SUPPORTING INFORMATION

Water-Soluble Ruthenium Alkylidenes: Synthesis, Characterization, and Application to Olefin Metathesis in Water

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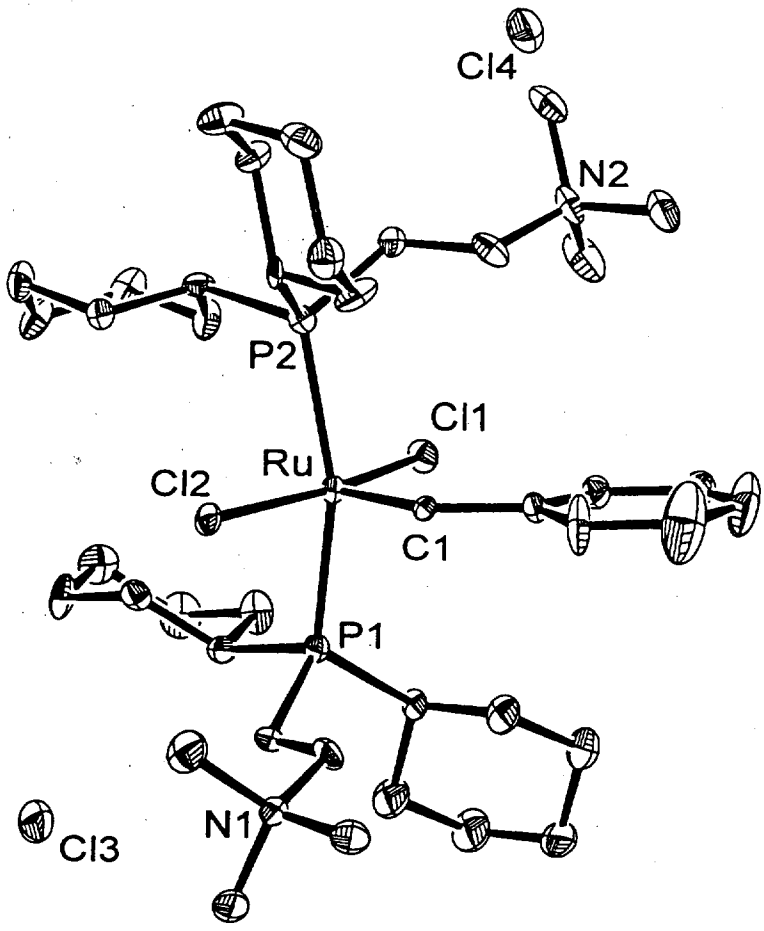
Additional details of the X-ray structural determination for alkylidene **6**, including details of the data collection and structural refinement, atomic coordinates, bond lengths and angles, thermal displacement parameters, and hydrogen atomic coordinates (16 pages).



ORTEP drawing of alkylidene 6 (solvent molecules and hydrogen atoms omitted for clarity). Thermal ellipsoids are drawn at 50% probability.

Supporting Information

Table 1. Crystal data and structure refinement for DML1A.

Empirical formula	$C_{44.78}H_{77.93}Cl_{11.57}N_2P_2Ru$ {$[C_{41}H_{58}N_2P_2Cl_2Ru][Cl_2]\cdot 3.8CH_2Cl_2$]}
Formula weight	1217.61 (883.78·333.82)
Crystallization Solvent	Dichloromethane/methanol/petroleum ether
Crystal Habit	Fragment
Crystal size	0.41 x 0.33 x 0.07 mm^3
Crystal color	Dichroic; purple and orange

Data Collection

Preliminary Photos	None
Type of diffractometer	CAD-4
Wavelength	0.71073 Å MoKα
Data Collection Temperature	85 K
θ range for reflections used in lattice determination	12.6 to 13.8°
Unit cell dimensions	a = 13.958(6) Å b = 25.919(11) Å β= 101.45(3)° c = 16.819(5) Å
Volume	5964(2) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/n$
Density (calculated)	1.356 Mg/m^3
F(000)	2525
θ range for data collection	1.57 to 24.97°
Completeness to θ = 24.97°	100.0 %
Index ranges	$-16 \le h \le 16, -30 \le k \le 27, -19 \le l \le 19$
Data collection scan type	ω scans
Reflections collected	21914
Independent reflections	10474 [R_{int}= 0.051; GOF_{merge}= 1.00]
Absorption coefficient	0.866 mm^{-1}
Absorption correction	None
Number of standards	3 reflections measured every 75min.
Variation of standards	-1.5%.

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Patterson method
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric calculated sites
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	10474 / 19 / 565
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	2.306
Final R indices [$I>2\sigma(I)$]	R1 = 0.0897, *w*R2 = 0.1518
R indices (all data)	R1 = 0.1464, *w*R2 = 0.1600
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.006
Average shift/error	0.000
Largest diff. peak and hole	2.642 and -1.460 e.Å^{-3}

