Table 1. Crystal data and structure refinement for complex **3**.

| | | |
|---|---|---|
| Identification code | nosod | |
| Empirical formula | C34 H19 Au F15 O2 P | |
| Formula weight | 972.43 | |
| Temperature | 143(2) K | |
| Wavelength | 0.71073 ≈ | |
| Crystal system | Triclinic | |
| Space group | P -1 | |
| Unit cell dimensions | a = 10.5562(10) ≈ | α= 109.378(3)∞ |
| | b = 10.5950(10) ≈ | β= 104.321(3)∞ |
| | c = 15.7468(14) ≈ | γ = 91.630(3)∞ |
| Volume | 1598.0(3) ≈$^3$ | |
| Z | 2 | |
| Density (calculated) | 2.021 Mg/m$^3$ | |
| Absorption coefficient | 4.775 mm$^{-1}$ | |
| F(000) | 936 | |
| Crystal size | 0.31 x 0.14 x 0.13 mm$^3$ | |
| Theta range for data collection | 1.42 to 30.03∞ | |
| Index ranges | -14<=h<=14, -14<=k<=14, -21<=l<=22 | |
| Reflections collected | 28899 | |
| Independent reflections | 9287 [R(int) = 0.0387] | |
| Completeness to theta = 30.00∞ | 99.3 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.802 and 0.611 | |
| Refinement method | Full-matrix least-squares on F$^2$ | |
| Data / restraints / parameters | 9287 / 146 / 480 | |
| Goodness-of-fit on F$^2$ | 1.023 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0299, wR2 = 0.0682 | |
| R indices (all data) | R1 = 0.0369, wR2 = 0.0700 | |
| Largest diff. peak and hole | 1.596 and -2.842 e.≈$^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters for complex **3** (≈$^2$x $10^3$). U(eq) is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Au | 2831.7(1) | 5360.4(1) | 2587.5(1) | 22.1(1) |
| P | 1083.2(8) | 3677.5(8) | 2277.3(6) | 24.6(2) |
| C(1) | 1063(4) | 2075(3) | 1345(3) | 35.9(7) |
| C(2) | 1537(4) | 954(4) | 1687(3) | 43.0(8) |
| C(3) | 3115(5) | 603(6) | 2879(5) | 78.9(18) |
| C(4) | 2388(5) | -227(5) | 424(4) | 67.9(15) |
| O(1) | 2742(3) | 1396(3) | 2313(2) | 46.5(7) |
| O(2) | 1502(3) | -262(3) | 947(3) | 56.7(8) |
| C(11) | 1089(3) | 3406(3) | 3354(2) | 25.3(6) |
| C(12) | 2090(3) | 4016(4) | 4166(2) | 34.8(7) |
| C(13) | 2063(4) | 3771(4) | 4973(3) | 41.7(9) |
| C(14) | 1041(3) | 2924(4) | 4968(3) | 35.3(7) |
| C(15) | 37(3) | 2323(3) | 4172(2) | 31.0(7) |
| C(16) | 46(3) | 2559(3) | 3357(2) | 28.6(6) |
| C(21) | -525(3) | 4216(3) | 1914(2) | 26.3(6) |
| C(22) | -1094(3) | 4032(4) | 982(2) | 32.6(7) |
| C(23) | -2260(3) | 4564(4) | 725(2) | 36.3(7) |
| C(24) | -2849(3) | 5284(4) | 1390(3) | 36.3(7) |
| C(25) | -2297(3) | 5469(4) | 2321(3) | 33.2(7) |
| C(26) | -1136(3) | 4942(3) | 2587(2) | 28.8(6) |
| C(31) | 4327(3) | 6911(3) | 2976(2) | 24.9(6) |
| C(32) | 4704(3) | 7362(3) | 2350(2) | 30.2(6) |
| C(33) | 5657(4) | 8445(4) | 2611(3) | 40.0(8) |
| C(34) | 6250(4) | 9118(4) | 3538(3) | 40.8(8) |
| C(35) | 5897(3) | 8701(4) | 4188(2) | 36.2(7) |
| C(36) | 4948(3) | 7611(4) | 3912(2) | 33.5(7) |
| F(1) | 4121(2) | 6749(3) | 1427.1(16) | 49.8(6) |
| F(2) | 5944(3) | 8876(3) | 1963(2) | 78.3(10) |
| F(3) | 7159(3) | 10179(3) | 3811(2) | 63.1(7) |
| F(4) | 6467(3) | 9381(3) | 5102.2(17) | 58.0(7) |
| F(5) | 4631(3) | 7259(3) | 4583.2(16) | 56.8(7) |
| C(41) | 1529(3) | 6783(3) | 2641(2) | 22.4(5) |

| | | | | |
|---|---|---|---|---|
| C(42) | 864(3) | 6892(3) | 1806(2) | 26.0(6) |
| C(43) | -65(3) | 7769(3) | 1729(2) | 30.1(7) |
| C(44) | -329(3) | 8599(3) | 2531(2) | 32.4(7) |
| C(45) | 336(4) | 8526(3) | 3388(2) | 33.3(7) |
| C(46) | 1239(3) | 7626(3) | 3427(2) | 27.8(6) |
| F(6) | 1080(2) | 6072(2) | 1001.3(14) | 38.7(5) |
| F(7) | -725(2) | 7808(2) | 895.0(15) | 44.8(5) |
| F(8) | -1226(2) | 9455(2) | 2478.8(18) | 49.3(6) |
| F(9) | 67(3) | 9318(2) | 4171.4(16) | 53.2(6) |
| F(10) | 1833(2) | 7557(2) | 4275.6(14) | 40.4(5) |
| C(51) | 4196(3) | 4010(3) | 2366(2) | 28.9(6) |
| C(52) | 5097(3) | 3729(3) | 3053(3) | 34.0(7) |
| C(53) | 6026(3) | 2870(4) | 2862(3) | 44.5(9) |
| C(54) | 6074(3) | 2247(4) | 1966(3) | 46.7(10) |
| C(55) | 5192(4) | 2500(4) | 1247(3) | 41.9(9) |
| C(56) | 4278(3) | 3380(3) | 1464(3) | 32.8(7) |
| F(11) | 5091(2) | 4312(3) | 3962.3(16) | 45.4(5) |
| F(12) | 6903(3) | 2648(3) | 3572(2) | 69.5(8) |
| F(13) | 6979(2) | 1418(3) | 1767(2) | 65.1(8) |
| F(14) | 5229(3) | 1903(3) | 359(2) | 60.3(7) |
| F(15) | 3439(2) | 3602(2) | 743.6(16) | 43.8(5) |

