Synthesis and Characterization of Bimetallic Ruthenium Complexes with $(CH)_6$ and Related Bridges

Sheng Hua Liu,[a] Haiping Xia[a], Tin Bin Wen,[a] Zhongyuan Zhou,[b] and Guochen Jia*,[a]

[a]Department of Chemistry, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong and [b]Department of Applied Biology & Chemical Technology, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong

Supporting information available

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for {[Ru(*t*-BuNC)$_3$(PPh$_3$)$_2$]$_2$(μ-COCH=CHCH=CHCH=CHCO)}(BPh$_4$)$_2$·6CH$_2$Cl$_2$

Table S2. Bond lengths [Å] for {[Ru(*t*-BuNC)$_3$(PPh$_3$)$_2$]$_2$(μ-COCH=CHCH=CHCH=CHCO)}(BPh$_4$)$_2$·6CH$_2$Cl$_2$

Table S3. Bond angles [°] for {[Ru(*t*-BuNC)$_3$(PPh$_3$)$_2$]$_2$(μ-COCH=CHCH=CHCH=CHCO)}(BPh$_4$)$_2$·6CH$_2$Cl$_2$

Table S4. Anisotropic displacement parameters ($Å^2$x 10^3) {[Ru(*t*-BuNC)$_3$(PPh$_3$)$_2$]$_2$(μ-COCH=CHCH=CHCH=CHCO)}(BPh$_4$)$_2$·6CH$_2$Cl$_2$

Table S5. Hydrogen coordinates (x10^4) and isotropic displacement parameters ($Å^2$x 10^3) for {[Ru(*t*-BuNC)$_3$(PPh$_3$)$_2$]$_2$(μ-COCH=CHCH=CHCH=CHCO)}(BPh$_4$)$_2$·6CH$_2$Cl$_2$

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for {[Ru(*t*-BuNC)$_3$(PPh$_3$)$_2$]$_2$(μ-COCH=CHCH=CHCH=CHCO)}(BPh$_4$)$_2$·6CH$_2$Cl$_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

Atom	x	y	z	U(eq)
Ru(1)	4622(1)	2635(1)	1179(1)	31(1)
P(1)	6487(1)	2319(1)	1144(1)	35(1)
P(2)	2819(1)	3007(1)	1255(1)	39(1)
O(1)	4150(2)	2599(1)	400(1)	65(1)
C(1)	4353(3)	3037(2)	652(1)	40(1)
C(2)	4442(3)	3878(2)	563(1)	44(1)
C(3)	4682(3)	4110(2)	257(1)	47(1)
C(4)	4857(3)	4895(2)	153(1)	50(1)
C(11)	5174(3)	3677(2)	1339(1)	36(1)
N(1)	5514(2)	4289(2)	1419(1)	50(1)
C(13)	5961(4)	5058(2)	1513(1)	69(1)
C(14)	5050(5)	5522(3)	1633(2)	138(3)
C(15)	6314(5)	5410(3)	1193(1)	121(2)
C(16)	6912(6)	4961(3)	1806(2)	152(3)
C(21)	4052(3)	1647(2)	946(1)	35(1)
N(2)	3702(2)	1121(2)	780(1)	42(1)
C(23)	3278(3)	601(2)	490(1)	49(1)
C(24)	3060(5)	-188(2)	646(1)	118(2)
C(25)	2242(4)	952(3)	297(1)	106(2)
C(26)	4155(4)	537(3)	260(1)	93(2)
C(31)	4826(3)	2094(2)	1656(1)	41(1)
N(3)	4939(3)	1724(2)	1909(1)	55(1)
C(33)	5137(4)	1287(3)	2239(1)	80(1)
C(34)	6136(5)	781(3)	2226(2)	124(2)
C(35)	5316(6)	1878(3)	2535(1)	141(3)
C(36)	4121(5)	778(3)	2251(1)	127(2)
C(41)	6715(3)	1362(2)	959(1)	41(1)
C(42)	6384(3)	710(2)	1125(1)	58(1)
C(43)	6602(4)	-27(2)	1014(1)	73(1)
C(44)	7147(4)	-124(3)	734(1)	78(1)
C(45)	7456(3)	511(3)	560(1)	71(1)

