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Supporting information_ X-Ray Tables

Allene-derived gold and platinum complexes: synthesis and first applications in catalysis.

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Crystal data and structure refinement for [ClAu(C8H3N-Ph-1,-C5H3N-Me-1,-Ph-3,-Me-7)], compound 2a

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^4). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor. E.s.ds are in parentheses.

	x	y	z	U(eq)
Au	4419.1(2)	5143.2(2)	6974.4(2)	140.7(4)
Cl	5814.1(6)	3999.1(6)	7770.3(5)	242.6(15)
N(1)	2042.3(18)	7351.9(19)	5174.0(17)	157(4)
C(2)	1840(2)	7388(2)	6013(2)	160(5)
C(3)	999(2)	8002(2)	6057(2)	185(5)
C(4)	374(2)	8558(3)	5240(2)	219(6)
C(5)	604(2)	8506(3)	4401(2)	212(6)
C(6)	1457(2)	7906(2)	4362(2)	194(6)
C(7)	1745(3)	7906(3)	3481(2)	244(6)
C(8)	2588(2)	6685(2)	6734.9(19)	146(5)
C(9)	3233(2)	6171(2)	6345.0(19)	152(5)
C(10)	2964(2)	6587(2)	5307.0(19)	165(5)
C(11)	2627(2)	6664(2)	7743.2(19)	160(5)
C(12)	2702(3)	7656(3)	8244(2)	239(6)
C(13)	2747(3)	7672(3)	9195(2)	270(7)
C(14)	2722(2)	6688(3)	9662(2)	234(6)
C(15)	2641(2)	5694(3)	9173(2)	229(6)
C(16)	2606(2)	5682(2)	8226(2)	195(6)
C(21)	3886(2)	7282(2)	5244(2)	186(5)
C(22)	4263(3)	7212(3)	4490(2)	247(6)
C(23)	5078(3)	7894(3)	4477(3)	302(7)
C(24)	5513(3)	8661(3)	5200(3)	327(8)
C(25)	5141(3)	8742(3)	5966(3)	310(7)
C(26)	4330(3)	8052(3)	5977(2)	235(6)
C(31)	2606(2)	5601(2)	4619.8(19)	188(5)
N(32)	1570(2)	5451(2)	4205(2)	268(6)
C(33)	1218(3)	4571(3)	3607(3)	326(7)
C(34)	1891(3)	3836(3)	3414(2)	333(8)
C(35)	2961(3)	3982(3)	3861(2)	275(7)
C(36)	3337(3)	4872(3)	4483(2)	233(6)
C(37)	58(3)	4465(4)	3174(4)	519(11)

Table 2. Molecular dimensions. Bond lengths are in Ångstroms, angles in degrees. E.s.ds are in parentheses.

Au-C(9)	1.986(3)	C(9)-Au-Cl	177.29(8)
Au-Cl	2.3031(7)		
N(1)-C(6)	1.358(3)	C(13)-C(14)	1.383(5)
N(1)-C(2)	1.367(4)	C(14)-C(15)	1.387(5)
N(1)-C(10)	1.514(4)	C(15)-C(16)	1.388(4)
C(2)-C(3)	1.385(4)	C(21)-C(22)	1.389(4)
C(2)-C(8)	1.457(4)	C(21)-C(26)	1.393(4)
C(3)-C(4)	1.380(4)	C(22)-C(23)	1.388(5)
C(4)-C(5)	1.387(4)	C(23)-C(24)	1.379(5)
C(5)-C(6)	1.388(4)	C(24)-C(25)	1.402(5)
C(6)-C(7)	1.491(4)	C(25)-C(26)	1.388(5)
C(8)-C(9)	1.360(4)	C(31)-N(32)	1.333(4)
C(8)-C(11)	1.476(4)	C(31)-C(36)	1.397(4)
C(9)-C(10)	1.532(4)	N(32)-C(33)	1.358(5)
C(10)-C(31)	1.530(4)	C(33)-C(34)	1.378(6)
C(10)-C(21)	1.541(4)	C(33)-C(37)	1.481(6)
C(11)-C(16)	1.391(4)	C(34)-C(35)	1.378(5)
C(11)-C(12)	1.395(4)	C(35)-C(36)	1.390(4)
C(12)-C(13)	1.388(4)		
C(6)-N(1)-C(2)	123.0(2)	C(16)-C(11)-C(8)	122.3(3)
C(6)-N(1)-C(10)	127.8(2)	C(12)-C(11)-C(8)	119.6(3)
C(2)-N(1)-C(10)	109.2(2)	C(13)-C(12)-C(11)	121.4(3)
N(1)-C(2)-C(3)	119.9(2)	C(14)-C(13)-C(12)	119.7(3)
N(1)-C(2)-C(8)	109.5(2)	C(13)-C(14)-C(15)	119.7(3)
C(3)-C(2)-C(8)	130.6(3)	C(14)-C(15)-C(16)	120.3(3)
C(4)-C(3)-C(2)	118.6(3)	C(15)-C(16)-C(11)	120.8(3)
C(3)-C(4)-C(5)	119.9(3)	C(22)-C(21)-C(26)	119.1(3)
C(4)-C(5)-C(6)	121.4(3)	C(22)-C(21)-C(10)	124.0(3)
N(1)-C(6)-C(5)	117.1(3)	C(26)-C(21)-C(10)	116.9(3)
N(1)-C(6)-C(7)	121.3(3)	C(23)-C(22)-C(21)	120.1(3)
C(5)-C(6)-C(7)	121.5(3)	C(24)-C(23)-C(22)	120.8(3)
C(9)-C(8)-C(2)	110.0(2)	C(23)-C(24)-C(25)	119.8(3)
C(9)-C(8)-C(11)	128.9(2)	C(26)-C(25)-C(24)	119.1(3)
C(2)-C(8)-C(11)	121.0(2)	C(25)-C(26)-C(21)	121.1(3)
C(8)-C(9)-C(10)	108.5(2)	N(32)-C(31)-C(36)	122.6(3)
C(8)-C(9)-Au	128.7(2)	N(32)-C(31)-C(10)	116.4(3)
C(10)-C(9)-Au	122.57(19)	C(36)-C(31)-C(10)	120.9(3)
N(1)-C(10)-C(31)	109.8(2)	C(31)-N(32)-C(33)	118.4(3)
N(1)-C(10)-C(9)	102.7(2)	N(32)-C(33)-C(34)	122.3(3)
C(31)-C(10)-C(9)	108.5(2)	N(32)-C(33)-C(37)	115.0(4)
N(1)-C(10)-C(21)	108.3(2)	C(34)-C(33)-C(37)	122.6(4)
C(31)-C(10)-C(21)	117.2(2)	C(35)-C(34)-C(33)	119.0(3)
C(9)-C(10)-C(21)	109.5(2)	C(34)-C(35)-C(36)	119.5(3)
C(16)-C(11)-C(12)	118.1(3)	C(35)-C(36)-C(31)	118.2(3)

Table 3. Anisotropic displacement parameters ($Å^2$ x 10^4) for the expression:

$$\exp\{-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})\}$$

E.s.ds are in parentheses.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au	159.3(5)	142.0(5)	118.2(5)	7.9(3)	46.7(4)	29.0(4)
Cl	256(4)	276(4)	187(3)	49(3)	69(3)	129(3)
N(1)	154(11)	160(11)	148(11)	14(8)	43(9)	20(8)
C(2)	175(13)	172(13)	134(12)	23(9)	55(10)	4(10)
C(3)	186(13)	192(13)	192(13)	36(10)	85(11)	26(10)
C(4)	145(13)	212(14)	289(15)	42(12)	64(11)	42(10)
C(5)	168(13)	220(14)	200(14)	55(11)	9(11)	18(11)
C(6)	212(14)	175(13)	165(13)	35(10)	29(11)	5(11)
C(7)	313(17)	242(15)	173(14)	65(11)	82(12)	65(12)
C(8)	157(12)	148(12)	122(11)	21(9)	38(10)	18(9)
C(9)	159(12)	168(13)	132(12)	-6(9)	56(10)	-9(10)
C(10)	197(13)	170(13)	147(12)	36(10)	83(11)	52(10)
C(11)	142(12)	220(14)	120(12)	12(10)	49(10)	24(10)
C(12)	350(17)	173(14)	195(14)	17(11)	100(13)	51(12)
C(13)	354(18)	279(16)	172(14)	-37(12)	90(13)	62(13)
C(14)	209(14)	371(18)	124(12)	29(11)	64(11)	79(12)
C(15)	227(14)	266(16)	197(14)	74(11)	80(12)	27(12)
C(16)	221(14)	185(14)	184(13)	12(10)	77(11)	14(11)
C(21)	198(13)	173(13)	217(14)	50(10)	110(11)	33(10)
C(22)	255(15)	275(16)	230(15)	64(12)	111(13)	58(12)
C(23)	318(18)	325(18)	362(18)	124(14)	241(15)	76(14)
C(24)	335(19)	250(17)	480(20)	92(15)	251(17)	48(14)
C(25)	337(18)	234(16)	400(19)	-7(14)	181(16)	-11(13)
C(26)	301(16)	198(14)	277(15)	23(12)	189(13)	36(12)
C(31)	281(15)	173(13)	114(12)	28(10)	76(11)	13(11)
N(32)	291(14)	256(13)	232(13)	41(11)	63(11)	11(11)
C(33)	354(19)	320(18)	255(16)	32(14)	50(14)	-58(15)
C(34)	530(20)	218(16)	209(15)	-2(12)	85(15)	-48(15)
C(35)	470(20)	198(15)	165(14)	-1(11)	122(14)	49(13)
C(36)	323(17)	216(14)	171(13)	5(11)	101(12)	44(12)
C(37)	380(20)	540(30)	540(30)	-20(20)	38(19)	-190(20)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3). All hydrogen atoms were included in idealised positions with U(iso)'s set at 1.2*U(eq) or, for the methyl group hydrogen atoms, 1.5*U(eq) of the parent carbon atoms.

	x	y	z	U(iso)
H(3)	859	8040	6627	22
H(4)	-200	8966	5251	26
H(5)	177	8882	3853	25
H(7A)	2330	8395	3577	37
H(7B)	1155	8151	2936	37
H(7C)	1937	7170	3363	37
H(12)	2722	8320	7934	29
H(13)	2795	8342	9517	32
H(14)	2758	6693	10301	28
H(15)	2610	5033	9482	27
H(16)	2569	5010	7910	23
H(22)	3970	6706	3993	30
H(23)	5334	7834	3976	36
H(24)	6052	9122	5180	39
H(25)	5433	9252	6459	37
H(26)	4079	8104	6482	28
H(34)	1628	3251	2988	40
H(35)	3428	3488	3747	33
H(36)	4056	4979	4801	28
H(37A)	-222	4351	3677	78
H(37B)	-121	3847	2739	78
H(37C)	-235	5129	2826	78

Table 5. Torsion angles, in degrees. E.s.ds are in parentheses.

