Table 1. Crystal data and structure refinement for $(PCy_3)_2Cl_2Ru=C(H)OEt$ (5).

Empirical formula	$C_{39}H_{72}Cl_2OP_2Ru \bullet C_7H_8$
Formula weight	883.01
Crystallization Solvent	Toluene
Crystal Habit	Striated blade
Crystal size	0.22 x 0.14 x 0.10 mm^3
Crystal color	Red

Data Collection

Preliminary Photos	Rotation
Type of diffractometer	CCD area detector
Wavelength	0.71073 Å MoKα
Data Collection Temperature	98(2) K
θ range for 17832 reflections used in lattice determination	2.22 to 24.27°
Unit cell dimensions	a = 10.5761(19)Å b = 36.738(7)Å β= 97.887(4)° c = 23.418(4)Å
Volume	9013(3) $Å^3$
Z	8
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.301 Mg/m^3
F(000)	3776
Data collection program	Bruker SMART
θ range for data collection	1.76 to 25.42°
Completeness to θ = 25.42°	98.5 %
Index ranges	$-12 \le h \le 12, -44 \le k \le 43, -28 \le l \le 27$
Data collection scan type	ω scans at 4 ϕ settings
Data reduction program	Bruker SAINT v6.2
Reflections collected	159532
Independent reflections	16393 [R_{int}= 0.2098]
Absorption coefficient	0.570 mm^{-1}
Absorption correction	None

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Calculated geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	16393 / 0 / 941
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.134
Final R indices [$I>2\sigma(I)$, 9497 reflections]	R1 = 0.0530, *w*R2 = 0.0817
R indices (all data)	R1 = 0.1049, *w*R2 = 0.0884
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	1.187 and -1.147 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

The crystallographic data has been deposited in the Cambridge Database (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 152443.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $(PCy_3)_2Cl_2Ru=C(H)OEt$ (5). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	2016(1)	4878(1)	2568(1)	19(1)
Cl(1)	3684(1)	5310(1)	2518(1)	28(1)
Cl(2)	446(1)	4413(1)	2530(1)	26(1)
P(1)	3420(1)	4480(1)	3143(1)	25(1)
P(2)	794(1)	5190(1)	1783(1)	20(1)
O(1A)	474(3)	5110(1)	3379(1)	49(1)
C(1A)	1488(4)	5142(1)	3144(2)	33(1)
C(2A)	214(5)	5394(1)	3792(2)	49(2)
C(3A)	576(6)	5266(2)	4370(2)	70(2)
C(4A)	1037(4)	5682(1)	1756(2)	23(1)
C(5A)	434(5)	5877(1)	1213(2)	32(1)
C(6A)	896(5)	6271(1)	1204(2)	37(1)
C(7A)	636(5)	6475(1)	1737(2)	37(1)
C(8A)	1216(4)	6280(1)	2274(2)	32(1)
C(9A)	748(4)	5896(1)	2285(2)	28(1)
C(10A)	1328(4)	5035(1)	1108(2)	20(1)
C(11A)	1225(4)	4624(1)	1045(2)	30(1)
C(12A)	1646(5)	4492(1)	490(2)	43(2)
C(13A)	2963(5)	4624(1)	430(2)	38(1)
C(14A)	3060(4)	5032(1)	475(2)	36(1)
C(15A)	2658(4)	5162(1)	1039(2)	27(1)
C(16A)	-900(4)	5081(1)	1688(2)	23(1)
C(17A)	-1687(4)	5145(1)	1104(2)	37(1)
C(18A)	-3005(4)	4975(1)	1096(2)	38(1)
C(19A)	-3678(4)	5116(1)	1570(2)	37(1)
C(20A)	-2900(4)	5059(1)	2145(2)	39(1)
C(21A)	-1586(4)	5231(1)	2162(2)	36(1)
C(22A)	2732(4)	4174(1)	3632(2)	25(1)
C(23A)	3639(5)	3881(1)	3920(2)	46(2)
C(24A)	2925(5)	3607(1)	4235(2)	56(2)
C(25A)	2243(6)	3784(2)	4672(2)	58(2)
C(26A)	1344(5)	4071(2)	4392(2)	54(2)
C(27A)	2011(5)	4350(1)	4073(2)	45(2)
C(28A)	4068(4)	4164(1)	2649(2)	23(1)
C(29A)	3153(4)	3868(1)	2393(2)	27(1)
C(30A)	3780(5)	3617(1)	2005(2)	34(1)
C(31A)	4301(5)	3823(1)	1533(2)	36(1)
C(32A)	5187(5)	4117(1)	1774(2)	40(1)
C(33A)	4565(4)	4372(1)	2165(2)	29(1)
C(34A)	4841(4)	4700(1)	3534(2)	36(1)
C(35A)	6042(5)	4521(2)	3607(3)	91(3)
C(36A)	7163(5)	4748(1)	3874(2)	53(2)
C(37A)	6883(6)	4960(2)	4384(3)	82(2)
C(38A)	5682(5)	5145(2)	4294(2)	57(2)
C(39A)	4588(4)	4923(1)	4024(2)	38(1)
Ru(2)	2388(1)	7547(1)	3330(1)	19(1)
Cl(3)	4029(1)	7984(1)	3375(1)	35(1)
Cl(4)	631(1)	7147(1)	3366(1)	26(1)

P(3)	3567(1)	7224(1)	4107(1)	19(1)
P(4)	1080(1)	7973(1)	2757(1)	24(1)
C(1B)	2838(4)	7271(1)	2747(2)	35(1)
O(1B)	3866(3)	7274(1)	2516(1)	47(1)
C(2B)	3961(6)	6999(2)	2065(3)	92(3)
C(3B)	5002(7)	7031(2)	1846(3)	160(5)
C(4B)	5275(4)	7327(1)	4214(2)	21(1)
C(5B)	5975(4)	7190(1)	3734(2)	36(1)
C(6B)	7257(4)	7371(2)	3759(2)	42(2)
C(7B)	8038(4)	7323(2)	4331(2)	44(2)
C(8B)	7341(4)	7439(2)	4815(2)	50(2)
C(9B)	6061(4)	7257(2)	4790(2)	43(2)
C(10B)	3036(4)	7380(1)	4775(2)	22(1)
C(11B)	1681(4)	7264(1)	4835(2)	26(1)
C(12B)	1267(4)	7396(1)	5395(2)	30(1)
C(13B)	1395(5)	7805(2)	5454(2)	46(2)
C(14B)	2733(5)	7922(1)	5395(2)	43(2)
C(15B)	3159(4)	7791(1)	4841(2)	31(1)
C(16B)	3290(4)	6731(1)	4128(2)	20(1)
C(17B)	3620(5)	6525(1)	3606(2)	30(1)
C(18B)	3151(5)	6134(1)	3605(2)	35(1)
C(19B)	3685(5)	5944(1)	4157(2)	35(1)
C(20B)	3385(5)	6147(1)	4674(2)	38(1)
C(21B)	3871(5)	6536(1)	4676(2)	31(1)
C(22B)	-391(4)	7777(1)	2370(2)	27(1)
C(23B)	-1519(5)	8030(1)	2230(2)	47(2)
C(24B)	-2701(5)	7820(2)	1987(2)	56(2)
C(25B)	-2451(5)	7600(2)	1450(2)	63(2)
C(26B)	-1335(5)	7353(1)	1596(2)	47(2)
C(27B)	-159(4)	7558(1)	1854(2)	33(1)
C(28B)	1880(4)	8255(1)	2267(2)	28(1)
C(29B)	2669(5)	8037(1)	1891(2)	38(1)
C(30B)	3439(5)	8285(2)	1543(2)	51(2)
C(31B)	2616(6)	8564(2)	1210(2)	60(2)
C(32B)	1876(6)	8779(2)	1597(2)	60(2)
C(33B)	1060(5)	8535(1)	1913(2)	42(2)
C(34B)	504(4)	8314(1)	3241(2)	31(1)
C(35B)	1505(5)	8587(1)	3498(2)	41(2)
C(36B)	980(5)	8847(1)	3898(2)	50(2)
C(37B)	438(5)	8644(1)	4374(2)	45(2)
C(38B)	-578(5)	8382(2)	4125(2)	53(2)
C(39B)	-79(4)	8117(1)	3709(2)	36(1)
C(1C)	9245(6)	6332(2)	3940(3)	86(2)
C(2C)	8192(6)	6260(2)	3447(3)	55(2)
C(3C)	7271(6)	6007(2)	3527(3)	62(2)
C(4C)	6356(6)	5929(2)	3061(3)	62(2)
C(5C)	6329(6)	6085(2)	2535(3)	67(2)
C(6C)	7238(7)	6339(2)	2481(3)	73(2)
C(7C)	8167(6)	6425(2)	2923(3)	65(2)
C(1D)	2435(6)	3466(2)	9458(3)	96(3)
C(2D)	3640(9)	3621(3)	9564(4)	111(3)
C(3D)	4446(10)	3598(3)	9991(4)	136(4)
C(4D)	5670(10)	3781(3)	10132(4)	132(4)
C(5D)	6193(9)	3990(2)	9774(4)	103(3)

C(6D)	5345(10)	4017(3)	9257(5)	149(4)
C(7D)	4091(9)	3860(2)	9174(4)	108(3)

Table 3. Selected bond lengths [Å] and angles [°] for $(PCy_3)_2Cl_2Ru=C(H)OEt$ (5).

Ru(1)-C(1A)	1.812(5)	C(1A)-Ru(1)-P(1)	98.07(14)
Ru(1)-P(1)	2.3683(13)	C(1A)-Ru(1)-Cl(1)	89.17(16)
Ru(1)-Cl(1)	2.3886(12)	P(1)-Ru(1)-Cl(1)	91.66(5)
Ru(1)-P(2)	2.3904(13)	C(1A)-Ru(1)-P(2)	97.26(14)
Ru(1)-Cl(2)	2.3749(12)	P(1)-Ru(1)-P(2)	164.67(4)
Ru(2)-C(1B)	1.817(5)	Cl(1)-Ru(1)-P(2)	88.16(4)
Ru(2)-Cl(3)	2.3569(13)	C(1A)-Ru(1)-Cl(2)	97.33(16)
Ru(2)-P(4)	2.3780(13)	P(1)-Ru(1)-Cl(2)	87.58(4)
Ru(2)-Cl(4)	2.3803(12)	Cl(1)-Ru(1)-Cl(2)	173.50(4)
Ru(2)-P(3)	2.3772(13)	P(2)-Ru(1)-Cl(2)	90.87(4)
		C(1B)-Ru(2)-Cl(3)	98.41(16)
		C(1B)-Ru(2)-P(4)	97.78(14)
		Cl(3)-Ru(2)-P(4)	86.78(5)
		C(1B)-Ru(2)-Cl(4)	88.15(16)
		Cl(3)-Ru(2)-Cl(4)	173.41(5)
		P(4)-Ru(2)-Cl(4)	91.73(4)
		C(1B)-Ru(2)-P(3)	97.56(14)
		Cl(3)-Ru(2)-P(3)	90.05(4)
		P(4)-Ru(2)-P(3)	164.64(4)
		Cl(4)-Ru(2)-P(3)	89.70(4)

Table 4. Bond lengths [Å] and angles [°] for $(PCy_3)_2Cl_2Ru=C(H)OEt$ (5).

Ru(1)-C(1A)	1.812(5)	C(14A)-H(14B)	0.9900
Ru(1)-P(1)	2.3683(13)	C(15A)-H(15A)	0.9900
Ru(1)-Cl(1)	2.3886(12)	C(15A)-H(15B)	0.9900
Ru(1)-P(2)	2.3904(13)	C(16A)-C(21A)	1.513(5)
Ru(1)-Cl(2)	2.3749(12)	C(16A)-C(17A)	1.517(6)
P(1)-C(22A)	1.826(4)	C(16A)-H(16A)	1.0000
P(1)-C(34A)	1.837(5)	C(17A)-C(18A)	1.525(5)
P(1)-C(28A)	1.835(4)	C(17A)-H(17A)	0.9900
P(2)-C(4A)	1.828(4)	C(17A)-H(17B)	0.9900
P(2)-C(16A)	1.820(4)	C(18A)-C(19A)	1.491(6)
P(2)-C(10A)	1.839(4)	C(18A)-H(18A)	0.9900
O(1A)-C(1A)	1.275(5)	C(18A)-H(18B)	0.9900
O(1A)-C(2A)	1.474(5)	C(19A)-C(20A)	1.494(6)
C(1A)-H(1A)	0.9500	C(19A)-H(19A)	0.9900
C(2A)-C(3A)	1.434(6)	C(19A)-H(19B)	0.9900
C(2A)-H(2A1)	0.9900	C(20A)-C(21A)	1.522(5)
C(2A)-H(2A2)	0.9900	C(20A)-H(20A)	0.9900
C(3A)-H(3A1)	0.9800	C(20A)-H(20B)	0.9900
C(3A)-H(3A2)	0.9800	C(21A)-H(21A)	0.9900
C(3A)-H(3A3)	0.9800	C(21A)-H(21B)	0.9900
C(4A)-C(5A)	1.521(6)	C(22A)-C(27A)	1.511(6)
C(4A)-C(9A)	1.533(5)	C(22A)-C(23A)	1.534(6)
C(4A)-H(4A)	1.0000	C(22A)-H(22A)	1.0000
C(5A)-C(6A)	1.527(6)	C(23A)-C(24A)	1.510(6)
C(5A)-H(5A1)	0.9900	C(23A)-H(23A)	0.9900
C(5A)-H(5A2)	0.9900	C(23A)-H(23B)	0.9900
C(6A)-C(7A)	1.513(6)	C(24A)-C(25A)	1.482(7)
C(6A)-H(6A1)	0.9900	C(24A)-H(24A)	0.9900
C(6A)-H(6A2)	0.9900	C(24A)-H(24B)	0.9900
C(7A)-C(8A)	1.503(6)	C(25A)-C(26A)	1.509(7)
C(7A)-H(7A1)	0.9900	C(25A)-H(25A)	0.9900
C(7A)-H(7A2)	0.9900	C(25A)-H(25B)	0.9900
C(8A)-C(9A)	1.497(5)	C(26A)-C(27A)	1.499(6)
C(8A)-H(8A1)	0.9900	C(26A)-H(26A)	0.9900
C(8A)-H(8A2)	0.9900	C(26A)-H(26B)	0.9900
C(9A)-H(9A1)	0.9900	C(27A)-H(27A)	0.9900
C(9A)-H(9A2)	0.9900	C(27A)-H(27B)	0.9900
C(10A)-C(11A)	1.520(5)	C(28A)-C(33A)	1.519(5)
C(10A)-C(15A)	1.513(5)	C(28A)-C(29A)	1.525(5)
C(10A)-H(10A)	1.0000	C(28A)-H(28A)	1.0000
C(11A)-C(12A)	1.510(6)	C(29A)-C(30A)	1.512(5)
C(11A)-H(11A)	0.9900	C(29A)-H(29A)	0.9900
C(11A)-H(11B)	0.9900	C(29A)-H(29B)	0.9900
C(12A)-C(13A)	1.500(6)	C(30A)-C(31A)	1.505(6)
C(12A)-H(12A)	0.9900	C(30A)-H(30A)	0.9900
C(12A)-H(12B)	0.9900	C(30A)-H(30B)	0.9900
C(13A)-C(14A)	1.504(6)	C(31A)-C(32A)	1.490(6)
C(13A)-H(13A)	0.9900	C(31A)-H(31A)	0.9900
C(13A)-H(13B)	0.9900	C(31A)-H(31B)	0.9900
C(14A)-C(15A)	1.519(5)	C(32A)-C(33A)	1.520(6)
C(14A)-H(14A)	0.9900	C(32A)-H(32A)	0.9900