Table 3. Bond lengths [Å] and angles [°] for complex **3**.

| | |
|---|---|
| Au-C(41) | 2.065(3) |
| Au-C(51) | 2.068(3) |
| Au-C(31) | 2.067(3) |
| Au-P | 2.3692(8) |
| P-C(11) | 1.810(3) |
| P-C(21) | 1.824(3) |
| P-C(1) | 1.835(4) |
| C(1)-C(2) | 1.509(5) |
| C(2)-O(1) | 1.360(5) |
| C(2)-O(2) | 1.414(5) |
| C(3)-O(1) | 1.414(5) |
| C(4)-O(2) | 1.398(6) |
| C(11)-C(12) | 1.383(4) |
| C(11)-C(16) | 1.402(4) |
| C(12)-C(13) | 1.384(5) |
| C(13)-C(14) | 1.381(5) |
| C(14)-C(15) | 1.369(5) |
| C(15)-C(16) | 1.389(4) |
| C(21)-C(22) | 1.386(4) |
| C(21)-C(26) | 1.397(4) |
| C(22)-C(23) | 1.394(5) |
| C(23)-C(24) | 1.372(5) |
| C(24)-C(25) | 1.381(5) |
| C(25)-C(26) | 1.389(4) |
| C(31)-C(32) | 1.362(4) |
| C(31)-C(36) | 1.386(4) |
| C(32)-F(1) | 1.349(4) |
| C(32)-C(33) | 1.383(5) |
| C(33)-F(2) | 1.341(4) |
| C(33)-C(34) | 1.365(5) |
| C(34)-F(3) | 1.336(4) |
| C(34)-C(35) | 1.365(5) |
| C(35)-F(4) | 1.346(4) |
| C(35)-C(36) | 1.383(5) |
| C(36)-F(5) | 1.340(4) |
| C(41)-C(42) | 1.373(4) |

| | |
|---|---|
| C(41)-C(46) | 1.376(4) |
| C(42)-F(6) | 1.355(4) |
| C(42)-C(43) | 1.381(4) |
| C(43)-F(7) | 1.341(4) |
| C(43)-C(44) | 1.377(5) |
| C(44)-F(8) | 1.336(4) |
| C(44)-C(45) | 1.387(5) |
| C(45)-F(9) | 1.343(4) |
| C(45)-C(46) | 1.373(4) |
| C(46)-F(10) | 1.355(3) |
| C(51)-C(52) | 1.372(4) |
| C(51)-C(56) | 1.380(5) |
| C(52)-F(11) | 1.361(4) |
| C(52)-C(53) | 1.376(5) |
| C(53)-F(12) | 1.356(4) |
| C(53)-C(54) | 1.360(6) |
| C(54)-F(13) | 1.339(4) |
| C(54)-C(55) | 1.383(6) |
| C(55)-F(14) | 1.341(5) |
| C(55)-C(56) | 1.386(5) |
| C(56)-F(15) | 1.349(4) |

| | |
|---|---|
| C(41)-Au-C(51) | 171.15(11) |
| C(41)-Au-C(31) | 87.62(11) |
| C(51)-Au-C(31) | 88.60(11) |
| C(41)-Au-P | 90.17(8) |
| C(51)-Au-P | 94.24(9) |
| C(31)-Au-P | 174.78(9) |
| C(11)-P-C(21) | 104.40(14) |
| C(11)-P-C(1) | 110.70(16) |
| C(21)-P-C(1) | 104.54(16) |
| C(11)-P-Au | 108.92(11) |
| C(21)-P-Au | 112.12(10) |
| C(1)-P-Au | 115.56(12) |
| C(2)-C(1)-P | 114.5(3) |
| O(1)-C(2)-O(2) | 113.8(3) |
| O(1)-C(2)-C(1) | 108.7(3) |
| O(2)-C(2)-C(1) | 112.7(4) |

| | |
|---|---|
| C(2)-O(1)-C(3) | 113.6(4) |
| C(4)-O(2)-C(2) | 115.0(3) |
| C(12)-C(11)-C(16) | 119.8(3) |
| C(12)-C(11)-P | 121.6(2) |
| C(16)-C(11)-P | 118.6(2) |
| C(11)-C(12)-C(13) | 119.7(3) |
| C(14)-C(13)-C(12) | 120.2(3) |
| C(15)-C(14)-C(13) | 120.7(3) |
| C(14)-C(15)-C(16) | 119.9(3) |
| C(15)-C(16)-C(11) | 119.6(3) |
| C(22)-C(21)-C(26) | 119.1(3) |
| C(22)-C(21)-P | 120.6(2) |
| C(26)-C(21)-P | 120.0(2) |
| C(21)-C(22)-C(23) | 120.0(3) |
| C(24)-C(23)-C(22) | 120.5(3) |
| C(23)-C(24)-C(25) | 120.0(3) |
| C(24)-C(25)-C(26) | 120.1(3) |
| C(25)-C(26)-C(21) | 120.2(3) |
| C(32)-C(31)-C(36) | 116.2(3) |
| C(32)-C(31)-Au | 123.0(2) |
| C(36)-C(31)-Au | 120.7(2) |
| F(1)-C(32)-C(31) | 119.5(3) |
| F(1)-C(32)-C(33) | 117.4(3) |
| C(31)-C(32)-C(33) | 123.2(3) |
| F(2)-C(33)-C(34) | 120.2(3) |
| F(2)-C(33)-C(32) | 120.3(3) |
| C(34)-C(33)-C(32) | 119.4(3) |
| F(3)-C(34)-C(33) | 120.7(3) |
| F(3)-C(34)-C(35) | 120.0(4) |
| C(33)-C(34)-C(35) | 119.3(3) |
| F(4)-C(35)-C(34) | 119.1(3) |
| F(4)-C(35)-C(36) | 120.5(3) |
| C(34)-C(35)-C(36) | 120.4(3) |
| F(5)-C(36)-C(35) | 117.7(3) |
| F(5)-C(36)-C(31) | 120.7(3) |
| C(35)-C(36)-C(31) | 121.6(3) |
| C(42)-C(41)-C(46) | 116.2(3) |
| C(42)-C(41)-Au | 117.0(2) |

