

Isolation, X-ray Crystal Structure and Reactivity of a New C-H Carbene Complex of (5,10,15,20-tetraphenylporphyrinato)ruthenium(II)

Paul Le Maux,^a Thierry Roisnel,^b Irène Nicolas^a and Gérard Simonneaux^{a*}

^a*Ingénierie Chimique et Molécules pour le Vivant*, ^b*Centre de Diffractométrie, UMR 6226,*
Université de Rennes I, Campus de Beaulieu, 35042 Rennes Cedex, France

Supporting information

Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	3174(1)	4856(1)	3083(1)	10(1)
N(1)	1539(3)	4783(3)	2639(1)	15(1)
N(2)	2885(3)	3154(3)	2594(1)	13(1)
N(3)	4655(3)	4772(3)	3591(1)	12(1)
N(4)	3316(3)	6429(3)	3635(1)	13(1)
C(1)	2509(4)	7050(3)	3600(2)	15(1)
C(2)	1445(4)	6710(3)	3188(2)	15(1)
C(3)	994(4)	5655(3)	2743(2)	16(1)
C(4)	-115(4)	5313(4)	2333(2)	20(1)
C(5)	-224(4)	4255(4)	1974(2)	19(1)
C(6)	811(3)	3923(3)	2170(2)	15(1)
C(7)	1007(3)	2857(3)	1918(2)	14(1)
C(8)	1977(3)	2508(3)	2122(2)	15(1)
C(9)	2221(4)	1447(3)	1858(2)	17(1)
C(10)	3256(4)	1451(3)	2169(2)	15(1)
C(11)	3682(3)	2522(3)	2632(2)	14(1)
C(12)	4742(3)	2853(3)	3046(2)	15(1)
C(13)	5184(3)	3900(3)	3487(2)	13(1)
C(14)	6323(3)	4268(3)	3897(2)	15(1)
C(15)	6492(4)	5371(4)	4227(2)	16(1)
C(16)	5445(3)	5694(3)	4040(2)	14(1)
C(17)	5283(3)	6792(3)	4271(2)	15(1)
C(18)	4254(3)	7090(3)	4088(2)	14(1)
C(19)	3988(4)	8131(4)	4370(2)	18(1)
C(20)	2915(4)	8102(4)	4071(2)	18(1)
C(21)	694(4)	7529(3)	3206(2)	16(1)
C(22)	1310(4)	8775(4)	3027(2)	17(1)
C(23)	592(4)	9507(4)	3020(2)	21(1)
C(24)	-738(4)	8996(4)	3193(2)	20(1)
C(25)	-1348(4)	7760(4)	3374(2)	22(1)
C(26)	-630(4)	7032(4)	3380(2)	21(1)
C(71)	179(4)	2110(4)	1373(2)	17(1)
C(72)	382(4)	2722(4)	870(2)	28(1)
C(73)	-415(5)	2044(5)	365(2)	38(1)

C(74)	-1422(5)	753(5)	361(2)	37(1)
C(75)	-1631(4)	159(4)	860(2)	27(1)
C(76)	-835(4)	820(4)	1361(2)	21(1)
C(121)	5460(3)	2011(3)	2986(2)	16(1)
C(122)	5124(4)	971(4)	3315(2)	21(1)
C(123)	5700(4)	116(4)	3207(2)	22(1)
C(124)	6628(4)	302(4)	2779(2)	24(1)
C(125)	7002(4)	1356(4)	2468(2)	27(1)
C(126)	6427(4)	2206(4)	2570(2)	24(1)
C(171)	6348(3)	7772(3)	4704(2)	14(1)
C(172)	6507(4)	7496(4)	5263(2)	18(1)
C(173)	7540(4)	8424(4)	5650(2)	21(1)
C(174)	8422(4)	9626(4)	5480(2)	21(1)
C(175)	8268(4)	9917(4)	4930(2)	23(1)
C(176)	7228(4)	8999(4)	4547(2)	18(1)
C(31)	4429(4)	5973(3)	2626(2)	16(1)
C(32)	4365(3)	5903(3)	1985(2)	16(1)
O(33)	3528(3)	5047(3)	1648(1)	20(1)
O(34)	5420(2)	6994(2)	1808(1)	17(1)
C(35)	5517(4)	7000(3)	1199(2)	16(1)
C(36)	4748(4)	7445(4)	890(2)	18(1)
C(37)	3729(4)	7941(4)	1121(2)	22(1)
C(37A)	4172(5)	9329(5)	949(2)	37(1)
C(37B)	3551(4)	8043(4)	1778(2)	28(1)
C(37C)	2304(4)	7001(5)	836(2)	39(1)
C(38)	4954(4)	7460(4)	290(2)	21(1)
C(39)	5828(4)	7057(4)	15(2)	20(1)
C(40)	6078(5)	7155(5)	-616(2)	31(1)
C(41)	6558(4)	6612(4)	344(2)	21(1)
C(42)	6440(4)	6582(4)	941(2)	19(1)
C(43)	7387(4)	6227(4)	1297(2)	22(1)
C(43A)	8121(5)	5630(5)	892(2)	39(1)
C(43B)	8471(4)	7510(4)	1632(2)	35(1)
C(43C)	6661(4)	5230(4)	1727(2)	24(1)
O(51)	1539(3)	3562(3)	3713(1)	19(1)
C(51)	1378(4)	4035(4)	4295(2)	25(1)
C(52)	20(5)	4096(5)	4263(2)	37(1)
C(53)	-753(4)	3151(5)	3721(2)	36(1)
C(54)	192(4)	2592(4)	3514(2)	25(1)

Table 2. Bond lengths [Å] and angles [deg] for **1**.