C(32A)-H(32B)	0.9900	C(8B)-H(8B2)	0.9900
C(33A)-H(33A)	0.9900	C(9B)-H(9B1)	0.9900
C(33A)-H(33B)	0.9900	C(9B)-H(9B2)	0.9900
C(34A)-C(35A)	1.419(6)	C(10B)-C(15B)	1.520(5)
C(34A)-C(39A)	1.464(6)	C(10B)-C(11B)	1.520(5)
C(34A)-H(34A)	1.0000	C(10B)-H(10B)	1.0000
C(35A)-C(36A)	1.512(6)	C(11B)-C(12B)	1.517(5)
C(35A)-H(35A)	0.9900	C(11B)-H(11C)	0.9900
C(35A)-H(35B)	0.9900	C(11B)-H(11D)	0.9900
C(36A)-C(37A)	1.489(7)	C(12B)-C(13B)	1.513(6)
C(36A)-H(36A)	0.9900	C(12B)-H(12C)	0.9900
C(36A)-H(36B)	0.9900	C(12B)-H(12D)	0.9900
C(37A)-C(38A)	1.430(7)	C(13B)-C(14B)	1.503(6)
C(37A)-H(37A)	0.9900	C(13B)-H(13C)	0.9900
C(37A)-H(37B)	0.9900	C(13B)-H(13D)	0.9900
C(38A)-C(39A)	1.485(6)	C(14B)-C(15B)	1.510(5)
C(38A)-H(38A)	0.9900	C(14B)-H(14C)	0.9900
C(38A)-H(38B)	0.9900	C(14B)-H(14D)	0.9900
C(39A)-H(39A)	0.9900	C(15B)-H(15C)	0.9900
C(39A)-H(39B)	0.9900	C(15B)-H(15D)	0.9900
Ru(2)-C(1B)	1.817(5)	C(16B)-C(21B)	1.524(6)
Ru(2)-Cl(3)	2.3569(13)	C(16B)-C(17B)	1.517(5)
Ru(2)-P(4)	2.3780(13)	C(16B)-H(16B)	1.0000
Ru(2)-Cl(4)	2.3803(12)	C(17B)-C(18B)	1.520(6)
Ru(2)-P(3)	2.3772(13)	C(17B)-H(17C)	0.9900
P(3)-C(10B)	1.828(4)	C(17B)-H(17D)	0.9900
P(3)-C(16B)	1.837(4)	C(18B)-C(19B)	1.509(6)
P(3)-C(4B)	1.828(4)	C(18B)-H(18C)	0.9900
P(4)-C(28B)	1.837(4)	C(18B)-H(18D)	0.9900
P(4)-C(22B)	1.837(5)	C(19B)-C(20B)	1.492(6)
P(4)-C(34B)	1.847(4)	C(19B)-H(19C)	0.9900
C(1B)-O(1B)	1.280(5)	C(19B)-H(19D)	0.9900
C(1B)-H(1B)	0.9500	C(20B)-C(21B)	1.518(6)
O(1B)-C(2B)	1.475(6)	C(20B)-H(20C)	0.9900
C(2B)-C(3B)	1.281(7)	C(20B)-H(20D)	0.9900
C(2B)-H(2B1)	0.9900	C(21B)-H(21C)	0.9900
C(2B)-H(2B2)	0.9900	C(21B)-H(21D)	0.9900
C(3B)-H(3B1)	0.9800	C(22B)-C(27B)	1.501(5)
C(3B)-H(3B2)	0.9800	C(22B)-C(23B)	1.510(6)
C(3B)-H(3B3)	0.9800	C(22B)-H(22B)	1.0000
C(4B)-C(9B)	1.507(6)	C(23B)-C(24B)	1.512(6)
C(4B)-C(5B)	1.513(5)	C(23B)-H(23C)	0.9900
C(4B)-H(4B)	1.0000	C(23B)-H(23D)	0.9900
C(5B)-C(6B)	1.503(6)	C(24B)-C(25B)	1.548(6)
C(5B)-H(5B1)	0.9900	C(24B)-H(24C)	0.9900
C(5B)-H(5B2)	0.9900	C(24B)-H(24D)	0.9900
C(6B)-C(7B)	1.485(6)	C(25B)-C(26B)	1.490(6)
C(6B)-H(6B1)	0.9900	C(25B)-H(25C)	0.9900
C(6B)-H(6B2)	0.9900	C(25B)-H(25D)	0.9900
C(7B)-C(8B)	1.494(6)	C(26B)-C(27B)	1.507(6)
C(7B)-H(7B1)	0.9900	C(26B)-H(26C)	0.9900
C(7B)-H(7B2)	0.9900	C(26B)-H(26D)	0.9900
C(8B)-C(9B)	1.504(6)	C(27B)-H(27C)	0.9900
C(8B)-H(8B1)	0.9900	C(27B)-H(27D)	0.9900

C(28B)-C(33B)	1.517(6)	C(2D)-C(7D)	1.396(10)
C(28B)-C(29B)	1.521(6)	C(3D)-C(4D)	1.455(11)
C(28B)-H(28B)	1.0000	C(3D)-H(3D)	0.9500
C(29B)-C(30B)	1.530(6)	C(4D)-C(5D)	1.313(10)
C(29B)-H(29C)	0.9900	C(4D)-H(4D)	0.9500
C(29B)-H(29D)	0.9900	C(5D)-C(6D)	1.408(10)
C(30B)-C(31B)	1.493(7)	C(5D)-H(5D)	0.9500
C(30B)-H(30C)	0.9900	C(6D)-C(7D)	1.435(10)
C(30B)-H(30D)	0.9900	C(6D)-H(6D)	0.9500
C(31B)-C(32B)	1.499(7)	C(7D)-H(7D)	0.9500
C(31B)-H(31C)	0.9900		
C(31B)-H(31D)	0.9900	C(1A)-Ru(1)-P(1)	98.07(14)
C(32B)-C(33B)	1.508(6)	C(1A)-Ru(1)-Cl(1)	89.17(16)
C(32B)-H(32C)	0.9900	P(1)-Ru(1)-Cl(1)	91.66(5)
C(32B)-H(32D)	0.9900	C(1A)-Ru(1)-P(2)	97.26(14)
C(33B)-H(33C)	0.9900	P(1)-Ru(1)-P(2)	164.67(4)
C(33B)-H(33D)	0.9900	Cl(1)-Ru(1)-P(2)	88.16(4)
C(34B)-C(35B)	1.520(6)	C(1A)-Ru(1)-Cl(2)	97.33(16)
C(34B)-C(39B)	1.514(6)	P(1)-Ru(1)-Cl(2)	87.58(4)
C(34B)-H(34B)	1.0000	Cl(1)-Ru(1)-Cl(2)	173.50(4)
C(35B)-C(36B)	1.498(6)	P(2)-Ru(1)-Cl(2)	90.87(4)
C(35B)-H(35C)	0.9900	C(22A)-P(1)-C(34A)	109.1(2)
C(35B)-H(35D)	0.9900	C(22A)-P(1)-C(28A)	102.9(2)
C(36B)-C(37B)	1.517(6)	C(34A)-P(1)-C(28A)	104.0(2)
C(36B)-H(36C)	0.9900	C(22A)-P(1)-Ru(1)	117.64(15)
C(36B)-H(36D)	0.9900	C(34A)-P(1)-Ru(1)	114.68(17)
C(37B)-C(38B)	1.501(6)	C(28A)-P(1)-Ru(1)	106.92(15)
C(37B)-H(37C)	0.9900	C(4A)-P(2)-C(16A)	110.8(2)
C(37B)-H(37D)	0.9900	C(4A)-P(2)-C(10A)	102.43(19)
C(38B)-C(39B)	1.523(6)	C(16A)-P(2)-C(10A)	103.8(2)
C(38B)-H(38C)	0.9900	C(4A)-P(2)-Ru(1)	115.96(15)
C(38B)-H(38D)	0.9900	C(16A)-P(2)-Ru(1)	114.06(14)
C(39B)-H(39C)	0.9900	C(10A)-P(2)-Ru(1)	108.33(14)
C(39B)-H(39D)	0.9900	C(1A)-O(1A)-C(2A)	117.4(4)
C(1C)-C(2C)	1.514(8)	O(1A)-C(1A)-Ru(1)	129.4(4)
C(1C)-H(1C1)	0.9800	O(1A)-C(1A)-H(1A)	115.3
C(1C)-H(1C2)	0.9800	Ru(1)-C(1A)-H(1A)	115.3
C(1C)-H(1C3)	0.9800	C(3A)-C(2A)-O(1A)	109.8(4)
C(2C)-C(7C)	1.367(8)	C(3A)-C(2A)-H(2A1)	109.7
C(2C)-C(3C)	1.377(7)	O(1A)-C(2A)-H(2A1)	109.7
C(3C)-C(4C)	1.386(8)	C(3A)-C(2A)-H(2A2)	109.7
C(3C)-H(3C)	0.9500	O(1A)-C(2A)-H(2A2)	109.7
C(4C)-C(5C)	1.356(8)	H(2A1)-C(2A)-H(2A2)	108.2
C(4C)-H(4C)	0.9500	C(2A)-C(3A)-H(3A1)	109.5
C(5C)-C(6C)	1.358(8)	C(2A)-C(3A)-H(3A2)	109.5
C(5C)-H(5C)	0.9500	H(3A1)-C(3A)-H(3A2)	109.5
C(6C)-C(7C)	1.362(8)	C(2A)-C(3A)-H(3A3)	109.5
C(6C)-H(6C)	0.9500	H(3A1)-C(3A)-H(3A3)	109.5
C(7C)-H(7C)	0.9500	H(3A2)-C(3A)-H(3A3)	109.5
C(1D)-C(2D)	1.387(10)	C(5A)-C(4A)-C(9A)	109.1(4)
C(1D)-H(1D1)	0.9800	C(5A)-C(4A)-P(2)	116.7(3)
C(1D)-H(1D2)	0.9800	C(9A)-C(4A)-P(2)	115.7(3)
C(1D)-H(1D3)	0.9800	C(5A)-C(4A)-H(4A)	104.6
C(2D)-C(3D)	1.226(10)	C(9A)-C(4A)-H(4A)	104.6

P(2)-C(4A)-H(4A)	104.6	H(13A)-C(13A)-H(13B)	107.9
C(6A)-C(5A)-C(4A)	111.0(4)	C(13A)-C(14A)-C(15A)	110.4(4)
C(6A)-C(5A)-H(5A1)	109.4	C(13A)-C(14A)-H(14A)	109.6
C(4A)-C(5A)-H(5A1)	109.4	C(15A)-C(14A)-H(14A)	109.6
C(6A)-C(5A)-H(5A2)	109.4	C(13A)-C(14A)-H(14B)	109.6
C(4A)-C(5A)-H(5A2)	109.4	C(15A)-C(14A)-H(14B)	109.6
H(5A1)-C(5A)-H(5A2)	108.0	H(14A)-C(14A)-H(14B)	108.1
C(7A)-C(6A)-C(5A)	111.3(4)	C(10A)-C(15A)-C(14A)	111.9(4)
C(7A)-C(6A)-H(6A1)	109.4	C(10A)-C(15A)-H(15A)	109.2
C(5A)-C(6A)-H(6A1)	109.4	C(14A)-C(15A)-H(15A)	109.2
C(7A)-C(6A)-H(6A2)	109.4	C(10A)-C(15A)-H(15B)	109.2
C(5A)-C(6A)-H(6A2)	109.4	C(14A)-C(15A)-H(15B)	109.2
H(6A1)-C(6A)-H(6A2)	108.0	H(15A)-C(15A)-H(15B)	107.9
C(6A)-C(7A)-C(8A)	110.7(4)	C(21A)-C(16A)-C(17A)	110.3(4)
C(6A)-C(7A)-H(7A1)	109.5	C(21A)-C(16A)-P(2)	113.1(3)
C(8A)-C(7A)-H(7A1)	109.5	C(17A)-C(16A)-P(2)	119.0(3)
C(6A)-C(7A)-H(7A2)	109.5	C(21A)-C(16A)-H(16A)	104.2
C(8A)-C(7A)-H(7A2)	109.5	C(17A)-C(16A)-H(16A)	104.2
H(7A1)-C(7A)-H(7A2)	108.1	P(2)-C(16A)-H(16A)	104.2
C(9A)-C(8A)-C(7A)	111.4(4)	C(18A)-C(17A)-C(16A)	109.6(4)
C(9A)-C(8A)-H(8A1)	109.3	C(18A)-C(17A)-H(17A)	109.7
C(7A)-C(8A)-H(8A1)	109.3	C(16A)-C(17A)-H(17A)	109.7
C(9A)-C(8A)-H(8A2)	109.3	C(18A)-C(17A)-H(17B)	109.7
C(7A)-C(8A)-H(8A2)	109.3	C(16A)-C(17A)-H(17B)	109.7
H(8A1)-C(8A)-H(8A2)	108.0	H(17A)-C(17A)-H(17B)	108.2
C(8A)-C(9A)-C(4A)	111.4(4)	C(17A)-C(18A)-C(19A)	112.2(4)
C(8A)-C(9A)-H(9A1)	109.3	C(17A)-C(18A)-H(18A)	109.2
C(4A)-C(9A)-H(9A1)	109.3	C(19A)-C(18A)-H(18A)	109.2
C(8A)-C(9A)-H(9A2)	109.3	C(17A)-C(18A)-H(18B)	109.2
C(4A)-C(9A)-H(9A2)	109.3	C(19A)-C(18A)-H(18B)	109.2
H(9A1)-C(9A)-H(9A2)	108.0	H(18A)-C(18A)-H(18B)	107.9
C(11A)-C(10A)-C(15A)	110.5(4)	C(18A)-C(19A)-C(20A)	111.3(4)
C(11A)-C(10A)-P(2)	111.4(3)	C(18A)-C(19A)-H(19A)	109.4
C(15A)-C(10A)-P(2)	113.4(3)	C(20A)-C(19A)-H(19A)	109.4
C(11A)-C(10A)-H(10A)	107.0	C(18A)-C(19A)-H(19B)	109.4
C(15A)-C(10A)-H(10A)	107.0	C(20A)-C(19A)-H(19B)	109.4
P(2)-C(10A)-H(10A)	107.0	H(19A)-C(19A)-H(19B)	108.0
C(12A)-C(11A)-C(10A)	112.2(4)	C(21A)-C(20A)-C(19A)	110.8(4)
C(12A)-C(11A)-H(11A)	109.2	C(21A)-C(20A)-H(20A)	109.5
C(10A)-C(11A)-H(11A)	109.2	C(19A)-C(20A)-H(20A)	109.5
C(12A)-C(11A)-H(11B)	109.2	C(21A)-C(20A)-H(20B)	109.5
C(10A)-C(11A)-H(11B)	109.2	C(19A)-C(20A)-H(20B)	109.5
H(11A)-C(11A)-H(11B)	107.9	H(20A)-C(20A)-H(20B)	108.1
C(11A)-C(12A)-C(13A)	111.3(4)	C(16A)-C(21A)-C(20A)	110.9(4)
C(11A)-C(12A)-H(12A)	109.4	C(16A)-C(21A)-H(21A)	109.5
C(13A)-C(12A)-H(12A)	109.4	C(20A)-C(21A)-H(21A)	109.5
C(11A)-C(12A)-H(12B)	109.4	C(16A)-C(21A)-H(21B)	109.5
C(13A)-C(12A)-H(12B)	109.4	C(20A)-C(21A)-H(21B)	109.5
H(12A)-C(12A)-H(12B)	108.0	H(21A)-C(21A)-H(21B)	108.0
C(14A)-C(13A)-C(12A)	111.9(4)	C(27A)-C(22A)-C(23A)	110.1(4)
C(14A)-C(13A)-H(13A)	109.2	C(27A)-C(22A)-P(1)	116.6(3)
C(12A)-C(13A)-H(13A)	109.2	C(23A)-C(22A)-P(1)	115.3(3)
C(14A)-C(13A)-H(13B)	109.2	C(27A)-C(22A)-H(22A)	104.4
C(12A)-C(13A)-H(13B)	109.2	C(23A)-C(22A)-H(22A)	104.4