C(6)-N(1)-C(2)-C(3)	0.7(4)	C(16)-C(11)-C(12)-C(13)	-0.5(5)
C(10)-N(1)-C(2)-C(3)	-177.4(3)	C(8)-C(11)-C(12)-C(13)	-179.5(3)
C(6)-N(1)-C(2)-C(8)	178.5(3)	C(11)-C(12)-C(13)-C(14)	0.2(5)
C(10)-N(1)-C(2)-C(8)	0.4(3)	C(12)-C(13)-C(14)-C(15)	-0.6(5)
N(1)-C(2)-C(3)-C(4)	0.7(4)	C(13)-C(14)-C(15)-C(16)	1.2(5)
C(8)-C(2)-C(3)-C(4)	-176.6(3)	C(14)-C(15)-C(16)-C(11)	-1.5(5)
C(2)-C(3)-C(4)-C(5)	-0.9(5)	C(12)-C(11)-C(16)-C(15)	1.1(4)
C(3)-C(4)-C(5)-C(6)	-0.2(5)	C(8)-C(11)-C(16)-C(15)	-179.8(3)
C(2)-N(1)-C(6)-C(5)	-1.7(4)	N(1)-C(10)-C(21)-C(22)	-111.3(3)
C(10)-N(1)-C(6)-C(5)	176.0(3)	C(31)-C(10)-C(21)-C(22)	13.5(4)
C(2)-N(1)-C(6)-C(7)	175.9(3)	C(9)-C(10)-C(21)-C(22)	137.5(3)
C(10)-N(1)-C(6)-C(7)	-6.4(4)	N(1)-C(10)-C(21)-C(26)	66.3(3)
C(4)-C(5)-C(6)-N(1)	1.5(4)	C(31)-C(10)-C(21)-C(26)	-169.0(3)
C(4)-C(5)-C(6)-C(7)	-176.2(3)	C(9)-C(10)-C(21)-C(26)	-44.9(3)
N(1)-C(2)-C(8)-C(9)	-2.4(3)	C(26)-C(21)-C(22)-C(23)	0.6(5)
C(3)-C(2)-C(8)-C(9)	175.1(3)	C(10)-C(21)-C(22)-C(23)	178.1(3)
N(1)-C(2)-C(8)-C(11)	173.2(2)	C(21)-C(22)-C(23)-C(24)	-1.0(5)
C(3)-C(2)-C(8)-C(11)	-9.3(5)	C(22)-C(23)-C(24)-C(25)	1.0(5)
C(2)-C(8)-C(9)-C(10)	3.3(3)	C(23)-C(24)-C(25)-C(26)	-0.5(5)
C(11)-C(8)-C(9)-C(10)	-171.8(3)	C(24)-C(25)-C(26)-C(21)	0.1(5)
C(2)-C(8)-C(9)-Au	178.6(2)	C(22)-C(21)-C(26)-C(25)	-0.2(5)
C(11)-C(8)-C(9)-Au	3.5(5)	C(10)-C(21)-C(26)-C(25)	-177.8(3)
C(6)-N(1)-C(10)-C(31)	-61.2(4)	N(1)-C(10)-C(31)-N(32)	-14.0(3)
C(2)-N(1)-C(10)-C(31)	116.7(2)	C(9)-C(10)-C(31)-N(32)	97.5(3)
C(6)-N(1)-C(10)-C(9)	-176.5(3)	C(21)-C(10)-C(31)-N(32)	-138.0(3)
C(2)-N(1)-C(10)-C(9)	1.5(3)	N(1)-C(10)-C(31)-C(36)	169.2(3)
C(6)-N(1)-C(10)-C(21)	67.8(4)	C(9)-C(10)-C(31)-C(36)	-79.3(3)
C(2)-N(1)-C(10)-C(21)	-114.3(2)	C(21)-C(10)-C(31)-C(36)	45.2(4)
C(8)-C(9)-C(10)-N(1)	-2.9(3)	C(36)-C(31)-N(32)-C(33)	-1.8(5)
Au-C(9)-C(10)-N(1)	-178.60(18)	C(10)-C(31)-N(32)-C(33)	-178.5(3)
C(8)-C(9)-C(10)-C(31)	-119.1(3)	C(31)-N(32)-C(33)-C(34)	-0.3(5)
Au-C(9)-C(10)-C(31)	65.3(3)	C(31)-N(32)-C(33)-C(37)	-179.9(3)
C(8)-C(9)-C(10)-C(21)	111.9(3)	N(32)-C(33)-C(34)-C(35)	1.7(5)
Au-C(9)-C(10)-C(21)	-63.7(3)	C(37)-C(33)-C(34)-C(35)	-178.8(4)
C(9)-C(8)-C(11)-C(16)	-55.6(4)	C(33)-C(34)-C(35)-C(36)	-0.9(5)
C(2)-C(8)-C(11)-C(16)	129.7(3)	C(34)-C(35)-C(36)-C(31)	-1.0(5)
C(9)-C(8)-C(11)-C(12)	123.4(3)	N(32)-C(31)-C(36)-C(35)	2.5(4)
C(2)-C(8)-C(11)-C(12)	-51.3(4)	C(10)-C(31)-C(36)-C(35)	179.0(3)

Table 6. Hydrogen bonds, in Ångstroms and degrees.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(3)-H(3)...Cl#1	0.93	2.96	3.692(3)	136.2
C(7)-H(7C)...N(32)	0.96	2.56	3.194(4)	123.4
C(34)-H(34)...Cl#2	0.93	2.91	3.716(4)	145.6

Symmetry transformations used to generate equivalent atoms:
#1 : ½-x, y+½, 1½-z #2 : x-½, ½-y, z-½

Crystal data and structure refinement for [$AuCl_3$(Ph-1,MePyr-1,Ph-3,7-Me-pyridoindolium)], CH_2Cl_2, compound 3a

Table 1. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters (A^2 x 10^4). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor. E.s.ds are in parentheses.

	x	y	z	U(eq)
Au	21547(2)	60742(2)	29008(2)	172.9(3)
Cl(1)	41389(6)	57632(5)	26400(3)	260.3(13)
Cl(2)	1630(6)	61823(5)	32352(4)	280.8(13)
Cl(3)	14108(7)	59504(5)	15788(3)	310.5(15)
N(1)	35007(19)	69497(13)	51945(11)	181(4)
C(2)	32290(20)	60737(16)	53217(13)	189(4)
C(3)	34100(30)	57280(18)	60619(14)	244(5)
C(4)	38630(30)	62871(19)	66643(15)	295(6)
C(5)	41390(30)	71701(19)	65182(14)	277(6)
C(6)	39710(20)	75105(17)	57684(14)	221(5)
C(7)	42970(30)	84507(18)	56051(15)	283(6)
C(8)	27890(20)	56455(16)	45902(13)	179(4)
C(9)	28090(20)	62475(15)	40186(13)	173(4)
C(10)	32580(20)	71601(15)	43340(13)	170(4)
C(11)	23470(20)	47155(15)	45275(13)	191(5)
C(12)	28300(30)	41237(17)	40135(15)	246(5)
C(13)	23720(30)	32587(18)	39350(16)	324(6)
C(14)	14150(30)	29865(18)	43542(17)	354(7)
C(15)	9380(30)	35664(19)	48671(16)	311(6)
C(16)	14120(20)	44248(17)	49567(14)	232(5)
C(21)	44780(20)	74783(17)	40477(13)	192(5)
C(22)	46220(30)	83300(19)	37632(14)	264(5)
C(23)	57540(30)	85940(20)	35218(17)	374(7)
C(24)	67350(30)	79940(30)	35539(18)	427(8)
C(25)	66060(30)	71520(20)	38444(18)	391(7)
C(26)	54840(20)	68958(19)	40938(15)	271(6)
C(31)	21450(20)	77954(15)	41658(14)	186(5)
N(32)	19070(20)	79739(14)	34052(12)	228(4)
C(35)	3810(30)	86096(19)	44670(20)	346(7)
C(36)	14130(20)	80897(17)	47168(16)	256(5)
C(33)	8900(30)	84594(18)	31668(17)	297(6)
C(34)	1130(30)	87910(18)	36910(20)	351(7)
C(37)	6300(30)	86140(20)	23167(19)	469(9)
C(51)	81620(30)	57390(20)	15623(18)	355(7)
Cl(52)	76115(8)	55702(6)	5715(5)	451(2)
Cl(53)	69351(8)	57645(9)	21330(5)	634(3)

Table 2. Molecular dimensions. Bond lengths are in Ångstroms, angles in degrees. E.s.ds are in parentheses.