| | |
|---|---|
| C(46)-C(41)-Au | 126.8(2) |
| F(6)-C(42)-C(41) | 119.3(3) |
| F(6)-C(42)-C(43) | 117.1(3) |
| C(41)-C(42)-C(43) | 123.5(3) |
| F(7)-C(43)-C(44) | 119.8(3) |
| F(7)-C(43)-C(42) | 121.5(3) |
| C(44)-C(43)-C(42) | 118.7(3) |
| F(8)-C(44)-C(43) | 120.1(3) |
| F(8)-C(44)-C(45) | 120.6(3) |
| C(43)-C(44)-C(45) | 119.3(3) |
| F(9)-C(45)-C(46) | 120.6(3) |
| F(9)-C(45)-C(44) | 119.6(3) |
| C(46)-C(45)-C(44) | 119.8(3) |
| F(10)-C(46)-C(45) | 117.8(3) |
| F(10)-C(46)-C(41) | 119.7(3) |
| C(45)-C(46)-C(41) | 122.5(3) |
| C(52)-C(51)-C(56) | 115.8(3) |
| C(52)-C(51)-Au | 125.4(3) |
| C(56)-C(51)-Au | 118.6(2) |
| F(11)-C(52)-C(51) | 119.8(3) |
| F(11)-C(52)-C(53) | 117.7(3) |
| C(51)-C(52)-C(53) | 122.6(4) |
| F(12)-C(53)-C(54) | 119.7(4) |
| F(12)-C(53)-C(52) | 119.8(4) |
| C(54)-C(53)-C(52) | 120.5(4) |
| F(13)-C(54)-C(53) | 121.3(4) |
| F(13)-C(54)-C(55) | 119.4(4) |
| C(53)-C(54)-C(55) | 119.3(3) |
| F(14)-C(55)-C(54) | 120.3(3) |
| F(14)-C(55)-C(56) | 121.0(4) |
| C(54)-C(55)-C(56) | 118.8(4) |
| F(15)-C(56)-C(51) | 120.1(3) |
| F(15)-C(56)-C(55) | 116.9(3) |
| C(51)-C(56)-C(55) | 123.1(3) |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\approx^2$x $10^3$) for complex **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[ h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12} ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Au | 19.6(1) | 23.1(1) | 22.9(1) | 8.7(1) | 4.0(1) | 1.0(1) |
| P | 24.4(4) | 23.2(4) | 25.1(4) | 7.4(3) | 6.2(3) | 0.3(3) |
| C(1) | 36.2(18) | 30.2(17) | 37.3(19) | 6.9(15) | 9.6(15) | 3.2(14) |
| C(2) | 36.5(19) | 35.5(19) | 51(2) | 7.6(17) | 11.3(17) | 7.8(15) |
| C(3) | 53(3) | 96(4) | 116(5) | 79(4) | 13(3) | 23(3) |
| C(4) | 61(3) | 48(3) | 76(4) | -10(2) | 30(3) | -11(2) |
| O(1) | 43.4(15) | 41.9(15) | 53.2(17) | 19.5(14) | 6.9(13) | 9.0(12) |
| O(2) | 46.6(17) | 33.9(15) | 78(2) | 2.7(15) | 19.5(16) | 4.5(13) |
| C(11) | 23.7(14) | 26.9(15) | 27.9(15) | 13.0(13) | 6.4(12) | 6.0(11) |
| C(12) | 23.8(15) | 45(2) | 33.0(18) | 15.2(16) | 1.2(13) | -7.3(13) |
| C(13) | 33.5(18) | 56(2) | 29.4(18) | 17.9(17) | -4.5(14) | -8.6(16) |
| C(14) | 36.4(18) | 42(2) | 31.4(17) | 18.6(16) | 8.7(14) | 4.0(15) |
| C(15) | 32.0(16) | 29.5(16) | 35.1(18) | 15.2(14) | 10.1(14) | 2.1(13) |
| C(16) | 24.4(14) | 28.6(16) | 30.3(16) | 10.2(13) | 3.3(12) | 0.6(12) |
| C(21) | 23.7(14) | 26.7(15) | 27.7(16) | 11.4(13) | 3.3(12) | -1.7(11) |
| C(22) | 31.1(16) | 38.3(18) | 26.4(16) | 10.3(14) | 5.6(13) | 6.0(14) |
| C(23) | 29.6(16) | 46(2) | 28.0(17) | 13.4(15) | -2.1(13) | 5.8(14) |
| C(24) | 25.5(15) | 44(2) | 40.3(19) | 18.7(17) | 4.3(14) | 5.7(14) |
| C(25) | 30.3(16) | 35.8(18) | 37.4(18) | 15.8(15) | 11.9(14) | 8.3(14) |
| C(26) | 28.0(15) | 30.8(16) | 28.6(16) | 12.7(13) | 6.1(13) | 3.7(12) |
| C(31) | 20.4(13) | 24.7(14) | 29.1(15) | 11.1(12) | 3.0(12) | 6.3(11) |
| C(32) | 24.4(14) | 33.8(17) | 29.5(16) | 11.2(14) | 2.4(12) | -1.9(12) |
| C(33) | 33.2(18) | 46(2) | 44(2) | 21.5(18) | 8.9(16) | -5.7(15) |
| C(34) | 29.0(17) | 31.0(18) | 55(2) | 10.4(17) | 6.5(16) | -5.3(14) |
| C(35) | 30.2(17) | 32.6(17) | 31.7(18) | -2.8(14) | 3.2(14) | -2.6(13) |
| C(36) | 30.0(16) | 36.1(18) | 30.7(17) | 8.9(14) | 6.0(14) | -1.9(13) |
| F(1) | 43.0(13) | 71.4(17) | 30.0(11) | 18.4(11) | 3.2(10) | -18.8(11) |
| F(2) | 72.1(19) | 100(2) | 67.9(19) | 46.5(18) | 9.2(15) | -40.7(17) |
| F(3) | 51.5(15) | 48.8(15) | 76.2(19) | 14.4(14) | 8.7(14) | -26.2(12) |
| F(4) | 48.7(14) | 60.9(16) | 37.9(13) | -8.3(12) | 3.0(11) | -17.8(12) |
| F(5) | 55.5(15) | 77.4(18) | 28.2(12) | 16.2(12) | 1.9(10) | -24.9(13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(41) | 19.7(13) | 21.8(13) | 23.9(14) | 7.0(11) | 4.7(11) | 0.2(10) |
| C(42) | 22.8(14) | 32.1(16) | 23.6(15) | 10.6(13) | 5.9(12) | 1.8(12) |
| C(43) | 26.2(15) | 35.1(17) | 28.0(16) | 15.1(14) | 0.4(12) | 1.2(13) |
| C(44) | 33.9(17) | 22.6(15) | 40.7(19) | 12.2(14) | 8.1(15) | 7.4(13) |
| C(45) | 46(2) | 23.0(15) | 32.3(17) | 7.8(13) | 16.2(15) | 7.0(14) |
| C(46) | 33.9(16) | 24.7(15) | 24.1(15) | 9.7(12) | 5.2(13) | 0.7(12) |
| F(6) | 39.2(11) | 53.6(13) | 23.8(10) | 11.5(9) | 11.5(9) | 13.5(10) |
| F(7) | 42.9(12) | 55.5(14) | 36.4(12) | 24.3(11) | -0.7(10) | 11.7(10) |
| F(8) | 52.4(14) | 35.4(12) | 58.1(15) | 16.4(11) | 9.4(12) | 22.7(10) |
| F(9) | 85.4(19) | 37.5(12) | 39.0(13) | 8.3(10) | 25.6(13) | 29.8(13) |
| F(10) | 58.6(14) | 39.6(12) | 22.0(10) | 11.5(9) | 7.1(9) | 13.5(10) |
| C(51) | 21.3(13) | 23.4(15) | 41.3(18) | 11.1(13) | 7.5(13) | 1.5(11) |
| C(52) | 23.1(15) | 35.2(18) | 46(2) | 19.2(16) | 6.5(14) | 0.4(13) |
| C(53) | 20.6(15) | 44(2) | 73(3) | 31(2) | 4.5(17) | 4.7(14) |
| C(54) | 24.4(16) | 30.7(18) | 84(3) | 16(2) | 16.7(19) | 6.8(14) |
| C(55) | 29.7(17) | 29.8(18) | 60(2) | 5.6(17) | 16.1(17) | 1.2(14) |
| C(56) | 26.2(15) | 28.3(16) | 42.1(19) | 9.2(15) | 10.3(14) | 3.8(12) |
| F(11) | 29.6(11) | 64.5(15) | 45.0(13) | 28.4(12) | 2.2(10) | 5.5(10) |
| F(12) | 38.3(13) | 81(2) | 98(2) | 52.9(19) | 3.2(14) | 22.5(13) |
| F(13) | 34.1(12) | 46.0(14) | 113(2) | 21.5(15) | 24.0(15) | 21.3(11) |
| F(14) | 51.7(15) | 51.8(15) | 65.7(18) | -4.4(13) | 28.8(14) | 12.2(12) |
| F(15) | 43.2(12) | 51.2(14) | 36.2(12) | 12.2(10) | 12.6(10) | 14.2(10) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (≈$^2$x $10^3$) for complex **3**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1A) | 153 | 1782 | 936 | 43 |
| H(1B) | 1623 | 2228 | 960 | 43 |
| H(2) | 919 | 774 | 2034 | 52 |
| H(3A) | 2490 | 634 | 3252 | 95 |
| H(3B) | 4001 | 955 | 3297 | 95 |
| H(3C) | 3111 | -332 | 2480 | 95 |
| H(4A) | 2163 | 427 | 108 | 81 |
| H(4B) | 2337 | -1122 | -45 | 81 |
| H(4C) | 3284 | 41 | 840 | 81 |
| H(12) | 2792 | 4600 | 4171 | 42 |
| H(13) | 2751 | 4187 | 5531 | 50 |
| H(14) | 1034 | 2757 | 5524 | 42 |
| H(15) | -664 | 1746 | 4177 | 37 |
| H(16) | -652 | 2149 | 2804 | 34 |
| H(22) | -688 | 3542 | 518 | 39 |
| H(23) | -2651 | 4428 | 85 | 44 |
| H(24) | -3637 | 5656 | 1210 | 44 |
| H(25) | -2711 | 5958 | 2780 | 40 |
| H(26) | -755 | 5074 | 3228 | 35 |