P(1)-C(22A)-H(22A)	104.4	H(31A)-C(31A)-H(31B)	108.0
C(22A)-C(23A)-C(24A)	111.0(4)	C(33A)-C(32A)-C(31A)	111.9(4)
C(22A)-C(23A)-H(23A)	109.4	C(33A)-C(32A)-H(32A)	109.2
C(24A)-C(23A)-H(23A)	109.4	C(31A)-C(32A)-H(32A)	109.2
C(22A)-C(23A)-H(23B)	109.4	C(33A)-C(32A)-H(32B)	109.2
C(24A)-C(23A)-H(23B)	109.4	C(31A)-C(32A)-H(32B)	109.2
H(23A)-C(23A)-H(23B)	108.0	H(32A)-C(32A)-H(32B)	107.9
C(25A)-C(24A)-C(23A)	111.7(5)	C(28A)-C(33A)-C(32A)	111.3(4)
C(25A)-C(24A)-H(24A)	109.3	C(28A)-C(33A)-H(33A)	109.4
C(23A)-C(24A)-H(24A)	109.3	C(32A)-C(33A)-H(33A)	109.4
C(25A)-C(24A)-H(24B)	109.3	C(28A)-C(33A)-H(33B)	109.4
C(23A)-C(24A)-H(24B)	109.3	C(32A)-C(33A)-H(33B)	109.4
H(24A)-C(24A)-H(24B)	108.0	H(33A)-C(33A)-H(33B)	108.0
C(24A)-C(25A)-C(26A)	110.0(4)	C(35A)-C(34A)-C(39A)	114.9(4)
C(24A)-C(25A)-H(25A)	109.7	C(35A)-C(34A)-P(1)	120.9(4)
C(26A)-C(25A)-H(25A)	109.7	C(39A)-C(34A)-P(1)	114.3(3)
C(24A)-C(25A)-H(25B)	109.7	C(35A)-C(34A)-H(34A)	100.6
C(26A)-C(25A)-H(25B)	109.7	C(39A)-C(34A)-H(34A)	100.6
H(25A)-C(25A)-H(25B)	108.2	P(1)-C(34A)-H(34A)	100.6
C(27A)-C(26A)-C(25A)	112.6(5)	C(34A)-C(35A)-C(36A)	115.7(5)
C(27A)-C(26A)-H(26A)	109.1	C(34A)-C(35A)-H(35A)	108.4
C(25A)-C(26A)-H(26A)	109.1	C(36A)-C(35A)-H(35A)	108.4
C(27A)-C(26A)-H(26B)	109.1	C(34A)-C(35A)-H(35B)	108.4
C(25A)-C(26A)-H(26B)	109.1	C(36A)-C(35A)-H(35B)	108.4
H(26A)-C(26A)-H(26B)	107.8	H(35A)-C(35A)-H(35B)	107.4
C(22A)-C(27A)-C(26A)	111.3(4)	C(37A)-C(36A)-C(35A)	112.9(5)
C(22A)-C(27A)-H(27A)	109.4	C(37A)-C(36A)-H(36A)	109.0
C(26A)-C(27A)-H(27A)	109.4	C(35A)-C(36A)-H(36A)	109.0
C(22A)-C(27A)-H(27B)	109.4	C(37A)-C(36A)-H(36B)	109.0
C(26A)-C(27A)-H(27B)	109.4	C(35A)-C(36A)-H(36B)	109.0
H(27A)-C(27A)-H(27B)	108.0	H(36A)-C(36A)-H(36B)	107.8
C(33A)-C(28A)-C(29A)	109.4(4)	C(38A)-C(37A)-C(36A)	113.6(5)
C(33A)-C(28A)-P(1)	110.5(3)	C(38A)-C(37A)-H(37A)	108.8
C(29A)-C(28A)-P(1)	115.3(3)	C(36A)-C(37A)-H(37A)	108.8
C(33A)-C(28A)-H(28A)	107.1	C(38A)-C(37A)-H(37B)	108.8
C(29A)-C(28A)-H(28A)	107.1	C(36A)-C(37A)-H(37B)	108.8
P(1)-C(28A)-H(28A)	107.1	H(37A)-C(37A)-H(37B)	107.7
C(30A)-C(29A)-C(28A)	111.4(4)	C(37A)-C(38A)-C(39A)	115.2(5)
C(30A)-C(29A)-H(29A)	109.4	C(37A)-C(38A)-H(38A)	108.5
C(28A)-C(29A)-H(29A)	109.4	C(39A)-C(38A)-H(38A)	108.5
C(30A)-C(29A)-H(29B)	109.4	C(37A)-C(38A)-H(38B)	108.5
C(28A)-C(29A)-H(29B)	109.4	C(39A)-C(38A)-H(38B)	108.5
H(29A)-C(29A)-H(29B)	108.0	H(38A)-C(38A)-H(38B)	107.5
C(31A)-C(30A)-C(29A)	111.7(4)	C(34A)-C(39A)-C(38A)	115.2(4)
C(31A)-C(30A)-H(30A)	109.3	C(34A)-C(39A)-H(39A)	108.5
C(29A)-C(30A)-H(30A)	109.3	C(38A)-C(39A)-H(39A)	108.5
C(31A)-C(30A)-H(30B)	109.3	C(34A)-C(39A)-H(39B)	108.5
C(29A)-C(30A)-H(30B)	109.3	C(38A)-C(39A)-H(39B)	108.5
H(30A)-C(30A)-H(30B)	107.9	H(39A)-C(39A)-H(39B)	107.5
C(30A)-C(31A)-C(32A)	111.2(4)	C(1B)-Ru(2)-Cl(3)	98.41(16)
C(30A)-C(31A)-H(31A)	109.4	C(1B)-Ru(2)-P(4)	97.78(14)
C(32A)-C(31A)-H(31A)	109.4	Cl(3)-Ru(2)-P(4)	86.78(5)
C(30A)-C(31A)-H(31B)	109.4	C(1B)-Ru(2)-Cl(4)	88.15(16)
C(32A)-C(31A)-H(31B)	109.4	Cl(3)-Ru(2)-Cl(4)	173.41(5)

P(4)-Ru(2)-Cl(4)	91.73(4)	C(8B)-C(7B)-H(7B2)	109.1
C(1B)-Ru(2)-P(3)	97.56(14)	C(6B)-C(7B)-H(7B2)	109.1
Cl(3)-Ru(2)-P(3)	90.05(4)	H(7B1)-C(7B)-H(7B2)	107.9
P(4)-Ru(2)-P(3)	164.64(4)	C(7B)-C(8B)-C(9B)	112.4(4)
Cl(4)-Ru(2)-P(3)	89.70(4)	C(7B)-C(8B)-H(8B1)	109.1
C(10B)-P(3)-C(16B)	102.62(19)	C(9B)-C(8B)-H(8B1)	109.1
C(10B)-P(3)-C(4B)	103.33(19)	C(7B)-C(8B)-H(8B2)	109.1
C(16B)-P(3)-C(4B)	111.0(2)	C(9B)-C(8B)-H(8B2)	109.1
C(10B)-P(3)-Ru(2)	107.88(14)	H(8B1)-C(8B)-H(8B2)	107.9
C(16B)-P(3)-Ru(2)	116.40(15)	C(4B)-C(9B)-C(8B)	109.9(4)
C(4B)-P(3)-Ru(2)	113.98(14)	C(4B)-C(9B)-H(9B1)	109.7
C(28B)-P(4)-C(22B)	110.1(2)	C(8B)-C(9B)-H(9B1)	109.7
C(28B)-P(4)-C(34B)	102.7(2)	C(4B)-C(9B)-H(9B2)	109.7
C(22B)-P(4)-C(34B)	103.9(2)	C(8B)-C(9B)-H(9B2)	109.7
C(28B)-P(4)-Ru(2)	116.24(16)	H(9B1)-C(9B)-H(9B2)	108.2
C(22B)-P(4)-Ru(2)	114.13(15)	C(15B)-C(10B)-C(11B)	109.7(4)
C(34B)-P(4)-Ru(2)	108.39(15)	C(15B)-C(10B)-P(3)	111.6(3)
O(1B)-C(1B)-Ru(2)	129.7(4)	C(11B)-C(10B)-P(3)	113.3(3)
O(1B)-C(1B)-H(1B)	115.1	C(15B)-C(10B)-H(10B)	107.3
Ru(2)-C(1B)-H(1B)	115.1	C(11B)-C(10B)-H(10B)	107.3
C(1B)-O(1B)-C(2B)	116.2(4)	P(3)-C(10B)-H(10B)	107.3
C(3B)-C(2B)-O(1B)	111.7(6)	C(12B)-C(11B)-C(10B)	112.2(4)
C(3B)-C(2B)-H(2B1)	109.3	C(12B)-C(11B)-H(11C)	109.2
O(1B)-C(2B)-H(2B1)	109.3	C(10B)-C(11B)-H(11C)	109.2
C(3B)-C(2B)-H(2B2)	109.3	C(12B)-C(11B)-H(11D)	109.2
O(1B)-C(2B)-H(2B2)	109.3	C(10B)-C(11B)-H(11D)	109.2
H(2B1)-C(2B)-H(2B2)	107.9	H(11C)-C(11B)-H(11D)	107.9
C(2B)-C(3B)-H(3B1)	109.5	C(11B)-C(12B)-C(13B)	111.3(4)
C(2B)-C(3B)-H(3B2)	109.5	C(11B)-C(12B)-H(12C)	109.4
H(3B1)-C(3B)-H(3B2)	109.5	C(13B)-C(12B)-H(12C)	109.4
C(2B)-C(3B)-H(3B3)	109.5	C(11B)-C(12B)-H(12D)	109.4
H(3B1)-C(3B)-H(3B3)	109.5	C(13B)-C(12B)-H(12D)	109.4
H(3B2)-C(3B)-H(3B3)	109.5	H(12C)-C(12B)-H(12D)	108.0
C(9B)-C(4B)-C(5B)	110.0(4)	C(14B)-C(13B)-C(12B)	110.5(4)
C(9B)-C(4B)-P(3)	120.1(3)	C(14B)-C(13B)-H(13C)	109.6
C(5B)-C(4B)-P(3)	113.8(3)	C(12B)-C(13B)-H(13C)	109.6
C(9B)-C(4B)-H(4B)	103.6	C(14B)-C(13B)-H(13D)	109.6
C(5B)-C(4B)-H(4B)	103.6	C(12B)-C(13B)-H(13D)	109.6
P(3)-C(4B)-H(4B)	103.6	H(13C)-C(13B)-H(13D)	108.1
C(6B)-C(5B)-C(4B)	110.8(4)	C(13B)-C(14B)-C(15B)	112.5(4)
C(6B)-C(5B)-H(5B1)	109.5	C(13B)-C(14B)-H(14C)	109.1
C(4B)-C(5B)-H(5B1)	109.5	C(15B)-C(14B)-H(14C)	109.1
C(6B)-C(5B)-H(5B2)	109.5	C(13B)-C(14B)-H(14D)	109.1
C(4B)-C(5B)-H(5B2)	109.5	C(15B)-C(14B)-H(14D)	109.1
H(5B1)-C(5B)-H(5B2)	108.1	H(14C)-C(14B)-H(14D)	107.8
C(5B)-C(6B)-C(7B)	111.7(4)	C(10B)-C(15B)-C(14B)	111.9(4)
C(5B)-C(6B)-H(6B1)	109.3	C(10B)-C(15B)-H(15C)	109.2
C(7B)-C(6B)-H(6B1)	109.3	C(14B)-C(15B)-H(15C)	109.2
C(5B)-C(6B)-H(6B2)	109.3	C(10B)-C(15B)-H(15D)	109.2
C(7B)-C(6B)-H(6B2)	109.3	C(14B)-C(15B)-H(15D)	109.2
H(6B1)-C(6B)-H(6B2)	107.9	H(15C)-C(15B)-H(15D)	107.9
C(8B)-C(7B)-C(6B)	112.3(4)	C(21B)-C(16B)-C(17B)	109.5(4)
C(8B)-C(7B)-H(7B1)	109.1	C(21B)-C(16B)-P(3)	116.0(3)
C(6B)-C(7B)-H(7B1)	109.1	C(17B)-C(16B)-P(3)	114.4(3)