Au-C(9)	2.004(2)	C(9)-Au-Cl(1)	88.94(7)
Au-Cl(1)	2.2819(7)	C(9)-Au-Cl(2)	89.13(7)
Au-Cl(2)	2.2900(7)	Cl(1)-Au-Cl(2)	171.72(2)
Au-Cl(3)	2.3502(6)	C(9)-Au-Cl(3)	176.99(7)
		Cl(1)-Au-Cl(3)	90.93(2)
		Cl(2)-Au-Cl(3)	91.42(2)
N(1)-C(6)	1.357(3)	C(13)-C(14)	1.387(4)
N(1)-C(2)	1.368(3)	C(14)-C(15)	1.383(4)
N(1)-C(10)	1.519(3)	C(15)-C(16)	1.386(4)
C(2)-C(3)	1.378(3)	C(21)-C(22)	1.383(4)
C(2)-C(8)	1.453(3)	C(21)-C(26)	1.387(4)
C(3)-C(4)	1.385(4)	C(22)-C(23)	1.390(4)
C(4)-C(5)	1.385(4)	C(23)-C(24)	1.383(5)
C(5)-C(6)	1.389(3)	C(24)-C(25)	1.371(5)
C(6)-C(7)	1.486(4)	C(25)-C(26)	1.383(4)
C(8)-C(9)	1.342(3)	C(31)-N(32)	1.342(3)
C(8)-C(11)	1.472(3)	C(31)-C(36)	1.377(3)
C(9)-C(10)	1.531(3)	N(32)-C(33)	1.342(3)
C(10)-C(21)	1.533(3)	C(35)-C(34)	1.372(5)
C(10)-C(31)	1.533(3)	C(35)-C(36)	1.387(4)
C(11)-C(16)	1.388(3)	C(33)-C(34)	1.394(4)
C(11)-C(12)	1.398(3)	C(33)-C(37)	1.488(4)
C(12)-C(13)	1.388(4)		
C(6)-N(1)-C(2)	123.0(2)	C(16)-C(11)-C(8)	120.4(2)
C(6)-N(1)-C(10)	127.0(2)	C(12)-C(11)-C(8)	120.5(2)
C(2)-N(1)-C(10)	109.92(18)	C(13)-C(12)-C(11)	120.1(3)
N(1)-C(2)-C(3)	120.0(2)	C(14)-C(13)-C(12)	120.0(3)
N(1)-C(2)-C(8)	109.7(2)	C(15)-C(14)-C(13)	120.2(3)
C(3)-C(2)-C(8)	130.2(2)	C(14)-C(15)-C(16)	119.8(3)
C(2)-C(3)-C(4)	118.5(2)	C(15)-C(16)-C(11)	120.8(2)
C(3)-C(4)-C(5)	120.3(2)	C(22)-C(21)-C(26)	118.9(2)
C(4)-C(5)-C(6)	120.9(2)	C(22)-C(21)-C(10)	122.5(2)
N(1)-C(6)-C(5)	117.3(2)	C(26)-C(21)-C(10)	118.6(2)
N(1)-C(6)-C(7)	121.6(2)	C(21)-C(22)-C(23)	120.4(3)
C(5)-C(6)-C(7)	121.1(2)	C(24)-C(23)-C(22)	119.7(3)
C(9)-C(8)-C(2)	108.5(2)	C(25)-C(24)-C(23)	120.3(3)
C(9)-C(8)-C(11)	127.8(2)	C(24)-C(25)-C(26)	119.9(3)
C(2)-C(8)-C(11)	123.6(2)	C(25)-C(26)-C(21)	120.8(3)
C(8)-C(9)-C(10)	111.5(2)	N(32)-C(31)-C(36)	123.8(2)
C(8)-C(9)-Au	126.48(18)	N(32)-C(31)-C(10)	111.7(2)
C(10)-C(9)-Au	121.63(16)	C(36)-C(31)-C(10)	124.3(2)
N(1)-C(10)-C(9)	100.30(17)	C(33)-N(32)-C(31)	118.1(2)
N(1)-C(10)-C(21)	108.79(18)	C(34)-C(35)-C(36)	119.4(3)
C(9)-C(10)-C(21)	114.24(19)	C(31)-C(36)-C(35)	117.7(3)
N(1)-C(10)-C(31)	111.19(18)	N(32)-C(33)-C(34)	121.4(3)
C(9)-C(10)-C(31)	106.08(19)	N(32)-C(33)-C(37)	116.6(3)
C(21)-C(10)-C(31)	115.25(19)	C(34)-C(33)-C(37)	122.0(3)
C(16)-C(11)-C(12)	119.1(2)	C(35)-C(34)-C(33)	119.6(3)
C(51)-Cl(53)	1.737(3)	Cl(53)-C(51)-Cl(52)	111.19(17)
C(51)-Cl(52)	1.772(3)		

Table 3. Anisotropic displacement parameters ($Å^2$ x 10^4) for the expression:

$$\exp\{-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})\}$$

E.s.ds are in parentheses.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au	207.0(5)	179.2(4)	133.5(4)	2.9(3)	23.6(3)	-35.4(4)
Cl(1)	258(3)	325(3)	209(3)	-5(2)	75(2)	30(3)
Cl(2)	206(3)	393(4)	247(3)	-32(3)	39(2)	-59(3)
Cl(3)	323(4)	447(4)	156(3)	-7(2)	-2(2)	-140(3)
N(1)	211(10)	197(10)	137(9)	11(7)	31(8)	-10(8)
C(2)	201(11)	203(11)	165(10)	20(9)	25(9)	20(9)
C(3)	313(14)	234(12)	185(11)	42(9)	35(10)	25(11)
C(4)	362(16)	359(15)	156(11)	28(10)	-4(11)	25(12)
C(5)	320(15)	333(15)	174(12)	-37(10)	3(10)	-14(12)
C(6)	221(12)	254(13)	187(11)	-45(9)	25(10)	-24(10)
C(7)	357(15)	267(14)	224(12)	-55(10)	26(11)	-100(11)
C(8)	197(12)	181(11)	161(10)	1(8)	29(9)	17(9)
C(9)	171(11)	178(11)	176(11)	-14(8)	40(9)	-1(8)
C(10)	193(11)	175(11)	140(10)	11(8)	13(9)	-2(9)
C(11)	233(12)	153(11)	182(11)	20(8)	8(9)	18(9)
C(12)	304(14)	202(12)	244(12)	5(9)	80(11)	15(10)
C(13)	467(18)	210(13)	304(14)	-55(11)	84(13)	17(12)
C(14)	520(20)	182(13)	368(16)	2(11)	72(14)	-89(12)
C(15)	398(17)	251(13)	300(14)	38(11)	117(12)	-83(12)
C(16)	273(14)	213(12)	217(12)	9(9)	56(10)	-6(10)
C(21)	169(11)	270(12)	133(10)	-2(9)	-3(9)	-36(9)
C(22)	250(13)	303(14)	228(12)	35(10)	-16(10)	-61(11)
C(23)	322(16)	467(18)	319(15)	109(13)	-27(13)	-163(14)
C(24)	211(15)	690(20)	380(17)	46(15)	28(12)	-153(15)
C(25)	186(14)	570(20)	414(17)	-3(15)	2(12)	40(13)
C(26)	220(13)	325(15)	262(13)	27(10)	-6(10)	7(11)
C(31)	175(11)	139(11)	242(12)	-3(9)	16(9)	-26(9)
N(32)	209(11)	188(10)	272(11)	7(8)	-41(9)	-15(8)
C(35)	265(15)	215(13)	580(20)	-23(13)	158(14)	-4(11)
C(36)	245(13)	191(12)	346(14)	-9(10)	93(11)	-27(10)
C(33)	237(14)	214(13)	413(16)	30(11)	-77(12)	-34(10)
C(34)	201(13)	199(14)	640(20)	47(12)	-8(13)	3(10)
C(37)	440(20)	470(19)	443(19)	74(15)	-182(16)	88(16)
C(51)	285(15)	365(16)	433(17)	68(13)	115(13)	79(13)
Cl(52)	401(4)	499(5)	464(4)	-70(4)	89(4)	-8(4)
Cl(53)	329(5)	1128(9)	473(5)	140(5)	167(4)	76(5)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3). All hydrogen atoms were included in idealised positions with U(iso)'s set at 1.2*U(eq) or, for the methyl group hydrogen atoms, 1.5*U(eq) of the parent carbon atoms.

	x	y	z	U(iso)
H(3)	3231	5133	6155	29
H(4)	3983	6069	7169	35
H(5)	4441	7540	6927	33
H(7A)	3666	8701	5233	42
H(7B)	5088	8467	5400	42
H(7C)	4346	8791	6076	42
H(12)	3459	4310	3724	30
H(13)	2706	2862	3601	39
H(14)	1094	2412	4290	42
H(15)	302	3381	5151	37
H(16)	1099	4810	5308	28
H(22)	3957	8729	3733	32
H(23)	5851	9170	3339	45
H(24)	7484	8163	3378	51
H(25)	7272	6754	3874	47
H(26)	5403	6326	4295	33
H(35)	-125	8833	4823	41
H(36)	1604	7945	5238	31
H(34)	-582	9133	3517	42
H(37A)	552	8050	2052	70
H(37B)	1303	8947	2139	70
H(37C)	-134	8943	2210	70
H(51A)	8732	5261	1738	43
H(51B)	8617	6298	1619	43

Table 5. Torsion angles, in degrees. E.s.ds are in parentheses.

C(6)-N(1)-C(2)-C(3)	1.2(4)	C(16)-C(11)-C(12)-C(13)	0.2(4)
C(10)-N(1)-C(2)-C(3)	178.4(2)	C(8)-C(11)-C(12)-C(13)	-177.4(2)
C(6)-N(1)-C(2)-C(8)	-177.8(2)	C(11)-C(12)-C(13)-C(14)	1.4(4)
C(10)-N(1)-C(2)-C(8)	-0.5(3)	C(12)-C(13)-C(14)-C(15)	-1.8(5)
N(1)-C(2)-C(3)-C(4)	0.2(4)	C(13)-C(14)-C(15)-C(16)	0.6(5)
C(8)-C(2)-C(3)-C(4)	179.0(3)	C(14)-C(15)-C(16)-C(11)	1.1(4)
C(2)-C(3)-C(4)-C(5)	-0.7(4)	C(12)-C(11)-C(16)-C(15)	-1.4(4)
C(3)-C(4)-C(5)-C(6)	-0.2(4)	C(8)-C(11)-C(16)-C(15)	176.1(2)
C(2)-N(1)-C(6)-C(5)	-2.0(4)	N(1)-C(10)-C(21)-C(22)	-116.4(2)
C(10)-N(1)-C(6)-C(5)	-178.8(2)	C(9)-C(10)-C(21)-C(22)	132.5(2)
C(2)-N(1)-C(6)-C(7)	177.8(2)	C(31)-C(10)-C(21)-C(22)	9.2(3)
C(10)-N(1)-C(6)-C(7)	1.1(4)	N(1)-C(10)-C(21)-C(26)	62.0(3)
C(4)-C(5)-C(6)-N(1)	1.5(4)	C(9)-C(10)-C(21)-C(26)	-49.1(3)
C(4)-C(5)-C(6)-C(7)	-178.4(3)	C(31)-C(10)-C(21)-C(26)	-172.3(2)
N(1)-C(2)-C(8)-C(9)	0.9(3)	C(26)-C(21)-C(22)-C(23)	0.5(4)
C(3)-C(2)-C(8)-C(9)	-177.9(3)	C(10)-C(21)-C(22)-C(23)	178.9(2)
N(1)-C(2)-C(8)-C(11)	-176.3(2)	C(21)-C(22)-C(23)-C(24)	1.1(4)
C(3)-C(2)-C(8)-C(11)	4.9(4)	C(22)-C(23)-C(24)-C(25)	-2.0(5)
C(2)-C(8)-C(9)-C(10)	-1.0(3)	C(23)-C(24)-C(25)-C(26)	1.1(5)
C(11)-C(8)-C(9)-C(10)	176.1(2)	C(24)-C(25)-C(26)-C(21)	0.6(4)
C(2)-C(8)-C(9)-Au	-173.81(17)	C(22)-C(21)-C(26)-C(25)	-1.4(4)
C(11)-C(8)-C(9)-Au	3.2(4)	C(10)-C(21)-C(26)-C(25)	-179.9(2)
C(6)-N(1)-C(10)-C(9)	177.1(2)	N(1)-C(10)-C(31)-N(32)	-178.91(19)
C(2)-N(1)-C(10)-C(9)	0.0(2)	C(9)-C(10)-C(31)-N(32)	-70.8(2)
C(6)-N(1)-C(10)-C(21)	56.9(3)	C(21)-C(10)-C(31)-N(32)	56.7(3)
C(2)-N(1)-C(10)-C(21)	-120.2(2)	N(1)-C(10)-C(31)-C(36)	-3.9(3)
C(6)-N(1)-C(10)-C(31)	-71.0(3)	C(9)-C(10)-C(31)-C(36)	104.2(3)
C(2)-N(1)-C(10)-C(31)	111.8(2)	C(21)-C(10)-C(31)-C(36)	-128.3(2)
C(8)-C(9)-C(10)-N(1)	0.6(3)	C(36)-C(31)-N(32)-C(33)	-0.7(4)
Au-C(9)-C(10)-N(1)	173.87(15)	C(10)-C(31)-N(32)-C(33)	174.3(2)
C(8)-C(9)-C(10)-C(21)	116.8(2)	N(32)-C(31)-C(36)-C(35)	-0.8(4)
Au-C(9)-C(10)-C(21)	-70.0(2)	C(10)-C(31)-C(36)-C(35)	-175.2(2)
C(8)-C(9)-C(10)-C(31)	-115.2(2)	C(34)-C(35)-C(36)-C(31)	1.6(4)
Au-C(9)-C(10)-C(31)	58.1(2)	C(31)-N(32)-C(33)-C(34)	1.6(4)
C(9)-C(8)-C(11)-C(16)	-122.8(3)	C(31)-N(32)-C(33)-C(37)	-177.7(2)
C(2)-C(8)-C(11)-C(16)	53.9(3)	C(36)-C(35)-C(34)-C(33)	-0.8(4)
C(9)-C(8)-C(11)-C(12)	54.8(4)	N(32)-C(33)-C(34)-C(35)	-0.9(4)
C(2)-C(8)-C(11)-C(12)	-128.6(3)	C(37)-C(33)-C(34)-C(35)	178.4(3)