C(46)	7242(3)	1260(2)	670(1)	53(1)
C(51)	7278(3)	2998(2)	911(1)	44(1)
C(52)	8193(3)	3390(2)	1086(1)	61(1)
C(53)	8759(4)	3914(2)	901(2)	82(2)
C(54)	8433(5)	4026(3)	552(2)	92(2)
C(55)	7536(4)	3643(3)	376(1)	85(2)
C(56)	6955(3)	3131(2)	556(1)	59(1)
C(61)	7379(3)	2266(2)	1573(1)	42(1)
C(62)	7218(3)	2763(2)	1843(1)	55(1)
C(63)	7943(4)	2781(3)	2158(1)	72(1)
C(64)	8832(4)	2300(3)	2205(1)	81(1)
C(65)	9011(4)	1797(3)	1946(1)	76(1)
C(66)	8291(3)	1781(2)	1629(1)	56(1)
C(71)	1786(3)	2235(2)	1183(1)	52(1)
C(72)	831(3)	2278(2)	939(1)	73(1)
C(73)	66(4)	1674(3)	900(2)	98(2)
C(74)	268(5)	1037(3)	1110(2)	97(2)
C(75)	1186(4)	973(2)	1354(2)	90(2)
C(76)	1958(3)	1572(2)	1386(1)	70(1)
C(81)	2666(3)	3311(2)	1703(1)	49(1)
C(82)	1618(4)	3359(2)	1796(1)	70(1)
C(83)	1489(5)	3621(3)	2130(2)	89(2)
C(84)	2378(6)	3818(3)	2370(2)	90(2)
C(85)	3412(5)	3768(2)	2285(1)	86(2)
C(86)	3552(4)	3521(2)	1949(1)	61(1)
C(91)	2226(3)	3828(2)	989(1)	49(1)
C(92)	1964(3)	3770(2)	629(1)	64(1)
C(93)	1557(4)	4400(3)	425(1)	95(2)
C(94)	1436(5)	5101(4)	584(2)	110(2)
C(95)	1716(5)	5179(3)	937(2)	99(2)
C(96)	2109(3)	4552(2)	1145(1)	66(1)
B(1)	1243(4)	8027(2)	1405(1)	53(1)
C(111)	877(3)	8169(2)	983(1)	60(1)
C(112)	1074(4)	7609(3)	741(1)	98(2)
C(113)	850(5)	7721(4)	380(2)	116(2)
C(114)	415(5)	8415(4)	248(1)	107(2)
C(115)	201(4)	8977(3)	475(2)	97(2)
C(116)	432(4)	8858(3)	833(1)	76(1)

C(121)	631(3)	8626(2)	1650(1)	57(1)
C(122)	-462(4)	8837(2)	1569(1)	78(1)
C(123)	-980(5)	9327(3)	1781(2)	94(2)
C(124)	-429(6)	9617(3)	2079(2)	96(2)
C(125)	631(5)	9421(3)	2175(1)	97(2)
C(126)	1164(4)	8934(3)	1966(1)	81(1)
C(131)	914(3)	7151(2)	1523(1)	53(1)
C(132)	56(4)	6725(3)	1337(1)	73(1)
C(133)	-266(4)	5995(3)	1445(2)	90(2)
C(134)	282(5)	5664(3)	1746(2)	92(2)
C(135)	1105(4)	6067(3)	1939(2)	91(2)
C(136)	1408(4)	6796(3)	1831(1)	74(1)
C(141)	2579(3)	8179(2)	1475(1)	53(1)
C(142)	3378(4)	7611(2)	1519(1)	76(1)
C(143)	4494(4)	7772(3)	1564(1)	96(2)
C(144)	4866(4)	8522(3)	1569(1)	90(2)
C(145)	4105(4)	9095(3)	1519(1)	88(2)
C(146)	2998(4)	8932(2)	1475(1)	75(1)
C(01)	2316(8)	2809(4)	-397(2)	204(4)
Cl(1)	2825(2)	2392(1)	-790(1)	220(1)
Cl(2)	2190(2)	3778(1)	-481(1)	195(1)
C(02)	8574(4)	7228(3)	2059(1)	94(2)
Cl(3)	7348(1)	7389(1)	1794(1)	155(1)
Cl(4)	8447(1)	6597(1)	2398(1)	135(1)
C(03)	6083(6)	2298(3)	-634(2)	130(2)
Cl(5)	5741(2)	1965(1)	-253(1)	167(1)
Cl(6)	6197(2)	3303(1)	-644(1)	146(1)