Ru(1)-C(31)	1.839(4)
Ru(1)-N(1)	2.042(3)
Ru(1)-N(2)	2.053(3)
Ru(1)-N(4)	2.054(3)
Ru(1)-N(3)	2.057(3)
Ru(1)-O(51)	2.376(3)
N(1)-C(6)	1.365(5)
N(1)-C(3)	1.390(4)
N(2)-C(8)	1.382(5)
N(2)-C(11)	1.383(4)
N(3)-C(13)	1.377(4)
N(3)-C(16)	1.380(4)
N(4)-C(18)	1.369(4)
N(4)-C(1)	1.381(4)
C(1)-C(2)	1.396(5)
C(1)-C(20)	1.448(5)
C(2)-C(3)	1.409(5)
C(2)-C(21)	1.511(5)
C(3)-C(4)	1.428(5)
C(4)-C(5)	1.362(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.448(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.413(5)
C(7)-C(8)	1.399(5)
C(7)-C(71)	1.495(5)
C(8)-C(9)	1.447(5)
C(9)-C(10)	1.349(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.449(5)
C(10)-H(10)	0.9500
C(11)-C(12)	1.396(5)
C(12)-C(13)	1.397(5)
C(12)-C(121)	1.505(5)
C(13)-C(14)	1.447(5)
C(14)-C(15)	1.351(5)
C(14)-H(14)	0.9500
C(15)-C(16)	1.446(5)
C(15)-H(15)	0.9500
C(16)-C(17)	1.410(5)
C(17)-C(18)	1.406(5)
C(17)-C(171)	1.492(5)
C(18)-C(19)	1.453(5)
C(19)-C(20)	1.357(5)
C(19)-H(19)	0.9500

C(20) -H(20)	0.9500
C(21) -C(26)	1.387(5)
C(21) -C(22)	1.395(5)
C(22) -C(23)	1.398(5)
C(22) -H(22)	0.9500
C(23) -C(24)	1.390(5)
C(23) -H(23)	0.9500
C(24) -C(25)	1.388(5)
C(24) -H(24)	0.9500
C(25) -C(26)	1.393(5)
C(25) -H(25)	0.9500
C(26) -H(26)	0.9500
C(71) -C(72)	1.394(5)
C(71) -C(76)	1.398(5)
C(72) -C(73)	1.393(6)
C(72) -H(72)	0.9500
C(73) -C(74)	1.399(6)
C(73) -H(73)	0.9500
C(74) -C(75)	1.373(6)
C(74) -H(74)	0.9500
C(75) -C(76)	1.381(5)
C(75) -H(75)	0.9500
C(76) -H(76)	0.9500
C(121) -C(126)	1.397(5)
C(121) -C(122)	1.398(5)
C(122) -C(123)	1.400(5)
C(122) -H(122)	0.9500
C(123) -C(124)	1.388(6)
C(123) -H(123)	0.9500
C(124) -C(125)	1.379(6)
C(124) -H(124)	0.9500
C(125) -C(126)	1.393(5)
C(125) -H(125)	0.9500
C(126) -H(126)	0.9500
C(171) -C(176)	1.396(5)
C(171) -C(172)	1.396(5)
C(172) -C(173)	1.395(5)
C(172) -H(172)	0.9500
C(173) -C(174)	1.388(6)
C(173) -H(173)	0.9500
C(174) -C(175)	1.380(6)
C(174) -H(174)	0.9500
C(175) -C(176)	1.389(5)
C(175) -H(175)	0.9500
C(176) -H(176)	0.9500
C(31) -C(32)	1.480(5)
C(31) -H(31)	0.9500
C(32) -O(33)	1.205(4)
C(32) -O(34)	1.377(4)
O(34) -C(35)	1.415(4)
C(35) -C(36)	1.404(5)
C(35) -C(42)	1.421(5)
C(36) -C(38)	1.410(5)
C(36) -C(37)	1.550(5)
C(37) -C(37B)	1.534(6)
C(37) -C(37A)	1.546(6)
C(37) -C(37C)	1.547(6)
C(37A) -H(37A)	0.9800
C(37A) -H(37B)	0.9800
C(37A) -H(37C)	0.9800
C(37B) -H(37D)	0.9800

C(37B) - H(37E)	0.9800
C(37B) - H(37F)	0.9800
C(37C) - H(37G)	0.9800
C(37C) - H(37H)	0.9800
C(37C) - H(37I)	0.9800
C(38) - C(39)	1.379(5)
C(38) - H(38)	0.9500
C(39) - C(41)	1.398(5)
C(39) - C(40)	1.494(5)
C(40) - H(40A)	0.9800
C(40) - H(40B)	0.9800
C(40) - H(40C)	0.9800
C(41) - C(42)	1.393(5)
C(41) - H(41)	0.9500
C(42) - C(43)	1.550(5)
C(43) - C(43C)	1.539(5)
C(43) - C(43B)	1.543(6)
C(43) - C(43A)	1.545(6)
C(43A) - H(43A)	0.9800
C(43A) - H(43B)	0.9800
C(43A) - H(43C)	0.9800
C(43B) - H(43D)	0.9800
C(43B) - H(43E)	0.9800
C(43B) - H(43F)	0.9800
C(43C) - H(43G)	0.9800
C(43C) - H(43H)	0.9800
C(43C) - H(43I)	0.9800
O(51) - C(54)	1.437(4)
O(51) - C(51)	1.446(4)
C(51) - C(52)	1.535(6)
C(51) - H(51A)	0.9900
C(51) - H(51B)	0.9900
C(52) - C(53)	1.538(6)
C(52) - H(52A)	0.9900
C(52) - H(52B)	0.9900
C(53) - C(54)	1.511(6)
C(53) - H(53A)	0.9900
C(53) - H(53B)	0.9900
C(54) - H(54A)	0.9900
C(54) - H(54B)	0.9900

C(31) - Ru(1) - N(1)	94.40(14)
C(31) - Ru(1) - N(2)	96.39(14)
N(1) - Ru(1) - N(2)	89.10(12)
C(31) - Ru(1) - N(4)	90.02(14)
N(1) - Ru(1) - N(4)	90.70(12)
N(2) - Ru(1) - N(4)	173.58(12)
C(31) - Ru(1) - N(3)	92.52(14)
N(1) - Ru(1) - N(3)	173.08(12)
N(2) - Ru(1) - N(3)	89.88(11)
N(4) - Ru(1) - N(3)	89.55(11)
C(31) - Ru(1) - O(51)	175.38(13)
N(1) - Ru(1) - O(51)	84.69(11)
N(2) - Ru(1) - O(51)	88.13(10)
N(4) - Ru(1) - O(51)	85.47(10)
N(3) - Ru(1) - O(51)	88.43(10)
C(6) - N(1) - C(3)	106.7(3)
C(6) - N(1) - Ru(1)	127.4(2)
C(3) - N(1) - Ru(1)	125.9(2)
C(8) - N(2) - C(11)	106.6(3)
C(8) - N(2) - Ru(1)	127.1(2)