Crystal data and structure refinement for [$Cl_2Pt\{6\text{-}Me\text{-}Pyr\text{-}C_9H_4\text{-}(^tBu)\text{-}Pyr\text{-}Me\}].CHCl_3$, compound 5

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^4). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor. E.s.ds are in parentheses.

	x	y	z	U(eq)
Pt	2479.7(2)	6864.9(2)	2777.6(2)	200.9(8)
Cl(2)	2195.8(14)	7613.8(13)	4579.3(10)	269(3)
Cl(3)	755.2(16)	8006.5(15)	2433.2(11)	332(3)
C(1)	4159(6)	3806(5)	2309(4)	225(9)
C(2)	5249(5)	4561(4)	3137(4)	204(9)
C(3)	6385(6)	4118(5)	3484(4)	258(10)
C(4)	6481(6)	2952(5)	2979(4)	285(11)
C(5)	5459(7)	2245(5)	2133(4)	282(11)
C(6)	4298(7)	2663(5)	1798(4)	277(11)
C(8)	4912(6)	5752(4)	3502(4)	196(9)
C(9)	3617(6)	5728(5)	2995(4)	207(9)
C(10)	2975(5)	4489(4)	2192(4)	197(9)
C(11)	6001(5)	6815(5)	4145(4)	216(9)
N(12)	5519(5)	7699(4)	4849(3)	207(8)
C(13)	6390(6)	8750(5)	5448(4)	242(10)
C(14)	7895(6)	8959(5)	5367(4)	256(10)
C(15)	8455(6)	8097(6)	4666(4)	280(11)
C(16)	7514(6)	7023(5)	4064(4)	265(10)
C(17)	5681(6)	9628(5)	6171(4)	285(11)
C(21)	1390(6)	3821(5)	2444(4)	263(10)
C(22)	1438(7)	3893(7)	3641(5)	388(15)
C(23)	972(8)	2486(6)	1791(6)	422(16)
C(24)	141(6)	4361(6)	2157(6)	364(13)
C(31)	2916(5)	4823(5)	1143(4)	209(9)
N(32)	2755(4)	5969(4)	1232(3)	180(8)
C(33)	2784(5)	6365(5)	348(4)	229(9)
C(34)	2927(6)	5618(5)	-655(4)	263(10)
C(35)	3046(7)	4453(6)	-756(4)	300(12)
C(36)	3047(6)	4045(5)	155(4)	274(10)
C(37)	2725(7)	7633(5)	435(5)	308(11)
C(41)	2147(7)	10825(5)	7965(5)	308(11)
Cl(42)	1608.7(17)	9562.8(13)	6835.7(11)	334(3)
Cl(43)	3929.9(17)	11663.0(14)	7851.7(14)	384(3)
Cl(44)	2135(3)	10360.3(18)	9149.2(14)	553(5)

Table 2. Molecular dimensions. Bond lengths are in Ångstroms, angles in degrees. E.s.ds are in parentheses.

Pt-C(9)	1.963(5)	C(9)-Pt-N(32)	77.41(18)
Pt-N(32)	2.056(4)	C(9)-Pt-Cl(2)	95.02(14)
Pt-Cl(2)	2.3138(12)	N(32)-Pt-Cl(2)	171.48(12)
Pt-Cl(3)	2.4247(13)	C(9)-Pt-Cl(3)	171.26(15)
		N(32)-Pt-Cl(3)	100.37(12)
		Cl(2)-Pt-Cl(3)	86.53(5)
C(1)-C(6)	1.378(8)	N(12)-H(12)	0.80(9)
C(1)-C(2)	1.419(7)	C(13)-C(14)	1.382(8)
C(1)-C(10)	1.534(7)	C(13)-C(17)	1.490(8)
C(2)-C(3)	1.397(7)	C(14)-C(15)	1.382(8)
C(2)-C(8)	1.472(7)	C(15)-C(16)	1.393(8)
C(3)-C(4)	1.388(8)	C(21)-C(24)	1.531(8)
C(4)-C(5)	1.385(8)	C(21)-C(22)	1.532(8)
C(5)-C(6)	1.392(8)	C(21)-C(23)	1.540(9)
C(8)-C(9)	1.351(7)	C(31)-N(32)	1.376(7)
C(8)-C(11)	1.464(7)	C(31)-C(36)	1.393(7)
C(9)-C(10)	1.538(7)	N(32)-C(33)	1.349(6)
C(10)-C(31)	1.519(6)	C(33)-C(34)	1.394(7)
C(10)-C(21)	1.601(7)	C(33)-C(37)	1.492(8)
C(11)-N(12)	1.362(6)	C(34)-C(35)	1.382(9)
C(11)-C(16)	1.389(7)	C(35)-C(36)	1.391(7)
N(12)-C(13)	1.349(7)		
C(6)-C(1)-C(2)	119.2(5)	C(13)-N(12)-H(12)	117(6)
C(6)-C(1)-C(10)	132.5(5)	C(11)-N(12)-H(12)	118(6)
C(2)-C(1)-C(10)	108.3(4)	N(12)-C(13)-C(14)	118.5(5)
C(3)-C(2)-C(1)	120.3(5)	N(12)-C(13)-C(17)	118.3(5)
C(3)-C(2)-C(8)	130.8(5)	C(14)-C(13)-C(17)	123.2(5)
C(1)-C(2)-C(8)	108.9(4)	C(13)-C(14)-C(15)	119.2(5)
C(4)-C(3)-C(2)	119.5(5)	C(14)-C(15)-C(16)	120.3(5)
C(5)-C(4)-C(3)	119.7(5)	C(11)-C(16)-C(15)	120.5(5)
C(4)-C(5)-C(6)	121.3(5)	C(24)-C(21)-C(22)	109.2(5)
C(1)-C(6)-C(5)	119.8(5)	C(24)-C(21)-C(23)	105.8(5)
C(9)-C(8)-C(11)	127.1(5)	C(22)-C(21)-C(23)	108.6(5)
C(9)-C(8)-C(2)	109.6(4)	C(24)-C(21)-C(10)	113.1(5)
C(11)-C(8)-C(2)	122.2(4)	C(22)-C(21)-C(10)	108.8(4)
C(8)-C(9)-C(10)	110.9(4)	C(23)-C(21)-C(10)	111.3(5)
C(8)-C(9)-Pt	138.7(4)	N(32)-C(31)-C(36)	121.5(4)
C(10)-C(9)-Pt	109.2(3)	N(32)-C(31)-C(10)	115.4(4)
C(31)-C(10)-C(1)	114.5(4)	C(36)-C(31)-C(10)	123.0(5)
C(31)-C(10)-C(9)	101.3(4)	C(33)-N(32)-C(31)	119.3(4)
C(1)-C(10)-C(9)	102.1(4)	C(33)-N(32)-Pt	128.4(4)
C(31)-C(10)-C(21)	112.5(4)	C(31)-N(32)-Pt	112.4(3)
C(1)-C(10)-C(21)	111.8(4)	N(32)-C(33)-C(34)	120.9(5)
C(9)-C(10)-C(21)	113.8(4)	N(32)-C(33)-C(37)	120.4(5)
N(12)-C(11)-C(16)	116.4(5)	C(34)-C(33)-C(37)	118.6(5)
N(12)-C(11)-C(8)	118.9(4)	C(35)-C(34)-C(33)	120.1(5)
C(16)-C(11)-C(8)	124.7(5)	C(34)-C(35)-C(36)	119.3(5)
C(13)-N(12)-C(11)	125.1(5)	C(35)-C(36)-C(31)	118.8(5)
C(41)-Cl(42)	1.761(6)	Cl(42)-C(41)-Cl(44)	110.1(3)
C(41)-Cl(44)	1.765(6)	Cl(42)-C(41)-Cl(43)	109.7(3)
C(41)-Cl(43)	1.769(6)	Cl(44)-C(41)-Cl(43)	110.3(3)