Table S2. Bond lengths [Å] for {[Ru(*t*-BuNC)$_3$(PPh$_3$)$_2$]$_2$(μ-COCH=CHCH=CHCH=CHCO)}(BPh$_4$)$_2$·6CH$_2$Cl$_2$

Ru(1)-P(1)	2.3799(9)	Ru(1)-P(2)	2.3682(9)
Ru(1)-C(1)	2.118(3)	Ru(1)-C(11)	1.980(3)
Ru(1)-C(21)	1.996(3)	Ru(1)-C(31)	2.038(4)
O(1)-C(1)	1.224(4)	C(1)-C(2)	1.494(4)
C(2)-C(3)	1.322(4)	C(3)-C(4)	1.433(4)
C(4)-C(4)#1	1.334(6)		
C(11)-N(1)	1.156(4)	N(1)-C(13)	1.454(4)
C(21)-N(2)	1.151(4)	N(2)-C(23)	1.460(4)
C(31)-N(3)	1.155(4)	N(3)-C(33)	1.462(5)
C(13)-C(15)	1.495(6)	C(23)-C(24)	1.526(5)
C(13)-C(16)	1.499(7)	C(33)-C(34)	1.513(7)
C(13)-C(14)	1.506(6)	C(33)-C(35)	1.517(6)
C(23)-C(25)	1.495(5)	C(33)-C(36)	1.531(6)
C(23)-C(26)	1.502(5)		
P(1)-C(61)	1.832(3)	P(2)-C(91)	1.825(4)
P(1)-C(41)	1.834(3)	P(2)-C(71)	1.828(4)
P(1)-C(51)	1.840(3)	P(2)-C(81)	1.841(4)
C(41)-C(42)	1.383(5)	C(71)-C(76)	1.381(5)
C(41)-C(46)	1.384(4)	C(71)-C(72)	1.383(6)
C(42)-C(43)	1.378(5)	C(72)-C(73)	1.393(6)
C(43)-C(44)	1.369(6)	C(73)-C(74)	1.362(7)
C(44)-C(45)	1.365(6)	C(74)-C(75)	1.353(7)
C(45)-C(46)	1.393(5)	C(75)-C(76)	1.393(6)
C(51)-C(56)	1.379(5)	C(81)-C(86)	1.372(5)
C(51)-C(52)	1.389(5)	C(81)-C(82)	1.392(5)
C(52)-C(53)	1.401(5)	C(82)-C(83)	1.397(6)
C(53)-C(54)	1.354(6)	C(83)-C(84)	1.356(7)
C(54)-C(55)	1.367(7)	C(84)-C(85)	1.363(6)
C(55)-C(56)	1.387(5)	C(85)-C(86)	1.399(5)
C(61)-C(66)	1.386(4)	C(91)-C(92)	1.378(5)
C(61)-C(62)	1.386(4)	C(91)-C(96)	1.400(5)
C(62)-C(63)	1.386(5)	C(92)-C(93)	1.383(6)
C(63)-C(64)	1.359(6)	C(93)-C(94)	1.371(7)
C(64)-C(65)	1.365(6)	C(94)-C(95)	1.353(7)

C(65)-C(66)	1.387(5)	C(95)-C(96)	1.383(6)
B(1)-C(111)	1.632(6)	B(1)-C(131)	1.643(6)
B(1)-C(121)	1.655(6)	B(1)-C(141)	1.641(6)
C(111)-C(112)	1.389(5)	C(131)-C(132)	1.384(5)
C(111)-C(116)	1.392(5)	C(131)-C(136)	1.384(5)
C(112)-C(113)	1.386(7)	C(132)-C(133)	1.400(6)
C(113)-C(114)	1.371(7)	C(133)-C(134)	1.367(7)
C(114)-C(115)	1.356(7)	C(134)-C(135)	1.347(7)
C(115)-C(116)	1.378(6)	C(135)-C(136)	1.390(6)
C(121)-C(122)	1.378(5)	C(141)-C(142)	1.376(5)
C(121)-C(126)	1.392(6)	C(141)-C(146)	1.394(5)
C(122)-C(123)	1.394(6)	C(142)-C(143)	1.383(6)
C(123)-C(124)	1.334(7)	C(143)-C(144)	1.367(6)
C(124)-C(125)	1.340(7)	C(144)-C(145)	1.352(6)
C(125)-C(126)	1.396(6)	C(145)-C(146)	1.372(6)
C(01)-Cl(1)	1.871(8)	C(01)-Cl(2)	1.699(7)
C(02)-Cl(3)	1.702(5)	C(02)-Cl(4)	1.724(5)
C(03)-Cl(5)	1.689(5)	C(03)-Cl(6)	1.735(5)

