

# ORGANOMETALLICS

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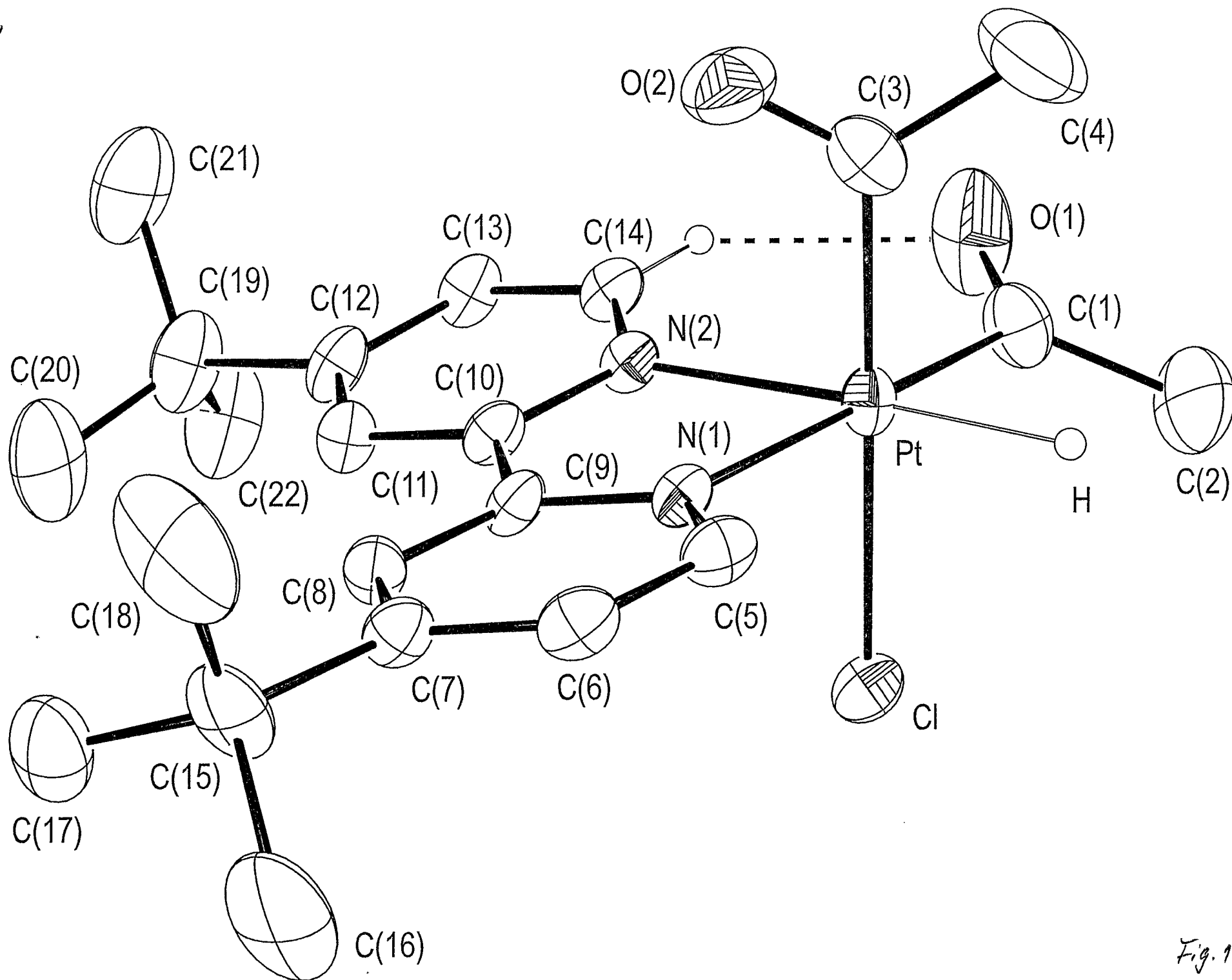


Fig. 1

Table 1. Crystal data and structure refinement for 1.