Table 3. Anisotropic displacement parameters ($Å^2$ x 10^4) for the expression:

$$\exp\{-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})\}$$

E.s.ds are in parentheses.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pt	208.0(12)	273.1(13)	123.2(11)	48.1(8)	-11.0(7)	72.6(8)
Cl(2)	255(6)	401(7)	144(5)	22(5)	6(4)	130(5)
Cl(3)	358(7)	467(8)	234(6)	93(5)	7(5)	234(6)
C(1)	270(20)	280(20)	140(20)	80(18)	8(17)	68(19)
C(2)	250(20)	240(20)	130(20)	63(17)	-3(16)	70(17)
C(3)	300(30)	350(30)	160(20)	102(19)	-1(18)	120(20)
C(4)	370(30)	330(30)	240(30)	150(20)	70(20)	180(20)
C(5)	400(30)	290(30)	200(20)	80(20)	60(20)	150(20)
C(6)	410(30)	240(20)	200(20)	97(19)	-10(20)	60(20)
C(8)	280(20)	240(20)	79(19)	57(16)	-24(16)	79(18)
C(9)	260(20)	270(20)	79(19)	16(16)	36(16)	64(18)
C(10)	230(20)	240(20)	130(20)	68(16)	-13(16)	35(17)
C(11)	240(20)	310(30)	100(20)	72(17)	4(16)	68(18)
N(12)	175(19)	270(20)	159(19)	57(15)	-13(14)	34(15)
C(13)	280(20)	280(20)	160(20)	90(18)	-3(18)	27(19)
C(14)	270(20)	290(30)	180(20)	54(19)	-28(18)	18(19)
C(15)	220(20)	420(30)	200(20)	110(20)	-23(18)	60(20)
C(16)	240(20)	400(30)	180(20)	110(20)	25(18)	70(20)
C(17)	350(30)	270(30)	210(20)	40(19)	0(20)	50(20)
C(21)	250(20)	350(30)	190(20)	110(20)	-2(18)	20(20)
C(22)	330(30)	640(40)	230(30)	240(30)	50(20)	30(30)
C(23)	410(30)	350(30)	400(40)	50(30)	0(30)	-60(30)
C(24)	220(30)	480(40)	410(30)	210(30)	0(20)	20(20)
C(31)	240(20)	250(20)	140(20)	74(17)	-9(16)	54(17)
N(32)	160(18)	200(18)	149(18)	1(14)	-4(14)	38(14)
C(33)	220(20)	330(30)	130(20)	88(18)	-2(16)	49(18)
C(34)	280(30)	390(30)	130(20)	90(20)	2(18)	90(20)
C(35)	420(30)	360(30)	110(20)	40(20)	0(20)	100(20)
C(36)	390(30)	290(30)	140(20)	42(18)	-29(19)	110(20)
C(37)	400(30)	330(30)	250(30)	140(20)	40(20)	130(20)
C(41)	340(30)	320(30)	240(30)	30(20)	-20(20)	100(20)
Cl(42)	392(7)	334(7)	225(6)	17(5)	-61(5)	67(5)
Cl(43)	331(7)	347(7)	431(9)	57(6)	-20(6)	67(5)
Cl(44)	829(14)	489(10)	222(8)	54(7)	-37(8)	-25(9)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3). The pyridinium hydrogen atom was located in a difference map and was refined freely. The remaining hydrogen atoms were included in idealised positions with U(iso)'s set at 1.2*U(eq) or, for the methyl group hydrogen atoms, 1.5*U(eq) of the parent carbon atoms.

	x	y	z	U(iso)
H(3)	7072	4602	4049	31
H(4)	7229	2647	3209	34
H(5)	5549	1475	1781	34
H(6)	3618	2173	1232	33
H(14)	8524	9670	5779	31
H(15)	9464	8235	4597	34
H(16)	7901	6442	3605	32
H(17A)	5783	9566	6891	43
H(17B)	4652	9453	5932	43
H(17C)	6151	10429	6156	43
H(22A)	2220	3556	3825	58
H(22B)	1612	4720	4057	58
H(22C)	513	3450	3792	58
H(23A)	1723	2099	1941	63
H(23B)	45	2098	1988	63
H(23C)	889	2428	1039	63
H(24A)	106	4317	1407	55
H(24B)	-783	3917	2310	55
H(24C)	316	5187	2575	55
H(34)	2942	5903	-1257	32
H(35)	3126	3948	-1426	36
H(36)	3133	3267	104	33
H(37A)	3137	8137	1135	46
H(37B)	1717	7671	325	46
H(37C)	3283	7906	-100	46
H(12)	4660(100)	7590(80)	4920(70)	50(20)
H(41)	1446	11335	7996	37

Table 5. Torsion angles, in degrees. E.s.ds are in parentheses.

C(6)-C(1)-C(2)-C(3)	-4.8(8)	C(11)-N(12)-C(13)-C(14)	-1.1(8)
C(10)-C(1)-C(2)-C(3)	173.7(5)	C(11)-N(12)-C(13)-C(17)	179.3(5)
C(6)-C(1)-C(2)-C(8)	176.2(5)	N(12)-C(13)-C(14)-C(15)	1.0(8)
C(10)-C(1)-C(2)-C(8)	-5.3(5)	C(17)-C(13)-C(14)-C(15)	-179.4(5)
C(1)-C(2)-C(3)-C(4)	3.0(8)	C(13)-C(14)-C(15)-C(16)	-1.1(8)
C(8)-C(2)-C(3)-C(4)	-178.3(5)	N(12)-C(11)-C(16)-C(15)	-1.2(8)
C(2)-C(3)-C(4)-C(5)	0.5(8)	C(8)-C(11)-C(16)-C(15)	176.2(5)
C(3)-C(4)-C(5)-C(6)	-2.3(9)	C(14)-C(15)-C(16)-C(11)	1.3(8)
C(2)-C(1)-C(6)-C(5)	3.1(8)	C(31)-C(10)-C(21)-C(24)	-40.0(6)
C(10)-C(1)-C(6)-C(5)	-175.1(5)	C(1)-C(10)-C(21)-C(24)	-170.5(5)
C(4)-C(5)-C(6)-C(1)	0.5(9)	C(9)-C(10)-C(21)-C(24)	74.5(6)
C(3)-C(2)-C(8)-C(9)	-174.2(5)	C(31)-C(10)-C(21)-C(22)	-161.4(5)
C(1)-C(2)-C(8)-C(9)	4.6(6)	C(1)-C(10)-C(21)-C(22)	68.1(6)
C(3)-C(2)-C(8)-C(11)	16.9(8)	C(9)-C(10)-C(21)-C(22)	-46.9(6)
C(1)-C(2)-C(8)-C(11)	-164.3(4)	C(31)-C(10)-C(21)-C(23)	79.0(6)
C(11)-C(8)-C(9)-C(10)	166.2(5)	C(1)-C(10)-C(21)-C(23)	-51.6(6)
C(2)-C(8)-C(9)-C(10)	-1.9(6)	C(9)-C(10)-C(21)-C(23)	-166.5(5)
C(11)-C(8)-C(9)-Pt	0.7(9)	C(1)-C(10)-C(31)-N(32)	-137.0(5)
C(2)-C(8)-C(9)-Pt	-167.4(4)	C(9)-C(10)-C(31)-N(32)	-28.0(5)
C(6)-C(1)-C(10)-C(31)	-69.3(7)	C(21)-C(10)-C(31)-N(32)	93.8(5)
C(2)-C(1)-C(10)-C(31)	112.5(5)	C(1)-C(10)-C(31)-C(36)	41.6(7)
C(6)-C(1)-C(10)-C(9)	-177.8(6)	C(9)-C(10)-C(31)-C(36)	150.6(5)
C(2)-C(1)-C(10)-C(9)	4.0(5)	C(21)-C(10)-C(31)-C(36)	-87.5(6)
C(6)-C(1)-C(10)-C(21)	60.2(7)	C(36)-C(31)-N(32)-C(33)	-2.7(7)
C(2)-C(1)-C(10)-C(21)	-118.0(5)	C(10)-C(31)-N(32)-C(33)	175.9(4)
C(8)-C(9)-C(10)-C(31)	-119.6(4)	C(36)-C(31)-N(32)-Pt	177.0(4)
Pt-C(9)-C(10)-C(31)	50.3(4)	C(10)-C(31)-N(32)-Pt	-4.4(5)
C(8)-C(9)-C(10)-C(1)	-1.2(5)	C(31)-N(32)-C(33)-C(34)	2.1(7)
Pt-C(9)-C(10)-C(1)	168.7(3)	Pt-N(32)-C(33)-C(34)	-177.6(4)
C(8)-C(9)-C(10)-C(21)	119.4(5)	C(31)-N(32)-C(33)-C(37)	-175.4(5)
Pt-C(9)-C(10)-C(21)	-70.6(4)	Pt-N(32)-C(33)-C(37)	5.0(7)
C(9)-C(8)-C(11)-N(12)	43.0(7)	N(32)-C(33)-C(34)-C(35)	-0.2(8)
C(2)-C(8)-C(11)-N(12)	-150.2(5)	C(37)-C(33)-C(34)-C(35)	177.3(5)
C(9)-C(8)-C(11)-C(16)	-134.3(6)	C(33)-C(34)-C(35)-C(36)	-1.1(9)
C(2)-C(8)-C(11)-C(16)	32.5(7)	C(34)-C(35)-C(36)-C(31)	0.4(9)
C(16)-C(11)-N(12)-C(13)	1.2(7)	N(32)-C(31)-C(36)-C(35)	1.5(8)
C(8)-C(11)-N(12)-C(13)	-176.4(5)	C(10)-C(31)-C(36)-C(35)	-177.1(5)

Table 6. Hydrogen bonds, in Ångstroms and degrees.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(17)-H(17B)...Cl(2)	0.96	2.94	3.755(6)	144.1
C(17)-H(17C)...Cl(2)#1	0.96	2.89	3.808(6)	160.6
C(41)-H(41)...Cl(3)#2	0.98	2.45	3.391(6)	159.9
N(12)-H(12)...Cl(2)	0.80(9)	2.33(9)	3.086(5)	158(8)

Symmetry transformations used to generate equivalent atoms:
#1 : 1-x, 2-y, 1-z #2 : -x, 2-y, 1-z

Crystal data and structure refinement for
[$AuCl_3$(C_8H_3N-Ph-1,-C_5H_3N-Me-1,-^{t}Bu-3,-Me-7)], compound 3b''

Table 1. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$ x 10^4). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor. E.s.ds are in parentheses.