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

Table S3. Bond angles [°] for {[Ru(*t*-BuNC)$_3$(PPh$_3$)$_2$]$_2$(μ-COCH=CHCH=CHCH=CHCO)}(BPh$_4$)$_2$·6CH$_2$Cl$_2$

P(2)-Ru(1)-P(1)	175.43(3)	C(31)-Ru(1)-C(1)	171.72(13)
C(11)-Ru(1)-C(21)	171.55(12)	C(11)-Ru(1)-C(1)	89.81(13)
C(21)-Ru(1)-C(1)	81.76(13)	C(11)-Ru(1)-C(31)	98.41(13)
C(21)-Ru(1)-C(31)	90.00(13)		
C(1)-Ru(1)-P(1)	91.45(9)	C(1)-Ru(1)-P(2)	91.34(9)
C(11)-Ru(1)-P(1)	86.53(9)	C(11)-Ru(1)-P(2)	89.86(9)
C(21)-Ru(1)-P(1)	92.97(9)	C(21)-Ru(1)-P(2)	91.01(9)
C(31)-Ru(1)-P(1)	88.02(9)	C(31)-Ru(1)-P(2)	89.73(9)
O(1)-C(1)-Ru(1)	122.7(2)	O(1)-C(1)-C(2)	115.2(3)
C(2)-C(1)-Ru(1)	122.0(2)	C(3)-C(2)-C(1)	122.2(3)
C(2)-C(3)-C(4)	126.6(3)	C(4)#1-C(4)-C(3)	125.0(4)
N(1)-C(11)-Ru(1)	177.0(3)	C(11)-N(1)-C(13)	178.4(4)
N(2)-C(21)-Ru(1)	173.0(3)	C(21)-N(2)-C(23)	164.1(3)
N(3)-C(31)-Ru(1)	173.7(3)	C(31)-N(3)-C(33)	176.5(4)
N(1)-C(13)-C(14)	106.7(4)	C(15)-C(13)-C(16)	111.7(5)
N(1)-C(13)-C(15)	108.2(3)	C(15)-C(13)-C(14)	111.4(4)
N(1)-C(13)-C(16)	107.7(4)	C(16)-C(13)-C(14)	110.9(5)
N(2)-C(23)-C(24)	107.8(3)	C(25)-C(23)-C(26)	111.7(4)
N(2)-C(23)-C(25)	107.7(3)	C(25)-C(23)-C(24)	111.5(4)
N(2)-C(23)-C(26)	107.1(3)	C(26)-C(23)-C(24)	110.8(4)
N(3)-C(33)-C(34)	106.8(4)	C(34)-C(33)-C(35)	113.0(5)
N(3)-C(33)-C(35)	107.0(4)	C(34)-C(33)-C(36)	110.0(4)
N(3)-C(33)-C(36)	107.2(4)	C(35)-C(33)-C(36)	112.5(4)
C(61)-P(1)-Ru(1)	113.81(11)	C(91)-P(2)-Ru(1)	115.96(11)
C(41)-P(1)-Ru(1)	115.81(11)	C(71)-P(2)-Ru(1)	115.17(11)
C(51)-P(1)-Ru(1)	118.06(11)	C(81)-P(2)-Ru(1)	115.45(14)
C(61)-P(1)-C(41)	101.48(15)	C(91)-P(2)-C(71)	105.69(18)
C(61)-P(1)-C(51)	100.60(16)	C(91)-P(2)-C(81)	102.39(17)
C(41)-P(1)-C(51)	104.76(15)	C(71)-P(2)-C(81)	100.20(17)
C(42)-C(41)-C(46)	118.6(3)	C(76)-C(71)-C(72)	117.8(4)
C(42)-C(41)-P(1)	118.2(3)	C(76)-C(71)-P(2)	118.3(3)
C(46)-C(41)-P(1)	123.1(3)	C(72)-C(71)-P(2)	123.9(3)
C(43)-C(42)-C(41)	121.1(4)	C(71)-C(72)-C(73)	121.2(5)
C(44)-C(43)-C(42)	120.0(4)	C(74)-C(73)-C(72)	118.7(5)