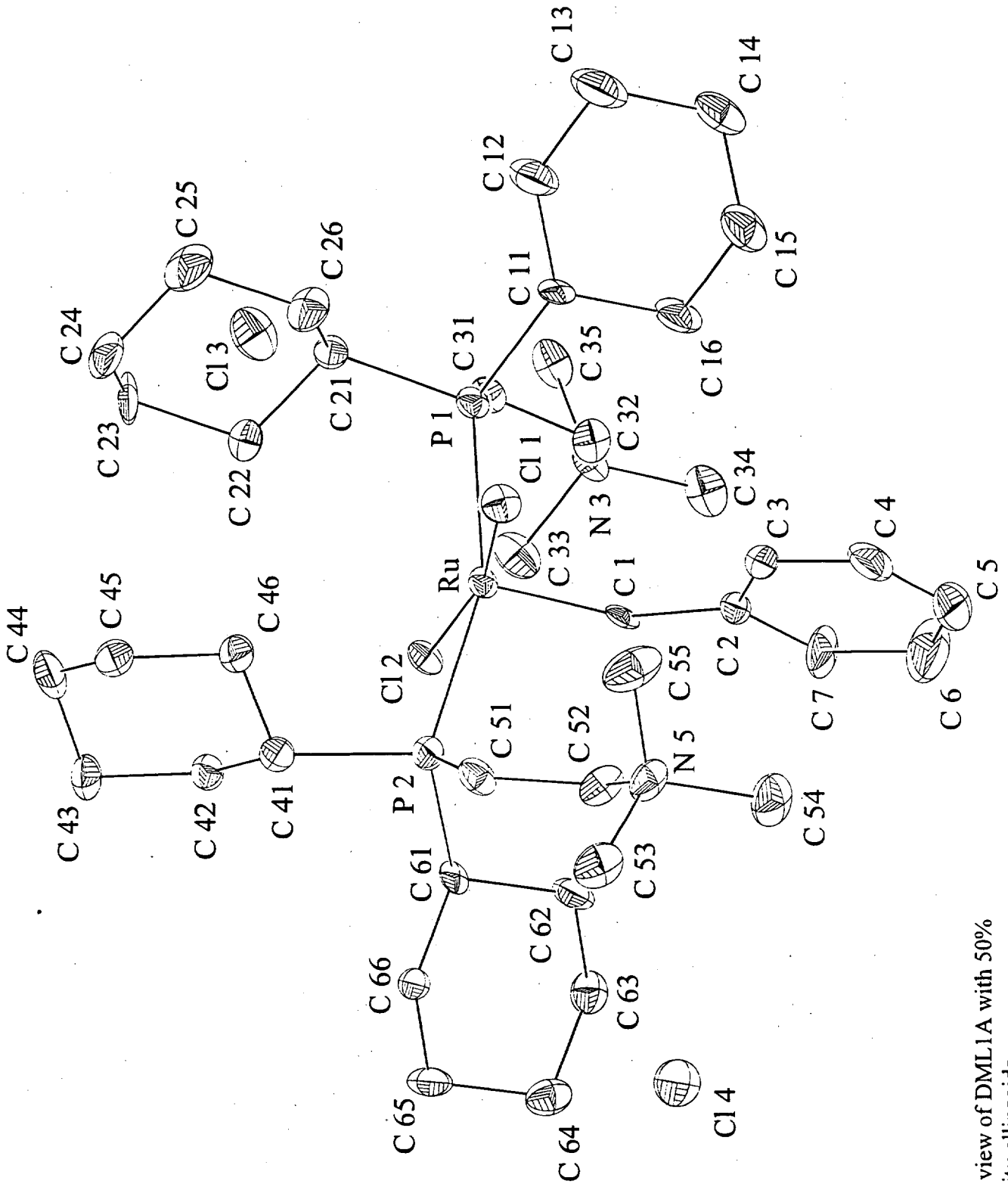
Special Refinement Details

This crystal contains disordered solvent molecules. These are modeled as six molecules of dichlormethane with partial occupancies which altogether add to 3.8 full occupancy molecules.

The variances [$\sigma^2(Fo^2)$] were derived from counting statistics plus an additional term, $(0.014I)^2$, and the variances of the merged data were obtained by propagation of error plus the addition of another term, $(0.014\langle I\rangle)^2$.

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.



Labeled view of DML1A with 50% probability ellipsoids.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for DML1A. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ru	5396(1)	7834(1)	7623(1)	15(1)	1
Cl(1)	5487(2)	7675(1)	9038(1)	21(1)	1
Cl(2)	4951(2)	7986(1)	6190(1)	18(1)	1
Cl(3)	3287(2)	9755(1)	5928(1)	35(1)	1
Cl(4)	7365(2)	5313(1)	7366(1)	33(1)	1
P(1)	5214(2)	8732(1)	7866(1)	17(1)	1
P(2)	4987(2)	6948(1)	7334(1)	17(1)	1
N(3)	6354(5)	9362(3)	5948(4)	20(2)	1
N(5)	6928(5)	6199(3)	9184(4)	25(2)	1
C(1)	6666(5)	7828(3)	7518(4)	15(2)	1
C(2)	7650(6)	7759(3)	8044(5)	17(2)	1
C(3)	7840(6)	7686(3)	8866(5)	22(2)	1
C(4)	8794(7)	7608(3)	9293(6)	33(3)	1
C(5)	9562(7)	7611(4)	8897(6)	51(3)	1
C(6)	9386(7)	7698(5)	8070(7)	66(4)	1
C(7)	8448(6)	7773(4)	7646(6)	38(3)	1
C(11)	5896(6)	9030(3)	8805(5)	17(2)	1
C(12)	5636(7)	9593(3)	8925(5)	39(3)	1
C(13)	6162(7)	9790(4)	9763(6)	50(3)	1
C(14)	7246(7)	9727(3)	9860(5)	33(3)	1
C(15)	7511(7)	9168(3)	9714(5)	34(3)	1
C(16)	6990(6)	8980(3)	8890(5)	30(2)	1
C(21)	3926(6)	8863(3)	7891(5)	19(2)	1
C(22)	3230(5)	8585(3)	7206(5)	20(2)	1
C(23)	2166(6)	8691(4)	7231(5)	30(2)	1
C(24)	1928(6)	8558(4)	8031(5)	32(3)	1
C(25)	2605(6)	8827(4)	8722(5)	37(3)	1
C(26)	3684(6)	8711(4)	8728(5)	29(2)	1
C(31)	5371(6)	9162(3)	7028(5)	19(2)	1
C(32)	6330(6)	9122(3)	6774(5)	21(2)	1
C(33)	5751(6)	9068(3)	5262(5)	30(2)	1
C(34)	7396(6)	9371(3)	5835(5)	28(2)	1
C(35)	5968(6)	9898(3)	5913(5)	26(2)	1
C(41)	3650(6)	6841(3)	7220(5)	18(2)	1
C(42)	3066(5)	7038(3)	6390(5)	20(2)	1
C(43)	1988(6)	6928(3)	6308(5)	28(2)	1
C(44)	1599(6)	7159(4)	7003(5)	33(2)	1
C(45)	2147(6)	6957(4)	7818(5)	31(3)	1
C(46)	3230(6)	7062(3)	7909(5)	28(2)	1
C(51)	5416(6)	6496(3)	8168(5)	22(2)	1
C(52)	6531(6)	6474(3)	8389(5)	23(2)	1
C(53)	6522(6)	5669(3)	9176(5)	31(3)	1
C(54)	8025(6)	6174(3)	9272(5)	35(3)	1
C(55)	6714(7)	6492(4)	9900(5)	41(3)	1
C(61)	5300(6)	6677(3)	6418(5)	16(2)	1
C(62)	6383(6)	6727(3)	6363(5)	26(2)	1
C(63)	6587(6)	6536(3)	5557(5)	25(2)	1

