

ORGANOMETALLICS

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Table 18. Crystal data and structure refinement.

Identification code	yice
Empirical formula	C ₆₁ H ₅₆ PRu
Formula weight	921.10
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P $\bar{1}$
Unit cell dimensions	$a = 10.2582(1) \text{ Å}$ $\alpha = 101.0450(1)^\circ$ $b = 15.8273(2) \text{ Å}$ $\beta = 107.5713(2)^\circ$ $c = 16.9688(2) \text{ Å}$ $\gamma = 108.5520(1)^\circ$
Volume, Z	2360.54(4) Å ³ , 2
Density (calculated)	1.296 Mg/m ³
Absorption coefficient	0.406 mm ⁻¹
F(000)	962
Crystal size	0.30 x 0.30 x 0.20 mm
Crystal color	yellow
θ range for data collection	1.33 to 28.27 ^o
Limiting indices	$-10 \leq h \leq 13$, $-19 \leq k \leq 20$, $-20 \leq l \leq 22$
Reflections collected	13928
Independent reflections	10101 ($R_{\text{int}} = 0.0485$)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10096 / 0 / 568
Goodness-of-fit on F^2	0.938
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0508$, $wR2 = 0.1046$
R indices (all data)	$R1 = 0.0883$, $wR2 = 0.1580$
Largest diff. peak and hole	0.598 and -1.179 eÅ ⁻³

Table 2S. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$]. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ru	3979.4(3)	11767.6(2)	13028.8(2)	20(1)
P	5724(1)	13225(1)	13209(1)	22(1)
C(1)	4244(4)	11827(3)	14394(2)	25(1)
C(2)	3477(4)	10874(3)	13850(2)	27(1)
C(3)	2083(4)	10765(3)	13228(2)	26(1)
C(4)	1966(4)	11652(3)	13384(2)	26(1)
C(5)	3301(4)	12312(3)	14103(2)	26(1)
C(6)	5622(4)	12198(3)	15211(2)	38(1)
C(7)	3942(5)	10078(3)	13954(3)	40(1)
C(8)	855(5)	9836(3)	12626(3)	41(1)
C(9)	617(4)	11838(3)	12950(3)	38(1)
C(10)	3499(5)	13275(3)	14578(3)	37(1)
C(11)	5912(4)	10599(3)	12594(2)	23(1)
C(12)	4912(4)	11006(2)	12472(2)	20(1)
C(13)	3526(4)	10833(3)	11807(2)	23(1)
C(14)	3312(4)	11620(3)	11583(2)	23(1)
C(15)	7074(4)	10875(3)	13444(2)	24(1)
C(16)	8089(4)	11075(3)	14123(2)	28(1)
C(21)	10544(4)	11052(3)	14859(3)	34(1)
C(22)	11819(5)	11308(4)	15599(3)	43(1)
C(23)	11964(5)	11831(3)	16382(3)	47(1)
C(24)	10830(5)	12099(3)	16448(3)	48(1)
C(25)	9547(5)	11851(3)	15711(3)	39(1)
C(26)	9393(4)	11328(3)	14907(2)	28(1)
C(31)	4998(4)	9631(3)	11015(2)	32(1)
C(32)	4989(5)	8946(3)	10372(3)	41(1)
C(33)	5897(5)	8465(3)	10581(3)	41(1)
C(34)	6830(5)	8695(3)	11443(3)	44(1)
C(35)	6826(4)	9385(3)	12084(3)	33(1)
C(36)	5910(4)	9862(3)	11888(2)	24(1)
C(41)	474(4)	10891(3)	10878(2)	33(1)
C(42)	-865(5)	10906(3)	10365(3)	38(1)
C(43)	-859(5)	11595(4)	9981(3)	43(1)
C(44)	493(5)	12284(3)	10105(3)	43(1)
C(45)	1827(5)	12275(3)	10628(3)	36(1)
C(46)	1842(4)	11583(3)	11022(2)	24(1)
C(51)	3412(4)	13829(3)	12646(2)	28(1)
C(52)	2804(5)	14480(3)	12476(3)	36(1)
C(53)	3716(6)	15426(3)	12723(3)	45(1)
C(54)	5245(5)	15715(3)	13115(3)	40(1)
C(55)	5854(5)	15067(3)	13277(2)	33(1)
C(56)	4954(4)	14111(3)	13052(2)	24(1)
C(61)	6523(4)	13817(3)	11876(2)	31(1)
C(62)	7200(5)	13848(3)	11276(3)	39(1)
C(63)	8069(5)	13336(3)	11241(3)	38(1)
C(64)	8255(4)	12815(3)	11800(3)	35(1)
C(65)	7578(4)	12795(3)	12397(3)	32(1)