Table 1. Crystal data and structure refinement for complex 6.

| | |
|---|---|
| Identification code | nidls |
| Empirical formula | C52 H30 Au2 Cl3 F15 O P2 |
| Formula weight | 1517.98 |
| Temperature | 133(2) K |
| Wavelength | 0.71073 A |
| Crystal system, space group | Monoclinic, P 21/n |
| Unit cell dimensions | a = 19.863(3) A alpha = 90 deg.<br>b = 13.2995(18) A beta = 92.484(6)<br>c = 19.928(3) A gamma = 90 deg. |
| Volume | 5259.4(12) A^3 |
| Z, Calculated density | 4, 1.917 Mg/m^3 |
| Absorption coefficient | 5.877 mm^-1 |
| F(000) | 2896 |
| Crystal size | 0.50 x 0.10 x 0.05 mm |
| Theta range for data collection | 1.42 to 28.29 deg. |
| Limiting indices | -26<=h<=26, -17<=k<=17, -26<=l<=26 |
| Reflections collected / unique | 79626 / 13044 [R(int) = 0.0881] |
| Completeness to theta = 28.00 | 99.9 % |
| Absorption correction | SADABS |
| Max. and min. transmission | 0.928 and 0.597 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 13044 / 204 / 676 |
| Goodness-of-fit on F^2 | 1.028 |
| Final R indices [I>2sigma(I)] | R1 = 0.0519, wR2 = 0.1349 |
| R indices (all data) | R1 = 0.0844, wR2 = 0.1592 |
| Largest diff. peak and hole | 3.044 and -3.860 e.A^-3 |

