) . . . . ?  
 C11 Pt1 C1 C6 121(5) . . . . ?  
 N1 Pt1 C1 C2 165(3) . . . . ?  
 Cl2 Pt1 C1 C2 -18(2) . . . . ?  
 C11 Pt1 C1 C2 -69(6) . . . . ?  
 C6 C1 C2 C3 -9(4) . . . . ?  
 Pt1 C1 C2 C3 -179(2) . . . . ?  
 C1 C2 C3 C4 0(5) . . . . ?  
 C2 C3 C4 C5 8(5) . . . . ?  
 C3 C4 C5 C6 -8(5) . . . . ?  
 C4 C5 C6 C1 -1(5) . . . . ?  
 C4 C5 C6 C7 -178(3) . . . . ?  
 C2 C1 C6 C5 10(4) . . . . ?  
 Pt1 C1 C6 C5 -179(2) . . . . ?  
 C2 C1 C6 C7 -172(2) . . . . ?  
 Pt1 C1 C6 C7 -1(3) . . . . ?  
 C11 N1 C7 C8 -3(4) . . . . ?  
 Pt1 N1 C7 C8 167(2) . . . . ?  
 C11 N1 C7 C6 173(2) . . . . ?  
 Pt1 N1 C7 C6 -16(3) . . . . ?  
 C5 C6 C7 N1 -170(3) . . . . ?  
 C1 C6 C7 N1 12(3) . . . . ?  
 C5 C6 C7 C8 7(4) . . . . ?  
 C1 C6 C7 C8 -171(3) . . . . ?  
 N1 C7 C8 C9 -2(4) . . . . ?  
 C6 C7 C8 C9 -179(2) . . . . ?  
 C7 C8 C9 C10 4(4) . . . . ?  
 C7 C8 C9 C18 -178(2) . . . . ?  
 C8 C9 C10 C11 -1(4) . . . . ?  
 C18 C9 C10 C11 -179(3) . . . . ?  
 C9 C10 C11 N1 -4(4) . . . . ?  
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Refinement of F2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F2, conventional R-factors R are based on F, with F set to zero for negative F2. The threshold expression of F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F2 are statistically about twice as large as those based on F, and R-factors based on ALL data

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will be even larger.

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loop\_

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N21 N 0.5613(9) 0.9205(4) 0.8131(4) 0.0198(15) Uani 1 1 d . . .
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O21 O 0.6998(10) 0.7067(4) 0.6735(4) 0.049(2) Uani 1 1 d . . .
C101 C 0.0614(12) 0.9075(5) 0.8154(4) 0.0222(18) Uani 1 1 d . . .
C102 C -0.0091(11) 0.9002(6) 0.8839(5) 0.028(2) Uani 1 1 d . . .
H10C H -0.0269 0.8550 0.9034 0.034 Uiso 1 1 calc R . .
C103 C -0.0538(13) 0.9606(6) 0.9240(5) 0.032(2) Uani 1 1 d . . .
H10A H -0.0999 0.9555 0.9706 0.038 Uiso 1 1 calc R . .
C104 C -0.0310(12) 1.0268(6) 0.8961(5) 0.034(2) Uani 1 1 d . . .
H10B H -0.0647 1.0667 0.9228 0.040 Uiso 1 1 calc R . .
C105 C 0.0411(11) 1.0344(5) 0.8292(5) 0.027(2) Uani 1 1 d . . .
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 C117 C 0.2139(11) 0.7869(5) 0.6483(4) 0.0236(18) Uani 1 1 d . . .  
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 C201 C 0.5299(12) 0.7889(5) 0.8507(5) 0.029(2) Uani 1 1 d . . .  
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 C206 C 0.4715(10) 0.8397(5) 0.9002(4) 0.0273(18) Uani 1 1 d . . .  
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 C215 C 0.8091(12) 0.9629(6) 0.5775(5) 0.033(2) Uani 1 1 d . . .  
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 C216 C 0.7590(13) 0.9051(6) 0.6154(5) 0.030(2) Uani 1 1 d . . .  
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 C217 C 0.6883(12) 0.9113(5) 0.6838(5) 0.0234(19) Uani 1 1 d . . .  
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C108 0.026(4) 0.027(5) 0.030(5) 0.000(4) -0.004(4) -0.001(4)
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C111 0.023(4) 0.029(5) 0.019(4) -0.001(4) 0.001(3) -0.005(3)
C112 0.027(4) 0.029(5) 0.019(4) -0.004(4) 0.000(3) 0.003(4)
C113 0.038(5) 0.032(5) 0.030(4) -0.009(4) 0.009(4) -0.004(4)
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C115 0.034(5) 0.041(6) 0.037(5) -0.007(5) -0.007(4) -0.006(4)
C116 0.032(5) 0.024(5) 0.039(6) -0.001(4) -0.006(4) -0.004(4)
C117 0.030(4) 0.027(5) 0.014(4) -0.008(3) -0.004(3) -0.001(4)
C118 0.036(5) 0.038(6) 0.038(6) -0.002(5) -0.009(5) 0.000(4)
C201 0.030(5) 0.035(6) 0.022(4) -0.005(4) -0.001(3) 0.000(4)
C202 0.033(5) 0.032(6) 0.036(5) 0.003(4) 0.002(4) 0.002(4)
C203 0.034(5) 0.031(5) 0.045(6) 0.012(4) -0.001(4) -0.002(4)
C204 0.024(5) 0.044(7) 0.048(7) 0.023(5) 0.005(5) 0.008(4)
C205 0.032(4) 0.043(6) 0.029(4) 0.009(4) 0.005(4) 0.013(4)
C206 0.024(4) 0.033(5) 0.025(4) 0.001(4) -0.004(3) 0.005(4)
C207 0.014(4) 0.031(5) 0.019(4) 0.000(4) -0.006(3) 0.007(3)
C208 0.026(4) 0.038(6) 0.018(4) -0.006(4) 0.000(3) 0.000(4)
C209 0.028(5) 0.028(5) 0.031(5) -0.014(4) -0.004(4) -0.002(4)
C210 0.021(4) 0.028(5) 0.028(5) -0.006(4) -0.004(3) 0.000(4)
C211 0.020(4) 0.016(4) 0.025(5) -0.004(3) 0.000(3) 0.006(3)
C212 0.014(4) 0.027(5) 0.021(4) 0.000(3) -0.011(3) 0.002(4)
C213 0.024(4) 0.030(5) 0.030(5) 0.003(4) -0.008(4) -0.004(4)
C214 0.032(5) 0.029(5) 0.026(5) 0.006(4) -0.003(4) -0.004(4)
C215 0.021(4) 0.055(7) 0.023(5) 0.004(4) 0.003(4) -0.001(4)
C216 0.035(5) 0.032(6) 0.023(5) 0.003(4) -0.001(4) 0.004(4)
C217 0.019(4) 0.028(5) 0.023(5) -0.002(4) -0.007(3) 0.002(4)
C218 0.035(5) 0.037(6) 0.025(5) -0.001(4) -0.003(4) -0.002(4)

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\_geom\_special\_details

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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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loop\_

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Pt2 C201 2.084(9) . . ?  
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loop\_

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