

X-Ray Structure determination of (E)-7, (EE)-12b. Data were measured using the ω - 2θ scan technique with a scan angle of 1.5° and a variable scan rate with a maximum scan time of 60 s per reflection. Mo $K\alpha$ radiation was used with a graphite-crystal monochromator on a Nonius CAD4 single-crystal diffractometer. On all reflections, profile analysis was performed.¹ Multiple measured reflections were averaged and Lorentz and polarization corrections were applied. The structures were solved by Patterson methods using DIRDIF99.² Isotropic least-squares refinement on F^2 using SHELXL97.³ During the final stages of the refinements, all positional parameters and the anisotropic temperature factors of all the non-H atoms were refined. The H-atoms were refined isotropically as a mixture of independent and constrained refinement. A statistical disordered model accounting for BF_4^- and CH_2Cl_2 groups was refined for structure (EE)-12b. Atomic scattering factors were taken from International tables for X-ray Crystallography.⁴ Plots were made with the PLATON package.⁵ Geometrical calculations were made with PARST.⁶ Publication Material were made with WinGX.⁷ All calculations were made on the Scientific Computer Centre at the University of Oviedo.

Acknowledgments,

Support – Project BQU2000-0219

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Table 1. Crystal data and structure refinement for (E)-7.

Identification code	(E)-7
Empirical formula	C ₅₇ H ₄₉ B F ₄ O P ₂ Ru
Formula weight	999.78
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /c
Unit cell dimensions	a = 15.145(2) Å b = 15.228(4) Å c = 20.986(5) Å β = 98.99(2)°
Volume	4780.5(17) Å ³
Z	4
Density (calculated)	1.389 Mg/m ³
Absorption coefficient	0.451 mm ⁻¹
F(000)	2056
Crystal size	0.34 x 0.19 x 0.13 mm ³
Theta range for data collection	1.36 to 24.97°
Index ranges	-17 ≤ h ≤ 17, 0 ≤ k ≤ 18, 0 ≤ l ≤ 24
Reflections collected	8380
Independent reflections	8380 [R(int) = 0.1152]
Completeness to theta = 24.97°	95.9 %
Absorption correction	Empirical
Max. and min. transmission	0.9987 and 0.8524
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8380 / 0 / 599
Goodness-of-fit on F ²	1.003
Final R indices [I > 2σ(I)]	R1 = 0.0534, wR2 = 0.1147
R indices (all data)	R1 = 0.2164, wR2 = 0.1569
Largest diff. peak and hole	0.594 and -1.069 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)for (E)-7. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Ru(1)	1916(1)	1344(1)	1118(1)	36(1)
C(70)	1744(6)	203(5)	1822(4)	49(2)
C(71)	2581(6)	153(6)	1602(4)	58(2)
C(72)	3091(5)	867(6)	1842(4)	50(2)
C(73)	2559(6)	1432(5)	2175(3)	52(2)
C(74)	1732(6)	993(5)	2182(3)	49(2)
C(75)	1012(7)	1176(7)	2510(4)	77(3)
C(76)	344(8)	568(9)	2487(5)	93(4)
C(77)	340(7)	-200(8)	2130(6)	89(3)
C(78)	1018(7)	-391(6)	1795(5)	82(3)
C(710)	2899(7)	-645(6)	1266(5)	92(4)
C(720)	4077(5)	991(7)	1832(5)	83(3)
C(730)	2935(7)	2188(6)	2599(4)	78(3)
C(1)	2708(5)	2269(5)	789(3)	39(2)
C(2)	3198(5)	2317(5)	309(4)	43(2)
C(3)	1602(5)	746(6)	360(4)	56(2)
O(3)	1393(5)	309(4)	-98(3)	89(2)
P(1)	745(1)	2331(1)	860(1)	40(1)
C(11)	255(6)	2420(5)	17(4)	47(2)
C(12)	776(6)	2333(6)	-464(4)	64(3)
C(13)	417(8)	2414(6)	-1116(4)	79(3)
C(14)	-463(8)	2586(6)	-1291(5)	77(3)
C(15)	-1016(6)	2659(6)	-826(5)	69(3)
C(16)	-657(6)	2584(5)	-182(4)	59(2)
C(21)	-234(5)	2084(5)	1231(4)	43(2)
C(22)	-621(5)	2658(6)	1621(4)	54(2)
C(23)	-1384(6)	2416(7)	1863(4)	64(3)
C(24)	-1773(6)	1618(7)	1731(4)	72(3)
C(25)	-1411(6)	1042(7)	1330(5)	76(3)
C(26)	-646(5)	1286(6)	1086(4)	61(2)
C(31)	1001(5)	3468(5)	1087(4)	41(2)
C(32)	826(6)	4165(6)	670(4)	69(3)
C(33)	1079(7)	5007(6)	871(5)	83(3)
C(34)	1490(6)	5168(6)	1480(5)	68(3)
C(35)	1669(6)	4479(6)	1895(5)	69(3)
C(36)	1438(6)	3644(6)	1702(4)	63(2)
P(2)	3872(1)	3272(1)	223(1)	39(1)
C(41)	3389(5)	3938(4)	-446(3)	39(2)
C(42)	3884(6)	4383(5)	-849(4)	55(2)
C(43)	3493(7)	4935(6)	-1315(4)	68(3)
C(44)	2569(8)	5071(6)	-1409(4)	71(3)
C(45)	2069(6)	4635(6)	-1024(4)	68(3)
C(46)	2463(5)	4057(5)	-548(4)	53(2)
C(51)	3956(5)	3974(5)	922(3)	40(2)
C(52)	4253(5)	3640(6)	1525(4)	51(2)
C(53)	4320(5)	4197(6)	2071(4)	57(2)
C(54)	4071(6)	5065(6)	1980(5)	64(3)
C(55)	3778(6)	5392(6)	1378(5)	64(3)
C(56)	3727(5)	4851(5)	851(4)	50(2)
C(61)	4965(5)	2943(5)	99(4)	41(2)