Table 2. Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex 6.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Au(1) | 2408(1) | 4361(1) | 4258(1) | 22(1) |
| Au(2) | 5135(1) | 2437(1) | 3875(1) | 24(1) |
| P(1) | 3462(1) | 4746(2) | 4785(1) | 22(1) |
| P(2) | 5829(1) | 1376(2) | 3330(1) | 25(1) |
| C(1) | 4088(4) | 3961(6) | 4507(4) | 26(2) |
| C(2) | 4499(4) | 3385(6) | 4281(4) | 24(2) |
| C(11) | 3470(3) | 4618(6) | 5686(4) | 26(2) |
| C(12) | 4056(4) | 4875(6) | 6053(4) | 37(2) |
| C(13) | 4093(5) | 4749(8) | 6750(5) | 47(2) |
| C(14) | 3563(4) | 4368(7) | 7073(5) | 43(2) |
| C(15) | 2974(4) | 4104(7) | 6714(4) | 40(2) |
| C(16) | 2923(4) | 4243(6) | 6021(4) | 31(2) |
| C(21) | 3743(3) | 6011(6) | 4626(4) | 24(2) |
| C(22) | 4190(3) | 6195(6) | 4114(4) | 29(2) |
| C(23) | 4359(4) | 7170(6) | 3960(4) | 35(2) |
| C(24) | 4080(4) | 7972(6) | 4305(4) | 33(2) |
| C(25) | 3649(4) | 7799(6) | 4816(4) | 31(2) |
| C(26) | 3479(4) | 6815(6) | 4982(4) | 27(2) |
| C(31) | 5557(3) | 1229(6) | 2450(4) | 28(2) |
| C(32) | 5990(4) | 922(7) | 1960(4) | 42(2) |
| C(33) | 5752(5) | 803(8) | 1311(5) | 50(2) |
| C(34) | 5086(5) | 993(9) | 1125(5) | 54(3) |
| C(35) | 4649(5) | 1282(8) | 1610(5) | 47(2) |
| C(36) | 4881(4) | 1405(7) | 2261(4) | 36(2) |
| C(41) | 6687(4) | 1840(6) | 3315(4) | 33(2) |
| C(42) | 7234(4) | 1336(8) | 3610(4) | 42(2) |
| C(43) | 7878(4) | 1749(10) | 3627(5) | 57(3) |
| C(44) | 7965(5) | 2683(8) | 3316(6) | 65(3) |
| C(45) | 7433(5) | 3201(9) | 3015(7) | 67(3) |
| C(46) | 6786(5) | 2776(7) | 3026(6) | 53(3) |
| C(51) | 5908(4) | 126(6) | 3684(4) | 30(2) |
| C(52) | 6190(5) | -658(7) | 3330(5) | 48(2) |
| C(53) | 6242(5) | -1617(7) | 3613(6) | 54(3) |
| C(54) | 6027(5) | -1802(7) | 4250(5) | 48(2) |
| C(55) | 5749(4) | -1012(7) | 4602(5) | 43(2) |
| C(56) | 5686(4) | -49(6) | 4319(4) | 35(2) |
| C(61) | 1483(3) | 4026(6) | 3779(3) | 27(2) |
| C(62) | 956(4) | 3710(6) | 4132(4) | 40(2) |
| C(63) | 334(4) | 3491(7) | 3819(5) | 47(2) |
| C(64) | 254(4) | 3589(8) | 3135(4) | 48(2) |
| C(65) | 768(4) | 3913(7) | 2770(4) | 40(2) |
| C(66) | 1393(4) | 4123(6) | 3097(4) | 29(2) |
| F(1) | 1012(3) | 3597(5) | 4798(3) | 57(2) |
| F(2) | -190(3) | 3189(7) | 4185(4) | 80(2) |
| F(3) | -346(3) | 3380(6) | 2832(4) | 73(2) |
| F(4) | 682(3) | 4043(5) | 2106(3) | 57(2) |
| F(5) | 1894(3) | 4437(4) | 2722(2) | 39(1) |
| C(71) | 2646(4) | 2850(6) | 4219(3) | 30(2) |
| C(72) | 2493(4) | 2143(7) | 4691(4) | 40(2) |
| C(73) | 2672(5) | 1121(7) | 4619(5) | 53(2) |
| C(74) | 3002(5) | 828(7) | 4079(5) | 58(3) |
| C(75) | 3154(4) | 1488(7) | 3597(5) | 50(2) |

| | | | | |
|---|---|---|---|---|
| F(6) | 2177(3) | 2424(4) | 5247(3) | 53(2) |
| F(7) | 2532(4) | 467(5) | 5116(4) | 78(2) |
| F(8) | 3171(3) | -154(5) | 4014(5) | 85(3) |
| F(9) | 3482(3) | 1204(5) | 3046(4) | 73(2) |
| F(10) | 3141(3) | 3141(4) | 3176(3) | 45(1) |
| C(81) | 2144(3) | 5861(6) | 4225(3) | 24(2) |
| C(82) | 2373(3) | 6486(6) | 3733(4) | 31(2) |
| C(83) | 2233(4) | 7503(6) | 3690(5) | 40(2) |
| C(84) | 1833(4) | 7913(7) | 4175(4) | 45(2) |
| C(85) | 1580(4) | 7320(6) | 4683(5) | 41(2) |
| C(86) | 1748(4) | 6306(6) | 4692(4) | 30(2) |
| F(11) | 2766(2) | 6108(4) | 3257(2) | 41(1) |
| F(12) | 2473(3) | 8084(5) | 3220(3) | 59(2) |
| F(13) | 1689(3) | 8917(4) | 4174(4) | 63(2) |
| F(14) | 1189(3) | 7731(4) | 5134(3) | 52(2) |
| F(15) | 1499(3) | 5759(4) | 5195(3) | 42(1) |
| Cl(1) | 878(5) | -415(8) | 2657(5) | 236(5) |
| Cl(2) | 1395(5) | 1225(9) | 3206(6) | 256(5) |
| Cl(3) | 140(8) | 1036(9) | 3118(9) | 400(10) |
| C(99) | 470(50) | 1200(70) | 5650(40) | 160(40) |
| O(1) | 306(15) | 1650(20) | 5311(16) | 57(7) |
| C(99') | 1707(12) | 1110(20) | 6442(13) | 40(6) |
| O(1') | 1251(10) | 1269(15) | 6401(10) | 51(5) |
| C(99") | 821(14) | -180(20) | 5520(15) | 49(7) |
| O(1") | 988(11) | 371(17) | 5274(11) | 56(6) |

Table 3. Bond lengths [A] and angles [deg] for complex 6.