C(45)-C(44)-C(43)	119.8(4)	C(75)-C(74)-C(73)	122.1(5)
C(44)-C(45)-C(46)	120.8(4)	C(74)-C(75)-C(76)	118.8(5)
C(41)-C(46)-C(45)	119.6(4)	C(71)-C(76)-C(75)	121.4(5)
C(56)-C(51)-C(52)	118.8(3)	C(86)-C(81)-C(82)	118.2(4)
C(56)-C(51)-P(1)	119.8(3)	C(86)-C(81)-P(2)	122.2(3)
C(52)-C(51)-P(1)	121.4(3)	C(82)-C(81)-P(2)	119.5(3)
C(51)-C(52)-C(53)	119.7(4)	C(81)-C(82)-C(83)	120.0(5)
C(54)-C(53)-C(52)	120.2(5)	C(84)-C(83)-C(82)	120.7(5)
C(53)-C(54)-C(55)	120.7(4)	C(83)-C(84)-C(85)	120.1(5)
C(54)-C(55)-C(56)	119.8(5)	C(84)-C(85)-C(86)	119.8(5)
C(51)-C(56)-C(55)	120.7(4)	C(81)-C(86)-C(85)	121.1(4)
C(66)-C(61)-C(62)	117.6(3)	C(92)-C(91)-C(96)	118.2(4)
C(66)-C(61)-P(1)	121.6(3)	C(92)-C(91)-P(2)	121.1(3)
C(62)-C(61)-P(1)	120.6(3)	C(96)-C(91)-P(2)	120.5(3)
C(63)-C(62)-C(61)	121.4(4)	C(91)-C(92)-C(93)	121.3(4)
C(64)-C(63)-C(62)	119.7(4)	C(94)-C(93)-C(92)	119.4(5)
C(63)-C(64)-C(65)	120.5(4)	C(95)-C(94)-C(93)	120.6(5)
C(64)-C(65)-C(66)	120.1(4)	C(94)-C(95)-C(96)	120.8(5)
C(61)-C(66)-C(65)	120.8(4)	C(95)-C(96)-C(91)	119.7(5)
C(111)-B(1)-C(141)	104.5(3)	C(111)-B(1)-C(121)	113.2(3)
C(111)-B(1)-C(131)	111.7(3)	C(141)-B(1)-C(121)	109.9(3)
C(141)-B(1)-C(131)	112.6(3)	C(131)-B(1)-C(121)	105.1(3)
C(112)-C(111)-C(116)	114.2(4)	C(132)-C(131)-C(136)	113.7(4)
C(112)-C(111)-B(1)	121.0(4)	C(132)-C(131)-B(1)	122.9(4)
C(116)-C(111)-B(1)	124.7(4)	C(136)-C(131)-B(1)	123.1(4)
C(113)-C(112)-C(111)	123.3(5)	C(131)-C(132)-C(133)	123.4(5)
C(114)-C(113)-C(112)	119.7(5)	C(134)-C(133)-C(132)	120.0(5)
C(115)-C(114)-C(113)	119.2(5)	C(135)-C(134)-C(133)	118.5(5)
C(114)-C(115)-C(116)	120.4(5)	C(134)-C(135)-C(136)	120.9(5)
C(115)-C(116)-C(111)	123.2(5)	C(131)-C(136)-C(135)	123.4(5)
C(122)-C(121)-C(126)	113.7(4)	C(142)-C(141)-C(146)	113.8(4)
C(122)-C(121)-B(1)	123.4(4)	C(142)-C(141)-B(1)	125.6(4)
C(126)-C(121)-B(1)	122.8(4)	C(146)-C(141)-B(1)	120.5(4)
C(121)-C(122)-C(123)	123.1(5)	C(141)-C(142)-C(143)	123.1(4)
C(124)-C(123)-C(122)	120.9(5)	C(144)-C(143)-C(142)	120.9(4)
C(123)-C(124)-C(125)	118.8(5)	C(145)-C(144)-C(143)	117.7(5)
C(124)-C(125)-C(126)	121.1(5)	C(144)-C(145)-C(146)	121.2(4)
C(121)-C(126)-C(125)	122.4(5)	C(145)-C(146)-C(141)	123.3(4)