C(11) - N(2) - Ru(1)	125.9(2)
C(13) - N(3) - C(16)	107.2(3)
C(13) - N(3) - Ru(1)	125.9(2)
C(16) - N(3) - Ru(1)	126.1(2)
C(18) - N(4) - C(1)	107.2(3)
C(18) - N(4) - Ru(1)	126.8(2)
C(1) - N(4) - Ru(1)	125.9(2)
N(4) - C(1) - C(2)	126.0(3)
N(4) - C(1) - C(20)	109.2(3)
C(2) - C(1) - C(20)	124.8(3)
C(1) - C(2) - C(3)	125.7(3)
C(1) - C(2) - C(21)	118.7(3)
C(3) - C(2) - C(21)	115.6(3)
N(1) - C(3) - C(2)	125.7(3)
N(1) - C(3) - C(4)	109.8(3)
C(2) - C(3) - C(4)	124.5(3)
C(5) - C(4) - C(3)	106.9(3)
C(5) - C(4) - H(4)	126.6
C(3) - C(4) - H(4)	126.6
C(4) - C(5) - C(6)	107.4(3)
C(4) - C(5) - H(5)	126.3
C(6) - C(5) - H(5)	126.3
N(1) - C(6) - C(7)	126.0(3)
N(1) - C(6) - C(5)	109.3(3)
C(7) - C(6) - C(5)	124.8(3)
C(8) - C(7) - C(6)	124.7(3)
C(8) - C(7) - C(71)	118.1(3)
C(6) - C(7) - C(71)	117.1(3)
N(2) - C(8) - C(7)	125.3(3)
N(2) - C(8) - C(9)	109.2(3)
C(7) - C(8) - C(9)	125.4(3)
C(10) - C(9) - C(8)	107.6(3)
C(10) - C(9) - H(9)	126.2
C(8) - C(9) - H(9)	126.2
C(9) - C(10) - C(11)	107.3(3)
C(9) - C(10) - H(10)	126.4
C(11) - C(10) - H(10)	126.4
N(2) - C(11) - C(12)	126.1(3)
N(2) - C(11) - C(10)	109.3(3)
C(12) - C(11) - C(10)	124.5(3)
C(11) - C(12) - C(13)	125.2(3)
C(11) - C(12) - C(121)	115.4(3)
C(13) - C(12) - C(121)	119.3(3)
N(3) - C(13) - C(12)	126.3(3)
N(3) - C(13) - C(14)	109.1(3)
C(12) - C(13) - C(14)	124.6(3)
C(15) - C(14) - C(13)	107.3(3)
C(15) - C(14) - H(14)	126.4
C(13) - C(14) - H(14)	126.4
C(14) - C(15) - C(16)	107.6(3)
C(14) - C(15) - H(15)	126.2
C(16) - C(15) - H(15)	126.2
N(3) - C(16) - C(17)	125.9(3)
N(3) - C(16) - C(15)	108.8(3)
C(17) - C(16) - C(15)	125.3(3)
C(18) - C(17) - C(16)	124.8(3)
C(18) - C(17) - C(171)	117.1(3)
C(16) - C(17) - C(171)	117.8(3)
N(4) - C(18) - C(17)	126.0(3)
N(4) - C(18) - C(19)	109.1(3)
C(17) - C(18) - C(19)	124.9(3)

C(20) - C(19) - C(18)	107.3 (3)
C(20) - C(19) - H(19)	126.3
C(18) - C(19) - H(19)	126.3
C(19) - C(20) - C(1)	107.1 (3)
C(19) - C(20) - H(20)	126.5
C(1) - C(20) - H(20)	126.5
C(26) - C(21) - C(22)	119.3 (3)
C(26) - C(21) - C(2)	120.4 (3)
C(22) - C(21) - C(2)	120.3 (3)
C(21) - C(22) - C(23)	120.2 (3)
C(21) - C(22) - H(22)	119.9
C(23) - C(22) - H(22)	119.9
C(24) - C(23) - C(22)	120.1 (3)
C(24) - C(23) - H(23)	120.0
C(22) - C(23) - H(23)	120.0
C(25) - C(24) - C(23)	119.8 (3)
C(25) - C(24) - H(24)	120.1
C(23) - C(24) - H(24)	120.1
C(24) - C(25) - C(26)	120.0 (3)
C(24) - C(25) - H(25)	120.0
C(26) - C(25) - H(25)	120.0
C(21) - C(26) - C(25)	120.7 (3)
C(21) - C(26) - H(26)	119.6
C(25) - C(26) - H(26)	119.6
C(72) - C(71) - C(76)	119.0 (3)
C(72) - C(71) - C(7)	119.6 (3)
C(76) - C(71) - C(7)	121.4 (3)
C(73) - C(72) - C(71)	119.9 (4)
C(73) - C(72) - H(72)	120.1
C(71) - C(72) - H(72)	120.1
C(72) - C(73) - C(74)	120.3 (4)
C(72) - C(73) - H(73)	119.9
C(74) - C(73) - H(73)	119.9
C(75) - C(74) - C(73)	119.7 (4)
C(75) - C(74) - H(74)	120.2
C(73) - C(74) - H(74)	120.2
C(74) - C(75) - C(76)	120.4 (4)
C(74) - C(75) - H(75)	119.8
C(76) - C(75) - H(75)	119.8
C(75) - C(76) - C(71)	120.8 (4)
C(75) - C(76) - H(76)	119.6
C(71) - C(76) - H(76)	119.6
C(126) - C(121) - C(122)	118.3 (3)
C(126) - C(121) - C(12)	120.3 (3)
C(122) - C(121) - C(12)	121.3 (3)
C(121) - C(122) - C(123)	120.2 (4)
C(121) - C(122) - H(122)	119.9
C(123) - C(122) - H(122)	119.9
C(124) - C(123) - C(122)	120.7 (4)
C(124) - C(123) - H(123)	119.7
C(122) - C(123) - H(123)	119.7
C(125) - C(124) - C(123)	119.3 (4)
C(125) - C(124) - H(124)	120.3
C(123) - C(124) - H(124)	120.3
C(124) - C(125) - C(126)	120.4 (4)
C(124) - C(125) - H(125)	119.8
C(126) - C(125) - H(125)	119.8
C(125) - C(126) - C(121)	121.0 (4)
C(125) - C(126) - H(126)	119.5
C(121) - C(126) - H(126)	119.5
C(176) - C(171) - C(172)	118.5 (3)