C(66)	6714(4)	13306(3)	12452(2)	24(1)
C(71)	8382(4)	13506(3)	14549(3)	35(1)
C(72)	9523(5)	13911(3)	15384(3)	41(1)
C(73)	9504(5)	14628(3)	15980(3)	43(1)
C(74)	8377(5)	14941(3)	15756(3)	44(1)
C(75)	7265(4)	14544(3)	14919(2)	34(1)
C(76)	7253(4)	13818(3)	14299(2)	26(1)
C(81)	-2927(8)	12333(5)	7955(5)	82(2)
C(82)	-2884(7)	12921(6)	8661(4)	73(2)
C(83)	-1789(9)	13792(6)	9041(4)	80(2)
C(85)	-746(7)	13504(5)	8000(5)	77(2)
C(86)	-704(7)	14101(5)	8725(4)	77(2)
C(86)	-1868(8)	12625(5)	7623(4)	84(2)
C(91)	3781(8)	14157(5)	9640(5)	79(2)
C(92)	4072(8)	14760(6)	10428(5)	79(2)
C(93)	5275(9)	15588(6)	10776(4)	79(2)

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

Ru-C(12)	2.026(3)	Ru-C(13)	2.124(3)
Ru-C(2)	2.220(4)	Ru-C(1)	2.229(3)
Ru-C(3)	2.248(4)	Ru-C(5)	2.257(4)
Ru-C(4)	2.284(4)	Ru-C(14)	2.282(3)
Ru-P	2.3219(10)	P-C(56)	1.839(4)
P-C(76)	1.846(4)	P-C(66)	1.862(4)
C(1)-C(2)	1.421(6)	C(1)-C(5)	1.448(5)
C(1)-C(6)	1.497(5)	C(2)-C(3)	1.432(5)
C(2)-C(7)	1.505(5)	C(3)-C(4)	1.428(5)
C(3)-C(8)	1.504(6)	C(4)-C(5)	1.432(5)
C(4)-C(9)	1.507(5)	C(5)-C(10)	1.499(5)
C(11)-C(12)	1.361(5)	C(11)-C(15)	1.443(5)
C(11)-C(36)	1.502(5)	C(12)-C(13)	1.426(5)
C(13)-C(14)	1.431(5)	C(14)-C(46)	1.497(5)
C(15)-C(16)	1.199(5)	C(16)-C(26)	1.449(5)
C(21)-C(22)	1.388(5)	C(21)-C(26)	1.402(5)
C(22)-C(23)	1.363(7)	C(23)-C(24)	1.385(7)
C(24)-C(25)	1.393(5)	C(25)-C(26)	1.388(5)
C(31)-C(32)	1.378(5)	C(31)-C(36)	1.394(5)
C(32)-C(33)	1.389(6)	C(33)-C(34)	1.386(6)
C(34)-C(35)	1.387(6)	C(35)-C(36)	1.386(5)
C(41)-C(46)	1.394(5)	C(41)-C(42)	1.397(5)
C(42)-C(43)	1.373(6)	C(43)-C(44)	1.390(6)
C(44)-C(45)	1.393(5)	C(45)-C(46)	1.390(5)
C(51)-C(52)	1.396(5)	C(51)-C(56)	1.396(5)
C(52)-C(53)	1.387(6)	C(53)-C(54)	1.381(6)
C(54)-C(55)	1.390(6)	C(55)-C(56)	1.402(5)
C(61)-C(66)	1.392(5)	C(61)-C(62)	1.395(5)
C(62)-C(63)	1.388(6)	C(63)-C(64)	1.380(6)
C(64)-C(65)	1.392(5)	C(65)-C(66)	1.388(5)
C(71)-C(76)	1.383(5)	C(71)-C(72)	1.401(5)
C(72)-C(73)	1.378(6)	C(73)-C(74)	1.378(6)
C(74)-C(75)	1.392(5)	C(75)-C(76)	1.395(5)
C(81)-C(82)	1.348(9)	C(81)-C(86)	1.364(9)
C(82)-C(83)	1.348(9)	C(83)-C(86)	1.371(9)
C(85)-C(86)	1.365(9)	C(85)-C(86)	1.381(9)
C(91)-C(93)#1	1.368(8)	C(91)-C(92)	1.371(9)
C(92)-C(93)	1.350(9)	C(93)-C(91)#1	1.368(8)
C(12)-Ru-C(13)	40.11(13)	C(12)-Ru-C(2)	94.56(14)
C(13)-Ru-C(2)	106.1(2)	C(12)-Ru-C(1)	116.41(14)
C(13)-Ru-C(1)	142.2(2)	C(2)-Ru-C(1)	37.24(14)
C(12)-Ru-C(3)	107.80(14)	C(13)-Ru-C(3)	93.6(2)
C(2)-Ru-C(3)	37.37(13)	C(1)-Ru-C(3)	62.29(14)
C(12)-Ru-C(5)	153.85(14)	C(13)-Ru-C(5)	152.5(2)
C(2)-Ru-C(5)	62.06(14)	C(1)-Ru-C(5)	37.66(13)
C(3)-Ru-C(5)	61.48(14)	C(12)-Ru-C(4)	143.5(2)
C(13)-Ru-C(4)	116.02(14)	C(2)-Ru-C(4)	62.03(13)
C(1)-Ru-C(4)	62.37(13)	C(3)-Ru-C(4)	36.72(14)
C(5)-Ru-C(4)	36.75(13)	C(12)-Ru-C(14)	68.95(13)
C(13)-Ru-C(14)	37.70(13)	C(2)-Ru-C(14)	138.2(2)
C(1)-Ru-C(14)	170.91(13)	C(3)-Ru-C(14)	109.57(14)
C(5)-Ru-C(14)	136.15(13)	C(4)-Ru-C(14)	108.81(13)
C(12)-Ru-P	95.64(10)	C(13)-Ru-P	108.07(11)