Cl(2)-C(01)-Cl(1)	104.8(4)	Cl(3)-C(02)-Cl(4)	112.2(3)
Cl(5)-C(03)-Cl(6)	113.0(3)		

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

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) {[Ru(*t*-BuNC)$_3$(PPh$_3$)$_2$]$_2$(μ-COCH=CHCH=CHCH=CHCO)}(BPh$_4$)$_2$·6CH$_2$Cl$_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	34(1)	30(1)	30(1)	-1(1)	8(1)	0(1)
P(1)	35(1)	38(1)	34(1)	-3(1)	6(1)	2(1)
P(2)	38(1)	35(1)	46(1)	0(1)	15(1)	2(1)
O(1)	112(2)	47(2)	35(1)	0(1)	10(2)	-15(2)
C(1)	46(2)	38(2)	38(2)	4(2)	12(2)	0(2)
C(2)	54(2)	42(2)	38(2)	7(2)	10(2)	3(2)
C(3)	57(2)	41(2)	42(2)	6(2)	10(2)	-1(2)
C(4)	63(3)	44(2)	45(2)	9(2)	11(2)	1(2)
C(11)	41(2)	38(2)	31(2)	2(2)	7(2)	4(2)
N(1)	62(2)	38(2)	49(2)	-7(2)	10(2)	-6(2)
C(13)	94(4)	35(2)	75(3)	-15(2)	7(3)	-18(2)
C(14)	169(6)	58(3)	203(7)	-52(4)	78(6)	-6(3)
C(15)	185(6)	76(3)	114(5)	-9(3)	54(4)	-64(4)
C(16)	181(7)	83(4)	157(6)	-19(4)	-81(5)	-45(4)
C(21)	36(2)	33(2)	38(2)	7(2)	10(2)	1(2)
N(2)	46(2)	39(2)	42(2)	-6(1)	7(2)	-6(1)
C(23)	48(2)	49(2)	49(2)	-17(2)	7(2)	-11(2)
C(24)	186(6)	64(3)	105(4)	-18(3)	23(4)	-59(4)
C(25)	73(4)	131(4)	101(4)	-51(3)	-27(3)	27(3)
C(26)	67(3)	139(4)	75(3)	-55(3)	23(3)	-17(3)
C(31)	40(2)	44(2)	41(2)	-4(2)	12(2)	-1(2)
N(3)	68(2)	63(2)	36(2)	12(2)	7(2)	2(2)
C(33)	107(4)	89(3)	43(3)	29(3)	8(3)	-5(3)
C(34)	123(5)	120(4)	118(5)	63(4)	-12(4)	24(4)
C(35)	251(8)	125(5)	44(3)	13(3)	11(4)	-19(5)
C(36)	145(6)	151(5)	90(4)	45(4)	36(4)	-43(4)
C(41)	36(2)	39(2)	46(2)	-10(2)	0(2)	3(2)
C(42)	69(3)	46(2)	59(3)	-1(2)	13(2)	8(2)
C(43)	90(4)	41(2)	86(4)	1(2)	5(3)	8(2)
C(44)	73(3)	53(3)	102(4)	-29(3)	-6(3)	14(2)
C(45)	63(3)	80(3)	72(3)	-40(3)	13(2)	6(2)
C(46)	45(2)	60(2)	53(3)	-19(2)	5(2)	-1(2)