C(176) - C(171) - C(17)	119.4 (3)
C(172) - C(171) - C(17)	122.0 (3)
C(173) - C(172) - C(171)	120.4 (3)
C(173) - C(172) - H(172)	119.8
C(171) - C(172) - H(172)	119.8
C(174) - C(173) - C(172)	120.1 (4)
C(174) - C(173) - H(173)	120.0
C(172) - C(173) - H(173)	120.0
C(175) - C(174) - C(173)	120.2 (4)
C(175) - C(174) - H(174)	119.9
C(173) - C(174) - H(174)	119.9
C(174) - C(175) - C(176)	119.8 (4)
C(174) - C(175) - H(175)	120.1
C(176) - C(175) - H(175)	120.1
C(175) - C(176) - C(171)	121.1 (4)
C(175) - C(176) - H(176)	119.5
C(171) - C(176) - H(176)	119.5
C(32) - C(31) - Ru(1)	127.6 (3)
C(32) - C(31) - H(31)	116.2
Ru(1) - C(31) - H(31)	116.2
O(33) - C(32) - O(34)	122.6 (3)
O(33) - C(32) - C(31)	127.2 (3)
O(34) - C(32) - C(31)	110.2 (3)
C(32) - O(34) - C(35)	115.4 (3)
C(36) - C(35) - O(34)	119.5 (3)
C(36) - C(35) - C(42)	123.9 (3)
O(34) - C(35) - C(42)	116.6 (3)
C(35) - C(36) - C(38)	115.1 (3)
C(35) - C(36) - C(37)	128.7 (3)
C(38) - C(36) - C(37)	116.2 (3)
C(37B) - C(37) - C(37A)	105.9 (3)
C(37B) - C(37) - C(37C)	105.9 (3)
C(37A) - C(37) - C(37C)	109.5 (4)
C(37B) - C(37) - C(36)	118.1 (3)
C(37A) - C(37) - C(36)	108.9 (3)
C(37C) - C(37) - C(36)	108.3 (3)
C(37) - C(37A) - H(37A)	109.5
C(37) - C(37A) - H(37B)	109.5
H(37A) - C(37A) - H(37B)	109.5
C(37) - C(37A) - H(37C)	109.5
H(37A) - C(37A) - H(37C)	109.5
H(37B) - C(37A) - H(37C)	109.5
C(37) - C(37B) - H(37D)	109.5
C(37) - C(37B) - H(37E)	109.5
H(37D) - C(37B) - H(37E)	109.5
C(37) - C(37B) - H(37F)	109.5
H(37D) - C(37B) - H(37F)	109.5
H(37E) - C(37B) - H(37F)	109.5
C(37) - C(37C) - H(37G)	109.5
C(37) - C(37C) - H(37H)	109.5
H(37G) - C(37C) - H(37H)	109.5
C(37) - C(37C) - H(37I)	109.5
H(37G) - C(37C) - H(37I)	109.5
H(37H) - C(37C) - H(37I)	109.5
C(39) - C(38) - C(36)	123.6 (4)
C(39) - C(38) - H(38)	118.2
C(36) - C(38) - H(38)	118.2
C(38) - C(39) - C(41)	118.8 (4)
C(38) - C(39) - C(40)	122.1 (4)
C(41) - C(39) - C(40)	119.1 (4)
C(39) - C(40) - H(40A)	109.5

C(39) - C(40) - H(40B)	109.5
H(40A) - C(40) - H(40B)	109.5
C(39) - C(40) - H(40C)	109.5
H(40A) - C(40) - H(40C)	109.5
H(40B) - C(40) - H(40C)	109.5
C(42) - C(41) - C(39)	121.8(4)
C(42) - C(41) - H(41)	119.1
C(39) - C(41) - H(41)	119.1
C(41) - C(42) - C(35)	116.8(3)
C(41) - C(42) - C(43)	119.8(3)
C(35) - C(42) - C(43)	123.2(3)
C(43C) - C(43) - C(43B)	109.5(3)
C(43C) - C(43) - C(43A)	106.2(3)
C(43B) - C(43) - C(43A)	108.3(4)
C(43C) - C(43) - C(42)	114.6(3)
C(43B) - C(43) - C(42)	107.3(3)
C(43A) - C(43) - C(42)	110.8(3)
C(43) - C(43A) - H(43A)	109.5
C(43) - C(43A) - H(43B)	109.5
H(43A) - C(43A) - H(43B)	109.5
C(43) - C(43A) - H(43C)	109.5
H(43A) - C(43A) - H(43C)	109.5
H(43B) - C(43A) - H(43C)	109.5
C(43) - C(43B) - H(43D)	109.5
C(43) - C(43B) - H(43E)	109.5
H(43D) - C(43B) - H(43E)	109.5
C(43) - C(43B) - H(43F)	109.5
H(43D) - C(43B) - H(43F)	109.5
H(43E) - C(43B) - H(43F)	109.5
C(43) - C(43C) - H(43G)	109.5
C(43) - C(43C) - H(43H)	109.5
H(43G) - C(43C) - H(43H)	109.5
C(43) - C(43C) - H(43I)	109.5
H(43G) - C(43C) - H(43I)	109.5
H(43H) - C(43C) - H(43I)	109.5
C(54) - O(51) - C(51)	104.0(3)
C(54) - O(51) - Ru(1)	123.2(2)
C(51) - O(51) - Ru(1)	124.3(2)
O(51) - C(51) - C(52)	105.1(3)
O(51) - C(51) - H(51A)	110.7
C(52) - C(51) - H(51A)	110.7
O(51) - C(51) - H(51B)	110.7
C(52) - C(51) - H(51B)	110.7
H(51A) - C(51) - H(51B)	108.8
C(51) - C(52) - C(53)	104.2(3)
C(51) - C(52) - H(52A)	110.9
C(53) - C(52) - H(52A)	110.9
C(51) - C(52) - H(52B)	110.9
C(53) - C(52) - H(52B)	110.9
H(52A) - C(52) - H(52B)	108.9
C(54) - C(53) - C(52)	103.6(4)
C(54) - C(53) - H(53A)	111.0
C(52) - C(53) - H(53A)	111.0
C(54) - C(53) - H(53B)	111.0
C(52) - C(53) - H(53B)	111.0
H(53A) - C(53) - H(53B)	109.0
O(51) - C(54) - C(53)	106.1(3)
O(51) - C(54) - H(54A)	110.5
C(53) - C(54) - H(54A)	110.5
O(51) - C(54) - H(54B)	110.5
C(53) - C(54) - H(54B)	110.5