C(64)	6277(6)	5975(3)	5395(5)	27(2)	1
C(65)	5201(6)	5913(3)	5459(5)	26(2)	1
C(66)	4992(6)	6096(3)	6270(5)	19(2)	1
Cl(5)	7657(2)	7785(1)	5177(2)	57(1)	0.968(5)
Cl(6)	9595(2)	8156(1)	5880(2)	70(1)	0.968(5)
C(90)	8896(8)	7643(4)	5405(7)	72(4)	0.968(5)
Cl(7)	-493(2)	6216(1)	5949(2)	63(1)	0.863(6)
Cl(8A)	-869(4)	6538(2)	7444(3)	61(2)	0.604(4)
Cl(8B)	-240(20)	6302(10)	7757(6)	193(12)	0.259(2)
C(91)	-737(10)	5982(4)	6844(5)	80(6)	0.863(6)
Cl(9A)	4354(6)	4800(3)	6697(5)	70(3)	0.376(3)
Cl(9B)	4830(9)	4842(4)	7588(7)	149(5)	0.376(3)
Cl(10)	5783(4)	3989(2)	7030(4)	135(3)	0.751(6)
C(92)	5513(8)	4639(4)	6844(9)	97(7)	0.751(6)
Cl(11)	4043(7)	5671(3)	9400(6)	117(4)	0.451(5)
Cl(12)	5028(6)	4677(3)	9396(5)	105(4)	0.451(5)
C(93)	4069(13)	5080(6)	8860(10)	56(8)	0.451(5)
Cl(13)	2572(9)	5440(4)	7240(6)	111(5)	0.390(6)
Cl(14)	3407(7)	5839(4)	8851(5)	89(4)	0.390(6)
C(94)	3260(20)	5283(6)	8221(10)	81(11)	0.390(6)
Cl(15)	1791(13)	5386(7)	7216(10)	195(7)	0.356(7)
Cl(16)	84(11)	5830(8)	7678(10)	195(7)	0.356(7)
C(95)	900(30)	5301(12)	7790(30)	195(7)	0.356(7)

Table 3. Selected bond lengths [Å] and angles [°] for DML1A.

		Bond lengths	
Ru-P(1)	2.384(2)	Ru-Cl(1)	2.393(2)
Ru-P(2)	2.393(2)	Ru-Cl(2)	2.399(2)
Ru-C(1)	1.816(7)		
		Bond angles	
C(1)-Ru-P(1)	99.5(2)	P(1)-Ru-P(2)	160.39(8)
C(1)-Ru-P(2)	99.8(2)	P(1)-Ru-Cl(2)	89.81(7)
C(1)-Ru-Cl(1)	103.6(2)	P(2)-Ru-Cl(2)	87.07(8)
C(1)-Ru-Cl(2)	88.1(2)	Cl(1)-Ru-P(2)	90.03(8)
P(1)-Ru-Cl(1)	89.11(8)	Cl(1)-Ru-Cl(2)	168.26(8)
		Plane angles	
Pln(1)-Pln (2)	4.7(1)	Pln(2)-Pln(3)	87.8(2)

Pln(1) is the plane formed by Cl(1)-Ru-Cl(2).
Pln(2) is the plane formed by Ru-C1-C_{aryl}.
Pln(3) is the plane formed by P(1)-Ru-P(2).

Table 4. Bond lengths [Å] and angles [°] for DML1A.