C(21B)-C(16B)-H(16B)	105.3	C(26B)-C(25B)-H(25D)	109.5
C(17B)-C(16B)-H(16B)	105.3	C(24B)-C(25B)-H(25D)	109.5
P(3)-C(16B)-H(16B)	105.3	H(25C)-C(25B)-H(25D)	108.1
C(18B)-C(17B)-C(16B)	111.2(4)	C(25B)-C(26B)-C(27B)	111.9(4)
C(18B)-C(17B)-H(17C)	109.4	C(25B)-C(26B)-H(26C)	109.2
C(16B)-C(17B)-H(17C)	109.4	C(27B)-C(26B)-H(26C)	109.2
C(18B)-C(17B)-H(17D)	109.4	C(25B)-C(26B)-H(26D)	109.2
C(16B)-C(17B)-H(17D)	109.4	C(27B)-C(26B)-H(26D)	109.2
H(17C)-C(17B)-H(17D)	108.0	H(26C)-C(26B)-H(26D)	107.9
C(17B)-C(18B)-C(19B)	110.6(4)	C(22B)-C(27B)-C(26B)	112.0(4)
C(17B)-C(18B)-H(18C)	109.5	C(22B)-C(27B)-H(27C)	109.2
C(19B)-C(18B)-H(18C)	109.5	C(26B)-C(27B)-H(27C)	109.2
C(17B)-C(18B)-H(18D)	109.5	C(22B)-C(27B)-H(27D)	109.2
C(19B)-C(18B)-H(18D)	109.5	C(26B)-C(27B)-H(27D)	109.2
H(18C)-C(18B)-H(18D)	108.1	H(27C)-C(27B)-H(27D)	107.9
C(18B)-C(19B)-C(20B)	111.6(4)	C(33B)-C(28B)-C(29B)	111.0(4)
C(18B)-C(19B)-H(19C)	109.3	C(33B)-C(28B)-P(4)	116.5(3)
C(20B)-C(19B)-H(19C)	109.3	C(29B)-C(28B)-P(4)	113.6(3)
C(18B)-C(19B)-H(19D)	109.3	C(33B)-C(28B)-H(28B)	104.8
C(20B)-C(19B)-H(19D)	109.3	C(29B)-C(28B)-H(28B)	104.8
H(19C)-C(19B)-H(19D)	108.0	P(4)-C(28B)-H(28B)	104.8
C(19B)-C(20B)-C(21B)	111.2(4)	C(28B)-C(29B)-C(30B)	111.7(4)
C(19B)-C(20B)-H(20C)	109.4	C(28B)-C(29B)-H(29C)	109.3
C(21B)-C(20B)-H(20C)	109.4	C(30B)-C(29B)-H(29C)	109.3
C(19B)-C(20B)-H(20D)	109.4	C(28B)-C(29B)-H(29D)	109.3
C(21B)-C(20B)-H(20D)	109.4	C(30B)-C(29B)-H(29D)	109.3
H(20C)-C(20B)-H(20D)	108.0	H(29C)-C(29B)-H(29D)	107.9
C(16B)-C(21B)-C(20B)	110.0(4)	C(31B)-C(30B)-C(29B)	111.8(5)
C(16B)-C(21B)-H(21C)	109.7	C(31B)-C(30B)-H(30C)	109.3
C(20B)-C(21B)-H(21C)	109.7	C(29B)-C(30B)-H(30C)	109.3
C(16B)-C(21B)-H(21D)	109.7	C(31B)-C(30B)-H(30D)	109.3
C(20B)-C(21B)-H(21D)	109.7	C(29B)-C(30B)-H(30D)	109.3
H(21C)-C(21B)-H(21D)	108.2	H(30C)-C(30B)-H(30D)	107.9
C(27B)-C(22B)-C(23B)	111.6(4)	C(30B)-C(31B)-C(32B)	111.2(5)
C(27B)-C(22B)-P(4)	112.8(3)	C(30B)-C(31B)-H(31C)	109.4
C(23B)-C(22B)-P(4)	117.2(3)	C(32B)-C(31B)-H(31C)	109.4
C(27B)-C(22B)-H(22B)	104.6	C(30B)-C(31B)-H(31D)	109.4
C(23B)-C(22B)-H(22B)	104.6	C(32B)-C(31B)-H(31D)	109.4
P(4)-C(22B)-H(22B)	104.6	H(31C)-C(31B)-H(31D)	108.0
C(24B)-C(23B)-C(22B)	110.9(4)	C(31B)-C(32B)-C(33B)	111.4(5)
C(24B)-C(23B)-H(23C)	109.5	C(31B)-C(32B)-H(32C)	109.3
C(22B)-C(23B)-H(23C)	109.5	C(33B)-C(32B)-H(32C)	109.3
C(24B)-C(23B)-H(23D)	109.5	C(31B)-C(32B)-H(32D)	109.3
C(22B)-C(23B)-H(23D)	109.5	C(33B)-C(32B)-H(32D)	109.3
H(23C)-C(23B)-H(23D)	108.0	H(32C)-C(32B)-H(32D)	108.0
C(23B)-C(24B)-C(25B)	110.3(4)	C(28B)-C(33B)-C(32B)	110.3(4)
C(23B)-C(24B)-H(24C)	109.6	C(28B)-C(33B)-H(33C)	109.6
C(25B)-C(24B)-H(24C)	109.6	C(32B)-C(33B)-H(33C)	109.6
C(23B)-C(24B)-H(24D)	109.6	C(28B)-C(33B)-H(33D)	109.6
C(25B)-C(24B)-H(24D)	109.6	C(32B)-C(33B)-H(33D)	109.6
H(24C)-C(24B)-H(24D)	108.1	H(33C)-C(33B)-H(33D)	108.1
C(26B)-C(25B)-C(24B)	110.5(4)	C(35B)-C(34B)-C(39B)	111.0(4)
C(26B)-C(25B)-H(25C)	109.5	C(35B)-C(34B)-P(4)	114.8(3)
C(24B)-C(25B)-H(25C)	109.5	C(39B)-C(34B)-P(4)	108.7(3)

C(35B)-C(34B)-H(34B)	107.3
C(39B)-C(34B)-H(34B)	107.3
P(4)-C(34B)-H(34B)	107.3
C(34B)-C(35B)-C(36B)	111.8(4)
C(34B)-C(35B)-H(35C)	109.3
C(36B)-C(35B)-H(35C)	109.3
C(34B)-C(35B)-H(35D)	109.3
C(36B)-C(35B)-H(35D)	109.3
H(35C)-C(35B)-H(35D)	107.9
C(35B)-C(36B)-C(37B)	110.9(4)
C(35B)-C(36B)-H(36C)	109.5
C(37B)-C(36B)-H(36C)	109.5
C(35B)-C(36B)-H(36D)	109.5
C(37B)-C(36B)-H(36D)	109.5
H(36C)-C(36B)-H(36D)	108.1
C(38B)-C(37B)-C(36B)	110.6(4)
C(38B)-C(37B)-H(37C)	109.5
C(36B)-C(37B)-H(37C)	109.5
C(38B)-C(37B)-H(37D)	109.5
C(36B)-C(37B)-H(37D)	109.5
H(37C)-C(37B)-H(37D)	108.1
C(37B)-C(38B)-C(39B)	111.5(4)
C(37B)-C(38B)-H(38C)	109.3
C(39B)-C(38B)-H(38C)	109.3
C(37B)-C(38B)-H(38D)	109.3
C(39B)-C(38B)-H(38D)	109.3
H(38C)-C(38B)-H(38D)	108.0
C(34B)-C(39B)-C(38B)	111.7(4)
C(34B)-C(39B)-H(39C)	109.3
C(38B)-C(39B)-H(39C)	109.3
C(34B)-C(39B)-H(39D)	109.3
C(38B)-C(39B)-H(39D)	109.3
H(39C)-C(39B)-H(39D)	107.9
C(2C)-C(1C)-H(1C1)	109.5
C(2C)-C(1C)-H(1C2)	109.5
H(1C1)-C(1C)-H(1C2)	109.5
C(2C)-C(1C)-H(1C3)	109.5
H(1C1)-C(1C)-H(1C3)	109.5
H(1C2)-C(1C)-H(1C3)	109.5
C(7C)-C(2C)-C(3C)	119.7(6)
C(7C)-C(2C)-C(1C)	121.9(6)
C(3C)-C(2C)-C(1C)	118.4(7)
C(4C)-C(3C)-C(2C)	117.6(6)
C(4C)-C(3C)-H(3C)	121.2
C(2C)-C(3C)-H(3C)	121.2
C(3C)-C(4C)-C(5C)	123.5(6)
C(3C)-C(4C)-H(4C)	118.2
C(5C)-C(4C)-H(4C)	118.2
C(6C)-C(5C)-C(4C)	116.7(7)
C(6C)-C(5C)-H(5C)	121.7
C(4C)-C(5C)-H(5C)	121.7
C(7C)-C(6C)-C(5C)	122.3(7)
C(7C)-C(6C)-H(6C)	118.8
C(5C)-C(6C)-H(6C)	118.8
C(6C)-C(7C)-C(2C)	120.1(6)
C(6C)-C(7C)-H(7C)	119.9
C(2C)-C(7C)-H(7C)	119.9
C(2D)-C(1D)-H(1D1)	109.5
C(2D)-C(1D)-H(1D2)	109.5
H(1D1)-C(1D)-H(1D2)	109.5
C(2D)-C(1D)-H(1D3)	109.5
H(1D1)-C(1D)-H(1D3)	109.5
H(1D2)-C(1D)-H(1D3)	109.5
C(3D)-C(2D)-C(7D)	108.4(10)
C(3D)-C(2D)-C(1D)	129.5(11)
C(7D)-C(2D)-C(1D)	122.0(10)
C(4D)-C(3D)-C(2D)	130.5(12)
C(4D)-C(3D)-H(3D)	114.7
C(2D)-C(3D)-H(3D)	114.7
C(3D)-C(4D)-C(5D)	124.4(10)
C(3D)-C(4D)-H(4D)	117.8
C(5D)-C(4D)-H(4D)	117.8
C(4D)-C(5D)-C(6D)	108.5(10)
C(4D)-C(5D)-H(5D)	125.8
C(6D)-C(5D)-H(5D)	125.8
C(7D)-C(6D)-C(5D)	123.7(10)
C(7D)-C(6D)-H(6D)	118.2
C(5D)-C(6D)-H(6D)	118.2
C(6D)-C(7D)-C(2D)	123.9(9)
C(6D)-C(7D)-H(7D)	118.1
C(2D)-C(7D)-H(7D)	118.1

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for $(PCy_3)_2Cl_2Ru=C(H)OEt$ (5). 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}
Ru(1)	192(2)	174(2)	211(2)	-19(2)	22(2)	-8(2)
Cl(1)	242(7)	249(7)	342(8)	-25(6)	18(6)	-63(6)
Cl(2)	238(7)	226(7)	306(7)	53(6)	-10(5)	-40(5)
P(1)	243(8)	233(8)	257(8)	-20(6)	-14(6)	10(6)
P(2)	191(7)	180(7)	240(7)	25(6)	29(6)	-21(6)
O(1A)	590(30)	450(30)	460(20)	-60(20)	160(20)	-20(20)
C(1A)	180(30)	410(30)	440(30)	190(30)	120(30)	60(30)
C(2A)	650(40)	410(40)	430(40)	-190(30)	200(30)	150(30)
C(3A)	850(50)	860(50)	410(40)	-150(40)	170(40)	160(40)
C(4A)	220(30)	200(30)	250(30)	20(20)	0(20)	-40(20)
C(5A)	410(30)	260(30)	290(30)	40(20)	-10(30)	-50(30)
C(6A)	470(40)	250(30)	380(30)	120(30)	10(30)	-20(30)
C(7A)	390(30)	220(30)	450(40)	-10(30)	-50(30)	-40(30)
C(8A)	330(30)	220(30)	400(30)	-10(30)	40(30)	0(30)
C(9A)	350(30)	190(30)	290(30)	20(20)	10(20)	-40(20)
C(10A)	220(30)	140(30)	230(30)	10(20)	0(20)	-30(20)
C(11A)	340(30)	250(30)	320(30)	-80(30)	50(20)	-30(20)
C(12A)	620(40)	290(30)	400(40)	-100(30)	140(30)	-90(30)
C(13A)	550(40)	360(40)	250(30)	-50(30)	150(30)	40(30)
C(14A)	270(30)	480(40)	320(30)	20(30)	60(30)	-30(30)
C(15A)	280(30)	250(30)	300(30)	-80(20)	90(20)	-50(20)
C(16A)	200(30)	230(30)	250(30)	70(20)	-20(20)	-30(20)
C(17A)	190(30)	550(40)	370(30)	170(30)	20(20)	-60(30)
C(18A)	190(30)	640(40)	280(30)	160(30)	-90(20)	-150(30)
C(19A)	130(30)	460(40)	510(40)	90(30)	50(30)	-70(30)
C(20A)	180(30)	610(40)	390(30)	-100(30)	60(30)	-100(30)
C(21A)	210(30)	430(40)	430(30)	-110(30)	90(30)	-50(30)
C(22A)	320(30)	200(30)	220(30)	20(20)	0(20)	20(20)
C(23A)	550(40)	450(40)	350(30)	90(30)	-10(30)	190(30)
C(24A)	750(50)	420(40)	490(40)	240(30)	30(40)	130(30)
C(25A)	840(50)	620(50)	280(40)	130(30)	70(30)	-120(40)
C(26A)	700(50)	460(40)	520(40)	40(30)	330(40)	-30(30)
C(27A)	620(40)	350(40)	420(40)	10(30)	210(30)	0(30)
C(28A)	220(30)	150(30)	290(30)	0(20)	-50(20)	40(20)
C(29A)	300(30)	200(30)	310(30)	-50(20)	40(20)	-40(20)
C(30A)	440(30)	210(30)	370(30)	-50(30)	20(30)	20(30)
C(31A)	450(40)	300(30)	350(30)	-10(30)	130(30)	90(30)
C(32A)	490(40)	330(30)	410(30)	-90(30)	200(30)	-10(30)
C(33A)	300(30)	260(30)	330(30)	-60(30)	80(20)	-50(20)
C(34A)	250(30)	340(30)	470(40)	-230(30)	-50(30)	50(30)
C(35A)	350(40)	960(60)	1310(60)	-840(50)	-280(40)	110(40)
C(36A)	260(30)	490(40)	770(50)	-220(30)	-190(30)	70(30)
C(37A)	550(50)	930(60)	880(60)	-470(50)	-290(40)	-60(40)
C(38A)	400(40)	590(40)	670(40)	-340(30)	-120(30)	30(30)
C(39A)	320(30)	380(40)	410(30)	-50(30)	-50(30)	-70(30)
Ru(2)	212(2)	171(2)	196(2)	5(2)	36(2)	-1(2)
Cl(3)	321(8)	286(8)	417(8)	99(6)	-19(6)	-102(6)
Cl(4)	241(7)	252(7)	285(7)	50(6)	1(6)	-36(6)