Symmetry transformations used to generate equivalent atoms:

Table 3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ru(1)	10(1)	11(1)	12(1)	1(1)	-1(1)	7(1)
N(1)	14(1)	13(2)	18(2)	1(1)	-1(1)	7(1)
N(2)	12(1)	12(1)	16(2)	2(1)	1(1)	5(1)
N(3)	12(1)	11(1)	14(1)	2(1)	-1(1)	6(1)
N(4)	13(1)	13(1)	16(2)	1(1)	-1(1)	8(1)
C(1)	15(2)	15(2)	18(2)	3(1)	3(1)	9(1)
C(2)	14(2)	15(2)	19(2)	3(1)	1(1)	9(1)
C(3)	16(2)	14(2)	22(2)	4(1)	3(1)	9(1)
C(4)	18(2)	19(2)	27(2)	2(2)	-1(2)	12(2)
C(5)	16(2)	16(2)	24(2)	0(2)	-7(2)	8(2)
C(6)	14(2)	14(2)	18(2)	2(1)	-1(1)	6(1)
C(7)	13(2)	13(2)	15(2)	2(1)	0(1)	5(1)
C(8)	14(2)	12(2)	18(2)	3(1)	2(1)	5(1)
C(9)	17(2)	14(2)	18(2)	-1(1)	1(1)	7(1)
C(10)	18(2)	13(2)	17(2)	0(1)	3(1)	9(1)
C(11)	15(2)	13(2)	16(2)	2(1)	1(1)	6(1)
C(12)	14(2)	14(2)	17(2)	6(1)	2(1)	7(1)
C(13)	10(2)	12(2)	19(2)	4(1)	0(1)	5(1)
C(14)	12(2)	18(2)	18(2)	5(1)	-2(1)	9(1)
C(15)	14(2)	17(2)	17(2)	2(1)	-2(1)	7(1)
C(16)	13(2)	14(2)	14(2)	2(1)	0(1)	4(1)
C(17)	13(2)	15(2)	16(2)	3(1)	0(1)	6(1)
C(18)	15(2)	12(2)	13(2)	0(1)	-1(1)	6(1)
C(19)	18(2)	16(2)	19(2)	-4(1)	-2(1)	9(2)
C(20)	19(2)	17(2)	22(2)	-1(2)	2(2)	12(2)
C(21)	18(2)	14(2)	17(2)	-2(1)	-2(1)	10(2)
C(22)	16(2)	18(2)	18(2)	1(1)	2(1)	10(2)
C(23)	27(2)	17(2)	21(2)	3(2)	2(2)	13(2)
C(24)	21(2)	21(2)	24(2)	-2(2)	-4(2)	16(2)
C(25)	14(2)	24(2)	29(2)	1(2)	3(2)	10(2)
C(26)	18(2)	15(2)	30(2)	5(2)	1(2)	7(2)
C(71)	16(2)	17(2)	18(2)	1(1)	-1(1)	9(2)
C(72)	25(2)	24(2)	25(2)	7(2)	-5(2)	3(2)
C(73)	40(3)	39(3)	23(2)	8(2)	-8(2)	7(2)
C(74)	38(3)	33(2)	26(2)	-5(2)	-18(2)	6(2)
C(75)	22(2)	21(2)	31(2)	-1(2)	-8(2)	4(2)
C(76)	20(2)	20(2)	20(2)	2(2)	1(2)	8(2)
C(121)	13(2)	14(2)	20(2)	1(1)	-4(1)	6(1)