| | |
|---|---|
| Au(1)-C(81) | 2.063(8) |
| Au(1)-C(71) | 2.067(8) |
| Au(1)-C(61) | 2.082(7) |
| Au(1)-P(1) | 2.3572(18) |
| Au(2)-C(2) | 1.982(8) |
| Au(2)-P(2) | 2.280(2) |
| P(1)-C(1) | 1.733(8) |
| P(1)-C(11) | 1.803(8) |
| P(1)-C(21) | 1.804(8) |
| P(2)-C(51) | 1.809(8) |
| P(2)-C(41) | 1.815(8) |
| P(2)-C(31) | 1.823(8) |
| C(1)-C(2) | 1.220(11) |
| C(11)-C(16) | 1.391(9) |
| C(11)-C(12) | 1.391(9) |
| C(12)-C(13) | 1.398(11) |
| C(13)-C(14) | 1.356(11) |
| C(14)-C(15) | 1.389(11) |
| C(15)-C(16) | 1.392(11) |
| C(21)-C(26) | 1.397(9) |
| C(21)-C(22) | 1.403(9) |
| C(22)-C(23) | 1.378(11) |
| C(23)-C(24) | 1.396(10) |
| C(24)-C(25) | 1.379(10) |
| C(25)-C(26) | 1.395(10) |
| C(31)-C(32) | 1.391(10) |
| C(31)-C(36) | 1.397(9) |
| C(32)-C(33) | 1.367(12) |
| C(33)-C(34) | 1.382(12) |
| C(34)-C(35) | 1.381(12) |
| C(35)-C(36) | 1.366(11) |
| C(41)-C(42) | 1.387(10) |
| C(41)-C(46) | 1.388(11) |
| C(42)-C(43) | 1.391(11) |
| C(43)-C(44) | 1.403(13) |
| C(44)-C(45) | 1.377(13) |
| C(45)-C(46) | 1.405(12) |
| C(51)-C(56) | 1.378(10) |
| C(51)-C(52) | 1.390(10) |
| C(52)-C(53) | 1.398(12) |
| C(53)-C(54) | 1.379(12) |
| C(54)-C(55) | 1.390(12) |
| C(55)-C(56) | 1.402(11) |
| C(61)-C(62) | 1.352(10) |
| C(61)-C(66) | 1.370(9) |
| C(62)-F(1) | 1.336(9) |
| C(62)-C(63) | 1.391(10) |
| C(63)-F(2) | 1.358(10) |
| C(63)-C(64) | 1.370(11) |
| C(64)-F(3) | 1.341(10) |
| C(64)-C(65) | 1.351(11) |
| C(65)-F(4) | 1.338(9) |
| C(65)-C(66) | 1.403(10) |
| C(66)-F(5) | 1.338(9) |
| C(71)-C(72) | 1.374(10) |
| C(71)-C(76) | 1.377(11) |
| C(72)-F(6) | 1.349(10) |
| C(72)-C(73) | 1.413(12) |
| C(73)-C(74) | 1.343(12) |

| | |
|---|---|
| C(74)-C(75) | 1.344(12) |
| C(74)-F(8) | 1.356(11) |
| C(75)-F(9) | 1.355(11) |
| C(75)-C(76) | 1.413(11) |
| C(76)-F(10) | 1.343(10) |
| C(81)-C(86) | 1.377(10) |
| C(81)-C(82) | 1.379(9) |
| C(82)-F(11) | 1.352(9) |
| C(82)-C(83) | 1.383(11) |
| C(83)-F(12) | 1.320(10) |
| C(83)-C(84) | 1.389(11) |
| C(84)-F(13) | 1.365(11) |
| C(84)-C(85) | 1.394(11) |
| C(85)-F(14) | 1.331(10) |
| C(85)-C(86) | 1.389(11) |
| C(86)-F(15) | 1.350(9) |
| C(99)-O(1) | 0.95(3) |
| C(99)-O(1") | 1.71(10) |
| C(99)-C(99") | 1.99(9) |
| C(99')-O(1') | 0.93(2) |
| C(99")-O(1") | 0.95(2) |

| | |
|---|---|
| C(81)-Au(1)-C(71) | 175.8(3) |
| C(81)-Au(1)-C(61) | 88.5(3) |
| C(71)-Au(1)-C(61) | 88.5(3) |
| C(81)-Au(1)-P(1) | 91.36(18) |
| C(71)-Au(1)-P(1) | 91.56(19) |
| C(61)-Au(1)-P(1) | 179.12(19) |
| C(2)-Au(2)-P(2) | 175.7(2) |
| C(1)-P(1)-C(11) | 106.6(4) |
| C(1)-P(1)-C(21) | 105.9(4) |
| C(11)-P(1)-C(21) | 105.9(3) |
| C(1)-P(1)-Au(1) | 111.3(3) |
| C(11)-P(1)-Au(1) | 113.1(2) |
| C(21)-P(1)-Au(1) | 113.6(2) |
| C(51)-P(2)-C(41) | 104.6(4) |
| C(51)-P(2)-C(31) | 107.1(4) |
| C(41)-P(2)-C(31) | 105.0(3) |
| C(51)-P(2)-Au(2) | 115.3(3) |
| C(41)-P(2)-Au(2) | 112.7(3) |
| C(31)-P(2)-Au(2) | 111.4(2) |
| C(2)-C(1)-P(1) | 175.8(7) |
| C(1)-C(2)-Au(2) | 177.1(7) |
| C(16)-C(11)-C(12) | 119.2(8) |
| C(16)-C(11)-P(1) | 122.6(6) |
| C(12)-C(11)-P(1) | 118.1(6) |
| C(11)-C(12)-C(13) | 120.0(8) |
| C(14)-C(13)-C(12) | 120.5(8) |
| C(13)-C(14)-C(15) | 120.2(9) |
| C(14)-C(15)-C(16) | 120.0(8) |
| C(11)-C(16)-C(15) | 119.9(8) |
| C(26)-C(21)-C(22) | 119.9(7) |
| C(26)-C(21)-P(1) | 119.9(5) |
| C(22)-C(21)-P(1) | 120.0(6) |
| C(23)-C(22)-C(21) | 119.6(7) |
| C(22)-C(23)-C(24) | 120.3(8) |
| C(25)-C(24)-C(23) | 120.5(8) |
| C(24)-C(25)-C(26) | 119.8(8) |
| C(25)-C(26)-C(21) | 119.9(7) |
| C(32)-C(31)-C(36) | 118.5(8) |
| C(32)-C(31)-P(2) | 122.7(6) |
| C(36)-C(31)-P(2) | 118.8(6) |
| C(33)-C(32)-C(31) | 119.9(8) |