C(51)	37(2)	43(2)	53(2)	2(2)	14(2)	4(2)
C(52)	55(3)	54(2)	75(3)	1(2)	16(2)	-5(2)
C(53)	58(3)	62(3)	127(5)	0(3)	20(3)	-17(2)
C(54)	75(4)	85(4)	126(5)	35(4)	45(4)	-4(3)
C(55)	72(4)	107(4)	84(4)	37(3)	33(3)	8(3)
C(56)	50(3)	70(3)	59(3)	12(2)	18(2)	0(2)
C(61)	36(2)	49(2)	39(2)	-2(2)	1(2)	0(2)
C(62)	51(2)	61(2)	48(2)	-8(2)	-8(2)	4(2)
C(63)	70(3)	90(3)	49(3)	-18(2)	-9(2)	6(3)
C(64)	65(3)	109(4)	58(3)	-1(3)	-23(2)	-1(3)
C(65)	58(3)	96(3)	67(3)	1(3)	-15(2)	15(3)
C(66)	47(2)	68(3)	49(2)	-3(2)	-3(2)	10(2)
C(71)	39(2)	43(2)	80(3)	-5(2)	27(2)	-3(2)
C(72)	50(3)	71(3)	101(4)	-5(3)	20(3)	-5(2)
C(73)	59(3)	101(4)	137(5)	-38(4)	29(3)	-24(3)
C(74)	65(4)	67(3)	173(6)	-41(4)	63(4)	-18(3)
C(75)	72(4)	46(3)	162(6)	5(3)	52(4)	0(3)
C(76)	52(3)	50(2)	111(4)	8(2)	26(3)	-4(2)
C(81)	65(3)	34(2)	55(3)	-2(2)	31(2)	0(2)
C(82)	74(3)	67(3)	80(3)	7(2)	44(3)	10(2)
C(83)	110(5)	76(3)	98(4)	6(3)	73(4)	16(3)
C(84)	139(5)	70(3)	79(4)	-12(3)	67(4)	4(3)
C(85)	119(5)	76(3)	71(3)	-25(3)	42(3)	-12(3)
C(86)	75(3)	54(2)	60(3)	-14(2)	32(3)	-5(2)
C(91)	39(2)	47(2)	64(3)	10(2)	20(2)	5(2)
C(92)	50(3)	73(3)	69(3)	12(2)	12(2)	12(2)
C(93)	80(4)	121(5)	87(4)	47(4)	19(3)	27(3)
C(94)	97(4)	100(5)	138(6)	64(4)	38(4)	40(4)
C(95)	118(5)	54(3)	138(5)	27(3)	56(4)	24(3)
C(96)	71(3)	45(2)	86(3)	14(2)	28(3)	12(2)
B(1)	50(3)	55(3)	54(3)	4(2)	11(2)	10(2)
C(111)	47(2)	73(3)	59(3)	12(2)	4(2)	10(2)
C(112)	114(4)	121(4)	60(3)	8(3)	20(3)	54(3)
C(113)	128(5)	152(5)	70(4)	-8(4)	23(4)	48(4)
C(114)	92(4)	173(6)	53(4)	23(4)	1(3)	13(4)
C(115)	88(4)	117(4)	79(4)	30(4)	-8(3)	9(3)
C(116)	85(3)	79(3)	59(3)	13(2)	-2(3)	-1(3)
C(121)	64(3)	53(2)	57(3)	16(2)	17(2)	10(2)

C(122)	68(3)	76(3)	94(4)	0(3)	24(3)	10(3)
C(123)	83(4)	86(4)	123(5)	10(3)	50(4)	28(3)
C(124)	138(6)	68(3)	99(5)	6(3)	69(4)	26(4)
C(125)	135(5)	101(4)	60(3)	-4(3)	28(4)	22(4)
C(126)	87(4)	100(4)	56(3)	6(3)	13(3)	29(3)
C(131)	52(3)	55(2)	53(3)	2(2)	10(2)	10(2)
C(132)	74(3)	66(3)	76(3)	-3(2)	3(3)	8(3)
C(133)	81(4)	67(3)	120(5)	-19(3)	16(4)	-10(3)
C(134)	97(5)	62(3)	123(5)	15(3)	33(4)	1(3)
C(135)	83(4)	88(4)	101(4)	34(3)	9(3)	5(3)
C(136)	65(3)	82(3)	74(3)	18(3)	5(3)	-9(2)
C(141)	57(3)	58(3)	45(2)	10(2)	9(2)	6(2)
C(142)	60(3)	67(3)	103(4)	18(3)	19(3)	9(2)
C(143)	57(3)	90(4)	142(5)	39(3)	15(3)	17(3)
C(144)	57(3)	101(4)	111(4)	26(3)	9(3)	-4(3)
C(145)	80(4)	72(3)	113(4)	-1(3)	18(3)	-20(3)
C(146)	69(3)	62(3)	95(4)	4(3)	15(3)	8(2)
C(01)	331(12)	167(7)	91(5)	54(5)	-34(6)	26(7)
Cl(1)	226(3)	152(2)	256(3)	-20(2)	-38(2)	13(2)
Cl(2)	275(3)	170(2)	129(2)	-17(2)	-2(2)	9(2)
C(02)	69(3)	98(4)	111(4)	-21(3)	5(3)	-5(3)
Cl(3)	84(1)	131(1)	225(2)	3(1)	-52(1)	-2(1)
Cl(4)	118(1)	163(2)	121(1)	4(1)	7(1)	-56(1)
C(03)	186(7)	95(4)	128(5)	-8(4)	79(5)	-9(4)
Cl(5)	239(2)	160(2)	119(2)	6(1)	81(2)	-13(2)
Cl(6)	199(2)	92(1)	157(2)	-1(1)	54(2)	39(1)