Lengths			
Ru-C(1)	1.816(7)	C(21)-C(26)	1.561(10)
Ru-P(1)	2.384(2)	C(21)-H(21A)	0.9600
Ru-Cl(1)	2.393(2)	C(22)-C(23)	1.518(10)
Ru-P(2)	2.393(2)	C(22)-H(22A)	0.9600
Ru-Cl(2)	2.399(2)	C(22)-H(22B)	0.9598
P(1)-C(31)	1.844(8)	C(23)-C(24)	1.489(11)
P(1)-C(21)	1.838(8)	C(23)-H(23A)	0.9599
P(1)-C(11)	1.844(7)	C(23)-H(23B)	0.9601
P(2)-C(61)	1.823(8)	C(24)-C(25)	1.514(11)
P(2)-C(51)	1.836(8)	C(24)-H(24A)	0.9601
P(2)-C(41)	1.859(8)	C(24)-H(24B)	0.9600
N(3)-C(33)	1.495(9)	C(25)-C(26)	1.534(11)
N(3)-C(34)	1.503(10)	C(25)-H(25A)	0.9599
N(3)-C(35)	1.488(9)	C(25)-H(25B)	0.9601
N(3)-C(32)	1.529(9)	C(26)-H(26A)	0.9601
N(5)-C(53)	1.484(10)	C(26)-H(26B)	0.9599
N(5)-C(54)	1.510(10)	C(31)-C(32)	1.487(10)
N(5)-C(55)	1.502(10)	C(31)-H(31A)	0.9601
N(5)-C(52)	1.521(9)	C(31)-H(31B)	0.9600
C(1)-C(2)	1.490(10)	C(32)-H(32A)	0.9600
C(1)-H(1A)	0.9598	C(32)-H(32B)	0.9599
C(2)-C(3)	1.368(10)	C(33)-H(33A)	0.9600
C(2)-C(7)	1.410(11)	C(33)-H(33B)	0.9601
C(3)-C(4)	1.396(11)	C(33)-H(33C)	0.9600
C(3)-H(3A)	0.9600	C(34)-H(34A)	0.9600
C(4)-C(5)	1.370(12)	C(34)-H(34B)	0.9600
C(4)-H(4A)	0.9601	C(34)-H(34C)	0.9600
C(5)-C(6)	1.382(13)	C(35)-H(35A)	0.9600
C(5)-H(5A)	0.9601	C(35)-H(35B)	0.9600
C(6)-C(7)	1.374(12)	C(35)-H(35C)	0.9600
C(6)-H(6A)	0.9600	C(41)-C(46)	1.511(10)
C(7)-H(7A)	0.9601	C(41)-C(42)	1.557(10)
C(11)-C(16)	1.509(11)	C(41)-H(41A)	0.9599
C(11)-C(12)	1.528(10)	C(42)-C(43)	1.510(10)
C(11)-H(11A)	0.9599	C(42)-H(42A)	0.9600
C(12)-C(13)	1.541(11)	C(42)-H(42B)	0.9598
C(12)-H(12A)	0.9600	C(43)-C(44)	1.508(10)
C(12)-H(12B)	0.9599	C(43)-H(43A)	0.9598
C(13)-C(14)	1.498(12)	C(43)-H(43B)	0.9600
C(13)-H(13A)	0.9600	C(44)-C(45)	1.523(11)
C(13)-H(13B)	0.9598	C(44)-H(44A)	0.9600
C(14)-C(15)	1.527(11)	C(44)-H(44B)	0.9600
C(14)-H(14A)	0.9599	C(45)-C(46)	1.514(10)
C(14)-H(14B)	0.9599	C(45)-H(45A)	0.9600
C(15)-C(16)	1.512(10)	C(45)-H(45B)	0.9601
C(15)-H(15A)	0.9599	C(46)-H(46A)	0.9600
C(15)-H(15B)	0.9601	C(46)-H(46B)	0.9600
C(16)-H(16A)	0.9599	C(51)-C(52)	1.527(10)
C(16)-H(16B)	0.9600	C(51)-H(51A)	0.9601
C(21)-C(22)	1.532(10)	C(51)-H(51B)	0.9599
		C(52)-H(52A)	0.9600

C(52)-H(52B)	0.9600
C(53)-H(53A)	0.9601
C(53)-H(53B)	0.9601
C(53)-H(53C)	0.9599
C(54)-H(54A)	0.9601
C(54)-H(54B)	0.9600
C(54)-H(54C)	0.9601
C(55)-H(55A)	0.9600
C(55)-H(55B)	0.9600
C(55)-H(55C)	0.9600
C(61)-C(62)	1.538(10)
C(61)-C(66)	1.571(10)
C(61)-H(61A)	0.9600
C(62)-C(63)	1.523(10)
C(62)-H(62A)	0.9600
C(62)-H(62B)	0.9602
C(63)-C(64)	1.526(10)
C(63)-H(63A)	0.9600
C(63)-H(63B)	0.9599
C(64)-C(65)	1.535(10)
C(64)-H(64A)	0.9600
C(64)-H(64B)	0.9600
C(65)-C(66)	1.527(10)
C(65)-H(65A)	0.9601
C(65)-H(65B)	0.9599
C(66)-H(66A)	0.9601
C(66)-H(66B)	0.9600
Cl(5)-C(90)	1.734(11)
Cl(6)-C(90)	1.744(11)
C(90)-H(90A)	0.9601
C(90)-H(90B)	0.9599
Cl(7)-C(91)	1.719(9)
Cl(8A)-C(91)	1.789(8)
Cl(8B)-C(91)	1.759(9)
Cl(9A)-C(92)	1.641(9)
Cl(9B)-C(92)	1.797(9)
Cl(10)-C(92)	1.742(9)
Cl(11)-C(93)	1.785(10)
Cl(12)-C(93)	1.793(10)
Cl(13)-C(94)	1.783(10)
Cl(14)-C(94)	1.777(10)
Cl(15)-C(95)	1.725(10)
Cl(16)-C(95)	1.771(10)