	x	y	z	U(eq)
Au	34621(2)	63048(2)	84161(2)	113.5(2)
Cl(1)	20662(5)	54177(2)	75592(4)	184.2(9)
Cl(2)	49232(6)	71764(3)	92743(4)	210.0(10)
Cl(3)	18832(6)	64316(3)	93997(4)	221.4(10)
N(1)	59280(19)	65544(9)	63855(12)	150(3)
C(2)	69870(20)	62452(10)	71596(15)	164(4)
C(3)	84530(20)	62378(12)	71475(17)	214(4)
C(4)	87790(30)	65316(13)	63428(18)	249(5)
C(5)	76520(30)	68029(12)	55458(18)	251(5)
C(6)	61940(30)	68091(11)	55540(16)	196(4)
C(7)	49330(30)	70685(12)	46922(16)	247(5)
C(8)	63050(20)	60005(11)	79023(14)	154(4)
C(9)	48900(20)	62349(9)	76195(14)	130(3)
C(10)	44730(20)	65860(10)	65978(14)	131(3)
C(11)	71350(20)	55602(13)	87912(16)	225(4)
C(12)	78350(30)	49500(15)	84160(20)	363(6)
C(13)	83240(30)	59825(18)	95546(19)	389(7)
C(14)	60960(30)	52669(14)	93339(19)	294(5)
C(21)	33300(20)	61508(10)	58053(14)	140(3)
C(22)	19390(20)	63854(11)	52381(15)	188(4)
C(23)	9590(20)	59577(13)	45533(16)	242(5)
C(24)	13600(30)	52998(13)	44130(18)	263(5)
C(25)	27690(30)	50688(12)	49669(18)	257(5)
C(26)	37410(20)	54894(11)	56626(17)	203(4)
C(31)	40590(20)	73277(10)	67294(15)	172(4)
N(32)	27130(20)	74065(9)	68351(13)	189(3)
C(33)	22880(30)	80322(12)	70182(16)	235(4)
C(34)	32140(30)	85892(12)	71126(18)	290(5)
C(35)	46140(30)	85039(12)	70284(19)	302(5)
C(36)	50660(30)	78588(11)	68318(17)	241(4)
C(37)	7460(30)	80942(14)	71110(20)	334(6)

Table 2. Molecular dimensions. Bond lengths are in Ångstroms, angles in degrees. E.s.ds are in parentheses.

Au-C(9)	2.013(2)	Au-Cl(2)	2.2962(5)
Au-Cl(1)	2.2923(5)	Au-Cl(3)	2.3461(5)
C(9)-Au-Cl(1)	91.84(5)	C(9)-Au-Cl(3)	176.85(6)
C(9)-Au-Cl(2)	86.84(5)	Cl(1)-Au-Cl(3)	91.293(19)
Cl(1)-Au-Cl(2)	178.296(19)	Cl(2)-Au-Cl(3)	90.021(19)
N(1)-C(6)	1.366(3)	C(11)-C(14)	1.535(3)
N(1)-C(2)	1.370(3)	C(11)-C(12)	1.544(4)
N(1)-C(10)	1.499(3)	C(21)-C(22)	1.387(3)
C(2)-C(3)	1.392(3)	C(21)-C(26)	1.393(3)
C(2)-C(8)	1.471(3)	C(22)-C(23)	1.392(3)
C(3)-C(4)	1.389(3)	C(23)-C(24)	1.383(3)
C(4)-C(5)	1.389(4)	C(24)-C(25)	1.393(3)
C(5)-C(6)	1.384(3)	C(25)-C(26)	1.388(3)
C(6)-C(7)	1.499(3)	C(31)-N(32)	1.337(3)
C(8)-C(9)	1.352(3)	C(31)-C(36)	1.392(3)
C(8)-C(11)	1.522(3)	N(32)-C(33)	1.347(3)
C(9)-C(10)	1.531(3)	C(33)-C(34)	1.384(4)
C(10)-C(31)	1.540(3)	C(33)-C(37)	1.510(4)
C(10)-C(21)	1.546(3)	C(34)-C(35)	1.377(4)
C(11)-C(13)	1.534(4)	C(35)-C(36)	1.396(3)
C(6)-N(1)-C(2)	123.93(18)	C(8)-C(11)-C(13)	110.0(2)
C(6)-N(1)-C(10)	125.61(18)	C(8)-C(11)-C(14)	112.12(17)
C(2)-N(1)-C(10)	110.44(16)	C(13)-C(11)-C(14)	107.5(2)
N(1)-C(2)-C(3)	118.58(19)	C(8)-C(11)-C(12)	109.25(18)
N(1)-C(2)-C(8)	109.56(17)	C(13)-C(11)-C(12)	111.3(2)
C(3)-C(2)-C(8)	131.8(2)	C(14)-C(11)-C(12)	106.7(2)
C(4)-C(3)-C(2)	118.8(2)	C(22)-C(21)-C(26)	119.13(19)
C(5)-C(4)-C(3)	120.5(2)	C(22)-C(21)-C(10)	123.55(18)
C(6)-C(5)-C(4)	120.8(2)	C(26)-C(21)-C(10)	117.31(17)
N(1)-C(6)-C(5)	117.1(2)	C(21)-C(22)-C(23)	120.1(2)
N(1)-C(6)-C(7)	120.3(2)	C(24)-C(23)-C(22)	120.9(2)
C(5)-C(6)-C(7)	122.6(2)	C(23)-C(24)-C(25)	119.0(2)
C(9)-C(8)-C(2)	107.09(18)	C(26)-C(25)-C(24)	120.4(2)
C(9)-C(8)-C(11)	130.15(18)	C(25)-C(26)-C(21)	120.5(2)
C(2)-C(8)-C(11)	122.75(18)	N(32)-C(31)-C(36)	123.1(2)
C(8)-C(9)-C(10)	111.75(17)	N(32)-C(31)-C(10)	114.28(17)
C(8)-C(9)-Au	129.44(15)	C(36)-C(31)-C(10)	122.3(2)
C(10)-C(9)-Au	118.09(13)	C(31)-N(32)-C(33)	118.7(2)
N(1)-C(10)-C(9)	100.69(15)	N(32)-C(33)-C(34)	121.8(2)
N(1)-C(10)-C(31)	110.36(16)	N(32)-C(33)-C(37)	116.4(2)
C(9)-C(10)-C(31)	108.47(15)	C(34)-C(33)-C(37)	121.8(2)
N(1)-C(10)-C(21)	108.19(15)	C(35)-C(34)-C(33)	119.5(2)
C(9)-C(10)-C(21)	109.99(15)	C(34)-C(35)-C(36)	119.4(2)
C(31)-C(10)-C(21)	117.78(16)	C(31)-C(36)-C(35)	117.6(20

Table 3. Anisotropic displacement parameters ($Å^2$ x 10^4) for the expression:

$$\exp\{-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})\}$$

E.s.ds are in parentheses.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au	100.3(4)	116.6(4)	126.0(4)	9.7(2)	39.1(2)	-4.2(2)
Cl(1)	151(2)	144(2)	256(2)	-32(2)	61(2)	-55(2)
Cl(2)	235(2)	232(2)	177(2)	-88(2)	85(2)	-97(2)
Cl(3)	195(2)	256(3)	267(3)	9(2)	150(2)	23(2)
N(1)	173(8)	155(8)	135(7)	-16(6)	69(6)	-41(6)
C(2)	153(9)	195(10)	152(9)	-21(7)	58(7)	-42(7)
C(3)	163(10)	280(12)	223(10)	-34(8)	95(8)	-36(8)
C(4)	231(11)	275(11)	310(12)	-74(9)	184(9)	-77(9)
C(5)	350(13)	232(11)	246(11)	-18(9)	200(10)	-83(9)
C(6)	296(11)	156(9)	171(9)	-20(7)	122(8)	-64(8)
C(7)	359(13)	237(11)	162(10)	39(8)	105(9)	-44(9)
C(8)	133(8)	206(10)	129(8)	-4(7)	50(7)	-18(7)
C(9)	128(8)	127(9)	128(8)	1(6)	32(7)	-28(6)
C(10)	152(9)	127(8)	117(8)	1(7)	47(7)	-12(7)
C(11)	124(9)	374(13)	184(10)	98(9)	57(7)	71(8)
C(12)	344(14)	437(16)	364(14)	195(12)	190(11)	211(12)
C(13)	165(11)	790(20)	188(11)	8(12)	17(9)	-38(12)
C(14)	193(10)	434(15)	287(12)	227(11)	121(9)	135(10)
C(21)	150(9)	143(9)	119(8)	-14(7)	32(7)	-7(7)
C(22)	205(10)	202(10)	139(9)	11(7)	24(7)	54(8)
C(23)	177(10)	334(13)	170(10)	-42(9)	-8(8)	30(9)
C(24)	207(11)	312(12)	237(11)	-116(9)	20(9)	-45(9)
C(25)	246(11)	193(11)	307(12)	-106(9)	50(9)	-4(8)
C(26)	154(9)	186(10)	239(10)	-35(8)	18(8)	8(7)
C(31)	267(10)	130(9)	114(8)	0(7)	53(7)	-8(7)
N(32)	263(9)	163(8)	137(8)	11(6)	60(7)	38(7)
C(33)	348(12)	208(10)	135(9)	-5(8)	55(8)	79(9)
C(34)	523(16)	156(10)	199(11)	-21(8)	123(10)	29(10)
C(35)	530(16)	155(10)	248(11)	-21(9)	160(11)	-101(10)
C(36)	341(12)	186(10)	209(10)	-18(8)	105(9)	-64(9)
C(37)	407(15)	286(13)	324(13)	-53(10)	135(11)	125(11)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3). All hydrogen atoms were included in idealised positions with U(iso)'s set at 1.2*U(eq) or, for the methyl group hydrogen atoms, 1.5*U(eq) of the parent carbon atoms.

	x	y	z	U(iso)
H(3)	9201	6040	7669	26
H(4)	9758	6547	6338	30
H(5)	7881	6983	5000	30
H(7A)	4372	6692	4329	37
H(7B)	5322	7330	4255	37
H(7C)	4297	7349	4940	37
H(12A)	8360	4671	8975	55
H(12B)	7064	4688	7955	55
H(12C)	8515	5111	8084	55
H(13A)	8843	5701	10112	58
H(13B)	9018	6158	9244	58
H(13C)	7857	6352	9785	58
H(14A)	6662	4993	9888	44
H(14B)	5629	5631	9577	44
H(14C)	5347	4993	8877	44
H(22)	1660	6829	5316	23
H(23)	21	6117	4185	29
H(24)	699	5016	3956	32
H(25)	3060	4630	4870	31
H(26)	4674	5328	6036	24
H(34)	2892	9017	7232	35
H(35)	5253	8873	7102	36
H(36)	6005	7787	6771	29
H(37A)	23	8086	6456	50
H(37B)	667	8514	7437	50
H(37C)	569	7722	7499	50

Table 5. Torsion angles, in degrees. E.s.ds are in parentheses.

C(6)-N(1)-C(2)-C(3)	5.7(3)	C(2)-C(8)-C(11)-C(13)	71.2(3)
C(10)-N(1)-C(2)-C(3)	-172.88(18)	C(9)-C(8)-C(11)-C(14)	9.9(3)
C(6)-N(1)-C(2)-C(8)	-176.99(18)	C(2)-C(8)-C(11)-C(14)	-169.3(2)
C(10)-N(1)-C(2)-C(8)	4.4(2)	C(9)-C(8)-C(11)-C(12)	128.0(2)
N(1)-C(2)-C(3)-C(4)	-1.3(3)	C(2)-C(8)-C(11)-C(12)	-51.3(3)
C(8)-C(2)-C(3)-C(4)	-177.9(2)	N(1)-C(10)-C(21)-C(22)	-128.4(2)
C(2)-C(3)-C(4)-C(5)	-2.6(3)	C(9)-C(10)-C(21)-C(22)	122.4(2)
C(3)-C(4)-C(5)-C(6)	2.4(4)	C(31)-C(10)-C(21)-C(22)	-2.5(3)
C(2)-N(1)-C(6)-C(5)	-5.8(3)	N(1)-C(10)-C(21)-C(26)	51.4(2)
C(10)-N(1)-C(6)-C(5)	172.54(19)	C(9)-C(10)-C(21)-C(26)	-57.7(2)
C(2)-N(1)-C(6)-C(7)	173.10(19)	C(31)-C(10)-C(21)-C(26)	177.36(18)
C(10)-N(1)-C(6)-C(7)	-8.6(3)	C(26)-C(21)-C(22)-C(23)	1.5(3)
C(4)-C(5)-C(6)-N(1)	1.6(3)	C(10)-C(21)-C(22)-C(23)	-178.67(19)
C(4)-C(5)-C(6)-C(7)	-177.3(2)	C(21)-C(22)-C(23)-C(24)	-1.2(4)
N(1)-C(2)-C(8)-C(9)	-6.9(2)	C(22)-C(23)-C(24)-C(25)	-0.2(4)
C(3)-C(2)-C(8)-C(9)	169.9(2)	C(23)-C(24)-C(25)-C(26)	1.3(4)
N(1)-C(2)-C(8)-C(11)	172.49(19)	C(24)-C(25)-C(26)-C(21)	-1.0(4)
C(3)-C(2)-C(8)-C(11)	-10.7(4)	C(22)-C(21)-C(26)-C(25)	-0.4(3)
C(2)-C(8)-C(9)-C(10)	6.6(2)	C(10)-C(21)-C(26)-C(25)	179.7(2)
C(11)-C(8)-C(9)-C(10)	-172.8(2)	N(1)-C(10)-C(31)-N(32)	174.48(16)
C(2)-C(8)-C(9)-Au	-163.35(14)	C(9)-C(10)-C(31)-N(32)	-76.1(2)
C(11)-C(8)-C(9)-Au	17.3(3)	C(21)-C(10)-C(31)-N(32)	49.6(2)
C(6)-N(1)-C(10)-C(9)	-179.10(18)	N(1)-C(10)-C(31)-C(36)	-11.8(3)
C(2)-N(1)-C(10)-C(9)	-0.6(2)	C(9)-C(10)-C(31)-C(36)	97.7(2)
C(6)-N(1)-C(10)-C(31)	-64.6(2)	C(21)-C(10)-C(31)-C(36)	-136.6(2)
C(2)-N(1)-C(10)-C(31)	113.90(18)	C(36)-C(31)-N(32)-C(33)	2.2(3)
C(6)-N(1)-C(10)-C(21)	65.5(2)	C(10)-C(31)-N(32)-C(33)	175.85(17)
C(2)-N(1)-C(10)-C(21)	-115.92(18)	C(31)-N(32)-C(33)-C(34)	-0.9(3)
C(8)-C(9)-C(10)-N(1)	-3.9(2)	C(31)-N(32)-C(33)-C(37)	178.85(19)
Au-C(9)-C(10)-N(1)	167.28(12)	N(32)-C(33)-C(34)-C(35)	-0.7(4)
C(8)-C(9)-C(10)-C(31)	-119.78(19)	C(37)-C(33)-C(34)-C(35)	179.5(2)
Au-C(9)-C(10)-C(31)	51.41(19)	C(33)-C(34)-C(35)-C(36)	1.1(4)
C(8)-C(9)-C(10)-C(21)	110.10(19)	N(32)-C(31)-C(36)-C(35)	-1.7(3)
Au-C(9)-C(10)-C(21)	-78.72(18)	C(10)-C(31)-C(36)-C(35)	-174.9(2)
C(9)-C(8)-C(11)-C(13)	-109.6(3)	C(34)-C(35)-C(36)-C(31)	0.0(3)

Table 6. Hydrogen bonds, in Ångstroms and degrees.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(5)-H(5)...Cl(2)#1	0.93	2.96	3.778(2)	147.5
C(7)-H(7B)...Cl(3)#1	0.96	2.83	3.576(2)	135.6
C(34)-H(34)...Cl(1)#2	0.93	2.77	3.653(2)	158.0
C(22)-H(22)...Cl(2)#3	0.93	2.68	3.448(2)	140.5
C(13)-H(13B)...Cl(3)#4	0.96	2.71	3.554(3)	147.8

Symmetry transformations used to generate equivalent atoms:
#1 : x+½, 1½-y, z-½ #2 : ½-x, y+½, 1½-z

Crystal data and structure refinement for [AuCl(C$_8$H$_3$N-Ph-1,-C$_5$H$_3$N-Me-1,-$_t$Bu-3,-Me-7)], compound 2b''

Table 1. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters (Å^2 x 10^4). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor. E.s.ds are in parentheses.

	x	y	z	U(eq)
Au	40039(2)	-6339(2)	44653(2)	103.4(3)
Cl	20221(7)	-17600(8)	43329(3)	178(2)
N(1)	74510(20)	14240(20)	51137(11)	110(4)
C(2)	79920(30)	7840(30)	46207(12)	111(5)
C(3)	93810(30)	7760(30)	45549(14)	147(6)
C(4)	101560(30)	13890(30)	49927(16)	195(6)
C(5)	95660(30)	20680(30)	54706(15)	188(6)
C(6)	81900(30)	20920(30)	55336(14)	166(6)
C(7)	75530(40)	27910(40)	60556(17)	286(8)
C(8)	69500(30)	1200(30)	42729(12)	106(5)
C(9)	57680(30)	2530(30)	45757(12)	102(6)
C(10)	59760(30)	11300(30)	51409(13)	104(5)
C(11)	72630(30)	-6090(30)	36799(14)	137(6)
C(12)	78980(30)	3630(40)	32217(15)	193(6)
C(13)	81990(30)	-18000(30)	37948(16)	212(7)
C(14)	60090(30)	-11620(30)	33755(15)	175(6)
C(21)	57240(30)	3410(30)	57283(13)	117(5)
C(22)	62980(30)	-9220(30)	57747(15)	179(6)
C(23)	62040(40)	-16410(40)	63121(17)	228(7)
C(24)	54950(30)	-11400(30)	68013(15)	224(7)
C(25)	48910(40)	840(40)	67487(15)	224(7)
C(26)	50070(30)	8340(30)	62217(15)	175(6)
C(31)	51490(30)	24030(30)	50643(13)	127(5)
N(32)	57750(30)	34890(30)	48616(16)	283(7)
C(33)	50470(40)	46110(40)	47680(20)	345(10)
C(34)	36900(40)	46640(30)	48759(16)	217(7)
C(35)	30530(30)	35410(30)	50866(16)	195(6)
C(36)	37850(30)	23820(30)	51769(15)	157(6)
C(37)	57830(60)	58220(50)	45500(50)	990(40)

Table 2. Molecular dimensions. Bond lengths are in Ångstroms, angles in degrees. E.s.ds are in parentheses.

Au-C(9)	1.997(3)	C(9)-Au-Cl	177.11(9)
Au-Cl	2.3068(7)		
N(1)-C(6)	1.362(4)	C(11)-C(12)	1.541(4)
N(1)-C(2)	1.372(4)	C(11)-C(13)	1.542(5)
N(1)-C(10)	1.510(4)	C(21)-C(26)	1.393(4)
C(2)-C(3)	1.402(4)	C(21)-C(22)	1.396(4)
C(2)-C(8)	1.458(4)	C(22)-C(23)	1.388(5)
C(3)-C(4)	1.383(4)	C(23)-C(24)	1.384(5)
C(4)-C(5)	1.386(5)	C(24)-C(25)	1.375(5)
C(5)-C(6)	1.388(4)	C(25)-C(26)	1.387(5)
C(6)-C(7)	1.489(5)	C(31)-N(32)	1.335(4)
C(8)-C(9)	1.367(4)	C(31)-C(36)	1.392(4)
C(8)-C(11)	1.528(4)	N(32)-C(33)	1.358(5)
C(9)-C(10)	1.537(4)	C(33)-C(34)	1.384(5)
C(10)-C(31)	1.534(4)	C(33)-C(37)	1.502(6)
C(10)-C(21)	1.536(4)	C(34)-C(35)	1.376(5)
C(11)-C(14)	1.530(4)	C(35)-C(36)	1.391(4)
C(6)-N(1)-C(2)	123.4(3)	C(8)-C(11)-C(14)	112.2(2)
C(6)-N(1)-C(10)	127.1(2)	C(8)-C(11)-C(12)	109.9(2)
C(2)-N(1)-C(10)	109.1(2)	C(14)-C(11)-C(12)	106.5(3)
N(1)-C(2)-C(3)	118.6(3)	C(8)-C(11)-C(13)	110.9(3)
N(1)-C(2)-C(8)	110.2(2)	C(14)-C(11)-C(13)	106.9(3)
C(3)-C(2)-C(8)	131.1(3)	C(12)-C(11)-C(13)	110.3(3)
C(4)-C(3)-C(2)	119.1(3)	C(26)-C(21)-C(22)	118.6(3)
C(3)-C(4)-C(5)	120.4(3)	C(26)-C(21)-C(10)	123.8(3)
C(4)-C(5)-C(6)	120.6(3)	C(22)-C(21)-C(10)	117.5(3)
N(1)-C(6)-C(5)	117.8(3)	C(23)-C(22)-C(21)	120.4(3)
N(1)-C(6)-C(7)	121.4(3)	C(24)-C(23)-C(22)	120.5(3)
C(5)-C(6)-C(7)	120.8(3)	C(25)-C(24)-C(23)	119.0(3)
C(9)-C(8)-C(2)	108.8(2)	C(24)-C(25)-C(26)	121.2(3)
C(9)-C(8)-C(11)	129.9(3)	C(25)-C(26)-C(21)	120.1(3)
C(2)-C(8)-C(11)	121.3(2)	N(32)-C(31)-C(36)	122.4(3)
C(8)-C(9)-C(10)	109.4(2)	N(32)-C(31)-C(10)	117.5(3)
C(8)-C(9)-Au	131.8(2)	C(36)-C(31)-C(10)	120.0(3)
C(10)-C(9)-Au	118.32(19)	C(31)-N(32)-C(33)	118.3(3)
N(1)-C(10)-C(31)	111.3(2)	N(32)-C(33)-C(34)	122.4(3)
N(1)-C(10)-C(21)	107.2(2)	N(32)-C(33)-C(37)	117.0(4)
C(31)-C(10)-C(21)	115.7(2)	C(34)-C(33)-C(37)	120.5(3)
N(1)-C(10)-C(9)	102.3(2)	C(35)-C(34)-C(33)	118.9(3)
C(31)-C(10)-C(9)	108.3(2)	C(34)-C(35)-C(36)	119.2(3)
C(21)-C(10)-C(9)	111.2(2)	C(35)-C(36)-C(31)	118.8(3)