Table S5. Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for $\{[Ru(t\text{-}BuNC)_3(PPh_3)_2]_2(\mu\text{-}COCH{=}CHCH{=}CHCH{=}CHCO)\}(BPh_4)_2 \cdot 6CH_2Cl_2$

Atom	x	y	z	U(eq)
H(2A)	4326	4250	728	53
H(3A)	4743	3724	91	56
H(4A)	4764	5287	312	61
H(14A)	4857	5292	1842	207
H(14B)	4417	5524	1451	207
H(14C)	5295	6046	1682	207
H(15A)	6897	5104	1124	182
H(15B)	6572	5930	1246	182
H(15C)	5700	5422	1005	182
H(16A)	6655	4736	2006	228
H(16B)	7236	5459	1868	228
H(16C)	7453	4626	1730	228
H(24A)	2494	-136	790	177
H(24B)	3724	-375	787	177
H(24C)	2825	-551	460	177
H(25A)	2409	1442	198	159
H(25B)	1728	1031	457	159
H(25C)	1925	608	112	159
H(26A)	4273	1037	162	139
H(26B)	3923	174	73	139
H(26C)	4828	358	398	139
H(34A)	5978	420	2034	186
H(34B)	6313	500	2443	186
H(34C)	6750	1101	2192	186
H(35A)	4654	2175	2535	212
H(35B)	5908	2220	2502	212
H(35C)	5498	1613	2756	212
H(36A)	3482	1103	2244	190
H(36B)	4226	479	2464	190
H(36C)	4018	434	2052	190
H(42A)	6008	771	1315	69
H(43A)	6378	-459	1130	88
H(44A)	7307	-621	661	94

H(45A)	7814	443	367	86
H(46A)	7451	1689	549	64
H(52A)	8428	3305	1325	73
H(53A)	9361	4186	1019	98
H(54A)	8823	4367	430	110
H(55A)	7315	3726	137	102
H(56A)	6341	2874	437	70
H(62A)	6609	3092	1812	66
H(63A)	7823	3121	2336	86
H(64A)	9321	2314	2416	97
H(65A)	9617	1466	1981	92
H(66A)	8422	1440	1453	67
H(72A)	697	2718	798	87
H(73A)	-571	1706	734	117
H(74A)	-240	632	1085	116
H(75A)	1300	536	1498	108
H(76A)	2602	1525	1548	83
H(82A)	1004	3217	1634	84
H(83A)	786	3662	2189	106
H(84A)	2282	3987	2593	109
H(85A)	4022	3897	2451	103
H(86A)	4258	3498	1891	73
H(92A)	2064	3298	520	77
H(93A)	1367	4349	182	114
H(94A)	1160	5526	449	132
H(95A)	1643	5660	1041	119
H(96A)	2295	4612	1387	79
H(11A)	1370	7135	825	117
H(11B)	995	7328	228	139
H(11C)	269	8498	7	129
H(11D)	-104	9447	387	117
H(11E)	283	9257	981	91
H(12A)	-874	8644	1364	93
H(12B)	-1719	9454	1713	112
H(12C)	-775	9950	2218	116
H(12D)	1019	9612	2385	117
H(12E)	1901	8811	2040	97
H(13A)	-326	6936	1131	88

H(13B)	-852	5734	1312	107
H(13C)	90	5172	1816	110
H(13D)	1474	5855	2147	109
H(13E)	1973	7059	1973	89
H(14D)	3157	7093	1517	91
H(14E)	4999	7365	1592	116
H(14F)	5616	8634	1606	108
H(14G)	4335	9610	1515	106
H(14H)	2503	9344	1442	90
H(01A)	1611	2585	-369	244
H(01B)	2840	2713	-184	244
H(02A)	8867	7719	2156	112
H(02B)	9094	7014	1919	112
H(03A)	5527	2133	-828	156
H(03B)	6780	2069	-668	156