|                                   |                                                                                                               |
|-----------------------------------|---------------------------------------------------------------------------------------------------------------|
| Identification code               | ipds561                                                                                                       |
| Empirical formula                 | C22 H31 Cl N2 O2 Pt                                                                                           |
| Formula weight                    | 586.03                                                                                                        |
| Temperature                       | 220(2) K                                                                                                      |
| Wavelength                        | 0.71073 Å                                                                                                     |
| Crystal system                    | Orthorhombic                                                                                                  |
| Space group                       | P 2(1) n b                                                                                                    |
| Unit cell dimensions              | a = 10.937(3) Å    alpha = 90 deg.<br>b = 13.523(4) Å    beta = 90 deg.<br>c = 16.267(5) Å    gamma = 90 deg. |
| Volume                            | 2406.0(11) Å <sup>3</sup>                                                                                     |
| Z                                 | 4                                                                                                             |
| Density (calculated)              | 1.618 Mg/m <sup>3</sup>                                                                                       |
| Absorption coefficient            | 5.961 mm <sup>-1</sup>                                                                                        |
| F(000)                            | 1152                                                                                                          |
| Crystal size                      | 0.30 x 0.10 x 0.10 mm                                                                                         |
| Theta range for data collection   | 2.70 to 24.99 deg.                                                                                            |
| Index ranges                      | -12<=h<=12, -17<=k<=17, -20<=l<=20                                                                            |
| Reflections collected             | 14936                                                                                                         |
| Independent reflections           | 4004 [R(int) = 0.0809]                                                                                        |
| Absorption correction             | Numerically                                                                                                   |
| Max. and min. transmission        | 0.24 and 0.15                                                                                                 |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup>                                                                   |
| Data / restraints / parameters    | 4004 / 1 / 257                                                                                                |
| Goodness-of-fit on F <sup>2</sup> | 0.988                                                                                                         |
| Final R indices [I>2sigma(I)]     | R1 = 0.0296, wR2 = 0.0672                                                                                     |
| R indices (all data)              | R1 = 0.0395, wR2 = 0.0709                                                                                     |
| Absolute structure parameter      | -0.006(11)                                                                                                    |
| Largest diff. peak and hole       | 1.561 and -0.561 e.Å <sup>-3</sup>                                                                            |

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

|       | x        | y        | z        | U(eq)  |
|-------|----------|----------|----------|--------|
| C(1)  | 1007(9)  | 5832(6)  | 2591(6)  | 63(2)  |
| C(2)  | 155(13)  | 5478(10) | 3291(9)  | 111(4) |
| C(3)  | 1350(9)  | 4879(5)  | 1030(6)  | 58(2)  |
| C(4)  | 27(14)   | 4736(12) | 977(10)  | 124(6) |
| C(5)  | 3446(8)  | 2921(4)  | 1553(4)  | 45(2)  |
| C(6)  | 4382(8)  | 2337(5)  | 1254(4)  | 47(2)  |
| C(7)  | 5469(8)  | 2743(5)  | 1023(4)  | 43(2)  |
| C(8)  | 5590(7)  | 3762(5)  | 1110(4)  | 42(2)  |
| C(9)  | 4635(8)  | 4325(4)  | 1406(4)  | 38(2)  |
| C(10) | 4671(7)  | 5421(5)  | 1460(4)  | 40(2)  |
| C(11) | 5693(8)  | 5970(4)  | 1276(4)  | 45(2)  |
| C(12) | 5651(9)  | 6995(5)  | 1275(4)  | 49(2)  |
| C(13) | 4549(8)  | 7421(4)  | 1458(4)  | 48(2)  |
| C(14) | 3549(8)  | 6845(5)  | 1659(4)  | 44(2)  |
| C(15) | 6474(10) | 2091(6)  | 677(7)   | 64(3)  |
| C(16) | 6698(11) | 1198(7)  | 1236(10) | 136(6) |
| C(17) | 7709(9)  | 2606(8)  | 609(8)   | 84(4)  |
| C(18) | 6085(13) | 1778(10) | -197(8)  | 134(6) |
| C(19) | 6741(10) | 7635(6)  | 1051(6)  | 77(4)  |
| C(20) | 7914(13) | 7062(10) | 936(11)  | 113(5) |
| C(21) | 6435(14) | 8179(9)  | 231(9)   | 126(6) |
| C(22) | 6929(15) | 8424(7)  | 1702(7)  | 108(6) |
| Cl    | 3268(2)  | 4861(1)  | 3461(1)  | 53(1)  |
| N(1)  | 3574(6)  | 3903(4)  | 1638(3)  | 36(1)  |
| N(2)  | 3615(6)  | 5865(3)  | 1678(3)  | 36(1)  |
| O(1)  | 959(9)   | 6670(5)  | 2356(6)  | 116(3) |
| O(2)  | 1935(10) | 4992(4)  | 410(4)   | 80(3)  |
| Pt    | 2197(1)  | 4875(1)  | 2120(1)  | 40(1)  |

Table 3. Bond lengths [Å] and angles [deg] for 1.