Angles

C(1)-Ru-P(1)	99.5(2)
C(1)-Ru-Cl(1)	103.6(2)
P(1)-Ru-Cl(1)	89.11(8)
C(1)-Ru-P(2)	99.8(2)
P(1)-Ru-P(2)	160.39(8)
Cl(1)-Ru-P(2)	90.03(8)
C(1)-Ru-Cl(2)	88.1(2)
P(1)-Ru-Cl(2)	89.81(7)
Cl(1)-Ru-Cl(2)	168.26(8)
P(2)-Ru-Cl(2)	87.07(8)
C(31)-P(1)-C(21)	99.9(4)
C(31)-P(1)-C(11)	106.3(4)
C(21)-P(1)-C(11)	104.1(4)
C(31)-P(1)-Ru	115.3(3)
C(21)-P(1)-Ru	108.8(3)
C(11)-P(1)-Ru	120.1(3)
C(61)-P(2)-C(51)	107.6(4)
C(61)-P(2)-C(41)	105.1(4)
C(51)-P(2)-C(41)	98.7(4)
C(61)-P(2)-Ru	117.0(3)
C(51)-P(2)-Ru	115.4(3)
C(41)-P(2)-Ru	111.0(3)
C(33)-N(3)-C(34)	108.8(7)
C(33)-N(3)-C(35)	107.5(6)
C(34)-N(3)-C(35)	109.4(6)
C(33)-N(3)-C(32)	112.6(6)
C(34)-N(3)-C(32)	108.5(6)
C(35)-N(3)-C(32)	110.0(6)
C(53)-N(5)-C(54)	109.8(7)
C(53)-N(5)-C(55)	109.8(7)
C(54)-N(5)-C(55)	107.6(7)
C(53)-N(5)-C(52)	110.8(7)
C(54)-N(5)-C(52)	106.9(6)
C(55)-N(5)-C(52)	111.8(7)
C(2)-C(1)-Ru	138.2(6)
C(2)-C(1)-H(1A)	110.9
Ru-C(1)-H(1A)	110.9
C(3)-C(2)-C(7)	118.0(8)
C(3)-C(2)-C(1)	126.0(8)
C(7)-C(2)-C(1)	115.9(7)
C(2)-C(3)-C(4)	120.9(8)
C(2)-C(3)-H(3A)	119.0
C(4)-C(3)-H(3A)	120.1
C(5)-C(4)-C(3)	120.5(9)
C(5)-C(4)-H(4A)	119.5
C(3)-C(4)-H(4A)	120.0
C(6)-C(5)-C(4)	119.3(10)
C(6)-C(5)-H(5A)	120.2
C(4)-C(5)-H(5A)	120.4
C(5)-C(6)-C(7)	120.4(10)
C(5)-C(6)-H(6A)	119.4
C(7)-C(6)-H(6A)	120.1
C(6)-C(7)-C(2)	120.7(9)
C(6)-C(7)-H(7A)	120.0
C(2)-C(7)-H(7A)	119.3
C(16)-C(11)-C(12)	109.4(7)