P(3)	184(7)	183(7)	209(7)	-2(6)	20(6)	-4(6)
P(4)	286(8)	209(8)	204(7)	15(6)	6(6)	21(6)
C(1B)	210(30)	470(40)	370(30)	110(30)	120(30)	110(30)
O(1B)	460(30)	650(30)	320(20)	-50(20)	130(19)	90(20)
C(2B)	690(50)	1700(80)	460(40)	-670(50)	420(40)	-390(50)
C(3B)	660(60)	2530(120)	1570(90)	-1450(80)	20(60)	160(70)
C(4B)	180(30)	260(30)	180(30)	20(20)	20(20)	-40(20)
C(5B)	270(30)	450(40)	360(30)	-50(30)	70(30)	10(30)
C(6B)	160(30)	700(40)	420(30)	-130(30)	100(30)	-70(30)
C(7B)	200(30)	590(40)	520(40)	-30(30)	10(30)	40(30)
C(8B)	220(30)	990(50)	250(30)	40(30)	-70(20)	-130(30)
C(9B)	280(30)	680(40)	310(30)	70(30)	-20(30)	-40(30)
C(10B)	260(30)	190(30)	200(30)	0(20)	50(20)	60(20)
C(11B)	290(30)	260(30)	240(30)	30(20)	90(20)	10(20)
C(12B)	380(30)	330(30)	200(30)	70(20)	100(20)	60(30)
C(13B)	510(40)	630(40)	300(30)	-40(30)	210(30)	100(30)
C(14B)	730(40)	220(30)	360(30)	-90(30)	100(30)	-30(30)
C(15B)	380(30)	240(30)	320(30)	-90(20)	120(30)	-50(20)
C(16B)	190(30)	210(30)	220(30)	10(20)	70(20)	-40(20)
C(17B)	410(30)	240(30)	260(30)	-70(20)	80(30)	-30(30)
C(18B)	510(40)	180(30)	340(30)	-70(30)	10(30)	10(30)
C(19B)	490(40)	130(30)	420(40)	-40(30)	0(30)	20(30)
C(20B)	600(40)	180(30)	340(30)	60(30)	40(30)	20(30)
C(21B)	490(30)	180(30)	250(30)	20(20)	20(30)	60(30)
C(22B)	310(30)	220(30)	250(30)	20(20)	-10(20)	120(20)
C(23B)	400(40)	560(40)	400(40)	-70(30)	-130(30)	180(30)
C(24B)	300(30)	900(50)	440(40)	-280(30)	-90(30)	230(30)
C(25B)	390(40)	900(50)	530(40)	-200(40)	-200(30)	180(40)
C(26B)	440(40)	460(40)	460(40)	-170(30)	-90(30)	40(30)
C(27B)	240(30)	410(30)	310(30)	-30(30)	-10(20)	50(30)
C(28B)	330(30)	250(30)	260(30)	-20(20)	0(20)	-80(20)
C(29B)	520(40)	400(40)	200(30)	60(30)	10(30)	-120(30)
C(30B)	610(40)	660(40)	270(30)	100(30)	100(30)	-320(30)
C(31B)	720(50)	650(50)	430(40)	220(40)	60(40)	-240(40)
C(32B)	860(50)	370(40)	540(40)	280(30)	-80(40)	-110(40)
C(33B)	560(40)	300(30)	390(40)	120(30)	-10(30)	0(30)
C(34B)	390(30)	250(30)	280(30)	10(20)	-40(30)	160(30)
C(35B)	660(40)	170(30)	360(30)	-30(30)	-40(30)	-60(30)
C(36B)	720(50)	250(30)	470(40)	-150(30)	-130(30)	180(30)
C(37B)	470(40)	520(40)	330(40)	-250(30)	-20(30)	220(30)
C(38B)	510(40)	680(40)	400(40)	-200(30)	60(30)	180(30)
C(39B)	300(30)	490(40)	290(30)	-120(30)	40(30)	0(30)
C(1C)	910(60)	700(50)	1040(60)	-140(50)	390(50)	0(40)
C(2C)	360(40)	550(50)	740(50)	-210(40)	70(40)	20(30)
C(3C)	450(40)	670(50)	800(50)	-40(40)	270(40)	-180(40)
C(4C)	430(40)	530(50)	930(60)	-190(40)	230(40)	-120(30)
C(5C)	550(50)	620(50)	900(60)	-80(40)	300(40)	-80(40)
C(6C)	790(60)	780(60)	650(50)	-190(40)	130(40)	-70(50)
C(7C)	580(50)	570(50)	850(60)	-40(40)	290(40)	-110(40)
C(1D)	730(60)	1090(70)	1020(60)	-10(50)	-80(50)	-400(50)
C(2D)	940(80)	1380(90)	970(80)	260(70)	-40(60)	-180(70)
C(3D)	960(80)	1670(100)	1300(100)	-580(80)	-300(70)	480(80)
C(4D)	1270(90)	1850(110)	830(70)	30(70)	50(70)	120(80)
C(5D)	1090(80)	1070(70)	940(70)	460(60)	160(60)	-40(60)

C(6D)	1180(90)	1860(110)	1360(100)	140(80)	-90(80)	-430(80)
C(7D)	980(80)	880(70)	1390(90)	200(60)	190(70)	100(60)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $(PCy_3)_2Cl_2Ru=C(H)OEt$ (5).

	x	y	z	U_{iso}
H(1A)	2047	5332	3294	40
H(2A1)	702	5616	3727	58
H(2A2)	-706	5455	3732	58
H(3A1)	162	5032	4419	104
H(3A2)	307	5443	4642	104
H(3A3)	1505	5236	4443	104
H(4A)	1977	5712	1756	28
H(5A1)	656	5748	870	39
H(5A2)	-507	5874	1196	39
H(6A1)	1824	6274	1182	45
H(6A2)	457	6395	857	45
H(7A1)	-297	6497	1736	44
H(7A2)	998	6723	1733	44
H(8A1)	2157	6280	2293	39
H(8A2)	998	6411	2616	39
H(9A1)	-185	5897	2295	34
H(9A2)	1162	5774	2639	34
H(10A)	733	5144	784	24
H(11A)	1759	4507	1375	36
H(11B)	329	4550	1055	36
H(12A)	1039	4580	160	52
H(12B)	1636	4222	484	52
H(13A)	3583	4513	735	45
H(13B)	3187	4546	52	45
H(14A)	2506	5145	148	43
H(14B)	3951	5108	455	43
H(15A)	3270	5069	1364	33
H(15B)	2687	5431	1052	33
H(16A)	-925	4811	1741	28
H(17A)	-1774	5410	1030	45
H(17B)	-1253	5035	798	45
H(18A)	-2915	4707	1133	46
H(18B)	-3527	5027	721	46
H(19A)	-4507	4989	1560	44
H(19B)	-3853	5378	1510	44
H(20A)	-3345	5169	2448	47
H(20B)	-2806	4795	2224	47
H(21A)	-1677	5498	2118	43
H(21B)	-1074	5182	2541	43
H(22A)	2067	4034	3377	30
H(23A)	4311	3998	4196	55
H(23B)	4058	3755	3623	55
H(24A)	2301	3476	3953	67
H(24B)	3535	3426	4426	67
H(25A)	2868	3897	4974	70
H(25B)	1755	3598	4858	70
H(26A)	671	3952	4119	64
H(26B)	925	4194	4691	64

H(27A)	1375	4522	3878	54
H(27B)	2614	4489	4352	54
H(28A)	4816	4040	2874	28
H(29A)	2864	3724	2709	32
H(29B)	2392	3982	2170	32
H(30A)	4484	3483	2237	41
H(30B)	3149	3436	1831	41
H(31A)	3585	3931	1271	43
H(31B)	4760	3653	1306	43
H(32A)	5956	4006	1996	48
H(32B)	5463	4259	1454	48
H(33A)	5196	4555	2331	35
H(33B)	3850	4502	1935	35
H(34A)	4998	4894	3252	44
H(35A)	6219	4435	3226	109
H(35B)	5980	4304	3852	109
H(36A)	7899	4585	3993	64
H(36B)	7409	4918	3581	64
H(37A)	6891	4793	4716	99
H(37B)	7570	5141	4484	99
H(38A)	5766	5360	4047	68
H(38B)	5487	5235	4670	68
H(39A)	4315	4760	4321	45
H(39B)	3866	5088	3893	45
H(1B)	2217	7098	2590	41
H(2B1)	3920	6753	2232	110
H(2B2)	3227	7026	1756	110
H(3B1)	5056	7277	1688	240
H(3B2)	5016	6851	1538	240
H(3B3)	5730	6989	2146	240
H(4B)	5303	7597	4173	25
H(5B1)	6091	6923	3770	43
H(5B2)	5460	7241	3357	43
H(6B1)	7135	7634	3678	51
H(6B2)	7719	7265	3458	51
H(7B1)	8284	7064	4383	53
H(7B2)	8830	7469	4344	53
H(8B1)	7219	7706	4799	60
H(8B2)	7865	7379	5186	60
H(9B1)	6179	6991	4849	51
H(9B2)	5609	7352	5102	51
H(10B)	3614	7268	5102	26
H(11C)	1091	7363	4507	31
H(11D)	1625	6995	4819	31
H(12C)	1797	7277	5724	36
H(12D)	367	7325	5406	36
H(13C)	787	7925	5152	56
H(13D)	1182	7881	5835	56
H(14C)	3323	7826	5726	52
H(14D)	2781	8191	5409	52
H(15C)	2635	7910	4511	37
H(15D)	4059	7862	4835	37
H(16B)	2346	6703	4115	24
H(17C)	3224	6649	3251	36

H(17D)	4557	6527	3609	36
H(18C)	3420	6003	3272	42
H(18D)	2207	6131	3562	42
H(19C)	4623	5922	4175	42
H(19D)	3323	5696	4159	42
H(20C)	3783	6021	5027	45
H(20D)	2449	6149	4676	45
H(21C)	3639	6666	5017	37
H(21D)	4813	6535	4701	37
H(22B)	-674	7595	2643	32
H(23C)	-1678	8159	2584	56
H(23D)	-1324	8214	1946	56
H(24C)	-3417	7991	1879	67
H(24D)	-2946	7652	2284	67
H(25C)	-3217	7454	1307	76
H(25D)	-2284	7769	1140	76
H(26C)	-1158	7226	1242	56
H(26D)	-1545	7166	1873	56
H(27C)	540	7382	1969	39
H(27D)	115	7722	1559	39
H(28B)	2519	8401	2526	34
H(29C)	2094	7882	1624	45
H(29D)	3260	7875	2139	45
H(30C)	4114	8409	1808	61
H(30D)	3860	8135	1272	61
H(31C)	2016	8442	909	73
H(31D)	3158	8731	1017	73
H(32C)	1325	8957	1363	72
H(32D)	2477	8916	1880	72
H(33C)	597	8684	2170	51
H(33D)	420	8409	1632	51
H(34B)	-195	8455	3008	38
H(35C)	1821	8725	3183	49
H(35D)	2237	8454	3711	49
H(36C)	300	8996	3679	60
H(36D)	1666	9013	4070	60
H(37C)	1131	8510	4613	54
H(37D)	72	8820	4626	54
H(38C)	-1309	8519	3921	64
H(38D)	-887	8243	4442	64
H(39C)	572	7957	3925	43
H(39D)	-789	7961	3530	43
H(1C1)	10074	6323	3798	129
H(1C2)	9220	6147	4239	129
H(1C3)	9124	6573	4102	129
H(3C)	7262	5891	3889	75
H(4C)	5714	5756	3112	74
H(5C)	5705	6020	2220	80
H(6C)	7225	6461	2123	88
H(7C)	8798	6600	2866	78
H(1D1)	2471	3215	9600	144
H(1D2)	2142	3467	9042	144
H(1D3)	1840	3607	9657	144
H(3D)	4237	3434	10278	163

H(4D)	6120	3747	10508	159
H(5D)	7006	4103	9851	124
H(6D)	5619	4148	8946	179
H(7D)	3535	3923	8835	130

Table 7. Crystal data and structure refinement for $(PCy_3)_2Cl_2Ru=C(H)SPh$ (7).

Empirical formula	$C_{43}H_{72}Cl_2P_2RuS \cdot C_7H_8$
Formula weight	947.11
Crystallization Solvent	Toluene
Crystal Habit	Plate
Crystal size	1.66 x 0.28 x 0.19 mm^3
Crystal color	Deep purple

Data Collection

Preliminary Photos	Rotation	
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	98(2) K	
θ range for 17589 reflections used in lattice determination	2.21 to 28.19°	
Unit cell dimensions	a = 9.8211(5) Å b = 13.6315(7) Å c = 18.7911(10) Å	α= 83.4410(10)° β= 78.7320(10)° γ = 78.1900(10)°
Volume	2407.7(2) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.306 Mg/m^3	
F(000)	1008	
Data collection program	Bruker SMART	
θ range for data collection	1.53 to 28.34°	
Completeness to θ = 28.34°	91.7 %	
Index ranges	$-13 \le h \le 12$, $-17 \le k \le 17$, $-24 \le l \le 25$	
Data collection scan type	ω scans at 6 ϕ settings	
Data reduction program	Bruker SAINT v6.2	
Reflections collected	41923	
Independent reflections	11011 [R_{int}= 0.0526]	
Absorption coefficient	0.579 mm^{-1}	
Absorption correction	None	
Max. and min. transmission (theoretical)	0.9004 and 0.4455	

Table 7 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	11011 / 0 / 506
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.935
Final R indices [I>2σ(I), 8708 reflections]	R1 = 0.0482, *w*R2 = 0.0890
R indices (all data)	R1 = 0.0618, *w*R2 = 0.0906
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	7.640
Average shift/error	0.161
Largest diff. peak and hole	1.972 and -2.244 e.Å^{-3}

Special Refinement Details

One cyclohexal ring, C38 to C43, contains atomic ellipsoids that are significantly elongated which may suggest a possibly different orientation for that ring. The largest peaks in the difference map appear near this ring. No attempt was made to model any other configuration. Analysis of the data suggest no other remedy.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

The crystallographic data has been deposited in the Cambridge Database (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 154097.