C(2)-Ru-P	137.68(11)	C(1)-Ru-P	102.80(11)
C(3)-Ru-P	155.96(10)	C(5)-Ru-P	94.99(11)
C(4)-Ru-P	120.68(11)	C(14)-Ru-P	83.43(10)
C(56)-P-C(76)	103.0(2)	C(56)-P-C(66)	99.6(2)
C(76)-P-C(66)	103.5(2)	C(56)-P-Ru	114.53(13)
C(76)-P-Ru	115.39(12)	C(66)-P-Ru	118.49(13)
C(2)-C(1)-C(5)	107.1(3)	C(2)-C(1)-C(6)	125.1(4)
C(5)-C(1)-C(6)	126.8(4)	C(2)-C(1)-Ru	71.0(2)
C(5)-C(1)-Ru	72.2(2)	C(6)-C(1)-Ru	130.6(3)
C(1)-C(2)-C(3)	108.5(3)	C(1)-C(2)-C(7)	126.7(3)
C(3)-C(2)-C(7)	124.4(4)	C(1)-C(2)-Ru	71.7(2)
C(3)-C(2)-Ru	72.3(2)	C(7)-C(2)-Ru	126.8(3)
C(4)-C(3)-C(2)	108.5(3)	C(4)-C(3)-C(8)	126.0(3)
C(2)-C(3)-C(8)	124.6(4)	C(4)-C(3)-Ru	73.0(2)
C(2)-C(3)-Ru	70.3(2)	C(8)-C(3)-Ru	130.8(3)
C(3)-C(4)-C(5)	107.3(3)	C(3)-C(4)-C(9)	126.5(4)
C(5)-C(4)-C(9)	125.8(4)	C(3)-C(4)-Ru	70.3(2)
C(5)-C(4)-Ru	70.6(2)	C(9)-C(4)-Ru	129.9(3)
C(4)-C(5)-C(1)	108.5(3)	C(4)-C(5)-C(10)	123.9(4)
C(1)-C(5)-C(10)	126.3(4)	C(4)-C(5)-Ru	72.6(2)
C(1)-C(5)-Ru	70.1(2)	C(10)-C(5)-Ru	133.2(3)
C(12)-C(11)-C(15)	120.0(3)	C(12)-C(11)-C(36)	124.2(3)
C(15)-C(11)-C(36)	115.8(3)	C(11)-C(12)-C(13)	136.5(3)
C(11)-C(12)-Ru	147.0(3)	C(13)-C(12)-Ru	73.6(2)
C(12)-C(13)-C(14)	117.9(3)	C(12)-C(13)-Ru	66.3(2)
C(14)-C(13)-Ru	77.2(2)	C(13)-C(14)-C(46)	124.1(3)
C(13)-C(14)-Ru	65.1(2)	C(46)-C(14)-Ru	123.2(2)
C(16)-C(15)-C(11)	175.4(4)	C(15)-C(16)-C(26)	175.5(4)
C(22)-C(21)-C(26)	120.6(4)	C(23)-C(22)-C(21)	120.2(4)
C(22)-C(23)-C(24)	120.2(4)	C(23)-C(24)-C(25)	120.3(4)