C(16)-C(11)-P(1)	112.7(6)	C(23)-C(24)-H(24A)	107.6
C(12)-C(11)-P(1)	114.7(6)	C(25)-C(24)-H(24A)	108.4
C(16)-C(11)-H(11A)	105.3	C(23)-C(24)-H(24B)	110.2
C(12)-C(11)-H(11A)	106.9	C(25)-C(24)-H(24B)	110.8
P(1)-C(11)-H(11A)	107.2	H(24A)-C(24)-H(24B)	107.9
C(13)-C(12)-C(11)	110.8(8)	C(26)-C(25)-C(24)	112.2(7)
C(13)-C(12)-H(12A)	110.0	C(26)-C(25)-H(25A)	109.3
C(11)-C(12)-H(12A)	108.4	C(24)-C(25)-H(25A)	109.2
C(13)-C(12)-H(12B)	109.4	C(26)-C(25)-H(25B)	108.7
C(11)-C(12)-H(12B)	109.6	C(24)-C(25)-H(25B)	109.0
H(12A)-C(12)-H(12B)	108.6	H(25A)-C(25)-H(25B)	108.3
C(14)-C(13)-C(12)	110.5(8)	C(25)-C(26)-C(21)	109.4(7)
C(14)-C(13)-H(13A)	108.3	C(25)-C(26)-H(26A)	111.8
C(12)-C(13)-H(13A)	108.6	C(21)-C(26)-H(26A)	110.7
C(14)-C(13)-H(13B)	110.3	C(25)-C(26)-H(26B)	108.8
C(12)-C(13)-H(13B)	110.9	C(21)-C(26)-H(26B)	107.6
H(13A)-C(13)-H(13B)	108.1	H(26A)-C(26)-H(26B)	108.4
C(13)-C(14)-C(15)	111.0(8)	C(32)-C(31)-P(1)	115.3(6)
C(13)-C(14)-H(14A)	110.1	C(32)-C(31)-H(31A)	107.1
C(15)-C(14)-H(14A)	110.0	P(1)-C(31)-H(31A)	108.4
C(13)-C(14)-H(14B)	108.3	C(32)-C(31)-H(31B)	108.7
C(15)-C(14)-H(14B)	109.2	P(1)-C(31)-H(31B)	109.2
H(14A)-C(14)-H(14B)	108.1	H(31A)-C(31)-H(31B)	107.8
C(16)-C(15)-C(14)	111.4(7)	C(31)-C(32)-N(3)	114.6(7)
C(16)-C(15)-H(15A)	107.5	C(31)-C(32)-H(32A)	109.6
C(14)-C(15)-H(15A)	109.4	N(3)-C(32)-H(32A)	108.8
C(16)-C(15)-H(15B)	110.3	C(31)-C(32)-H(32B)	107.0
C(14)-C(15)-H(15B)	109.9	N(3)-C(32)-H(32B)	108.8
H(15A)-C(15)-H(15B)	108.3	H(32A)-C(32)-H(32B)	107.9
C(15)-C(16)-C(11)	110.7(8)	N(3)-C(33)-H(33A)	110.1
C(15)-C(16)-H(16A)	107.7	N(3)-C(33)-H(33B)	108.7
C(11)-C(16)-H(16A)	107.7	H(33A)-C(33)-H(33B)	109.5
C(15)-C(16)-H(16B)	111.9	N(3)-C(33)-H(33C)	109.6
C(11)-C(16)-H(16B)	110.2	H(33A)-C(33)-H(33C)	109.5
H(16A)-C(16)-H(16B)	108.4	H(33B)-C(33)-H(33C)	109.5
C(22)-C(21)-C(26)	110.0(7)	N(3)-C(34)-H(34A)	109.7
C(22)-C(21)-P(1)	111.9(6)	N(3)-C(34)-H(34B)	109.1
C(26)-C(21)-P(1)	111.2(6)	H(34A)-C(34)-H(34B)	109.5
C(22)-C(21)-H(21A)	107.7	N(3)-C(34)-H(34C)	109.6
C(26)-C(21)-H(21A)	107.5	H(34A)-C(34)-H(34C)	109.5
P(1)-C(21)-H(21A)	108.4	H(34B)-C(34)-H(34C)	109.5
C(23)-C(22)-C(21)	111.8(7)	N(3)-C(35)-H(35A)	110.9
C(23)-C(22)-H(22A)	108.2	N(3)-C(35)-H(35B)	108.2
C(21)-C(22)-H(22A)	107.6	H(35A)-C(35)-H(35B)	109.5
C(23)-C(22)-H(22B)	110.4	N(3)-C(35)-H(35C)	109.3
C(21)-C(22)-H(22B)	110.4	H(35A)-C(35)-H(35C)	109.5
H(22A)-C(22)-H(22B)	108.3	H(35B)-C(35)-H(35C)	109.5
C(24)-C(23)-C(22)	112.2(7)	C(46)-C(41)-C(42)	110.5(7)
C(24)-C(23)-H(23A)	110.3	C(46)-C(41)-P(2)	113.5(6)
C(22)-C(23)-H(23A)	110.5	C(42)-C(41)-P(2)	112.3(5)
C(24)-C(23)-H(23B)	107.8	C(46)-C(41)-H(41A)	106.8
C(22)-C(23)-H(23B)	107.9	C(42)-C(41)-H(41A)	106.4
H(23A)-C(23)-H(23B)	108.1	P(2)-C(41)-H(41A)	106.9
C(23)-C(24)-C(25)	111.7(8)	C(43)-C(42)-C(41)	110.7(7)

C(43)-C(42)-H(42A)	110.8
C(41)-C(42)-H(42A)	110.1
C(43)-C(42)-H(42B)	108.6
C(41)-C(42)-H(42B)	108.3
H(42A)-C(42)-H(42B)	108.2
C(42)-C(43)-C(44)	111.0(7)
C(42)-C(43)-H(43A)	108.6
C(44)-C(43)-H(43A)	108.2
C(42)-C(43)-H(43B)	109.8
C(44)-C(43)-H(43B)	110.9
H(43A)-C(43)-H(43B)	108.2
C(43)-C(44)-C(45)	111.5(8)
C(43)-C(44)-H(44A)	110.0
C(45)-C(44)-H(44A)	109.9
C(43)-C(44)-H(44B)	108.2
C(45)-C(44)-H(44B)	108.9
H(44A)-C(44)-H(44B)	108.2
C(46)-C(45)-C(44)	110.0(7)
C(46)-C(45)-H(45A)	109.4
C(44)-C(45)-H(45A)	108.7
C(46)-C(45)-H(45B)	110.3
C(44)-C(45)-H(45B)	110.2
H(45A)-C(45)-H(45B)	108.1
C(41)-C(46)-C(45)	112.6(7)
C(41)-C(46)-H(46A)	108.6
C(45)-C(46)-H(46A)	109.5
C(41)-C(46)-H(46B)	108.7
C(45)-C(46)-H(46B)	109.1
H(46A)-C(46)-H(46B)	108.2
C(52)-C(51)-P(2)	111.8(6)
C(52)-C(51)-H(51A)	109.2
P(2)-C(51)-H(51A)	109.2
C(52)-C(51)-H(51B)	108.5
P(2)-C(51)-H(51B)	109.8
H(51A)-C(51)-H(51B)	108.4
C(51)-C(52)-N(5)	114.0(7)
C(51)-C(52)-H(52A)	108.2
N(5)-C(52)-H(52A)	108.9
C(51)-C(52)-H(52B)	108.0
N(5)-C(52)-H(52B)	109.6
H(52A)-C(52)-H(52B)	108.0
N(5)-C(53)-H(53A)	110.7
N(5)-C(53)-H(53B)	108.2
H(53A)-C(53)-H(53B)	109.5
N(5)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
N(5)-C(54)-H(54A)	109.3
N(5)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
N(5)-C(54)-H(54C)	109.6
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
N(5)-C(55)-H(55A)	108.7
N(5)-C(55)-H(55B)	110.1
H(55A)-C(55)-H(55B)	109.5
N(5)-C(55)-H(55C)	109.6
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
C(62)-C(61)-C(66)	108.2(7)
C(62)-C(61)-P(2)	114.9(5)
C(66)-C(61)-P(2)	113.5(6)
C(62)-C(61)-H(61A)	106.0
C(66)-C(61)-H(61A)	106.6
P(2)-C(61)-H(61A)	107.0
C(61)-C(62)-C(63)	112.7(7)
C(61)-C(62)-H(62A)	107.7
C(63)-C(62)-H(62A)	108.3
C(61)-C(62)-H(62B)	109.7
C(63)-C(62)-H(62B)	110.1
H(62A)-C(62)-H(62B)	108.1
C(64)-C(63)-C(62)	111.8(7)
C(64)-C(63)-H(63A)	109.1
C(62)-C(63)-H(63A)	110.3
C(64)-C(63)-H(63B)	109.2
C(62)-C(63)-H(63B)	108.2
H(63A)-C(63)-H(63B)	108.1
C(65)-C(64)-C(63)	109.5(7)
C(65)-C(64)-H(64A)	109.0
C(63)-C(64)-H(64A)	109.7
C(65)-C(64)-H(64B)	109.6
C(63)-C(64)-H(64B)	110.7
H(64A)-C(64)-H(64B)	108.3
C(64)-C(65)-C(66)	113.1(7)
C(64)-C(65)-H(65A)	110.0
C(66)-C(65)-H(65A)	110.4
C(64)-C(65)-H(65B)	107.9
C(66)-C(65)-H(65B)	107.6
H(65A)-C(65)-H(65B)	107.6
C(65)-C(66)-C(61)	110.2(6)
C(65)-C(66)-H(66A)	109.9
C(61)-C(66)-H(66A)	109.7
C(65)-C(66)-H(66B)	109.2
C(61)-C(66)-H(66B)	109.2
H(66A)-C(66)-H(66B)	108.6
Cl(5)-C(90)-Cl(6)	112.5(6)
Cl(5)-C(90)-H(90A)	110.6
Cl(6)-C(90)-H(90A)	110.7
Cl(5)-C(90)-H(90B)	107.5
Cl(6)-C(90)-H(90B)	107.0
H(90A)-C(90)-H(90B)	108.3
Cl(8B)-C(91)-Cl(7)	119.2(8)
Cl(7)-C(91)-Cl(8A)	105.7(5)
Cl(9A)-C(92)-Cl(10)	116.4(8)
Cl(10)-C(92)-Cl(9B)	106.5(7)