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $(PCy_3)_2Cl_2Ru=C(H)SPh$ (7). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	8200(1)	7637(1)	7462(1)	17(1)
S(1)	9880(1)	5375(1)	7536(1)	30(1)
Cl(1)	9562(1)	8941(1)	7126(1)	21(1)
Cl(2)	6580(1)	6497(1)	7810(1)	23(1)
P(1)	8183(1)	7882(1)	8711(1)	17(1)
P(2)	7769(1)	7780(1)	6228(1)	18(1)
C(1)	9771(3)	6645(2)	7323(2)	19(1)
C(2)	11687(3)	4839(2)	7246(2)	26(1)
C(3)	12800(3)	5238(2)	7380(2)	30(1)
C(4)	14182(4)	4753(3)	7173(2)	40(1)
C(5)	14453(4)	3863(3)	6843(2)	46(1)
C(6)	13346(4)	3459(3)	6717(2)	42(1)
C(7)	11965(4)	3939(2)	6918(2)	35(1)
C(8)	6189(3)	8763(2)	6123(2)	18(1)
C(9)	6404(3)	9827(2)	6203(2)	21(1)
C(10)	5106(3)	10614(2)	6076(2)	26(1)
C(11)	3772(3)	10391(2)	6574(2)	26(1)
C(12)	3549(3)	9332(2)	6498(2)	28(1)
C(13)	4841(3)	8540(2)	6634(2)	23(1)
C(14)	7300(3)	6647(2)	5950(2)	20(1)
C(15)	6453(3)	6763(2)	5332(2)	25(1)
C(16)	6001(3)	5774(2)	5260(2)	28(1)
C(17)	7252(3)	4906(2)	5163(2)	33(1)
C(18)	8108(3)	4810(2)	5771(2)	29(1)
C(19)	8585(3)	5797(2)	5811(2)	24(1)
C(20)	9170(3)	8212(2)	5521(2)	18(1)
C(21)	10672(3)	7605(2)	5540(2)	22(1)
C(22)	11770(3)	8082(2)	4989(2)	25(1)
C(23)	11432(3)	8210(2)	4227(2)	27(1)
C(24)	9965(3)	8827(2)	4215(2)	27(1)
C(25)	8860(3)	8351(2)	4745(2)	26(1)
C(26)	6869(3)	9052(2)	8920(2)	19(1)
C(27)	5649(3)	9077(2)	8511(2)	24(1)
C(28)	4467(3)	9976(2)	8686(2)	37(1)
C(29)	5015(4)	10964(2)	8527(2)	37(1)
C(30)	6226(3)	10932(2)	8931(2)	27(1)
C(31)	7419(3)	10042(2)	8736(2)	27(1)
C(32)	9837(3)	8147(2)	8916(2)	18(1)
C(33)	9786(3)	8293(2)	9715(2)	23(1)
C(34)	11104(3)	8650(3)	9821(2)	30(1)
C(35)	12433(3)	7924(3)	9526(2)	30(1)
C(36)	12499(3)	7759(2)	8736(2)	26(1)
C(37)	11176(3)	7412(2)	8620(2)	21(1)
C(38)	7518(3)	6948(2)	9428(2)	34(1)
C(39)	8462(3)	5920(2)	9404(2)	25(1)
C(40)	7905(5)	5161(3)	9957(3)	83(2)
C(41)	6813(8)	5310(3)	10449(3)	164(4)
C(42)	5894(5)	6340(3)	10480(2)	69(2)

C(43)	6446(9)	7112(4)	9920(5)	288(8)
C(1A)	7275(5)	3567(4)	8040(4)	142(3)
C(2A)	8633(5)	2952(4)	8100(3)	85(2)
C(3A)	9582(6)	3153(3)	8454(3)	64(2)
C(4A)	10852(7)	2583(5)	8471(3)	84(2)
C(5A)	11234(5)	1682(4)	8170(3)	66(1)
C(6A)	10304(6)	1421(3)	7829(3)	66(1)
C(7A)	9021(5)	2002(3)	7763(2)	52(1)

Table 9. Selected bond lengths [Å] and angles [°] for $(PCy_3)_2Cl_2Ru=C(H)SPh$ (7).

Ru(1)-C(1)	1.830(3)	C(1)-Ru(1)-Cl(1)	92.56(9)
Ru(1)-Cl(1)	2.3951(8)	C(1)-Ru(1)-Cl(2)	94.61(9)
Ru(1)-Cl(2)	2.3966(8)	Cl(1)-Ru(1)-Cl(2)	172.81(3)
Ru(1)-P(1)	2.4045(9)	C(1)-Ru(1)-P(1)	98.43(9)
Ru(1)-P(2)	2.4167(9)	Cl(1)-Ru(1)-P(1)	87.55(3)
S(1)-C(1)	1.718(3)	Cl(2)-Ru(1)-P(1)	91.87(3)
S(1)-C(2)	1.778(3)	C(1)-Ru(1)-P(2)	95.95(9)
		Cl(1)-Ru(1)-P(2)	88.96(3)
		Cl(2)-Ru(1)-P(2)	89.83(3)
		P(1)-Ru(1)-P(2)	165.34(3)
		C(1)-S(1)-C(2)	105.07(15)
		S(1)-C(1)-Ru(1)	127.88(18)

Table 10. Bond lengths [Å] and angles [°] for $(PCy_3)_2Cl_2Ru=C(H)SPh$ (7).

Ru(1)-C(1)	1.830(3)	C(17)-C(18)	1.525(5)
Ru(1)-Cl(1)	2.3951(8)	C(17)-H(17A)	0.9900
Ru(1)-Cl(2)	2.3966(8)	C(17)-H(17B)	0.9900
Ru(1)-P(1)	2.4045(9)	C(18)-C(19)	1.527(4)
Ru(1)-P(2)	2.4167(9)	C(18)-H(18A)	0.9900
S(1)-C(1)	1.718(3)	C(18)-H(18B)	0.9900
S(1)-C(2)	1.778(3)	C(19)-H(19A)	0.9900
P(1)-C(32)	1.853(3)	C(19)-H(19B)	0.9900
P(1)-C(26)	1.861(3)	C(20)-C(25)	1.530(4)
P(1)-C(38)	1.862(3)	C(20)-C(21)	1.541(4)
P(2)-C(14)	1.855(3)	C(20)-H(20)	1.0000
P(2)-C(20)	1.856(3)	C(21)-C(22)	1.534(4)
P(2)-C(8)	1.857(3)	C(21)-H(21A)	0.9900
C(1)-H(1)	0.9500	C(21)-H(21B)	0.9900
C(2)-C(7)	1.389(4)	C(22)-C(23)	1.517(4)
C(2)-C(3)	1.391(4)	C(22)-H(22A)	0.9900
C(3)-C(4)	1.383(4)	C(22)-H(22B)	0.9900
C(3)-H(3)	0.9500	C(23)-C(24)	1.515(4)
C(4)-C(5)	1.380(5)	C(23)-H(23A)	0.9900
C(4)-H(4)	0.9500	C(23)-H(23B)	0.9900
C(5)-C(6)	1.385(5)	C(24)-C(25)	1.520(4)
C(5)-H(5)	0.9500	C(24)-H(24A)	0.9900
C(6)-C(7)	1.379(5)	C(24)-H(24B)	0.9900
C(6)-H(6)	0.9500	C(25)-H(25A)	0.9900
C(7)-H(7)	0.9500	C(25)-H(25B)	0.9900
C(8)-C(9)	1.536(4)	C(26)-C(31)	1.533(4)
C(8)-C(13)	1.539(4)	C(26)-C(27)	1.538(4)
C(8)-H(8)	1.0000	C(26)-H(26)	1.0000
C(9)-C(10)	1.528(4)	C(27)-C(28)	1.522(4)
C(9)-H(9A)	0.9900	C(27)-H(27A)	0.9900
C(9)-H(9B)	0.9900	C(27)-H(27B)	0.9900
C(10)-C(11)	1.518(4)	C(28)-C(29)	1.528(5)
C(10)-H(10A)	0.9900	C(28)-H(28A)	0.9900
C(10)-H(10B)	0.9900	C(28)-H(28B)	0.9900
C(11)-C(12)	1.530(4)	C(29)-C(30)	1.523(4)
C(11)-H(11A)	0.9900	C(29)-H(29A)	0.9900
C(11)-H(11B)	0.9900	C(29)-H(29B)	0.9900
C(12)-C(13)	1.531(4)	C(30)-C(31)	1.528(4)
C(12)-H(12A)	0.9900	C(30)-H(30A)	0.9900
C(12)-H(12B)	0.9900	C(30)-H(30B)	0.9900
C(13)-H(13A)	0.9900	C(31)-H(31A)	0.9900
C(13)-H(13B)	0.9900	C(31)-H(31B)	0.9900
C(14)-C(15)	1.531(4)	C(32)-C(33)	1.527(4)
C(14)-C(19)	1.532(4)	C(32)-C(37)	1.531(4)
C(14)-H(14)	1.0000	C(32)-H(32)	1.0000
C(15)-C(16)	1.532(4)	C(33)-C(34)	1.527(4)
C(15)-H(15A)	0.9900	C(33)-H(33A)	0.9900
C(15)-H(15B)	0.9900	C(33)-H(33B)	0.9900
C(16)-C(17)	1.519(4)	C(34)-C(35)	1.518(4)
C(16)-H(16A)	0.9900	C(34)-H(34A)	0.9900
C(16)-H(16B)	0.9900	C(34)-H(34B)	0.9900

C(35)-C(36)	1.515(4)	C(32)-P(1)-Ru(1)	116.13(10)
C(35)-H(35A)	0.9900	C(26)-P(1)-Ru(1)	105.98(10)
C(35)-H(35B)	0.9900	C(38)-P(1)-Ru(1)	118.10(13)
C(36)-C(37)	1.531(4)	C(14)-P(2)-C(20)	109.66(14)
C(36)-H(36A)	0.9900	C(14)-P(2)-C(8)	102.65(13)
C(36)-H(36B)	0.9900	C(20)-P(2)-C(8)	102.75(13)
C(37)-H(37A)	0.9900	C(14)-P(2)-Ru(1)	114.68(10)
C(37)-H(37B)	0.9900	C(20)-P(2)-Ru(1)	115.34(10)
C(38)-C(43)	1.259(5)	C(8)-P(2)-Ru(1)	110.34(10)
C(38)-C(39)	1.514(4)	S(1)-C(1)-Ru(1)	127.88(18)
C(38)-H(38)	1.0000	S(1)-C(1)-H(1)	116.1
C(39)-C(40)	1.488(4)	Ru(1)-C(1)-H(1)	116.1
C(39)-H(39A)	0.9900	C(7)-C(2)-C(3)	119.7(3)
C(39)-H(39B)	0.9900	C(7)-C(2)-S(1)	116.8(3)
C(40)-C(41)	1.270(5)	C(3)-C(2)-S(1)	123.3(3)
C(40)-H(40A)	0.9900	C(4)-C(3)-C(2)	120.3(3)
C(40)-H(40B)	0.9900	C(4)-C(3)-H(3)	119.9
C(41)-C(42)	1.506(5)	C(2)-C(3)-H(3)	119.8
C(41)-H(41A)	0.9900	C(5)-C(4)-C(3)	119.7(4)
C(41)-H(41B)	0.9900	C(5)-C(4)-H(4)	120.2
C(42)-C(43)	1.505(5)	C(3)-C(4)-H(4)	120.1
C(42)-H(42A)	0.9900	C(4)-C(5)-C(6)	120.1(3)
C(42)-H(42B)	0.9900	C(4)-C(5)-H(5)	120.0
C(43)-H(43A)	0.9900	C(6)-C(5)-H(5)	119.9
C(43)-H(43B)	0.9900	C(7)-C(6)-C(5)	120.6(3)
C(1A)-C(2A)	1.440(6)	C(7)-C(6)-H(6)	119.6
C(1A)-H(1A1)	0.9800	C(5)-C(6)-H(6)	119.7
C(1A)-H(1A2)	0.9800	C(6)-C(7)-C(2)	119.5(3)
C(1A)-H(1A3)	0.9800	C(6)-C(7)-H(7)	120.3
C(2A)-C(3A)	1.333(7)	C(2)-C(7)-H(7)	120.2
C(2A)-C(7A)	1.454(7)	C(9)-C(8)-C(13)	110.5(2)
C(3A)-C(4A)	1.332(7)	C(9)-C(8)-P(2)	113.1(2)
C(3A)-H(3A)	0.9500	C(13)-C(8)-P(2)	112.7(2)
C(4A)-C(5A)	1.363(7)	C(9)-C(8)-H(8)	106.7
C(4A)-H(4A)	0.9500	C(13)-C(8)-H(8)	106.7
C(5A)-C(6A)	1.337(6)	P(2)-C(8)-H(8)	106.7
C(5A)-H(5A)	0.9500	C(10)-C(9)-C(8)	111.2(2)
C(6A)-C(7A)	1.364(6)	C(10)-C(9)-H(9A)	109.4
C(6A)-H(6A)	0.9500	C(8)-C(9)-H(9A)	109.4
C(7A)-H(7A)	0.9500	C(10)-C(9)-H(9B)	109.4
		C(8)-C(9)-H(9B)	109.4
C(1)-Ru(1)-Cl(1)	92.56(9)	H(9A)-C(9)-H(9B)	108.0
C(1)-Ru(1)-Cl(2)	94.61(9)	C(11)-C(10)-C(9)	111.8(3)
Cl(1)-Ru(1)-Cl(2)	172.81(3)	C(11)-C(10)-H(10A)	109.3
C(1)-Ru(1)-P(1)	98.43(9)	C(9)-C(10)-H(10A)	109.2
Cl(1)-Ru(1)-P(1)	87.55(3)	C(11)-C(10)-H(10B)	109.3
Cl(2)-Ru(1)-P(1)	91.87(3)	C(9)-C(10)-H(10B)	109.2
C(1)-Ru(1)-P(2)	95.95(9)	H(10A)-C(10)-H(10B)	107.9
Cl(1)-Ru(1)-P(2)	88.96(3)	C(10)-C(11)-C(12)	111.2(3)
Cl(2)-Ru(1)-P(2)	89.83(3)	C(10)-C(11)-H(11A)	109.4
P(1)-Ru(1)-P(2)	165.34(3)	C(12)-C(11)-H(11A)	109.4
C(1)-S(1)-C(2)	105.07(15)	C(10)-C(11)-H(11B)	109.4
C(32)-P(1)-C(26)	103.79(13)	C(12)-C(11)-H(11B)	109.4
C(32)-P(1)-C(38)	108.55(16)	H(11A)-C(11)-H(11B)	108.0
C(26)-P(1)-C(38)	102.27(14)	C(11)-C(12)-C(13)	111.2(3)