| | |
|---|---|
| C(35)-C(34)-C(33) | 119.1(9) |
| C(36)-C(35)-C(34) | 120.1(8) |
| C(35)-C(36)-C(31) | 121.1(8) |
| C(42)-C(41)-C(46) | 119.1(8) |
| C(42)-C(41)-P(2) | 123.2(7) |
| C(46)-C(41)-P(2) | 117.6(6) |
| C(41)-C(42)-C(43) | 121.5(10) |
| C(42)-C(43)-C(44) | 118.1(9) |
| C(45)-C(44)-C(43) | 121.9(10) |
| C(44)-C(45)-C(46) | 118.4(11) |
| C(41)-C(46)-C(45) | 121.0(10) |
| C(56)-C(51)-C(52) | 119.4(8) |
| C(56)-C(51)-P(2) | 119.2(6) |
| C(52)-C(51)-P(2) | 121.4(7) |
| C(51)-C(52)-C(53) | 120.3(9) |
| C(54)-C(53)-C(52) | 120.9(9) |
| C(53)-C(54)-C(55) | 118.4(9) |
| C(54)-C(55)-C(56) | 121.2(9) |
| C(51)-C(56)-C(55) | 119.8(8) |
| C(62)-C(61)-C(66) | 118.4(7) |
| C(62)-C(61)-Au(1) | 121.0(5) |
| C(66)-C(61)-Au(1) | 120.6(5) |
| F(1)-C(62)-C(61) | 121.3(7) |
| F(1)-C(62)-C(63) | 117.1(7) |
| C(61)-C(62)-C(63) | 121.6(8) |
| F(2)-C(63)-C(64) | 120.3(7) |
| F(2)-C(63)-C(62) | 120.5(8) |
| C(64)-C(63)-C(62) | 119.2(8) |
| F(3)-C(64)-C(65) | 120.1(8) |
| F(3)-C(64)-C(63) | 119.3(7) |
| C(65)-C(64)-C(63) | 120.6(8) |
| F(4)-C(65)-C(64) | 120.5(7) |
| F(4)-C(65)-C(66) | 120.4(8) |
| C(64)-C(65)-C(66) | 119.1(7) |
| F(5)-C(66)-C(61) | 121.0(7) |
| F(5)-C(66)-C(65) | 117.8(7) |
| C(61)-C(66)-C(65) | 121.1(7) |
| C(72)-C(71)-C(76) | 116.6(8) |
| C(72)-C(71)-Au(1) | 125.6(6) |
| C(76)-C(71)-Au(1) | 117.8(6) |
| F(6)-C(72)-C(71) | 119.8(8) |
| F(6)-C(72)-C(73) | 118.5(8) |
| C(71)-C(72)-C(73) | 121.6(9) |
| C(74)-C(73)-F(7) | 121.5(9) |
| C(74)-C(73)-C(72) | 119.6(9) |
| F(7)-C(73)-C(72) | 118.8(10) |
| C(73)-C(74)-C(75) | 121.0(9) |
| C(73)-C(74)-F(8) | 119.2(9) |
| C(75)-C(74)-F(8) | 119.8(9) |
| C(74)-C(75)-F(9) | 121.8(8) |
| C(74)-C(75)-C(76) | 119.4(9) |
| F(9)-C(75)-C(76) | 118.8(9) |
| F(10)-C(76)-C(71) | 121.1(7) |
| F(10)-C(76)-C(75) | 117.2(8) |
| C(71)-C(76)-C(75) | 121.7(9) |
| C(86)-C(81)-C(82) | 115.9(7) |
| C(86)-C(81)-Au(1) | 123.1(5) |
| C(82)-C(81)-Au(1) | 121.0(5) |
| F(11)-C(82)-C(81) | 119.6(7) |
| F(11)-C(82)-C(83) | 116.2(7) |
| C(81)-C(82)-C(83) | 124.2(8) |
| F(12)-C(83)-C(82) | 122.5(9) |
| F(12)-C(83)-C(84) | 120.0(8) |