Table 3. Anisotropic displacement parameters ($Å^2$ x 10^4) for the expression:

$$\exp\{-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})\}$$

E.s.ds are in parentheses.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au	86.5(5)	107.9(5)	115.8(4)	2.9(4)	-11.1(4)	-9.2(4)
Cl	120(3)	197(3)	219(4)	3(3)	-10(2)	-57(3)
N(1)	82(11)	134(11)	114(11)	-1(9)	-3(8)	-25(9)
C(2)	119(12)	115(12)	100(13)	6(9)	6(9)	-1(10)
C(3)	116(12)	163(13)	162(15)	-10(11)	14(10)	-12(10)
C(4)	102(13)	235(16)	249(16)	9(13)	-25(12)	-21(12)
C(5)	155(15)	232(16)	177(15)	-26(12)	-42(11)	-68(12)
C(6)	156(14)	189(15)	154(14)	-12(11)	1(11)	-50(11)
C(7)	205(17)	410(20)	240(18)	-186(15)	30(13)	-104(15)
C(8)	103(12)	110(12)	106(12)	2(9)	-9(9)	-6(10)
C(9)	126(12)	98(12)	83(15)	19(9)	-18(9)	8(9)
C(10)	86(12)	123(13)	104(12)	5(10)	4(9)	-15(10)
C(11)	142(14)	135(13)	133(14)	-32(10)	20(11)	-25(11)
C(12)	246(16)	187(15)	146(14)	-22(11)	49(13)	-54(13)
C(13)	187(16)	156(15)	294(18)	-46(12)	13(13)	11(12)
C(14)	171(15)	224(16)	131(14)	-54(12)	-3(11)	-31(12)
C(21)	98(12)	144(13)	108(12)	21(10)	-4(10)	-23(10)
C(22)	195(15)	173(15)	168(14)	42(12)	25(12)	42(12)
C(23)	212(16)	194(16)	279(18)	93(13)	24(13)	42(13)
C(24)	242(16)	252(17)	177(17)	88(12)	-23(12)	-58(13)
C(25)	253(17)	273(17)	145(14)	20(12)	35(12)	-26(14)
C(26)	225(16)	140(14)	161(15)	2(11)	22(12)	10(12)
C(31)	145(13)	135(13)	102(12)	3(10)	1(10)	14(10)
N(32)	236(15)	164(14)	449(19)	107(13)	157(13)	44(12)
C(33)	280(20)	206(18)	540(30)	154(17)	226(18)	75(15)
C(34)	220(16)	178(15)	254(17)	54(13)	62(13)	83(13)
C(35)	140(14)	183(15)	264(17)	-24(12)	3(12)	27(12)
C(36)	134(14)	130(13)	208(15)	-13(11)	-8(11)	-9(11)
C(37)	510(30)	350(30)	2120(100)	630(50)	680(50)	240(20)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3). All hydrogen atoms were included in idealised positions with U(iso)'s set at 1.2*U(eq) or, for the methyl group hydrogen atoms, 1.5*U(eq) of the parent carbon atoms.

	x	y	z	U(iso)
H(3)	9775	365	4221	18
H(4)	11080	1346	4966	23
H(5)	10097	2512	5752	23
H(7A)	6776	3258	5917	43
H(7B)	8172	3415	6228	43
H(7C)	7301	2151	6359	43
H(12A)	8092	-101	2850	29
H(12B)	7289	1079	3140	29
H(12C)	8707	717	3389	29
H(13A)	8382	-2242	3417	32
H(13B)	9018	-1488	3969	32
H(13C)	7780	-2413	4070	32
H(14A)	6250	-1611	3006	26
H(14B)	5580	-1780	3645	26
H(14C)	5411	-444	3284	26
H(22)	6746	-1283	5443	21
H(23)	6620	-2466	6344	27
H(24)	5428	-1625	7160	27
H(25)	4396	415	7073	27
H(26)	4606	1667	6198	21
H(34)	3216	5445	4807	26
H(35)	2143	3557	5168	23
H(36)	3371	1606	5310	19
H(37A)	6561	5956	4797	149
H(37B)	5214	6588	4580	149
H(37C)	6045	5697	4134	149

Table 5. Torsion angles, in degrees. E.s.ds are in parentheses.

C(6)-N(1)-C(2)-C(3)	2.3(4)	C(2)-C(8)-C(11)-C(14)	-176.8(3)
C(10)-N(1)-C(2)-C(3)	-171.6(3)	C(9)-C(8)-C(11)-C(12)	123.4(3)
C(6)-N(1)-C(2)-C(8)	177.7(3)	C(2)-C(8)-C(11)-C(12)	-58.5(4)
C(10)-N(1)-C(2)-C(8)	3.8(3)	C(9)-C(8)-C(11)-C(13)	-114.4(3)
N(1)-C(2)-C(3)-C(4)	1.2(4)	C(2)-C(8)-C(11)-C(13)	63.7(4)
C(8)-C(2)-C(3)-C(4)	-173.1(3)	N(1)-C(10)-C(21)-C(26)	112.5(3)
C(2)-C(3)-C(4)-C(5)	-3.8(5)	C(31)-C(10)-C(21)-C(26)	-12.4(4)
C(3)-C(4)-C(5)-C(6)	3.0(5)	C(9)-C(10)-C(21)-C(26)	-136.5(3)
C(2)-N(1)-C(6)-C(5)	-3.0(5)	N(1)-C(10)-C(21)-C(22)	-64.8(3)
C(10)-N(1)-C(6)-C(5)	169.8(3)	C(31)-C(10)-C(21)-C(22)	170.4(3)
C(2)-N(1)-C(6)-C(7)	178.9(3)	C(9)-C(10)-C(21)-C(22)	46.3(3)
C(10)-N(1)-C(6)-C(7)	-8.3(5)	C(26)-C(21)-C(22)-C(23)	-2.8(5)
C(4)-C(5)-C(6)-N(1)	0.3(5)	C(10)-C(21)-C(22)-C(23)	174.6(3)
C(4)-C(5)-C(6)-C(7)	178.4(3)	C(21)-C(22)-C(23)-C(24)	2.6(5)
N(1)-C(2)-C(8)-C(9)	-4.9(3)	C(22)-C(23)-C(24)-C(25)	-0.4(5)
C(3)-C(2)-C(8)-C(9)	169.8(3)	C(23)-C(24)-C(25)-C(26)	-1.6(5)
N(1)-C(2)-C(8)-C(11)	176.7(3)	C(24)-C(25)-C(26)-C(21)	1.2(5)
C(3)-C(2)-C(8)-C(11)	-8.7(5)	C(22)-C(21)-C(26)-C(25)	1.0(5)
C(2)-C(8)-C(9)-C(10)	3.8(3)	C(10)-C(21)-C(26)-C(25)	-176.3(3)
C(11)-C(8)-C(9)-C(10)	-177.9(3)	N(1)-C(10)-C(31)-N(32)	13.8(4)
C(2)-C(8)-C(9)-Au	-167.7(2)	C(21)-C(10)-C(31)-N(32)	136.5(3)
C(11)-C(8)-C(9)-Au	10.6(5)	C(9)-C(10)-C(31)-N(32)	-97.9(3)
C(6)-N(1)-C(10)-C(31)	69.5(4)	N(1)-C(10)-C(31)-C(36)	-169.2(3)
C(2)-N(1)-C(10)-C(31)	-116.9(3)	C(21)-C(10)-C(31)-C(36)	-46.6(4)
C(6)-N(1)-C(10)-C(21)	-58.0(4)	C(9)-C(10)-C(31)-C(36)	79.0(3)
C(2)-N(1)-C(10)-C(21)	115.7(3)	C(36)-C(31)-N(32)-C(33)	0.5(5)
C(6)-N(1)-C(10)-C(9)	-175.0(3)	C(10)-C(31)-N(32)-C(33)	177.4(3)
C(2)-N(1)-C(10)-C(9)	-1.4(3)	C(31)-N(32)-C(33)-C(34)	0.0(7)
C(8)-C(9)-C(10)-N(1)	-1.6(3)	C(31)-N(32)-C(33)-C(37)	179.0(6)
Au-C(9)-C(10)-N(1)	171.25(17)	N(32)-C(33)-C(34)-C(35)	0.2(7)
C(8)-C(9)-C(10)-C(31)	116.1(3)	C(37)-C(33)-C(34)-C(35)	-178.8(6)
Au-C(9)-C(10)-C(31)	-71.1(3)	C(33)-C(34)-C(35)-C(36)	-0.9(6)
C(8)-C(9)-C(10)-C(21)	-115.7(3)	C(34)-C(35)-C(36)-C(31)	1.5(5)
Au-C(9)-C(10)-C(21)	57.1(3)	N(32)-C(31)-C(36)-C(35)	-1.3(5)
C(9)-C(8)-C(11)-C(14)	5.1(4)	C(10)-C(31)-C(36)-C(35)	-178.1(3)

Table 6. Hydrogen bonds, in Ångstroms and degrees.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(5)-H(5)...Cl#1	0.93	2.95	3.719(3)	141.4
C(7)-H(7A)...N(32)	0.96	2.54	3.251(5)	131.1

Symmetry transformation used to generate equivalent atoms:
#1 : 1-y, x, z+