C(26)-C(25)-C(24)	120.1(4)	C(25)-C(26)-C(21)	118.6(4)
C(25)-C(26)-C(16)	121.7(4)	C(21)-C(26)-C(16)	119.8(4)
C(32)-C(31)-C(36)	121.4(4)	C(31)-C(32)-C(33)	120.5(4)
C(34)-C(33)-C(32)	118.9(4)	C(35)-C(34)-C(33)	119.9(4)
C(34)-C(35)-C(36)	121.9(4)	C(35)-C(36)-C(31)	117.3(4)
C(35)-C(36)-C(11)	120.9(3)	C(31)-C(36)-C(11)	121.7(3)
C(46)-C(41)-C(42)	120.7(4)	C(43)-C(42)-C(41)	120.7(4)
C(42)-C(43)-C(44)	119.6(4)	C(43)-C(44)-C(45)	119.7(4)
C(46)-C(45)-C(44)	121.5(4)	C(45)-C(46)-C(41)	117.9(3)
C(45)-C(46)-C(14)	118.9(3)	C(41)-C(46)-C(14)	123.2(3)
C(52)-C(51)-C(56)	120.8(4)	C(53)-C(52)-C(51)	120.7(4)
C(54)-C(53)-C(52)	119.2(4)	C(53)-C(54)-C(55)	120.2(4)
C(54)-C(55)-C(56)	121.7(4)	C(51)-C(56)-C(55)	117.4(4)
C(51)-C(56)-P	119.7(3)	C(55)-C(56)-P	122.9(3)
C(66)-C(61)-C(62)	122.2(4)	C(63)-C(62)-C(61)	118.8(4)
C(64)-C(63)-C(62)	119.8(4)	C(63)-C(64)-C(65)	120.7(4)
C(66)-C(65)-C(64)	120.8(4)	C(65)-C(66)-C(61)	117.7(3)
C(65)-C(66)-P	120.6(3)	C(61)-C(66)-P	121.5(3)
C(76)-C(71)-C(72)	121.9(4)	C(73)-C(72)-C(71)	119.1(4)
C(74)-C(73)-C(72)	120.3(4)	C(73)-C(74)-C(75)	120.0(4)
C(74)-C(75)-C(76)	121.2(4)	C(71)-C(76)-C(75)	117.5(4)
C(71)-C(76)-P	120.3(3)	C(75)-C(76)-P	122.0(3)
C(82)-C(81)-C(86)	119.8(7)	C(81)-C(82)-C(83)	120.0(6)
C(82)-C(83)-C(86)	121.3(6)	C(86)-C(85)-C(86)	118.7(6)
C(83)-C(86)-C(85)	118.9(6)	C(81)-C(86)-C(85)	121.2(6)
C(93)#1-C(91)-C(92)	118.8(7)	C(93)-C(92)-C(91)	119.6(6)
C(92)-C(93)-C(91)#1	121.6(7)		