| | |
|---|---|
| F(13)-C(84)-C(83) | 120.6(8) |
| F(13)-C(84)-C(85) | 118.2(8) |
| C(83)-C(84)-C(85) | 121.2(8) |
| F(14)-C(85)-C(86) | 122.5(8) |
| F(14)-C(85)-C(84) | 119.8(8) |
| C(86)-C(85)-C(84) | 117.7(8) |
| F(15)-C(86)-C(81) | 120.6(7) |
| F(15)-C(86)-C(85) | 115.9(7) |
| C(81)-C(86)-C(85) | 123.6(8) |
| O(1)-C(99)-O(1") | 107(8) |
| O(1)-C(99)-C(99") | 127(9) |
| O(1")-C(99)-C(99") | 28.6(17) |
| O(1")-C(99")-C(99) | 59(3) |
| C(99")-O(1")-C(99) | 92(4) |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for complex 6. The anisotropic displacement factor exponent takes the form: -2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Au(1) | 19(1) | 23(1) | 25(1) | 0(1) | -3(1) | 1(1) |
| Au(2) | 21(1) | 24(1) | 28(1) | -1(1) | 0(1) | 4(1) |
| P(1) | 18(1) | 20(1) | 29(1) | -1(1) | -4(1) | 3(1) |
| P(2) | 23(1) | 25(1) | 26(1) | -2(1) | -2(1) | 5(1) |
| C(1) | 26(4) | 23(4) | 30(4) | 1(3) | -5(3) | 2(3) |
| C(2) | 21(3) | 23(4) | 29(4) | 3(3) | 0(3) | 1(3) |
| C(11) | 26(4) | 26(4) | 26(4) | 1(3) | 0(3) | 2(3) |
| C(12) | 26(4) | 43(5) | 40(4) | 8(4) | -3(3) | -9(4) |
| C(13) | 45(5) | 54(6) | 42(5) | 6(5) | -12(4) | -5(4) |
| C(14) | 53(5) | 46(6) | 29(4) | 3(4) | 2(3) | 9(4) |
| C(15) | 36(4) | 46(6) | 40(5) | 9(4) | 15(4) | 6(4) |
| C(16) | 23(3) | 33(5) | 39(4) | 0(4) | 6(3) | 3(3) |
| C(21) | 19(3) | 21(4) | 32(4) | 1(3) | -4(3) | 2(3) |
| C(22) | 22(3) | 29(4) | 36(4) | 0(3) | 2(3) | -1(3) |
| C(23) | 31(4) | 32(4) | 40(5) | 4(4) | 1(3) | -1(3) |
| C(24) | 39(4) | 21(4) | 39(5) | 7(3) | -8(3) | -7(3) |
| C(25) | 34(4) | 23(4) | 35(4) | -5(3) | -6(3) | -2(3) |
| C(26) | 29(4) | 24(4) | 28(4) | 1(3) | -7(3) | 2(3) |
| C(31) | 26(3) | 31(4) | 26(4) | 2(3) | -5(3) | -3(3) |
| C(32) | 31(4) | 57(6) | 39(5) | 0(4) | 0(3) | 4(4) |
| C(33) | 58(5) | 61(7) | 31(4) | -7(5) | 6(4) | -7(5) |
| C(34) | 65(6) | 70(8) | 26(4) | -5(5) | -7(4) | -11(6) |
| C(35) | 38(4) | 60(7) | 42(5) | 6(5) | -9(3) | -10(4) |
| C(36) | 28(4) | 46(6) | 34(4) | 8(4) | -4(3) | -4(4) |
| C(41) | 28(4) | 42(5) | 27(4) | -11(3) | 0(3) | -2(3) |
| C(42) | 31(4) | 62(6) | 33(5) | -5(4) | -2(3) | 2(4) |
| C(43) | 28(4) | 88(7) | 53(6) | -24(5) | -9(4) | -3(5) |
| C(44) | 25(4) | 83(7) | 86(9) | -42(6) | 6(5) | -14(4) |
| C(45) | 50(6) | 52(7) | 100(10) | -12(6) | 15(6) | -14(5) |
| C(46) | 34(4) | 37(5) | 88(8) | -6(5) | 11(5) | -3(4) |
| C(51) | 30(4) | 20(4) | 38(4) | -3(3) | -12(3) | 2(3) |
| C(52) | 61(6) | 43(5) | 39(5) | -1(4) | -4(4) | 28(5) |
| C(53) | 63(7) | 34(5) | 62(6) | -5(5) | -10(5) | 19(5) |
| C(54) | 47(5) | 30(5) | 65(6) | 12(4) | -23(4) | 0(4) |
| C(55) | 28(4) | 44(5) | 55(6) | 16(4) | -6(4) | -5(4) |
| C(56) | 28(4) | 32(4) | 44(5) | 1(4) | -3(3) | 2(3) |
| C(61) | 20(3) | 29(4) | 29(4) | -4(3) | -10(3) | -2(3) |
| C(62) | 23(4) | 59(6) | 37(4) | 1(4) | -1(3) | -3(4) |
| C(63) | 21(4) | 66(7) | 53(5) | -7(5) | -4(4) | -5(4) |
| C(64) | 21(4) | 63(7) | 57(5) | -12(5) | -13(4) | -4(4) |
| C(65) | 46(5) | 35(5) | 36(4) | -4(4) | -23(3) | 6(4) |
| C(66) | 24(3) | 30(4) | 34(4) | 3(3) | -3(3) | 2(3) |
| F(1) | 42(3) | 100(5) | 30(3) | 2(3) | 12(2) | -15(3) |
| F(2) | 30(3) | 127(7) | 83(5) | 8(5) | 10(3) | -25(4) |
| F(3) | 34(3) | 96(6) | 87(5) | -1(4) | -33(3) | -6(3) |
| F(4) | 66(4) | 64(4) | 38(3) | -4(3) | -29(3) | 4(3) |
| F(5) | 39(3) | 53(3) | 24(2) | 8(2) | 3(2) | -1(2) |
| C(71) | 31(4) | 23(4) | 34(4) | 0(3) | -13(3) | -2(3) |
| C(72) | 40(5) | 37(5) | 42(5) | 4(4) | -12(4) | -5(4) |
| C(73) | 49(6) | 29(5) | 77(7) | 20(5) | -26(4) | -11(4) |
| C(74) | 40(5) | 24(5) | 107(9) | -12(4) | -26(5) | 3(4) |
| C(75) | 29(4) | 37(5) | 83(7) | -26(4) | -5(4) | 2(4) |
| C(76) | 22(4) | 34(4) | 55(5) | -8(4) | -4(3) | 0(3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| F(7) | 95(5) | 44(4) | 93(6) | 27(4) | -35(4) | -19(4) |
| F(8) | 60(4) | 25(3) | 168(8) | -16(4) | -28(5) | 11(3) |
| F(9) | 50(4) | 55(4) | 117(6) | -44(4) | 19(4) | -3(3) |
| F(10) | 47(3) | 46(3) | 43(3) | -10(3) | 5(2) | -1(3) |
| C(81) | 20(3) | 24(4) | 27(4) | 3(3) | -11(3) | 0(3) |
| C(82) | 29(4) | 35(4) | 28(4) | 4(3) | -9(3) | -5(3) |
| C(83) | 40(5) | 31(4) | 49(5) | 13(4) | -15(4) | -6(4) |
| C(84) | 49(5) | 20(4) | 62(6) | 1(4) | -20(4) | 6(4) |
| C(85) | 34(5) | 37(5) | 52(5) | -11(4) | -6(4) | 8(4) |
| C(86) | 25(4) | 31(4) | 35(4) | 3(3) | -4(3) | -3(3) |
| F(11) | 41(3) | 50(3) | 32(3) | 3(2) | 5(2) | -4(2) |
| F(12) | 75(4) | 45(4) | 57(4) | 24(3) | -21(3) | -12(3) |
| F(13) | 70(4) | 34(3) | 82(5) | -2(3) | -21(3) | 16(3) |
| F(14) | 42(3) | 46(3) | 69(4) | -16(3) | 3(3) | 14(3) |
| F(15) | 44(3) | 41(3) | 42(3) | -2(2) | 12(2) | 5(2) |
| Cl(1) | 262(11) | 246(10) | 194(8) | -41(8) | -72(8) | 101(9) |
| Cl(2) | 179(8) | 308(14) | 281(13) | 13(11) | 3(8) | 38(9) |
| Cl(3) | 500(20) | 246(13) | 440(20) | -92(15) | -169(19) | -143(15) |

Table 5. Hydrogen coordinates ( x 10^4) and isotropic displacement parameters (A^2 x 10^3) for complex 6.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(12) | 4431 | 5137 | 5830 | 44 |
| H(13) | 4493 | 4931 | 6999 | 57 |
| H(14) | 3594 | 4282 | 7546 | 51 |
| H(15) | 2606 | 3829 | 6941 | 48 |
| H(16) | 2516 | 4082 | 5777 | 38 |
| H(22) | 4375 | 5650 | 3875 | 35 |
| H(23) | 4667 | 7298 | 3618 | 41 |
| H(24) | 4188 | 8643 | 4186 | 40 |
| H(25) | 3468 | 8347 | 5055 | 37 |
| H(26) | 3186 | 6691 | 5337 | 32 |
| H(32) | 6452 | 796 | 2076 | 51 |
| H(33) | 6051 | 586 | 981 | 60 |
| H(34) | 4930 | 925 | 670 | 65 |
| H(35) | 4187 | 1395 | 1492 | 56 |
| H(36) | 4579 | 1614 | 2590 | 44 |
| H(42) | 7168 | 693 | 3805 | 50 |
| H(43) | 8248 | 1408 | 3842 | 68 |
| H(44) | 8404 | 2966 | 3312 | 78 |
| H(45) | 7502 | 3832 | 2805 | 80 |
| H(46) | 6411 | 3134 | 2834 | 63 |
| H(52) | 6348 | -541 | 2893 | 57 |
| H(53) | 6427 | -2150 | 3363 | 64 |
| H(54) | 6068 | -2452 | 4444 | 58 |
| H(55) | 5598 | -1127 | 5041 | 51 |
| H(56) | 5491 | 481 | 4565 | 42 |