Cl(12)-C(93)-Cl(11)	109.4(7)		
		Cl(15)-C(95)-Cl(16)	111.4(9)
Cl(13)-C(94)-Cl(14)	110.1(8)		

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for DML1A. 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	140(4)	158(4)	134(4)	-1(3)	-10(3)	1(4)
Cl(1)	258(13)	243(13)	134(12)	16(9)	29(10)	10(10)
Cl(2)	205(12)	206(12)	106(11)	1(9)	-27(9)	-28(10)
Cl(3)	352(15)	384(16)	272(14)	66(12)	-41(12)	-52(13)
Cl(4)	337(15)	323(14)	295(14)	36(12)	-30(12)	68(12)
P(1)	178(13)	167(13)	138(12)	-8(10)	-15(10)	3(11)
P(2)	159(13)	161(13)	193(13)	2(10)	17(10)	12(11)
N(3)	210(40)	160(40)	200(40)	30(30)	-40(30)	-40(30)
N(5)	220(40)	270(50)	230(40)	50(40)	0(40)	120(40)
C(1)	190(50)	100(40)	100(40)	-40(40)	-60(40)	0(40)
C(2)	150(50)	150(50)	190(50)	-10(40)	-30(40)	30(40)
C(3)	170(50)	200(50)	260(50)	-50(40)	-10(40)	40(40)
C(4)	340(60)	270(60)	290(60)	-90(50)	-110(50)	0(50)
C(5)	250(70)	740(90)	460(70)	-300(70)	-140(60)	70(60)
C(6)	290(70)	1230(120)	450(80)	-310(80)	60(60)	110(70)
C(7)	150(50)	650(80)	290(60)	-80(60)	-80(40)	120(60)
C(11)	230(50)	180(50)	70(40)	-60(40)	-40(40)	30(40)
C(12)	410(70)	310(60)	390(70)	-160(50)	-80(50)	10(50)
C(13)	540(80)	330(70)	520(70)	-220(60)	-190(60)	40(60)
C(14)	410(70)	290(60)	220(60)	-40(50)	-70(50)	-70(50)
C(15)	340(60)	370(60)	260(60)	-30(50)	-90(50)	-40(50)
C(16)	360(60)	280(60)	210(50)	-110(40)	-80(50)	0(50)
C(21)	180(50)	160(50)	230(50)	0(40)	40(40)	0(40)
C(22)	170(50)	210(50)	210(50)	60(40)	60(40)	0(40)
C(23)	60(50)	480(70)	340(60)	-10(50)	-10(40)	-30(50)
C(24)	180(50)	340(60)	480(70)	-20(50)	170(50)	10(50)
C(25)	350(60)	510(70)	310(60)	-80(50)	170(50)	70(60)
C(26)	260(60)	450(70)	170(50)	-30(50)	80(40)	60(50)
C(31)	210(50)	120(50)	210(50)	40(40)	0(40)	-10(40)
C(32)	220(50)	190(50)	190(50)	100(40)	0(40)	30(40)
C(33)	360(60)	340(60)	170(50)	10(40)	20(50)	-80(50)
C(34)	290(60)	260(60)	300(60)	120(50)	30(50)	-70(50)
C(35)	270(60)	260(60)	240(50)	100(40)	20(40)	-90(50)
C(41)	190(50)	120(50)	260(50)	20(40)	70(40)	-20(40)
C(42)	160(50)	190(50)	230(50)	0(40)	0(40)	20(40)
C(43)	150(50)	360(60)	290(60)	-20(50)	-20(40)	20(50)
C(44)	180(50)	410(60)	370(60)	-80(50)	0(50)	-100(50)
C(45)	230(60)	430(60)	300(60)	-160(50)	100(50)	-10(50)
C(46)	180(50)	360(60)	260(50)	-100(50)	-10(40)	40(50)
C(51)	240(50)	190(50)	200(50)	10(40)	-50(40)	-20(40)
C(52)	290(60)	210(50)	210(50)	90(40)	90(40)	90(40)
C(53)	370(60)	240(60)	320(60)	100(50)	40(50)	120(50)
C(54)	250(60)	340(60)	410(60)	100(50)	-20(50)	90(50)
C(55)	530(70)	440(70)	250(60)	20(50)	40(50)	270(60)
C(61)	140(50)	190(50)	120(50)	-10(40)	-80(40)	20(40)
C(62)	280(60)	240(50)	290(60)	-130(50)	80(50)	-100(50)
C(63)	210(50)	300(60)	240(50)	20(40)	50(40)	0(50)

C(64)	340(60)	210(50)	240(60)	10(40)	50(50)	70(50)
C(65)	320(60)	190(50)	290(60)	-100(40)	130(50)	-50(50)
C(66)	150(50)	200(50)	230(50)	-60(40)	100(40)	-50(40)
Cl(5)	530(20)	600(20)	520(20)	-2(17)	-55(15)	-153(18)
Cl(6)	420(20)	990(30)	700(20)	-140(20)	139(18)	-180(20)
C(90)	650(90)	680(100)	990(110)	-340(80)	560(90)	-170(80)
Cl(7)	460(20)	530(20)	890(30)	-50(20)	140(20)	-119(19)
Cl(8A)	550(40)	530(30)	880(40)	-290(30)	450(30)	-180(30)
C(91)	1030(130)	500(100)	590(100)	-310(80)	-480(90)	90(90)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for DML1A.

	x	y	z	U_{iso}
H(1A)	6716	7875	6961	17
H(3A)	7306	7691	9148	26
H(4A)	8916	7554	9869	39
H(5A)	10218	7559	9192	61
H(6A)	9923	7697	7791	79
H(7A)	8332	7838	7073	46
H(11A)	5739	8840	9251	21
H(12A)	4941	9618	8878	47
H(12B)	5822	9802	8509	47
H(13A)	5948	9589	10174	60
H(13B)	6001	10145	9838	60
H(14A)	7567	9834	10392	39
H(14B)	7466	9945	9471	39
H(15A)	7314	8950	10115	41
H(15B)	8206	9136	9764	41
H(16A)	7184	9197	8488	36
H(16B)	7160	8630	8791	36
H(21A)	3813	9227	7820	22
H(22A)	3342	8221	7278	23
H(22B)	3366	8681	6689	23
H(23A)	1742	8509	6804	36
H(23B)	2053	9054	7144	36
H(24A)	2010	8192	8104	38
H(24B)	1258	8640	8034	38
H(25A)	2449	8719	9227	45
H(25B)	2503	9193	8669	45
H(26A)	4110	8888	9162	35
H(26B)	3793	8347	8799	35
H(31A)	5305	9512	7194	23
H(31B)	4861	9096	6566	23
H(32A)	6828	9281	7176	25
H(32B)	6481	8762	6756	25
H(33A)	5776	9233	4755	36
H(33B)	6007	8725	5262	36
H(33C)	5085	9054	5332	36
H(34A)	7426	9521	5319	34
H(34B)	7781	9573	6261	34
H(34C)	7647	9025	5858	34
H(35A)	5972	10052	5395	31
H(35B)	5310	9886	6002	31
H(35C)	6364	10101	6332	31
H(41A)	3551	6475	7226	22
H(42A)	3314	6883	5954	24
H(42B)	3154	7405	6366	24
H(43A)	1898	6561	6318	33
H(43B)	1636	7056	5797	33
H(44A)	914	7087	6942	39
H(44B)	1681	7527	6989	39

H(45A)	2041	6591	7840	38
H(45B)	1900	7115	8252	38
H(46A)	3343	7428	7932	33
H(46B)	3571	6914	8409	33
H(51A)	5167	6158	8012	27
H(51B)	5176	6600	8640	27
H(52A)	6762	6300	7959	28
H(52B)	6774	6822	8415	28
H(53A)	6769	5496	9680	38
H(53B)	5823	5695	9097	38
H(53C)	6695	5477	8738	38
H(54A)	8303	6004	9772	42
H(54B)	8184	5984	8826	42
H(54C)	8285	6517	9275	42
H(55A)	6979	6304	10385	50
H(55B)	7008	6828	9925	50
H(55C)	6020	6527	9850	50
H(61A)	4940	6868	5967	20
H(62A)	6757	6522	6789	32
H(62B)	6587	7079	6451	32
H(63A)	7270	6568	5548	30
H(63B)	6230	6749	5133	30
H(64A)	6673	5756	5789	32
H(64B)	6360	5870	4865	32
H(65A)	5002	5560	5361	31
H(65B)	4814	6119	5041	31
H(66A)	4309	6058	6274	22
H(66B)	5358	5889	6699	22
H(90A)[a]	9121	7538	4926	86
H(90B)[a]	8984	7360	5781	86

[a] Occupancy=0.968(5)