C(122)	19 (2)	21 (2)	25 (2)	6 (2)	0 (2)	9 (2)
C(123)	25 (2)	20 (2)	27 (2)	6 (2)	-4 (2)	14 (2)
C(124)	20 (2)	22 (2)	34 (2)	-2 (2)	-6 (2)	15 (2)
C(125)	25 (2)	29 (2)	35 (2)	6 (2)	10 (2)	18 (2)
C(126)	23 (2)	21 (2)	34 (2)	10 (2)	10 (2)	14 (2)
C(171)	12 (2)	17 (2)	15 (2)	-2 (1)	2 (1)	7 (1)
C(172)	20 (2)	16 (2)	19 (2)	1 (1)	0 (1)	8 (2)
C(173)	25 (2)	28 (2)	15 (2)	-4 (2)	-4 (2)	18 (2)
C(174)	15 (2)	23 (2)	25 (2)	-8 (2)	-6 (2)	12 (2)
C(175)	19 (2)	18 (2)	30 (2)	0 (2)	1 (2)	7 (2)
C(176)	20 (2)	18 (2)	16 (2)	1 (1)	1 (1)	8 (2)
C(31)	16 (2)	14 (2)	17 (2)	1 (1)	-2 (1)	6 (1)
C(32)	13 (2)	14 (2)	22 (2)	4 (1)	0 (1)	6 (1)
O(33)	20 (1)	20 (1)	17 (1)	1 (1)	1 (1)	6 (1)
O(34)	17 (1)	16 (1)	16 (1)	3 (1)	0 (1)	4 (1)
C(35)	16 (2)	14 (2)	16 (2)	2 (1)	-1 (1)	4 (1)
C(36)	18 (2)	16 (2)	18 (2)	2 (1)	0 (1)	6 (2)
C(37)	24 (2)	22 (2)	24 (2)	3 (2)	1 (2)	14 (2)
C(37A)	57 (3)	37 (3)	33 (3)	10 (2)	11 (2)	33 (2)
C(37B)	33 (2)	34 (2)	26 (2)	6 (2)	5 (2)	23 (2)
C(37C)	21 (2)	50 (3)	43 (3)	-8 (2)	-6 (2)	17 (2)
C(38)	21 (2)	20 (2)	21 (2)	3 (2)	-4 (2)	8 (2)
C(39)	24 (2)	14 (2)	17 (2)	-1 (1)	0 (2)	5 (2)
C(40)	35 (2)	38 (3)	21 (2)	4 (2)	2 (2)	17 (2)
C(41)	20 (2)	17 (2)	24 (2)	1 (2)	1 (2)	7 (2)
C(42)	18 (2)	16 (2)	20 (2)	3 (1)	-1 (1)	5 (2)
C(43)	20 (2)	23 (2)	27 (2)	8 (2)	0 (2)	11 (2)
C(43A)	45 (3)	53 (3)	39 (3)	18 (2)	12 (2)	38 (3)
C(43B)	26 (2)	29 (2)	47 (3)	13 (2)	-12 (2)	8 (2)
C(43C)	22 (2)	21 (2)	32 (2)	8 (2)	-1 (2)	11 (2)
O(51)	16 (1)	20 (1)	18 (1)	-1 (1)	1 (1)	7 (1)
C(51)	28 (2)	28 (2)	17 (2)	1 (2)	-1 (2)	10 (2)
C(52)	38 (3)	35 (3)	37 (3)	-4 (2)	7 (2)	17 (2)
C(53)	23 (2)	37 (3)	45 (3)	0 (2)	1 (2)	11 (2)
C(54)	21 (2)	22 (2)	27 (2)	1 (2)	2 (2)	5 (2)

Table 4. Torsion angles [deg] for **1**.

C(31)-Ru(1)-N(1)-C(6)	89.9(3)
N(2)-Ru(1)-N(1)-C(6)	-6.4(3)
N(4)-Ru(1)-N(1)-C(6)	180.0(3)
N(3)-Ru(1)-N(1)-C(6)	-88.0(10)
O(51)-Ru(1)-N(1)-C(6)	-94.6(3)
C(31)-Ru(1)-N(1)-C(3)	-86.7(3)
N(2)-Ru(1)-N(1)-C(3)	177.0(3)
N(4)-Ru(1)-N(1)-C(3)	3.4(3)
N(3)-Ru(1)-N(1)-C(3)	95.4(10)
O(51)-Ru(1)-N(1)-C(3)	88.8(3)
C(31)-Ru(1)-N(2)-C(8)	-87.2(3)
N(1)-Ru(1)-N(2)-C(8)	7.1(3)
N(4)-Ru(1)-N(2)-C(8)	95.3(11)
N(3)-Ru(1)-N(2)-C(8)	-179.7(3)
O(51)-Ru(1)-N(2)-C(8)	91.8(3)
C(31)-Ru(1)-N(2)-C(11)	84.2(3)
N(1)-Ru(1)-N(2)-C(11)	178.5(3)
N(4)-Ru(1)-N(2)-C(11)	-93.2(11)
N(3)-Ru(1)-N(2)-C(11)	-8.3(3)
O(51)-Ru(1)-N(2)-C(11)	-96.8(3)
C(31)-Ru(1)-N(3)-C(13)	-88.7(3)
N(1)-Ru(1)-N(3)-C(13)	89.2(10)
N(2)-Ru(1)-N(3)-C(13)	7.7(3)
N(4)-Ru(1)-N(3)-C(13)	-178.7(3)
O(51)-Ru(1)-N(3)-C(13)	95.8(3)
C(31)-Ru(1)-N(3)-C(16)	80.3(3)
N(1)-Ru(1)-N(3)-C(16)	-101.8(10)
N(2)-Ru(1)-N(3)-C(16)	176.7(3)
N(4)-Ru(1)-N(3)-C(16)	-9.7(3)
O(51)-Ru(1)-N(3)-C(16)	-95.2(3)
C(31)-Ru(1)-N(4)-C(18)	-85.3(3)
N(1)-Ru(1)-N(4)-C(18)	-179.7(3)
N(2)-Ru(1)-N(4)-C(18)	92.2(11)
N(3)-Ru(1)-N(4)-C(18)	7.3(3)
O(51)-Ru(1)-N(4)-C(18)	95.7(3)
C(31)-Ru(1)-N(4)-C(1)	91.8(3)
N(1)-Ru(1)-N(4)-C(1)	-2.6(3)
N(2)-Ru(1)-N(4)-C(1)	-90.7(11)
N(3)-Ru(1)-N(4)-C(1)	-175.6(3)
O(51)-Ru(1)-N(4)-C(1)	-87.2(3)
C(18)-N(4)-C(1)-C(2)	178.3(3)
Ru(1)-N(4)-C(1)-C(2)	0.8(5)
C(18)-N(4)-C(1)-C(20)	-3.1(4)
Ru(1)-N(4)-C(1)-C(20)	179.3(2)