C(11)-C(12)-H(12A)	109.4	C(20)-C(21)-H(21A)	109.6
C(13)-C(12)-H(12A)	109.4	C(22)-C(21)-H(21B)	109.4
C(11)-C(12)-H(12B)	109.3	C(20)-C(21)-H(21B)	109.4
C(13)-C(12)-H(12B)	109.4	H(21A)-C(21)-H(21B)	108.1
H(12A)-C(12)-H(12B)	108.0	C(23)-C(22)-C(21)	111.9(3)
C(12)-C(13)-C(8)	111.1(2)	C(23)-C(22)-H(22A)	109.2
C(12)-C(13)-H(13A)	109.4	C(21)-C(22)-H(22A)	109.2
C(8)-C(13)-H(13A)	109.4	C(23)-C(22)-H(22B)	109.3
C(12)-C(13)-H(13B)	109.4	C(21)-C(22)-H(22B)	109.2
C(8)-C(13)-H(13B)	109.4	H(22A)-C(22)-H(22B)	107.9
H(13A)-C(13)-H(13B)	108.0	C(22)-C(23)-C(24)	110.7(3)
C(15)-C(14)-C(19)	109.6(3)	C(22)-C(23)-H(23A)	109.5
C(15)-C(14)-P(2)	119.1(2)	C(24)-C(23)-H(23A)	109.5
C(19)-C(14)-P(2)	112.0(2)	C(22)-C(23)-H(23B)	109.5
C(15)-C(14)-H(14)	104.9	C(24)-C(23)-H(23B)	109.5
C(19)-C(14)-H(14)	105.0	H(23A)-C(23)-H(23B)	108.1
P(2)-C(14)-H(14)	104.9	C(23)-C(24)-C(25)	110.9(3)
C(14)-C(15)-C(16)	110.7(3)	C(23)-C(24)-H(24A)	109.4
C(14)-C(15)-H(15A)	109.5	C(25)-C(24)-H(24A)	109.4
C(16)-C(15)-H(15A)	109.5	C(23)-C(24)-H(24B)	109.5
C(14)-C(15)-H(15B)	109.6	C(25)-C(24)-H(24B)	109.5
C(16)-C(15)-H(15B)	109.5	H(24A)-C(24)-H(24B)	108.1
H(15A)-C(15)-H(15B)	108.1	C(24)-C(25)-C(20)	111.9(3)
C(17)-C(16)-C(15)	112.0(3)	C(24)-C(25)-H(25A)	109.3
C(17)-C(16)-H(16A)	109.2	C(20)-C(25)-H(25A)	109.2
C(15)-C(16)-H(16A)	109.2	C(24)-C(25)-H(25B)	109.3
C(17)-C(16)-H(16B)	109.2	C(20)-C(25)-H(25B)	109.2
C(15)-C(16)-H(16B)	109.2	H(25A)-C(25)-H(25B)	107.9
H(16A)-C(16)-H(16B)	107.9	C(31)-C(26)-C(27)	109.4(2)
C(16)-C(17)-C(18)	111.2(3)	C(31)-C(26)-P(1)	116.3(2)
C(16)-C(17)-H(17A)	109.4	C(27)-C(26)-P(1)	107.5(2)
C(18)-C(17)-H(17A)	109.4	C(31)-C(26)-H(26)	107.8
C(16)-C(17)-H(17B)	109.4	C(27)-C(26)-H(26)	107.8
C(18)-C(17)-H(17B)	109.4	P(1)-C(26)-H(26)	107.8
H(17A)-C(17)-H(17B)	108.0	C(28)-C(27)-C(26)	111.6(3)
C(17)-C(18)-C(19)	110.4(3)	C(28)-C(27)-H(27A)	109.4
C(17)-C(18)-H(18A)	109.6	C(26)-C(27)-H(27A)	109.3
C(19)-C(18)-H(18A)	109.6	C(28)-C(27)-H(27B)	109.3
C(17)-C(18)-H(18B)	109.6	C(26)-C(27)-H(27B)	109.3
C(19)-C(18)-H(18B)	109.6	H(27A)-C(27)-H(27B)	108.0
H(18A)-C(18)-H(18B)	108.1	C(27)-C(28)-C(29)	111.5(3)
C(18)-C(19)-C(14)	110.2(2)	C(27)-C(28)-H(28A)	109.4
C(18)-C(19)-H(19A)	109.6	C(29)-C(28)-H(28A)	109.3
C(14)-C(19)-H(19A)	109.6	C(27)-C(28)-H(28B)	109.2
C(18)-C(19)-H(19B)	109.6	C(29)-C(28)-H(28B)	109.3
C(14)-C(19)-H(19B)	109.6	H(28A)-C(28)-H(28B)	108.0
H(19A)-C(19)-H(19B)	108.1	C(30)-C(29)-C(28)	110.3(3)
C(25)-C(20)-C(21)	110.6(2)	C(30)-C(29)-H(29A)	109.6
C(25)-C(20)-P(2)	115.2(2)	C(28)-C(29)-H(29A)	109.6
C(21)-C(20)-P(2)	114.7(2)	C(30)-C(29)-H(29B)	109.6
C(25)-C(20)-H(20)	105.1	C(28)-C(29)-H(29B)	109.6
C(21)-C(20)-H(20)	105.0	H(29A)-C(29)-H(29B)	108.1
P(2)-C(20)-H(20)	105.0	C(29)-C(30)-C(31)	111.3(3)
C(22)-C(21)-C(20)	110.8(2)	C(29)-C(30)-H(30A)	109.4
C(22)-C(21)-H(21A)	109.5	C(31)-C(30)-H(30A)	109.4

C(29)-C(30)-H(30B)	109.4	C(38)-C(39)-H(39B)	110.3
C(31)-C(30)-H(30B)	109.4	H(39A)-C(39)-H(39B)	107.7
H(30A)-C(30)-H(30B)	108.0	C(41)-C(40)-C(39)	127.1(4)
C(30)-C(31)-C(26)	110.4(3)	C(41)-C(40)-H(40A)	105.4
C(30)-C(31)-H(31A)	109.6	C(39)-C(40)-H(40A)	105.5
C(26)-C(31)-H(31A)	109.6	C(41)-C(40)-H(40B)	105.7
C(30)-C(31)-H(31B)	109.6	C(39)-C(40)-H(40B)	105.5
C(26)-C(31)-H(31B)	109.5	H(40A)-C(40)-H(40B)	106.1
H(31A)-C(31)-H(31B)	108.1	C(40)-C(41)-C(42)	119.2(4)
C(33)-C(32)-C(37)	110.8(2)	C(40)-C(41)-H(41A)	107.3
C(33)-C(32)-P(1)	114.5(2)	C(42)-C(41)-H(41A)	107.4
C(37)-C(32)-P(1)	114.6(2)	C(40)-C(41)-H(41B)	107.7
C(33)-C(32)-H(32)	105.3	C(42)-C(41)-H(41B)	107.6
C(37)-C(32)-H(32)	105.3	H(41A)-C(41)-H(41B)	107.0
P(1)-C(32)-H(32)	105.3	C(41)-C(42)-C(43)	113.9(3)
C(34)-C(33)-C(32)	111.2(3)	C(41)-C(42)-H(42A)	108.9
C(34)-C(33)-H(33A)	109.4	C(43)-C(42)-H(42A)	109.1
C(32)-C(33)-H(33A)	109.4	C(41)-C(42)-H(42B)	108.7
C(34)-C(33)-H(33B)	109.4	C(43)-C(42)-H(42B)	108.4
C(32)-C(33)-H(33B)	109.4	H(42A)-C(42)-H(42B)	107.7
H(33A)-C(33)-H(33B)	108.0	C(38)-C(43)-C(42)	125.9(4)
C(35)-C(34)-C(33)	110.8(3)	C(38)-C(43)-H(43A)	104.7
C(35)-C(34)-H(34A)	109.5	C(42)-C(43)-H(43A)	106.1
C(33)-C(34)-H(34A)	109.5	C(38)-C(43)-H(43B)	107.1
C(35)-C(34)-H(34B)	109.4	C(42)-C(43)-H(43B)	105.5
C(33)-C(34)-H(34B)	109.5	H(43A)-C(43)-H(43B)	106.2
H(34A)-C(34)-H(34B)	108.0	C(2A)-C(1A)-H(1A1)	109.5
C(36)-C(35)-C(34)	111.7(3)	C(2A)-C(1A)-H(1A2)	109.5
C(36)-C(35)-H(35A)	109.3	H(1A1)-C(1A)-H(1A2)	109.5
C(34)-C(35)-H(35A)	109.3	C(2A)-C(1A)-H(1A3)	109.4
C(36)-C(35)-H(35B)	109.2	H(1A1)-C(1A)-H(1A3)	109.5
C(34)-C(35)-H(35B)	109.3	H(1A2)-C(1A)-H(1A3)	109.5
H(35A)-C(35)-H(35B)	107.9	C(3A)-C(2A)-C(1A)	126.3(7)
C(35)-C(36)-C(37)	111.8(3)	C(3A)-C(2A)-C(7A)	115.4(4)
C(35)-C(36)-H(36A)	109.3	C(1A)-C(2A)-C(7A)	118.2(7)
C(37)-C(36)-H(36A)	109.3	C(2A)-C(3A)-C(4A)	124.4(5)
C(35)-C(36)-H(36B)	109.2	C(2A)-C(3A)-H(3A)	117.9
C(37)-C(36)-H(36B)	109.3	C(4A)-C(3A)-H(3A)	117.8
H(36A)-C(36)-H(36B)	107.9	C(3A)-C(4A)-C(5A)	121.3(5)
C(32)-C(37)-C(36)	110.8(2)	C(3A)-C(4A)-H(4A)	119.3
C(32)-C(37)-H(37A)	109.5	C(5A)-C(4A)-H(4A)	119.4
C(36)-C(37)-H(37A)	109.5	C(6A)-C(5A)-C(4A)	117.0(5)
C(32)-C(37)-H(37B)	109.4	C(6A)-C(5A)-H(5A)	121.6
C(36)-C(37)-H(37B)	109.5	C(4A)-C(5A)-H(5A)	121.4
H(37A)-C(37)-H(37B)	108.1	C(5A)-C(6A)-C(7A)	123.9(5)
C(43)-C(38)-C(39)	120.2(3)	C(5A)-C(6A)-H(6A)	118.0
C(43)-C(38)-P(1)	126.6(3)	C(7A)-C(6A)-H(6A)	118.0
C(39)-C(38)-P(1)	113.1(2)	C(6A)-C(7A)-C(2A)	117.8(5)
C(43)-C(38)-H(38)	89.0	C(6A)-C(7A)-H(7A)	121.2
C(39)-C(38)-H(38)	88.8	C(2A)-C(7A)-H(7A)	121.0
P(1)-C(38)-H(38)	89.2		
C(40)-C(39)-C(38)	113.3(3)		
C(40)-C(39)-H(39A)	109.0		
C(38)-C(39)-H(39A)	107.5		
C(40)-C(39)-H(39B)	108.9		

Table 11. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for $(PCy_3)_2Cl_2Ru=C(H)SPh$ (7). 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}
Ru(1)	160(1)	137(1)	207(2)	-9(1)	-39(1)	-39(1)
S(1)	258(5)	177(4)	424(6)	13(4)	-16(4)	-13(4)
Cl(1)	237(4)	187(4)	224(4)	1(3)	-55(3)	-91(3)
Cl(2)	227(4)	231(4)	249(5)	-8(3)	-40(3)	-105(3)
P(1)	161(4)	157(4)	198(5)	-17(3)	-20(3)	-39(3)
P(2)	175(4)	159(4)	202(5)	-15(3)	-33(3)	-53(3)
C(1)	207(17)	211(16)	172(18)	-6(13)	-47(14)	-82(13)
C(2)	263(18)	214(17)	240(20)	15(14)	-2(15)	17(14)
C(3)	310(20)	254(18)	310(20)	-11(16)	-44(17)	11(16)
C(4)	300(20)	320(20)	510(30)	5(18)	-17(19)	-5(17)
C(5)	330(20)	390(20)	530(30)	-40(20)	90(20)	51(19)
C(6)	500(30)	260(20)	410(30)	-110(17)	60(20)	20(18)
C(7)	380(20)	270(19)	350(20)	-43(16)	1(18)	-52(17)
C(8)	164(16)	192(16)	191(18)	-26(13)	-53(13)	-25(13)
C(9)	201(17)	200(16)	227(19)	-30(14)	-34(14)	-32(13)
C(10)	243(18)	213(17)	300(20)	-42(15)	-63(15)	22(14)
C(11)	205(17)	300(19)	270(20)	-56(15)	-67(15)	32(14)
C(12)	180(17)	340(20)	310(20)	2(16)	-53(15)	-36(15)
C(13)	209(17)	237(17)	243(19)	-16(14)	-57(14)	-55(14)
C(14)	209(17)	167(15)	226(18)	-40(13)	-23(14)	-79(13)
C(15)	249(18)	260(18)	280(20)	-72(15)	-33(15)	-90(14)
C(16)	282(19)	295(19)	320(20)	-78(16)	-56(16)	-142(15)
C(17)	310(20)	245(18)	460(20)	-148(17)	-5(18)	-136(16)
C(18)	286(19)	178(17)	390(20)	-76(15)	14(17)	-72(14)
C(19)	257(18)	191(16)	300(20)	-62(14)	-36(15)	-53(14)
C(20)	191(16)	160(15)	182(17)	-9(13)	-13(13)	-73(13)
C(21)	190(17)	203(16)	241(19)	-14(14)	-11(14)	-38(13)
C(22)	218(17)	215(17)	300(20)	-27(15)	-15(15)	-64(14)
C(23)	301(19)	246(18)	260(20)	-59(15)	49(15)	-150(15)
C(24)	350(20)	276(18)	188(19)	-7(15)	-25(15)	-109(16)
C(25)	276(18)	263(18)	230(20)	-34(15)	-18(15)	-67(15)
C(26)	163(16)	191(16)	211(18)	-34(13)	-15(13)	-20(13)
C(27)	256(18)	210(17)	270(20)	-75(14)	-75(15)	-3(14)
C(28)	260(19)	300(20)	590(30)	-127(18)	-194(19)	32(16)
C(29)	380(20)	230(19)	520(30)	-78(17)	-190(20)	57(16)
C(30)	266(19)	176(16)	360(20)	-78(15)	-32(16)	-11(14)
C(31)	244(18)	178(16)	370(20)	-45(15)	-29(16)	-35(14)
C(32)	180(16)	185(16)	184(18)	-27(13)	-39(13)	-55(13)
C(33)	238(18)	268(18)	203(19)	-46(14)	-28(14)	-71(14)
C(34)	330(20)	380(20)	220(20)	-87(16)	-51(16)	-141(17)
C(35)	230(18)	420(20)	310(20)	-35(17)	-101(16)	-128(16)
C(36)	190(17)	315(19)	290(20)	-53(15)	-33(15)	-53(14)
C(37)	184(16)	238(17)	215(19)	-43(14)	-37(14)	-25(13)
C(38)	225(18)	251(19)	440(20)	109(16)	65(17)	2(15)
C(39)	273(18)	208(17)	240(20)	10(14)	-34(15)	-44(14)
C(40)	470(30)	340(20)	1310(50)	440(30)	290(30)	70(20)
C(41)	2170(80)	250(30)	1450(60)	260(30)	1490(60)	270(40)

C(42)	890(40)	270(20)	610(30)	60(20)	540(30)	-100(20)
C(43)	2930(100)	440(30)	3130(100)	870(50)	2880(90)	760(50)
C(1A)	540(30)	1160(50)	1770(70)	1070(50)	560(40)	300(30)
C(2A)	440(30)	880(40)	850(40)	650(40)	200(30)	70(30)
C(3A)	790(40)	440(30)	450(30)	10(20)	210(30)	80(30)
C(4A)	1280(60)	940(50)	410(30)	100(30)	-200(30)	-500(40)
C(5A)	520(30)	790(40)	590(30)	70(30)	-200(30)	60(30)
C(6A)	890(40)	460(30)	540(30)	-70(20)	180(30)	-220(30)
C(7A)	520(30)	570(30)	380(30)	110(20)	140(20)	-190(20)

Table 12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $(PCy_3)_2Cl_2Ru=C(H)SPh$ (7).

	x	y	z	U_{iso}
H(1)	10632	6858	7107	23
H(3)	12611	5846	7613	36
H(4)	14941	5032	7259	48
H(5)	15400	3527	6702	55
H(6)	13539	2846	6489	50
H(7)	11210	3655	6833	41
H(8)	6027	8757	5615	22
H(9A)	6588	9863	6698	25
H(9B)	7239	9974	5849	25
H(10A)	5254	11285	6161	31
H(10B)	4989	10631	5563	31
H(11A)	2948	10889	6452	32
H(11B)	3840	10455	7085	32
H(12A)	3371	9292	6002	33
H(12B)	2708	9191	6851	33
H(13A)	4689	7868	6555	27
H(13B)	4960	8532	7146	27
H(14)	6675	6393	6388	23
H(15A)	7038	6968	4869	30
H(15B)	5604	7297	5431	30
H(16A)	5321	5616	5700	34
H(16B)	5515	5853	4836	34
H(17A)	7867	5017	4688	39
H(17B)	6907	4273	5161	39
H(18A)	8945	4265	5680	34
H(18B)	7523	4631	6241	34
H(19A)	9202	5962	5348	29
H(19B)	9137	5725	6208	29
H(20)	9199	8901	5643	21
H(21A)	10888	7582	6035	26
H(21B)	10720	6907	5424	26
H(22A)	11803	8747	5142	30
H(22B)	12715	7653	4987	30
H(23A)	11489	7541	4054	32
H(23B)	12137	8547	3893	32
H(24A)	9751	8879	3717	32
H(24B)	9933	9515	4348	32
H(25A)	8836	7688	4585	31
H(25B)	7918	8781	4740	31
H(26)	6481	9002	9453	23
H(27A)	6013	9109	7980	29
H(27B)	5267	8450	8646	29
H(28A)	4033	9905	9206	44
H(28B)	3728	9989	8393	44
H(29A)	5347	11078	7997	45
H(29B)	4240	11528	8680	45

H(30A)	5869	10880	9462	32
H(30B)	6596	11565	8807	32
H(31A)	8186	10036	9009	32
H(31B)	7812	10111	8210	32
H(32)	9949	8812	8648	21
H(33A)	8936	8794	9888	28
H(33B)	9712	7650	10009	28
H(34A)	11129	9325	9565	35
H(34B)	11065	8705	10345	35
H(35A)	13272	8193	9573	36
H(35B)	12458	7272	9820	36
H(36A)	13343	7247	8575	31
H(36B)	12597	8394	8434	31
H(37A)	11221	7364	8094	25
H(37B)	11141	6736	8871	25
H(38)	6942	6757	9100	41
H(39A)	8574	5682	8914	29
H(39B)	9408	5979	9484	29
H(40A)	7764	4629	9677	99
H(40B)	8694	4855	10216	99
H(41A)	7125	5130	10925	197
H(41B)	6210	4830	10401	197
H(42A)	5804	6572	10970	83
H(42B)	4938	6291	10410	83
H(43A)	5650	7426	9668	345
H(43B)	6608	7639	10198	345
H(1A1)	6759	3731	8526	213
H(1A2)	6734	3199	7814	213
H(1A3)	7407	4188	7740	213
H(3A)	9336	3743	8712	77
H(4A)	11504	2809	8698	100
H(5A)	12122	1259	8201	79
H(6A)	10552	792	7619	79
H(7A)	8401	1792	7507	62

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Table 13. Torsion angles [°] for $(PCy_3)_2Cl_2Ru=C(H)SPh$ (7).

P(1)-Ru(1)-C(1)-H(1)	-96.0
P(1)-Ru(1)-C(1)-S(1)	84.0(2)

Table 14. Crystal data and structure refinement for $(PCy_3)_2Cl_2Ru=C(H)N(carbazole)$ (8).

Empirical formula	$C_{49}H_{75}Cl_2NP_2Ru$
Formula weight	912.01
Crystallization Solvent	Toluene/pentane
Crystal Habit	Trapezoidal
Crystal size	0.31 x 0.16 x 0.10 mm^3
Crystal color	Purple

Data Collection

Preliminary Photos	Rotation	
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	98(2) K	
θ range for 10189 reflections used in lattice determination	2.34 to 25.58°	
Unit cell dimensions	a = 12.6111(11) Å b = 14.3083(13) Å c = 17.0253(15) Å	α= 83.5180(10)° β= 74.7200(10)° γ = 77.7990(10)°
Volume	2891.2(4) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.048 Mg/m^3	
F(000)	968	
Data collection program	Bruker SMART	
θ range for data collection	1.70 to 28.48°	
Completeness to θ = 28.48°	91.5 %	
Index ranges	$-16 \le h \le 16, -19 \le k \le 18, -21 \le l \le 22$	
Data collection scan type	ω scans at 6 ϕ settings	
Data reduction program	Bruker SAINT v6.1	
Reflections collected	43255	
Independent reflections	13384 [R_{int}= 0.0629]	
Absorption coefficient	0.446 mm^{-1}	
Absorption correction	SADABS	
Max. and min. transmission	1.000 and 0.8590	

Table 14 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Patterson methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full Matrix least-squares on F^2
Data / restraints / parameters	13384 / 0 / 496
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.026
Final R indices [I>2σ(I), 8349 reflections]	R1 = 0.0637, *w*R2 = 0.2323
R indices (all data)	R1 = 0.1040, *w*R2 = 0.2557
Type of weighting scheme used	Calculated
Weighting scheme used	$w=1/[\sigma^2(Fo^2)+(0.1582P)^2+0.0000P]$ where $P=(Fo^2+2Fc^{\hat{}2\hat{}})/3$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	1.921 and -0.474 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

The crystallographic data has been deposited in the Cambridge Database (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 148805.

Table 15. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $(PCy_3)_2Cl_2Ru=C(H)N$(carbazole) (8). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru	7773(1)	7129(1)	7089(1)	29(1)
Cl(1)	8365(1)	5689(1)	6395(1)	40(1)
Cl(2)	7377(1)	8259(1)	8124(1)	40(1)
P(1)	6031(1)	6649(1)	7768(1)	31(1)
P(2)	9701(1)	7312(1)	6689(1)	31(1)
N	7010(4)	8460(3)	5710(3)	33(1)
C(1)	7247(5)	8177(4)	6449(3)	34(1)
C(2)	7047(5)	7944(5)	5029(4)	39(1)
C(3)	7296(5)	6972(5)	4933(4)	45(2)
C(4)	7269(7)	6676(6)	4202(5)	65(2)
C(5)	6995(7)	7325(7)	3571(5)	67(2)
C(6)	6748(6)	8279(7)	3675(4)	63(2)
C(7)	6768(5)	8617(5)	4412(4)	47(2)
C(8)	6546(5)	9551(5)	4701(4)	44(2)
C(9)	6238(6)	10459(6)	4349(5)	60(2)
C(10)	6072(6)	11253(5)	4794(5)	62(2)
C(11)	6225(6)	11149(5)	5573(5)	59(2)
C(12)	6524(5)	10238(4)	5956(5)	50(2)
C(13)	6691(5)	9446(4)	5486(4)	41(1)
C(14)	4877(5)	7595(4)	8248(4)	37(1)
C(15)	3826(5)	7244(5)	8743(4)	49(2)
C(16)	2988(6)	8038(6)	9229(5)	64(2)
C(17)	2688(6)	8908(6)	8677(5)	67(2)
C(18)	3736(6)	9259(5)	8166(5)	59(2)
C(19)	4559(6)	8468(4)	7692(4)	45(2)
C(20)	6234(5)	5810(4)	8662(4)	41(1)
C(21)	6454(7)	6297(5)	9345(4)	56(2)
C(22)	6564(7)	5544(6)	10067(4)	68(2)
C(23)	7463(7)	4679(7)	9806(5)	79(3)
C(24)	7252(7)	4208(6)	9129(5)	73(2)
C(25)	7183(6)	4923(5)	8386(5)	58(2)
C(26)	5517(5)	5927(4)	7160(3)	35(1)
C(27)	4774(5)	5219(4)	7598(4)	42(1)
C(28)	4639(6)	4587(5)	6975(4)	50(2)
C(29)	4203(6)	5173(5)	6280(4)	55(2)
C(30)	4904(6)	5903(5)	5880(4)	50(2)
C(31)	4993(5)	6551(4)	6513(4)	38(1)
C(32)	10503(5)	6890(4)	5677(3)	34(1)
C(33)	9948(5)	7302(4)	4991(3)	38(1)
C(34)	10531(6)	6775(5)	4220(4)	49(2)
C(35)	11771(6)	6789(5)	3974(4)	57(2)
C(36)	12335(6)	6434(6)	4660(4)	57(2)
C(37)	11742(5)	6960(5)	5417(4)	47(2)
C(38)	9880(5)	8537(4)	6796(3)	34(1)
C(39)	9513(5)	9246(4)	6130(4)	40(1)

C(40)	9416(5)	10275(4)	6330(4)	46(2)
C(41)	10534(6)	10436(5)	6427(5)	55(2)
C(42)	10954(7)	9708(5)	7077(5)	60(2)
C(43)	11014(6)	8686(5)	6891(5)	50(2)
C(44)	10486(5)	6547(4)	7384(4)	40(1)
C(45)	10682(6)	5487(5)	7285(5)	54(2)
C(46)	11332(6)	4908(5)	7877(5)	60(2)
C(47)	10766(6)	5110(6)	8743(4)	63(2)
C(48)	10557(8)	6152(7)	8860(5)	83(3)
C(49)	9878(7)	6757(6)	8279(4)	60(2)

Table 16. Selected bond lengths [Å] & angles [°] for $(PCy_3)_2Cl_2Ru=C(H)N$(carbazole) (8).

Ru-C(1)	1.863(6)	C(1)-Ru-Cl(1)	112.95(18)
Ru-Cl(1)	2.3742(15)	C(1)-Ru-P(1)	99.32(17)
Ru-P(1)	2.3994(15)	Cl(1)-Ru-P(1)	90.05(5)
Ru-P(2)	2.4082(15)	C(1)-Ru-P(2)	96.04(17)
Ru-Cl(2)	2.4088(15)	Cl(1)-Ru-P(2)	87.06(5)
		P(1)-Ru-P(2)	164.28(5)
		C(1)-Ru-Cl(2)	85.09(18)
		Cl(1)-Ru-Cl(2)	161.94(6)
		P(1)-Ru-Cl(2)	87.55(5)
		P(2)-Ru-Cl(2)	90.43(5)

Table 17. Bond lengths [Å] and angles [°] for $(PCy_3)_2Cl_2Ru=C(H)N(carbazole)$ (8).

Ru-C(1)	1.863(6)	C(19)-H(19A)	0.9900
Ru-Cl(1)	2.3742(15)	C(19)-H(19B)	0.9900
Ru-P(1)	2.3994(15)	C(20)-C(21)	1.533(9)
Ru-P(2)	2.4082(15)	C(20)-C(25)	1.569(9)
Ru-Cl(2)	2.4088(15)	C(20)-H(20)	1.0000
P(1)-C(14)	1.847(6)	C(21)-C(22)	1.556(9)
P(1)-C(26)	1.853(6)	C(21)-H(21A)	0.9900
P(1)-C(20)	1.866(6)	C(21)-H(21B)	0.9900
P(2)-C(32)	1.848(6)	C(22)-C(23)	1.509(12)
P(2)-C(38)	1.848(6)	C(22)-H(22A)	0.9900
P(2)-C(44)	1.856(6)	C(22)-H(22B)	0.9900
N-C(1)	1.366(7)	C(23)-C(24)	1.507(12)
N-C(13)	1.421(7)	C(23)-H(23A)	0.9900
N-C(2)	1.429(8)	C(23)-H(23B)	0.9900
C(1)-H(1)	0.9500	C(24)-C(25)	1.543(9)
C(2)-C(3)	1.379(9)	C(24)-H(24A)	0.9900
C(2)-C(7)	1.407(8)	C(24)-H(24B)	0.9900
C(3)-C(4)	1.370(9)	C(25)-H(25A)	0.9900
C(3)-H(3)	0.9500	C(25)-H(25B)	0.9900
C(4)-C(5)	1.403(11)	C(26)-C(27)	1.524(8)
C(4)-H(4A)	0.9500	C(26)-C(31)	1.536(7)
C(5)-C(6)	1.355(11)	C(26)-H(26)	1.0000
C(5)-H(5)	0.9500	C(27)-C(28)	1.533(9)
C(6)-C(7)	1.402(10)	C(27)-H(27A)	0.9900
C(6)-H(6)	0.9500	C(27)-H(27B)	0.9900
C(7)-C(8)	1.423(10)	C(28)-C(29)	1.525(10)
C(8)-C(13)	1.385(9)	C(28)-H(28A)	0.9900
C(8)-C(9)	1.389(9)	C(28)-H(28B)	0.9900
C(9)-C(10)	1.385(12)	C(29)-C(30)	1.500(9)
C(9)-H(9)	0.9500	C(29)-H(29A)	0.9900
C(10)-C(11)	1.376(11)	C(29)-H(29B)	0.9900
C(10)-H(10)	0.9500	C(30)-C(31)	1.537(8)
C(11)-C(12)	1.413(9)	C(30)-H(30A)	0.9900
C(11)-H(11)	0.9500	C(30)-H(30B)	0.9900
C(12)-C(13)	1.408(10)	C(31)-H(31A)	0.9900
C(12)-H(12)	0.9500	C(31)-H(31B)	0.9900
C(14)-C(15)	1.522(8)	C(32)-C(33)	1.518(8)
C(14)-C(19)	1.529(8)	C(32)-C(37)	1.529(8)
C(14)-H(14)	1.0000	C(32)-H(32)	1.0000
C(15)-C(16)	1.528(9)	C(33)-C(34)	1.521(8)
C(15)-H(15A)	0.9900	C(33)-H(33A)	0.9900
C(15)-H(15B)	0.9900	C(33)-H(33B)	0.9900
C(16)-C(17)	1.516(11)	C(34)-C(35)	1.512(10)
C(16)-H(16A)	0.9900	C(34)-H(34A)	0.9900
C(16)-H(16B)	0.9900	C(34)-H(34B)	0.9900
C(17)-C(18)	1.527(11)	C(35)-C(36)	1.509(10)
C(17)-H(17A)	0.9900	C(35)-H(35A)	0.9900
C(17)-H(17B)	0.9900	C(35)-H(35B)	0.9900
C(18)-C(19)	1.509(9)	C(36)-C(37)	1.503(9)
C(18)-H(18A)	0.9900	C(36)-H(36A)	0.9900
C(18)-H(18B)	0.9900	C(36)-H(36B)	0.9900