---

|              |           |
|--------------|-----------|
| C(1)-O(1)    | 1.196(11) |
| C(1)-C(2)    | 1.548(14) |
| C(1)-Pt      | 1.990(9)  |
| C(2)-H(2A)   | 0.97      |
| C(2)-H(2B)   | 0.97      |
| C(2)-H(2C)   | 0.97      |
| C(3)-O(2)    | 1.204(12) |
| C(3)-C(4)    | 1.46(2)   |
| C(3)-Pt      | 2.001(10) |
| C(4)-H(4A)   | 0.97      |
| C(4)-H(4B)   | 0.97      |
| C(4)-H(4C)   | 0.97      |
| C(5)-N(1)    | 1.343(8)  |
| C(5)-C(6)    | 1.381(11) |
| C(5)-H(5)    | 0.94      |
| C(6)-C(7)    | 1.363(11) |
| C(6)-H(6)    | 0.94      |
| C(7)-C(8)    | 1.391(9)  |
| C(7)-C(15)   | 1.518(11) |
| C(8)-C(9)    | 1.380(10) |
| C(8)-H(8)    | 0.94      |
| C(9)-N(1)    | 1.347(9)  |
| C(9)-C(10)   | 1.485(9)  |
| C(10)-N(2)   | 1.349(9)  |
| C(10)-C(11)  | 1.375(10) |
| C(11)-C(12)  | 1.387(9)  |
| C(11)-H(11)  | 0.94      |
| C(12)-C(13)  | 1.369(12) |
| C(12)-C(19)  | 1.518(12) |
| C(13)-C(14)  | 1.382(11) |
| C(13)-H(13)  | 0.94      |
| C(14)-N(2)   | 1.328(8)  |
| C(14)-H(14)  | 0.94      |
| C(15)-C(17)  | 1.524(14) |
| C(15)-C(16)  | 1.531(13) |
| C(15)-C(18)  | 1.54(2)   |
| C(16)-H(16A) | 0.97      |
| C(16)-H(16B) | 0.97      |
| C(16)-H(16C) | 0.97      |
| C(17)-H(17A) | 0.97      |
| C(17)-H(17B) | 0.97      |
| C(17)-H(17C) | 0.97      |
| C(18)-H(18A) | 0.97      |
| C(18)-H(18B) | 0.97      |
| C(18)-H(18C) | 0.97      |
| C(19)-C(20)  | 1.51(2)   |
| C(19)-C(22)  | 1.517(12) |
| C(19)-C(21)  | 1.56(2)   |
| C(20)-H(20A) | 0.97      |
| C(20)-H(20B) | 0.97      |
| C(20)-H(20C) | 0.97      |
| C(21)-H(21A) | 0.97      |
| C(21)-H(21B) | 0.97      |
| C(21)-H(21C) | 0.97      |
| C(22)-H(22A) | 0.97      |
| C(22)-H(22B) | 0.97      |
| C(22)-H(22C) | 0.97      |
| Cl-Pt        | 2.476(2)  |
| N(1)-Pt      | 2.147(6)  |
| N(2)-Pt      | 2.172(6)  |