N(4) - C(1) - C(2) - C(3)	1.4 (6)
C(20) - C(1) - C(2) - C(3)	-176.9 (3)
N(4) - C(1) - C(2) - C(21)	-178.2 (3)
C(20) - C(1) - C(2) - C(21)	3.4 (5)
C(6) - N(1) - C(3) - C(2)	-179.8 (3)
Ru(1) - N(1) - C(3) - C(2)	-2.6 (5)
C(6) - N(1) - C(3) - C(4)	0.9 (4)
Ru(1) - N(1) - C(3) - C(4)	178.1 (2)
C(1) - C(2) - C(3) - N(1)	-0.4 (6)
C(21) - C(2) - C(3) - N(1)	179.3 (3)
C(1) - C(2) - C(3) - C(4)	178.8 (4)
C(21) - C(2) - C(3) - C(4)	-1.6 (5)
N(1) - C(3) - C(4) - C(5)	-1.3 (4)
C(2) - C(3) - C(4) - C(5)	179.4 (3)
C(3) - C(4) - C(5) - C(6)	1.1 (4)
C(3) - N(1) - C(6) - C(7)	-179.1 (3)
Ru(1) - N(1) - C(6) - C(7)	3.8 (5)
C(3) - N(1) - C(6) - C(5)	-0.3 (4)
Ru(1) - N(1) - C(6) - C(5)	-177.4 (2)
C(4) - C(5) - C(6) - N(1)	-0.5 (4)
C(4) - C(5) - C(6) - C(7)	178.3 (3)
N(1) - C(6) - C(7) - C(8)	1.1 (6)
C(5) - C(6) - C(7) - C(8)	-177.6 (3)
N(1) - C(6) - C(7) - C(71)	-174.6 (3)
C(5) - C(6) - C(7) - C(71)	6.8 (5)
C(11) - N(2) - C(8) - C(7)	-178.0 (3)
Ru(1) - N(2) - C(8) - C(7)	-5.3 (5)
C(11) - N(2) - C(8) - C(9)	-0.1 (4)
Ru(1) - N(2) - C(8) - C(9)	172.6 (2)
C(6) - C(7) - C(8) - N(2)	-0.3 (6)
C(71) - C(7) - C(8) - N(2)	175.3 (3)
C(6) - C(7) - C(8) - C(9)	-177.9 (3)
C(71) - C(7) - C(8) - C(9)	-2.2 (5)
N(2) - C(8) - C(9) - C(10)	0.3 (4)
C(7) - C(8) - C(9) - C(10)	178.2 (3)
C(8) - C(9) - C(10) - C(11)	-0.3 (4)
C(8) - N(2) - C(11) - C(12)	179.6 (3)
Ru(1) - N(2) - C(11) - C(12)	6.8 (5)
C(8) - N(2) - C(11) - C(10)	-0.1 (4)
Ru(1) - N(2) - C(11) - C(10)	-172.9 (2)
C(9) - C(10) - C(11) - N(2)	0.2 (4)
C(9) - C(10) - C(11) - C(12)	-179.5 (3)
N(2) - C(11) - C(12) - C(13)	-1.1 (6)
C(10) - C(11) - C(12) - C(13)	178.6 (3)
N(2) - C(11) - C(12) - C(121)	-179.4 (3)
C(10) - C(11) - C(12) - C(121)	0.3 (5)
C(16) - N(3) - C(13) - C(12)	-176.1 (3)
Ru(1) - N(3) - C(13) - C(12)	-5.4 (5)
C(16) - N(3) - C(13) - C(14)	1.7 (4)
Ru(1) - N(3) - C(13) - C(14)	172.4 (2)
C(11) - C(12) - C(13) - N(3)	0.4 (6)
C(121) - C(12) - C(13) - N(3)	178.6 (3)
C(11) - C(12) - C(13) - C(14)	-177.1 (3)
C(121) - C(12) - C(13) - C(14)	1.1 (5)
N(3) - C(13) - C(14) - C(15)	-1.9 (4)
C(12) - C(13) - C(14) - C(15)	175.9 (3)
C(13) - C(14) - C(15) - C(16)	1.4 (4)
C(13) - N(3) - C(16) - C(17)	177.7 (3)
Ru(1) - N(3) - C(16) - C(17)	7.1 (5)
C(13) - N(3) - C(16) - C(15)	-0.9 (4)
Ru(1) - N(3) - C(16) - C(15)	-171.5 (2)

C(14) - C(15) - C(16) - N(3)	-0.3 (4)
C(14) - C(15) - C(16) - C(17)	-179.0 (3)
N(3) - C(16) - C(17) - C(18)	2.2 (6)
C(15) - C(16) - C(17) - C(18)	-179.4 (3)
N(3) - C(16) - C(17) - C(171)	-172.2 (3)
C(15) - C(16) - C(17) - C(171)	6.2 (5)
C(1) - N(4) - C(18) - C(17)	-179.2 (3)
Ru(1) - N(4) - C(18) - C(17)	-1.7 (5)
C(1) - N(4) - C(18) - C(19)	2.9 (4)
Ru(1) - N(4) - C(18) - C(19)	-179.6 (2)
C(16) - C(17) - C(18) - N(4)	-5.1 (6)
C(171) - C(17) - C(18) - N(4)	169.3 (3)
C(16) - C(17) - C(18) - C(19)	172.5 (3)
C(171) - C(17) - C(18) - C(19)	-13.1 (5)
N(4) - C(18) - C(19) - C(20)	-1.5 (4)
C(17) - C(18) - C(19) - C(20)	-179.5 (3)
C(18) - C(19) - C(20) - C(1)	-0.4 (4)
N(4) - C(1) - C(20) - C(19)	2.2 (4)
C(2) - C(1) - C(20) - C(19)	-179.3 (3)
C(1) - C(2) - C(21) - C(26)	-109.1 (4)
C(3) - C(2) - C(21) - C(26)	71.2 (5)
C(1) - C(2) - C(21) - C(22)	73.1 (5)
C(3) - C(2) - C(21) - C(22)	-106.6 (4)
C(26) - C(21) - C(22) - C(23)	-0.7 (6)
C(2) - C(21) - C(22) - C(23)	177.2 (3)
C(21) - C(22) - C(23) - C(24)	0.3 (6)
C(22) - C(23) - C(24) - C(25)	0.2 (6)
C(23) - C(24) - C(25) - C(26)	-0.3 (6)
C(22) - C(21) - C(26) - C(25)	0.6 (6)
C(2) - C(21) - C(26) - C(25)	-177.3 (3)
C(24) - C(25) - C(26) - C(21)	-0.1 (6)
C(8) - C(7) - C(71) - C(72)	-110.6 (4)
C(6) - C(7) - C(71) - C(72)	65.4 (5)
C(8) - C(7) - C(71) - C(76)	71.9 (5)
C(6) - C(7) - C(71) - C(76)	-112.1 (4)
C(76) - C(71) - C(72) - C(73)	-0.5 (6)
C(7) - C(71) - C(72) - C(73)	-178.1 (4)
C(71) - C(72) - C(73) - C(74)	0.3 (7)
C(72) - C(73) - C(74) - C(75)	0.6 (8)
C(73) - C(74) - C(75) - C(76)	-1.3 (7)
C(74) - C(75) - C(76) - C(71)	1.1 (6)
C(72) - C(71) - C(76) - C(75)	-0.2 (6)
C(7) - C(71) - C(76) - C(75)	177.3 (4)
C(11) - C(12) - C(121) - C(126)	78.7 (4)
C(13) - C(12) - C(121) - C(126)	-99.7 (4)
C(11) - C(12) - C(121) - C(122)	-97.3 (4)
C(13) - C(12) - C(121) - C(122)	84.3 (4)
C(126) - C(121) - C(122) - C(123)	-3.1 (6)
C(12) - C(121) - C(122) - C(123)	173.0 (3)
C(121) - C(122) - C(123) - C(124)	1.2 (6)
C(122) - C(123) - C(124) - C(125)	1.3 (6)
C(123) - C(124) - C(125) - C(126)	-1.8 (6)
C(124) - C(125) - C(126) - C(121)	-0.2 (7)
C(122) - C(121) - C(126) - C(125)	2.6 (6)
C(12) - C(121) - C(126) - C(125)	-173.5 (4)
C(18) - C(17) - C(171) - C(176)	-65.5 (4)
C(16) - C(17) - C(171) - C(176)	109.3 (4)
C(18) - C(17) - C(171) - C(172)	115.3 (4)
C(16) - C(17) - C(171) - C(172)	-69.9 (5)
C(176) - C(171) - C(172) - C(173)	-1.0 (5)
C(17) - C(171) - C(172) - C(173)	178.2 (3)