Table 4S. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$].

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Ru	16(1)	19(1)	20(1)	4(1)	4(1)	6(1)
P	19(1)	20(1)	22(1)	4(1)	5(1)	5(1)
C(1)	23(2)	32(2)	23(2)	13(2)	9(2)	9(2)
C(2)	24(2)	33(2)	25(2)	12(2)	9(2)	13(2)
C(3)	23(2)	27(2)	32(2)	14(2)	15(2)	10(2)
C(4)	24(2)	33(2)	27(2)	13(2)	14(2)	14(2)
C(5)	29(2)	26(2)	28(2)	9(2)	17(2)	12(2)
C(6)	31(2)	45(3)	25(2)	11(2)	5(2)	3(2)
C(7)	40(3)	39(3)	48(3)	25(2)	17(2)	18(2)
C(8)	32(2)	35(3)	45(3)	12(2)	12(2)	1(2)
C(9)	27(2)	56(3)	45(2)	25(2)	18(2)	25(2)
C(10)	45(3)	39(3)	34(2)	5(2)	23(2)	22(2)
C(11)	18(2)	24(2)	23(2)	5(2)	6(2)	6(2)
C(12)	19(2)	16(2)	20(2)	4(2)	6(1)	4(2)
C(13)	21(2)	24(2)	20(2)	2(2)	5(2)	10(2)
C(14)	21(2)	27(2)	20(2)	7(2)	8(2)	9(2)
C(15)	21(2)	21(2)	31(2)	10(2)	10(2)	10(2)
C(16)	23(2)	29(2)	28(2)	7(2)	7(2)	9(2)
C(21)	28(2)	42(3)	35(2)	16(2)	13(2)	15(2)
C(22)	22(2)	55(3)	55(3)	28(3)	12(2)	15(2)
C(23)	30(2)	45(3)	44(3)	21(2)	-6(2)	3(2)
C(24)	48(3)	43(3)	27(2)	2(2)	-2(2)	7(2)
C(25)	35(2)	46(3)	32(2)	6(2)	8(2)	19(2)
C(26)	20(2)	27(2)	30(2)	14(2)	5(2)	5(2)
C(31)	29(2)	39(3)	28(2)	8(2)	8(2)	20(2)
C(32)	41(3)	50(3)	24(2)	2(2)	9(2)	17(2)
C(33)	42(3)	34(3)	43(3)	-3(2)	19(2)	16(2)
C(34)	37(3)	43(3)	49(3)	2(2)	10(2)	25(2)
C(35)	28(2)	30(2)	34(2)	5(2)	4(2)	14(2)
C(36)	17(2)	24(2)	25(2)	5(2)	7(2)	5(2)
C(41)	28(2)	28(2)	29(2)	7(2)	1(2)	7(2)
C(42)	23(2)	40(3)	35(2)	1(2)	-1(2)	9(2)
C(43)	33(3)	54(3)	34(2)	7(2)	-2(2)	26(2)
C(44)	43(3)	47(3)	46(3)	23(2)	10(2)	27(2)
C(45)	30(2)	37(3)	36(2)	13(2)	8(2)	14(2)
C(46)	20(2)	28(2)	20(2)	2(2)	5(2)	11(2)
C(51)	31(2)	26(2)	25(2)	6(2)	11(2)	11(2)
C(52)	33(2)	45(3)	38(2)	15(2)	15(2)	24(2)
C(53)	57(3)	43(3)	55(3)	27(3)	28(3)	34(3)
C(54)	59(3)	22(2)	37(2)	9(2)	18(2)	14(2)
C(55)	34(2)	26(2)	31(2)	6(2)	8(2)	7(2)
C(56)	26(2)	21(2)	24(2)	6(2)	10(2)	9(2)
C(61)	30(2)	36(2)	34(2)	14(2)	14(2)	17(2)
C(62)	47(3)	44(3)	41(2)	26(2)	25(2)	23(2)
C(63)	39(3)	50(3)	34(2)	16(2)	22(2)	19(2)
C(64)	29(2)	49(3)	39(2)	14(2)	17(2)	25(2)
C(65)	33(2)	36(2)	33(2)	17(2)	13(2)	17(2)

C(66)	16(2)	24(2)	23(2)	4(2)	6(2)	2(2)
C(71)	30(2)	34(2)	32(2)	8(2)	4(2)	10(2)
C(72)	27(2)	44(3)	36(2)	13(2)	0(2)	8(2)
C(73)	33(2)	40(3)	30(2)	10(2)	-2(2)	-4(2)
C(74)	46(3)	40(3)	26(2)	-3(2)	8(2)	6(2)
C(75)	30(2)	35(2)	27(2)	6(2)	9(2)	7(2)
C(76)	23(2)	22(2)	23(2)	7(2)	4(2)	1(2)
C(81)	81(5)	52(4)	94(5)	19(4)	33(4)	8(4)
C(82)	73(4)	103(6)	77(4)	54(4)	45(4)	47(4)
C(83)	102(6)	93(6)	42(3)	11(4)	20(4)	49(5)
C(85)	61(4)	88(5)	90(5)	34(4)	41(4)	25(4)
C(86)	58(4)	54(4)	79(4)	14(4)	0(3)	4(3)
C(86)	105(6)	69(5)	73(4)	7(4)	42(4)	33(4)
C(91)	92(5)	80(5)	95(5)	48(5)	50(4)	47(4)
C(92)	103(6)	101(6)	104(5)	74(5)	74(5)	71(5)
C(93)	124(6)	92(6)	66(4)	45(4)	56(4)	68(5)

Table 5S. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$).

	x	y	z	U(eq)
H(6A)	5932(4)	12868(3)	15465(2)	58
H(6B)	6414(4)	12082(3)	15075(2)	58
H(6C)	5412(4)	11883(3)	15624(2)	58
H(7A)	3214(5)	9502(3)	13493(3)	60
H(7B)	3997(5)	10000(3)	14515(3)	60
H(7C)	4912(5)	10217(3)	13922(3)	60
H(8A)	1227(5)	9345(3)	12639(3)	62
H(8B)	516(5)	9865(3)	12037(3)	62
H(8C)	28(5)	9699(3)	12814(3)	62
H(9A)	840(4)	12501(3)	13176(3)	57
H(9B)	-216(4)	11470(3)	13069(3)	57
H(9C)	357(4)	11662(3)	12325(3)	57
H(10A)	4488(5)	13597(3)	15039(3)	56
H(10B)	2754(5)	13222(3)	14829(3)	56
H(10C)	3382(5)	13630(3)	14174(3)	56
H(13A)	2695(4)	10203(3)	11562(2)	28
H(14A)	4149(4)	12006(3)	11459(2)	27
H(21A)	10452(4)	10690(3)	14321(3)	40
H(22A)	12585(5)	11120(4)	15559(3)	52
H(23A)	12835(5)	12011(3)	16880(3)	57
H(24A)	10927(5)	12449(3)	16993(3)	58
H(25A)	8784(5)	12039(3)	15758(3)	47
H(31A)	4375(4)	9949(3)	10861(2)	38
H(32A)	4363(5)	8804(3)	9788(3)	49
H(33A)	5879(5)	7990(3)	10144(3)	50
H(34A)	7465(5)	8384(3)	11595(3)	53
H(35A)	7462(4)	9534(3)	12667(3)	39
H(41A)	452(4)	10408(3)	11129(2)	39
H(42A)	-1779(5)	10439(3)	10281(3)	46
H(43A)	-1764(5)	11601(4)	9637(3)	52
H(44A)	509(5)	12753(3)	9838(3)	52
H(45A)	2737(5)	12749(3)	10716(3)	43
H(51A)	2776(4)	13193(3)	12486(2)	33
H(52A)	1765(5)	14275(3)	12191(3)	44
H(53A)	3299(6)	15865(3)	12626(3)	53
H(54A)	5875(5)	16352(3)	13272(3)	48
H(55A)	6897(5)	15275(3)	13545(2)	40
H(61A)	5918(4)	14153(3)	11892(2)	37
H(62A)	7070(5)	14208(3)	10901(3)	47
H(63A)	8529(5)	13344(3)	10839(3)	46
H(64A)	8846(4)	12470(3)	11776(3)	42
H(65A)	7707(4)	12431(3)	12769(3)	39
H(71A)	8383(4)	13007(3)	14147(3)	42
H(72A)	10291(5)	13696(3)	15536(3)	49
H(73A)	10264(5)	14905(3)	16543(3)	52
H(74A)	8359(5)	15423(3)	16168(3)	53
H(75A)	6509(4)	14769(3)	14769(2)	40
H(81A)	-3685(8)	11723(5)	7692(5)	99

H(82A)	-3617(7)	12723(6)	8887(4)	87
H(83A)	-1768(9)	14196(6)	9534(4)	96
H(85A)	-16(7)	13698(5)	7769(5)	93
H(86A)	56(7)	14710(5)	8998(4)	92
H(86B)	-1911(8)	12215(5)	7127(4)	100
H(91A)	2947(8)	13578(5)	9389(5)	95
H(92A)	3439(8)	14598(6)	10726(5)	95
H(93A)	5468(9)	15999(6)	11316(4)	95