|                          |            |
|--------------------------|------------|
| Pt-H                     | 1.72 (5)   |
| O (1) -C (1) -C (2)      | 120.1 (9)  |
| O (1) -C (1) -Pt         | 121.5 (7)  |
| C (2) -C (1) -Pt         | 118.4 (7)  |
| C (1) -C (2) -H (2A)     | 109.5 (7)  |
| C (1) -C (2) -H (2B)     | 109.5 (6)  |
| H (2A) -C (2) -H (2B)    | 109.5      |
| C (1) -C (2) -H (2C)     | 109.5 (6)  |
| H (2A) -C (2) -H (2C)    | 109.5      |
| H (2B) -C (2) -H (2C)    | 109.5      |
| O (2) -C (3) -C (4)      | 119.6 (11) |
| O (2) -C (3) -Pt         | 119.8 (8)  |
| C (4) -C (3) -Pt         | 120.6 (9)  |
| C (3) -C (4) -H (4A)     | 109.5 (7)  |
| C (3) -C (4) -H (4B)     | 109.5 (7)  |
| H (4A) -C (4) -H (4B)    | 109.5      |
| C (3) -C (4) -H (4C)     | 109.5 (8)  |
| H (4A) -C (4) -H (4C)    | 109.5      |
| H (4B) -C (4) -H (4C)    | 109.5      |
| N (1) -C (5) -C (6)      | 121.7 (7)  |
| N (1) -C (5) -H (5)      | 119.2 (4)  |
| C (6) -C (5) -H (5)      | 119.2 (4)  |
| C (7) -C (6) -C (5)      | 120.8 (6)  |
| C (7) -C (6) -H (6)      | 119.6 (4)  |
| C (5) -C (6) -H (6)      | 119.6 (4)  |
| C (6) -C (7) -C (8)      | 117.0 (6)  |
| C (6) -C (7) -C (15)     | 120.0 (6)  |
| C (8) -C (7) -C (15)     | 123.0 (7)  |
| C (9) -C (8) -C (7)      | 120.7 (7)  |
| C (9) -C (8) -H (8)      | 119.7 (4)  |
| C (7) -C (8) -H (8)      | 119.7 (4)  |
| N (1) -C (9) -C (8)      | 121.1 (6)  |
| N (1) -C (9) -C (10)     | 115.4 (6)  |
| C (8) -C (9) -C (10)     | 123.5 (7)  |
| N (2) -C (10) -C (11)    | 120.9 (6)  |
| N (2) -C (10) -C (9)     | 115.9 (6)  |
| C (11) -C (10) -C (9)    | 123.2 (7)  |
| C (10) -C (11) -C (12)   | 120.9 (7)  |
| C (10) -C (11) -H (11)   | 119.6 (4)  |
| C (12) -C (11) -H (11)   | 119.6 (5)  |
| C (13) -C (12) -C (11)   | 116.7 (7)  |
| C (13) -C (12) -C (19)   | 120.3 (7)  |
| C (11) -C (12) -C (19)   | 123.0 (8)  |
| C (12) -C (13) -C (14)   | 120.8 (6)  |
| C (12) -C (13) -H (13)   | 119.6 (4)  |
| C (14) -C (13) -H (13)   | 119.6 (4)  |
| N (2) -C (14) -C (13)    | 121.7 (7)  |
| N (2) -C (14) -H (14)    | 119.2 (4)  |
| C (13) -C (14) -H (14)   | 119.2 (4)  |
| C (7) -C (15) -C (17)    | 113.8 (7)  |
| C (7) -C (15) -C (16)    | 110.8 (8)  |
| C (17) -C (15) -C (16)   | 105.2 (9)  |
| C (7) -C (15) -C (18)    | 107.5 (8)  |
| C (17) -C (15) -C (18)   | 107.6 (11) |
| C (16) -C (15) -C (18)   | 112.0 (10) |
| C (15) -C (16) -H (16A)  | 109.5 (6)  |
| C (15) -C (16) -H (16B)  | 109.5 (6)  |
| H (16A) -C (16) -H (16B) | 109.5      |
| C (15) -C (16) -H (16C)  | 109.5 (7)  |
| H (16A) -C (16) -H (16C) | 109.5      |
| H (16B) -C (16) -H (16C) | 109.5      |
| C (15) -C (17) -H (17A)  | 109.5 (6)  |
| C (15) -C (17) -H (17B)  | 109.5 (4)  |