C(171) - C(172) - C(173) - C(174)	-0.5 (6)
C(172) - C(173) - C(174) - C(175)	1.1 (6)
C(173) - C(174) - C(175) - C(176)	-0.1 (6)
C(174) - C(175) - C(176) - C(171)	-1.4 (6)
C(172) - C(171) - C(176) - C(175)	2.0 (5)
C(17) - C(171) - C(176) - C(175)	-177.2 (3)
N(1) - Ru(1) - C(31) - C(32)	-44.2 (3)
N(2) - Ru(1) - C(31) - C(32)	45.4 (3)
N(4) - Ru(1) - C(31) - C(32)	-134.9 (3)
N(3) - Ru(1) - C(31) - C(32)	135.5 (3)
O(51) - Ru(1) - C(31) - C(32)	-122.7 (15)
Ru(1) - C(31) - C(32) - O(33)	-6.0 (6)
Ru(1) - C(31) - C(32) - O(34)	173.3 (3)
O(33) - C(32) - O(34) - C(35)	-4.4 (5)
C(31) - C(32) - O(34) - C(35)	176.2 (3)
C(32) - O(34) - C(35) - C(36)	85.2 (4)
C(32) - O(34) - C(35) - C(42)	-96.7 (4)
O(34) - C(35) - C(36) - C(38)	177.7 (3)
C(42) - C(35) - C(36) - C(38)	-0.2 (5)
O(34) - C(35) - C(36) - C(37)	-1.2 (6)
C(42) - C(35) - C(36) - C(37)	-179.1 (4)
C(35) - C(36) - C(37) - C(37B)	3.4 (6)
C(38) - C(36) - C(37) - C(37B)	-175.4 (4)
C(35) - C(36) - C(37) - C(37A)	124.1 (4)
C(38) - C(36) - C(37) - C(37A)	-54.7 (5)
C(35) - C(36) - C(37) - C(37C)	-116.8 (4)
C(38) - C(36) - C(37) - C(37C)	64.3 (4)
C(35) - C(36) - C(38) - C(39)	0.7 (5)
C(37) - C(36) - C(38) - C(39)	179.8 (3)
C(36) - C(38) - C(39) - C(41)	-0.2 (6)
C(36) - C(38) - C(39) - C(40)	-176.5 (4)
C(38) - C(39) - C(41) - C(42)	-0.9 (6)
C(40) - C(39) - C(41) - C(42)	175.5 (4)
C(39) - C(41) - C(42) - C(35)	1.4 (5)
C(39) - C(41) - C(42) - C(43)	-173.2 (3)
C(36) - C(35) - C(42) - C(41)	-0.8 (5)
O(34) - C(35) - C(42) - C(41)	-178.8 (3)
C(36) - C(35) - C(42) - C(43)	173.6 (3)
O(34) - C(35) - C(42) - C(43)	-4.4 (5)
C(41) - C(42) - C(43) - C(43C)	-133.8 (4)
C(35) - C(42) - C(43) - C(43C)	52.0 (5)
C(41) - C(42) - C(43) - C(43B)	104.4 (4)
C(35) - C(42) - C(43) - C(43B)	-69.8 (5)
C(41) - C(42) - C(43) - C(43A)	-13.6 (5)
C(35) - C(42) - C(43) - C(43A)	172.2 (4)
C(31) - Ru(1) - O(51) - C(54)	113.5 (16)
N(1) - Ru(1) - O(51) - C(54)	34.7 (3)
N(2) - Ru(1) - O(51) - C(54)	-54.6 (3)
N(4) - Ru(1) - O(51) - C(54)	125.8 (3)
N(3) - Ru(1) - O(51) - C(54)	-144.5 (3)
C(31) - Ru(1) - O(51) - C(51)	-29.2 (17)
N(1) - Ru(1) - O(51) - C(51)	-108.1 (3)
N(2) - Ru(1) - O(51) - C(51)	162.7 (3)
N(4) - Ru(1) - O(51) - C(51)	-16.9 (3)
N(3) - Ru(1) - O(51) - C(51)	72.7 (3)
C(54) - O(51) - C(51) - C(52)	-38.8 (4)
Ru(1) - O(51) - C(51) - C(52)	109.7 (3)
O(51) - C(51) - C(52) - C(53)	21.6 (5)
C(51) - C(52) - C(53) - C(54)	2.7 (5)
C(51) - O(51) - C(54) - C(53)	41.3 (4)

Ru(1) - O(51) - C(54) - C(53)	-107.7(3)
C(52) - C(53) - C(54) - O(51)	-26.6(5)

Symmetry transformations used to generate equivalent atoms: