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Supporting information

Title : **Synthesis of Dinuclear and Trinuclear Ruthenium Cyclopropenyl Complexes**

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Figure: A Complete ORTEP drawing of
1,4-{[Ru]=C=C($CH_2CH=CH_2$)}$_2C_6H_4$,2I·6$CDCl_3$, (**2b**).

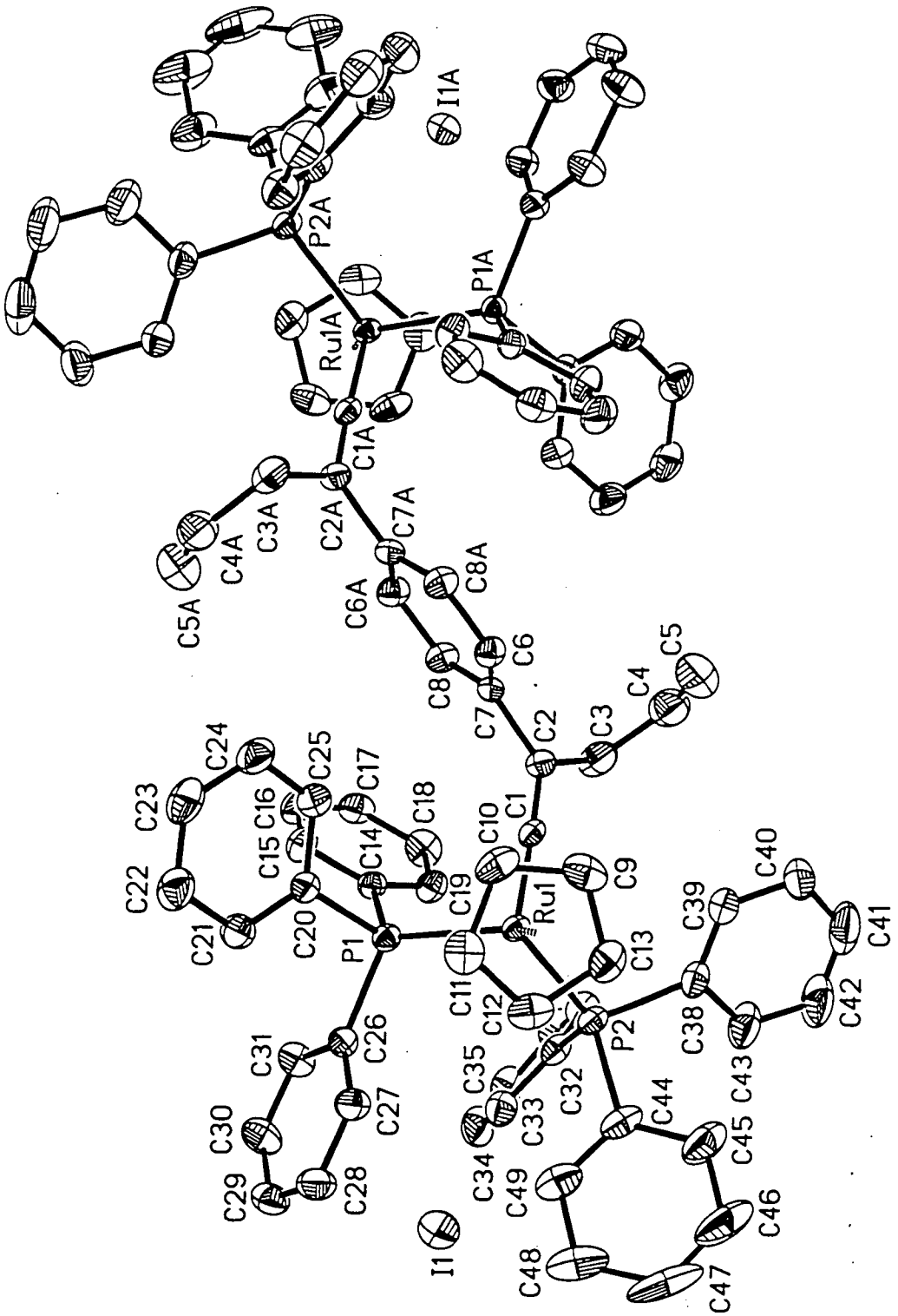
Table 1: Crystal data and structure refinement for **2b**.

Table 2: Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$Å^2 \times 10^3$] for **2b**. U(eq) is defined as one third of the trace of the orthogonalized I_{ij} tensor.

Table 3: Bond lengths [Å] and angles [deg] for **2b**.

Table 4: Anisotropic displacement parameters [$Å^2 \times 10^3$] for **2b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2U_{11}$ + ...+ $2hka^*b^*U_{12}$]

Table 5: hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$Å^2 \times 10^3$] for **2b**.


I1A
P2A
P1A
Ru1A
C1A
C2A
C3A
C4A
C5A
C7A
C6A
C8A
C6
C5
C4
C3
C2
C7
C8
C1
C10
C9
Ru1
C13
C11
C12
P2
C35
C32
C33
C34
C44
C45
C43
C46
C47
C48
C49
C38
C39
C40
C41
C42
P1
C26
C27
C28
C29
C30
C31
C20
C21
C22
C23
C24
C25
C16
C15
C14
C17
C18
C19
I1

Identification code	ic8802
Diffractometer used	Nonius KappaCCD
Empirical formula	$C_{104}H_{84}D_6Cl_{18}I_2P_4Ru_2$
Formula weight	2563.68
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 9.56600(10) Å alpha = 101.4130(10)° b = 15.20300(10) Å beta = 103.0790(10)° c = 20.8060(2) Å gamma = 103.8240(10)°
Volume, Z	2758.58(4) $Å^3$, 1
Density (calculated)	1.540 Mg/m^3
Absorption coefficient	1.372 mm^{-1}
F(000)	1274
Crystal size	0.40 x 0.20 x 0.15 mm
θ range for data collection	1.04 to 27.47°
Limiting indices	$-12 \le h \le 12$, $-19 \le k \le 19$, $-26 \le l \le 26$
Reflections collected	67315
Independent reflections	12612 (R_{int} = 0.0760)
Absorption correction	Multi-scan
Max. and min. transmission	0.874 and 0.653
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12547 / 0 / 587
Goodness-of-fit on F^2	1.020
Final R indices [I>2σ(I)]	R1 = 0.0531, wR2 = 0.1325
R indices (all data)	R1 = 0.0936, wR2 = 0.1630
Extinction coefficient	0.0025(4)
Largest diff. peak and hole	0.967 and -0.888 $eÅ^{-3}$

Note:

The solvent: $CDCl_3$

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Table 2. Atomic coordinates [x 10] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 8802. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	8022(1)	3024(1)	2498(1)	71(1)
Ru(1)	8281(1)	6990(1)	3008(1)	34(1)
P(1)	6373(1)	6765(1)	3548(1)	35(1)
P(2)	6888(1)	6734(1)	1855(1)	40(1)
C(1)	8531(4)	8268(3)	3283(2)	36(1)
C(2)	8827(5)	9177(3)	3530(2)	40(1)
C(3)	8443(7)	9793(4)	3062(3)	65(1)
C(4)	9721(12)	10463(5)	2973(4)	97(2)
C(5)	11062(13)	10496(7)	3150(5)	132(4)
C(6)	10786(5)	9536(3)	4659(2)	44(1)
C(7)	9444(5)	9606(3)	4286(2)	38(1)
C(8)	8656(5)	10081(3)	4642(2)	43(1)
C(9)	10746(5)	7188(4)	3203(3)	62(1)
C(10)	10324(6)	6915(4)	3748(3)	61(1)
C(11)	9330(6)	5988(4)	3491(3)	59(1)
C(12)	9142(5)	5708(4)	2791(3)	56(1)
C(13)	10001(6)	6462(4)	2608(3)	58(1)
C(14)	5481(4)	7701(3)	3707(2)	38(1)
C(15)	5107(6)	7963(4)	4313(2)	52(1)
C(16)	4505(6)	8692(4)	4425(3)	61(1)
C(17)	4224(5)	9165(3)	3944(3)	55(1)
C(18)	4529(6)	8900(4)	3332(3)	60(1)
C(19)	5152(5)	8172(3)	3222(2)	48(1)
C(20)	7154(5)	6679(3)	4420(2)	40(1)
C(21)	6684(6)	5886(4)	4632(2)	54(1)
C(22)	7358(7)	5856(4)	5291(3)	69(2)
C(23)	8477(7)	6616(5)	5734(3)	68(2)
C(24)	8937(6)	7418(4)	5531(3)	65(1)
C(25)	8289(5)	7453(4)	4876(2)	54(1)
C(26)	4828(5)	5676(3)	3183(2)	41(1)
C(27)	5143(5)	4850(3)	2940(2)	50(1)
C(28)	4036(6)	4001(4)	2697(3)	60(1)
C(29)	2584(6)	3964(4)	2709(3)	62(1)
C(30)	2245(6)	4771(4)	2951(3)	65(1)
C(31)	3359(5)	5630(3)	3190(3)	52(1)
C(32)	4942(5)	6787(3)	1617(2)	44(1)
C(33)	3737(5)	6050(4)	1579(3)	58(1)
C(34)	2272(6)	6110(5)	1401(3)	71(2)
C(35)	2022(6)	6911(5)	1263(3)	76(2)
C(36)	3209(7)	7660(5)	1319(3)	69(2)
C(37)	4663(6)	7598(4)	1493(3)	57(1)
C(38)	7804(5)	7572(4)	1439(2)	52(1)
C(39)	9149(6)	8242(4)	1768(3)	63(1)
C(40)	9819(8)	8851(5)	1432(4)	84(2)
C(41)	9124(11)	8764(6)	757(4)	100(2)
C(42)	7790(10)	8083(7)	417(4)	102(2)
C(43)	7128(7)	7516(5)	757(3)	82(2)
C(44)	6805(5)	5609(4)	1299(2)	54(1)
C(45)	7601(7)	5561(5)	820(3)	87(2)
C(46)	7545(11)	4702(8)	428(4)	126(4)
C(47)	6754(11)	3897(7)	495(4)	125(4)
C(48)	5974(9)	3901(5)	981(4)	99(2)

Cl(1)	7747(5)	3585(3)	4627(2)	203(2)
Cl(2)	4688(4)	2736(3)	3969(2)	185(2)
Cl(3)	6787(4)	1672(2)	4026(2)	172(2)
C(50)	6445(9)	2699(6)	3945(4)	92(2)
Cl(4)	4225(6)	537(3)	2036(2)	253(3)
Cl(5)	6200(4)	-30(2)	1301(2)	189(2)
Cl(6)	4076(5)	772(3)	720(2)	222(2)
C(51)	5182(9)	799(5)	1477(4)	106(3)
Cl(7)	8161(4)	1654(2)	344(2)	163(1)
Cl(8)	10926(4)	1729(2)	1260(1)	151(1)
Cl(9)	10615(4)	3303(2)	773(2)	159(1)
C(52)	9695(10)	2352(6)	1010(4)	111(3)

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Table 3. Bond lengths [Å] and angles [°]

Ru(1)-C(1)	1.853(4)	Ru(1)-C(9)	2.235(4)
Ru(1)-C(10)	2.240(4)	Ru(1)-C(13)	2.243(4)
Ru(1)-C(11)	2.285(5)	Ru(1)-C(12)	2.295(4)
Ru(1)-P(1)	2.3429(11)	Ru(1)-P(2)	2.3708(11)
P(1)-C(26)	1.824(4)	P(1)-C(14)	1.841(4)
P(1)-C(20)	1.842(4)	P(2)-C(44)	1.838(5)
P(2)-C(38)	1.839(5)	P(2)-C(32)	1.841(4)
C(1)-C(2)	1.311(6)	C(2)-C(7)	1.497(6)
C(2)-C(3)	1.525(7)	C(3)-C(4)	1.465(10)
C(4)-C(5)	1.237(12)	C(6)-C(8)#1	1.379(6)
C(6)-C(7)	1.382(6)	C(7)-C(8)	1.392(6)
C(8)-C(6)#1	1.379(6)	C(9)-C(10)	1.392(8)
C(9)-C(13)	1.392(7)	C(10)-C(11)	1.416(8)
C(11)-C(12)	1.391(7)	C(12)-C(13)	1.413(8)
C(14)-C(19)	1.371(6)	C(14)-C(15)	1.397(6)
C(15)-C(16)	1.370(7)	C(16)-C(17)	1.359(8)
C(17)-C(18)	1.375(7)	C(18)-C(19)	1.381(7)
C(20)-C(21)	1.375(6)	C(20)-C(25)	1.395(6)
C(21)-C(22)	1.392(7)	C(22)-C(23)	1.368(8)
C(23)-C(24)	1.375(8)	C(24)-C(25)	1.381(7)
C(26)-C(27)	1.386(6)	C(26)-C(31)	1.395(6)
C(27)-C(28)	1.374(7)	C(28)-C(29)	1.382(7)
C(29)-C(30)	1.373(7)	C(30)-C(31)	1.388(7)
C(32)-C(33)	1.377(7)	C(32)-C(37)	1.383(7)
C(33)-C(34)	1.397(7)	C(34)-C(35)	1.367(9)
C(35)-C(36)	1.367(9)	C(36)-C(37)	1.386(7)
C(38)-C(39)	1.365(7)	C(38)-C(43)	1.397(7)
C(39)-C(40)	1.389(8)	C(40)-C(41)	1.375(11)
C(41)-C(42)	1.367(11)	C(42)-C(43)	1.352(9)
C(44)-C(49)	1.381(8)	C(44)-C(45)	1.386(8)
C(45)-C(46)	1.379(10)	C(46)-C(47)	1.327(14)
C(47)-C(48)	1.385(13)	C(48)-C(49)	1.400(8)
Cl(1)-C(50)	1.738(9)	Cl(2)-C(50)	1.707(7)
Cl(3)-C(50)	1.701(7)	Cl(4)-C(51)	1.686(10)
Cl(5)-C(51)	1.798(9)	Cl(6)-C(51)	1.675(8)
Cl(7)-C(52)	1.719(9)	Cl(8)-C(52)	1.732(9)
Cl(9)-C(52)	1.728(10)		

C(1)-Ru(1)-C(9)	93.5(2)	C(1)-Ru(1)-C(10)	99.6(2)
C(9)-Ru(1)-C(10)	36.2(2)	C(1)-Ru(1)-C(13)	120.6(2)
C(9)-Ru(1)-C(13)	36.2(2)	C(10)-Ru(1)-C(13)	60.6(2)
C(1)-Ru(1)-C(11)	133.7(2)	C(9)-Ru(1)-C(11)	60.2(2)
C(10)-Ru(1)-C(11)	36.5(2)	C(13)-Ru(1)-C(11)	60.1(2)
C(1)-Ru(1)-C(12)	153.5(2)	C(9)-Ru(1)-C(12)	60.0(2)
C(10)-Ru(1)-C(12)	60.0(2)	C(13)-Ru(1)-C(12)	36.3(2)
C(11)-Ru(1)-C(12)	35.4(2)	C(1)-Ru(1)-P(1)	87.51(12)
C(9)-Ru(1)-P(1)	141.5(2)	C(10)-Ru(1)-P(1)	105.7(2)
C(13)-Ru(1)-P(1)	149.2(2)	C(11)-Ru(1)-P(1)	92.09(14)
C(12)-Ru(1)-P(1)	113.2(2)	C(1)-Ru(1)-P(2)	97.04(12)
C(9)-Ru(1)-P(2)	116.2(2)	C(10)-Ru(1)-P(2)	148.29(14)
C(13)-Ru(1)-P(2)	87.72(14)	C(11)-Ru(1)-P(2)	128.1(2)
C(12)-Ru(1)-P(2)	94.71(13)	P(1)-Ru(1)-P(2)	101.81(4)
C(26)-P(1)-C(14)	105.5(2)	C(26)-P(1)-C(20)	102.2(2)
C(14)-P(1)-C(20)	102.1(2)	C(26)-P(1)-Ru(1)	117.11(14)
C(14)-P(1)-Ru(1)	118.40(14)	C(20)-P(1)-Ru(1)	109.42(14)
C(44)-P(2)-C(38)	101.1(2)	C(44)-P(2)-C(32)	104.0(2)
C(38)-P(2)-C(32)	101.6(2)	C(44)-P(2)-Ru(1)	113.0(2)
C(38)-P(2)-Ru(1)	112.3(2)	C(32)-P(2)-Ru(1)	122.24(14)
C(2)-C(1)-Ru(1)	174.0(3)	C(1)-C(2)-C(7)	119.7(4)

C(4)-C(3)-C(2)	116.2(6)	C(5)-C(4)-C(3)	127.5(8)
C(8)#1-C(6)-C(7)	122.0(4)	C(6)-C(7)-C(8)	117.5(4)
C(6)-C(7)-C(2)	122.0(4)	C(8)-C(7)-C(2)	120.5(4)
C(6)#1-C(8)-C(7)	120.5(4)	C(10)-C(9)-C(13)	108.6(5)
C(10)-C(9)-Ru(1)	72.0(3)	C(13)-C(9)-Ru(1)	72.2(3)
C(9)-C(10)-C(11)	107.7(5)	C(9)-C(10)-Ru(1)	71.7(3)
C(11)-C(10)-Ru(1)	73.5(3)	C(12)-C(11)-C(10)	107.9(5)
C(12)-C(11)-Ru(1)	72.7(3)	C(10)-C(11)-Ru(1)	70.0(3)
C(11)-C(12)-C(13)	107.9(5)	C(11)-C(12)-Ru(1)	71.9(3)
C(13)-C(12)-Ru(1)	69.9(3)	C(9)-C(13)-C(12)	107.8(5)
C(9)-C(13)-Ru(1)	71.6(3)	C(12)-C(13)-Ru(1)	73.9(3)
C(19)-C(14)-C(15)	117.2(4)	C(19)-C(14)-P(1)	120.3(3)
C(15)-C(14)-P(1)	122.5(3)	C(16)-C(15)-C(14)	120.8(5)
C(17)-C(16)-C(15)	120.9(5)	C(16)-C(17)-C(18)	119.6(5)
C(17)-C(18)-C(19)	119.5(5)	C(14)-C(19)-C(18)	121.9(4)
C(21)-C(20)-C(25)	119.3(4)	C(21)-C(20)-P(1)	122.9(3)
C(25)-C(20)-P(1)	117.8(3)	C(20)-C(21)-C(22)	120.0(5)
C(23)-C(22)-C(21)	120.3(5)	C(22)-C(23)-C(24)	120.1(5)
C(23)-C(24)-C(25)	120.1(5)	C(24)-C(25)-C(20)	120.2(5)
C(27)-C(26)-C(31)	118.6(4)	C(27)-C(26)-P(1)	118.9(3)
C(31)-C(26)-P(1)	122.3(3)	C(28)-C(27)-C(26)	121.3(4)
C(27)-C(28)-C(29)	119.6(5)	C(30)-C(29)-C(28)	120.3(5)
C(29)-C(30)-C(31)	120.3(5)	C(30)-C(31)-C(26)	120.0(5)
C(33)-C(32)-C(37)	118.1(4)	C(33)-C(32)-P(2)	122.1(4)
C(37)-C(32)-P(2)	119.8(4)	C(32)-C(33)-C(34)	121.0(5)
C(35)-C(34)-C(33)	119.8(6)	C(36)-C(35)-C(34)	119.9(5)
C(35)-C(36)-C(37)	120.2(6)	C(32)-C(37)-C(36)	121.0(5)
C(39)-C(38)-C(43)	117.9(5)	C(39)-C(38)-P(2)	122.5(4)
C(43)-C(38)-P(2)	119.5(4)	C(38)-C(39)-C(40)	120.8(6)
C(41)-C(40)-C(39)	119.3(7)	C(42)-C(41)-C(40)	120.6(7)
C(43)-C(42)-C(41)	119.4(7)	C(42)-C(43)-C(38)	121.9(7)
C(49)-C(44)-C(45)	117.3(5)	C(49)-C(44)-P(2)	120.4(4)
C(45)-C(44)-P(2)	122.1(5)	C(46)-C(45)-C(44)	120.3(8)
C(47)-C(46)-C(45)	122.1(8)	C(46)-C(47)-C(48)	120.2(7)
C(47)-C(48)-C(49)	118.2(8)	C(44)-C(49)-C(48)	121.8(7)
Cl(3)-C(50)-Cl(2)	114.1(5)	Cl(3)-C(50)-Cl(1)	106.8(4)
Cl(2)-C(50)-Cl(1)	108.2(4)	Cl(6)-C(51)-Cl(4)	113.4(6)
Cl(6)-C(51)-Cl(5)	106.3(5)	Cl(4)-C(51)-Cl(5)	110.7(5)
Cl(7)-C(52)-Cl(9)	109.8(5)	Cl(7)-C(52)-Cl(8)	111.4(5)
Cl(9)-C(52)-Cl(8)	109.7(5)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+2,-z+1

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Table 4. Anisotropic displacement parameters (Å^2 x 10^3)

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
I(1)	66(1)	66(1)	67(1)	8(1)	21(1)	0(1)
Ru(1)	30(1)	36(1)	32(1)	2(1)	8(1)	11(1)
P(1)	34(1)	37(1)	34(1)	7(1)	10(1)	11(1)
P(2)	38(1)	47(1)	32(1)	2(1)	10(1)	14(1)
C(1)	37(2)	45(2)	27(2)	5(2)	11(2)	14(2)
C(2)	44(2)	36(2)	36(2)	4(2)	10(2)	10(2)
C(3)	96(4)	53(3)	45(3)	12(2)	14(3)	29(3)
C(4)	150(8)	56(4)	67(4)	17(3)	26(5)	4(5)
C(5)	136(8)	121(8)	103(7)	27(5)	38(6)	-28(7)
C(6)	40(2)	46(2)	45(2)	2(2)	15(2)	17(2)
C(7)	42(2)	28(2)	38(2)	3(2)	11(2)	5(2)
C(8)	39(2)	46(2)	42(2)	7(2)	6(2)	17(2)
C(9)	30(2)	61(3)	88(4)	11(3)	10(2)	14(2)
C(10)	50(3)	78(4)	45(3)	-2(3)	-6(2)	33(3)
C(11)	53(3)	71(3)	71(3)	31(3)	20(3)	37(3)
C(12)	44(2)	54(3)	67(3)	-1(2)	6(2)	29(2)
C(13)	50(3)	78(4)	61(3)	14(3)	28(2)	36(3)
C(14)	37(2)	39(2)	39(2)	7(2)	13(2)	11(2)
C(15)	60(3)	59(3)	46(3)	11(2)	25(2)	25(2)
C(16)	58(3)	72(3)	55(3)	2(3)	28(2)	24(3)
C(17)	46(3)	46(3)	69(3)	1(2)	19(2)	18(2)
C(18)	54(3)	62(3)	74(4)	22(3)	21(3)	28(3)
C(19)	55(3)	51(3)	47(3)	12(2)	20(2)	26(2)
C(20)	40(2)	45(2)	38(2)	12(2)	12(2)	14(2)
C(21)	57(3)	53(3)	47(3)	17(2)	9(2)	12(2)
C(22)	89(4)	72(4)	53(3)	30(3)	19(3)	29(3)
C(23)	71(4)	98(5)	42(3)	27(3)	9(3)	34(3)
C(24)	52(3)	83(4)	42(3)	3(3)	3(2)	9(3)
C(25)	54(3)	57(3)	44(3)	10(2)	10(2)	7(2)
C(26)	41(2)	41(2)	37(2)	10(2)	9(2)	9(2)
C(27)	41(2)	48(3)	58(3)	4(2)	18(2)	12(2)
C(28)	62(3)	46(3)	63(3)	2(2)	16(3)	10(2)
C(29)	51(3)	50(3)	65(3)	9(2)	4(2)	-1(2)
C(30)	39(3)	59(3)	90(4)	18(3)	12(3)	10(2)
C(31)	40(2)	48(3)	68(3)	15(2)	12(2)	16(2)
C(32)	43(2)	56(3)	30(2)	4(2)	8(2)	18(2)
C(33)	49(3)	71(3)	52(3)	15(2)	10(2)	18(2)
C(34)	46(3)	94(4)	68(4)	20(3)	19(3)	13(3)
C(35)	51(3)	119(6)	64(4)	23(4)	18(3)	39(4)
C(36)	67(4)	89(4)	67(3)	25(3)	20(3)	46(3)
C(37)	54(3)	65(3)	54(3)	16(2)	12(2)	25(2)
C(38)	54(3)	68(3)	43(3)	15(2)	24(2)	22(2)
C(39)	69(3)	65(3)	54(3)	10(3)	30(3)	11(3)
C(40)	99(5)	72(4)	88(5)	20(3)	58(4)	10(3)
C(41)	141(7)	106(6)	94(6)	54(5)	78(5)	46(5)
C(42)	120(6)	142(7)	68(4)	57(5)	45(4)	41(6)
C(43)	75(4)	125(6)	51(3)	31(4)	22(3)	27(4)
C(44)	48(3)	66(3)	39(2)	-8(2)	4(2)	26(2)
C(45)	74(4)	112(5)	64(4)	-15(3)	26(3)	34(4)
C(46)	118(7)	150(9)	91(6)	-43(6)	33(5)	65(7)
C(47)	130(7)	116(7)	84(5)	-58(5)	-25(5)	77(6)
C(48)	115(6)	65(4)	87(5)	-20(4)	-9(4)	36(4)

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Table 5. Hydrogen coordinates (x 10) and isotropic displacement parameters ($Å^2$ x 10^3)

	x	y	z	U(eq)
H(3A)	7840(7)	9386(4)	2614(3)	78
H(3B)	7826(7)	10142(4)	3241(3)	78
H(4A)	9499(12)	10915(5)	2759(4)	116
H(5A)	11349(13)	10061(7)	3367(5)	159
H(5B)	11782(13)	10956(7)	3067(5)	159
H(6A)	11330(5)	9220(3)	4432(2)	53
H(8A)	7747(5)	10139(3)	4408(2)	51
H(9A)	11505(5)	7770(4)	3237(3)	74
H(10A)	10735(6)	7270(4)	4231(3)	73
H(11A)	8907(6)	5597(4)	3764(3)	71
H(12A)	8556(5)	5088(4)	2483(3)	67
H(13A)	10145(6)	6447(4)	2155(3)	70
H(15A)	5268(6)	7639(4)	4645(2)	63
H(16A)	4286(6)	8866(4)	4837(3)	73
H(17A)	3829(5)	9664(3)	4028(3)	66
H(18A)	4316(6)	9208(4)	2995(3)	72
H(19A)	5355(5)	7997(3)	2806(2)	58
H(21A)	5916(6)	5370(4)	4335(2)	64
H(22A)	7046(7)	5316(4)	5431(3)	82
H(23A)	8928(7)	6590(5)	6172(3)	82
H(24A)	9686(6)	7938(4)	5836(3)	78
H(25A)	8609(5)	7995(4)	4739(2)	65
H(27A)	6123(5)	4870(3)	2941(2)	60
H(28A)	4262(6)	3456(4)	2526(3)	72
H(29A)	1835(6)	3390(4)	2553(3)	74
H(30A)	1265(6)	4742(4)	2955(3)	78
H(31A)	3125(5)	6175(3)	3355(3)	63
H(33A)	3901(5)	5504(4)	1673(3)	70
H(34A)	1468(6)	5607(5)	1377(3)	85
H(35A)	1045(6)	6947(5)	1130(3)	91
H(36A)	3040(7)	8213(5)	1241(3)	83
H(37A)	5462(6)	8110(4)	1526(3)	68
H(39A)	9624(6)	8293(4)	2222(3)	76
H(40A)	10729(8)	9313(5)	1661(4)	101
H(41A)	9565(11)	9171(6)	530(4)	120
H(42A)	7343(10)	8011(7)	-44(4)	123
H(43A)	6195(7)	7077(5)	530(3)	99
H(45A)	8175(7)	6111(5)	762(3)	104
H(46A)	8080(11)	4685(8)	106(4)	151
H(47A)	6723(11)	3330(7)	216(4)	150
H(48A)	5429(9)	3342(5)	1038(4)	119
H(49A)	5526(8)	4783(4)	1719(3)	92
H(50A)	6598(9)	2811(6)	3515(4)	110
H(51A)	5901(9)	1429(5)	1678(4)	127
H(52A)	9346(10)	2584(6)	1401(4)	134

Cl(1)	230(4)	180(3)	169(3)	-16(3)	26(3)	84(3)
Cl(2)	146(2)	352(5)	169(3)	159(3)	95(2)	156(3)
Cl(3)	275(4)	134(2)	238(3)	117(2)	185(3)	139(3)
C(50)	118(6)	117(6)	84(5)	47(4)	54(4)	73(5)
Cl(4)	283(5)	228(4)	210(4)	65(3)	119(4)	-45(4)
Cl(5)	190(3)	133(2)	263(4)	102(3)	38(3)	67(2)
Cl(6)	226(4)	260(5)	147(3)	26(3)	-46(3)	127(4)
C(51)	117(6)	71(4)	98(5)	31(4)	-10(5)	0(4)
Cl(7)	164(3)	174(3)	119(2)	7(2)	23(2)	37(2)
Cl(8)	208(3)	137(2)	123(2)	33(2)	37(2)	91(2)
Cl(9)	213(3)	135(2)	159(3)	50(2)	82(2)	69(2)
C(52)	130(7)	135(7)	74(5)	8(5)	35(5)	62(6)