|                     |           |
|---------------------|-----------|
| H(17A)-C(17)-H(17B) | 109.5     |
| C(15)-C(17)-H(17C)  | 109.5(7)  |
| H(17A)-C(17)-H(17C) | 109.5     |
| H(17B)-C(17)-H(17C) | 109.5     |
| C(15)-C(18)-H(18A)  | 109.5(6)  |
| C(15)-C(18)-H(18B)  | 109.5(7)  |
| H(18A)-C(18)-H(18B) | 109.5     |
| C(15)-C(18)-H(18C)  | 109.5(6)  |
| H(18A)-C(18)-H(18C) | 109.5     |
| H(18B)-C(18)-H(18C) | 109.5     |
| C(20)-C(19)-C(22)   | 109.4(11) |
| C(20)-C(19)-C(12)   | 113.9(7)  |
| C(22)-C(19)-C(12)   | 109.9(9)  |
| C(20)-C(19)-C(21)   | 108.6(11) |
| C(22)-C(19)-C(21)   | 107.1(9)  |
| C(12)-C(19)-C(21)   | 107.8(9)  |
| C(19)-C(20)-H(20A)  | 109.5(7)  |
| C(19)-C(20)-H(20B)  | 109.5(8)  |
| H(20A)-C(20)-H(20B) | 109.5     |
| C(19)-C(20)-H(20C)  | 109.5(5)  |
| H(20A)-C(20)-H(20C) | 109.5     |
| H(20B)-C(20)-H(20C) | 109.5     |
| C(19)-C(21)-H(21A)  | 109.5(7)  |
| C(19)-C(21)-H(21B)  | 109.5(6)  |
| H(21A)-C(21)-H(21B) | 109.5     |
| C(19)-C(21)-H(21C)  | 109.5(6)  |
| H(21A)-C(21)-H(21C) | 109.5     |
| H(21B)-C(21)-H(21C) | 109.5     |
| C(19)-C(22)-H(22A)  | 109.5(8)  |
| C(19)-C(22)-H(22B)  | 109.5(6)  |
| H(22A)-C(22)-H(22B) | 109.5     |
| C(19)-C(22)-H(22C)  | 109.5(7)  |
| H(22A)-C(22)-H(22C) | 109.5     |
| H(22B)-C(22)-H(22C) | 109.5     |
| C(5)-N(1)-C(9)      | 118.7(6)  |
| C(5)-N(1)-Pt        | 124.8(5)  |
| C(9)-N(1)-Pt        | 116.5(4)  |
| C(14)-N(2)-C(10)    | 119.0(6)  |
| C(14)-N(2)-Pt       | 125.8(5)  |
| C(10)-N(2)-Pt       | 115.1(4)  |
| C(1)-Pt-C(3)        | 92.1(4)   |
| C(1)-Pt-N(1)        | 176.3(3)  |
| C(3)-Pt-N(1)        | 90.2(3)   |
| C(1)-Pt-N(2)        | 101.1(3)  |
| C(3)-Pt-N(2)        | 92.0(3)   |
| N(1)-Pt-N(2)        | 75.9(2)   |
| C(1)-Pt-Cl          | 88.6(3)   |
| C(3)-Pt-Cl          | 179.3(3)  |
| N(1)-Pt-Cl          | 89.2(2)   |
| N(2)-Pt-Cl          | 87.6(2)   |
| C(1)-Pt-H           | 78(2)     |
| C(3)-Pt-H           | 91(2)     |
| N(1)-Pt-H           | 105(2)    |
| N(2)-Pt-H           | 177(2)    |
| Cl-Pt-H             | 90(2)     |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.  
The anisotropic displacement factor exponent takes the form:  
 $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

|       | U11     | U22     | U33     | U23      | U13    | U12    |
|-------|---------|---------|---------|----------|--------|--------|
| C(1)  | 52(6)   | 57(5)   | 81(7)   | -10(4)   | 8(5)   | 9(4)   |
| C(2)  | 87(11)  | 142(11) | 103(10) | 2(9)     | 45(8)  | 29(8)  |
| C(3)  | 53(7)   | 44(4)   | 78(7)   | -7(4)    | -7(5)  | 6(4)   |
| C(4)  | 67(12)  | 200(16) | 106(12) | -23(10)  | -32(8) | 16(10) |
| C(5)  | 57(6)   | 31(3)   | 47(4)   | 5(3)     | -3(4)  | -7(3)  |
| C(6)  | 65(6)   | 30(3)   | 46(4)   | 1(3)     | 1(4)   | 4(3)   |
| C(7)  | 52(6)   | 32(3)   | 43(4)   | 3(3)     | 5(3)   | 3(3)   |
| C(8)  | 42(5)   | 35(3)   | 49(4)   | 5(3)     | 7(3)   | 5(3)   |
| C(9)  | 52(6)   | 30(3)   | 33(4)   | 5(3)     | 12(3)  | 2(3)   |
| C(10) | 54(6)   | 29(3)   | 36(4)   | 1(3)     | 7(3)   | -1(3)  |
| C(11) | 49(6)   | 34(4)   | 51(4)   | -3(3)    | 10(4)  | -2(3)  |
| C(12) | 72(8)   | 37(4)   | 38(4)   | -10(3)   | 17(4)  | -8(4)  |
| C(13) | 68(6)   | 23(3)   | 51(5)   | -3(3)    | 14(4)  | -1(3)  |
| C(14) | 60(6)   | 34(4)   | 36(4)   | -4(3)    | 8(4)   | 7(3)   |
| C(15) | 50(7)   | 35(4)   | 108(8)  | 2(5)     | 6(5)   | 15(4)  |
| C(16) | 85(11)  | 60(5)   | 261(18) | 68(8)    | 39(9)  | 34(5)  |
| C(17) | 71(10)  | 62(7)   | 120(10) | 16(7)    | 28(6)  | 18(5)  |
| C(18) | 98(11)  | 186(13) | 120(10) | -107(10) | -5(8)  | 61(10) |
| C(19) | 94(11)  | 47(5)   | 92(8)   | -11(4)   | 29(5)  | -34(5) |
| C(20) | 85(12)  | 74(8)   | 178(15) | 0(9)     | 43(10) | -32(7) |
| C(21) | 138(14) | 99(8)   | 140(12) | 27(8)    | 49(10) | -43(8) |
| C(22) | 122(17) | 85(6)   | 116(8)  | -47(5)   | 40(9)  | -55(8) |
| Cl    | 68(2)   | 44(1)   | 47(1)   | 2(1)     | 2(1)   | -3(1)  |
| N(1)  | 43(4)   | 32(3)   | 32(3)   | 2(2)     | 3(3)   | -4(2)  |
| N(2)  | 47(4)   | 28(3)   | 34(3)   | -3(2)    | 7(3)   | 6(2)   |
| O(1)  | 103(7)  | 58(5)   | 188(10) | -3(5)    | 64(7)  | 26(4)  |
| O(2)  | 94(10)  | 94(4)   | 51(3)   | 4(2)     | -15(4) | -15(4) |
| Pt    | 38(1)   | 36(1)   | 45(1)   | -3(1)    | 8(1)   | -2(1)  |



Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.

|        | x        | y        | z        | U(eq) |
|--------|----------|----------|----------|-------|
| H(2A)  | 576(13)  | 5538(10) | 3813(9)  | 166   |
| H(2B)  | -68(13)  | 4793(10) | 3199(9)  | 166   |
| H(2C)  | -578(13) | 5883(10) | 3299(9)  | 166   |
| H(4A)  | -386(14) | 5271(12) | 1261(10) | 186   |
| H(4B)  | -191(14) | 4111(12) | 1231(10) | 186   |
| H(4C)  | -221(14) | 4730(12) | 404(10)  | 186   |
| H(5)   | 2701(8)  | 2623(4)  | 1700(4)  | 54    |
| H(6)   | 4268(8)  | 1650(5)  | 1210(4)  | 56    |
| H(8)   | 6331(7)  | 4069(5)  | 966(4)   | 51    |
| H(11)  | 6429(8)  | 5646(4)  | 1149(4)  | 54    |
| H(13)  | 4472(8)  | 8113(4)  | 1448(4)  | 57    |
| H(14)  | 2803(8)  | 7155(5)  | 1786(4)  | 52    |
| H(16A) | 7339(11) | 789(7)   | 1003(10) | 203   |
| H(16B) | 5952(11) | 814(7)   | 1282(10) | 203   |
| H(16C) | 6946(11) | 1425(7)  | 1776(10) | 203   |
| H(17A) | 7673(9)  | 3103(8)  | 179(8)   | 126   |
| H(17B) | 8334(9)  | 2124(8)  | 475(8)   | 126   |
| H(17C) | 7905(9)  | 2920(8)  | 1128(8)  | 126   |
| H(18A) | 6503(13) | 1171(10) | -347(8)  | 202   |
| H(18B) | 6299(13) | 2295(10) | -584(8)  | 202   |
| H(18C) | 5209(13) | 1669(10) | -209(8)  | 202   |
| H(20A) | 7791(13) | 6551(10) | 526(11)  | 169   |
| H(20B) | 8149(13) | 6760(10) | 1453(11) | 169   |
| H(20C) | 8555(13) | 7507(10) | 755(11)  | 169   |
| H(21A) | 5805(14) | 8669(9)  | 330(9)   | 188   |
| H(21B) | 6145(14) | 7703(9)  | -171(9)  | 188   |
| H(21C) | 7164(14) | 8502(9)  | 24(9)    | 188   |
| H(22A) | 6149(15) | 8722(7)  | 1839(7)  | 162   |
| H(22B) | 7478(15) | 8928(7)  | 1493(7)  | 162   |
| H(22C) | 7281(15) | 8126(7)  | 2190(7)  | 162   |
| H      | 1107(51) | 4096(33) | 2519(33) | 8(12) |