C(62)	5103(6)	2624(5)	-504(4)	53(2)
C(63)	5955(6)	2341(6)	-594(5)	66(3)
C(64)	6636(6)	2377(7)	-101(5)	79(3)
C(65)	6520(6)	2699(7)	501(5)	87(3)
C(66)	5684(5)	2988(6)	592(4)	65(3)
C(81)	3283(5)	1593(5)	-171(3)	43(2)
C(82)	3717(6)	827(6)	28(4)	60(2)
C(83)	3818(6)	165(6)	-405(5)	70(3)
C(84)	3510(7)	258(7)	-1051(5)	73(3)
C(85)	3091(7)	1022(7)	-1252(4)	72(3)
C(86)	2980(6)	1688(6)	-818(4)	59(2)
B(1)	6325(8)	2457(8)	2503(5)	63(3)
F(1)	7040(4)	2205(4)	2963(3)	87(2)
F(2)	5598(4)	2588(4)	2806(3)	103(2)
F(3)	6141(4)	1822(4)	2041(3)	94(2)
F(4)	6547(4)	3224(4)	2220(3)	96(2)

Table 3. Selected bond lengths [Å] and angles [°] for (E)-7.

Ru-C* 1.953(5)
 Δ 0.078(7)

C1 -Ru1 -C* 119.5(2)
 C3 -Ru1 -C* 121.4(3)
 P1 -Ru1 -C* 130.4(2)

FA 11.3(7)
 HA 6.0(4)
 DA 107.0(6)
 CA 155.4(3)

^a Δ = d(Ru1-C74), C(70)) - d(Ru1-C(71), C(73)).

^bFA(fold angle) = angle between normals to least-squares planes defined by C(71), C(72), C(73) and C(70), C(74), C(75), C(76), C(77), C(78).

^cHA(hinge angle) = angle between normals to least-squares planes defined by C(71), C(72), C(73) and C(71), C(74), C(70), C(73).

^dDA(dihedral angle) = angle between normals to least-squares planes defined by C*, Ru(1), C(1) and Ru(1), C(1), C(2).

^eCA(conformational angle) = angle between normals to least-squares planes defined by C**, C*, Ru(1) and C*, Ru(1), C(1).

C* = centroid of C(70), C(71), C(72), C(73), C(74).

C** = centroid of C(70), C(74), C(75), C(76), C(77), C(78).

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [Å] and angles [°] for (E)-7.

Ru(1)-C(3)	1.831(9)	C(22)-H(22)	0.9300
Ru(1)-C(1)	2.039(7)	C(23)-C(24)	1.358(12)
Ru(1)-C(71)	2.240(8)	C(23)-H(23)	0.9300
Ru(1)-C(72)	2.271(8)	C(24)-C(25)	1.388(12)
Ru(1)-C(73)	2.283(7)	C(24)-H(24)	0.9300
Ru(1)-C(70)	2.322(7)	C(25)-C(26)	1.389(10)
Ru(1)-P(1)	2.323(2)	C(25)-H(25)	0.9300
Ru(1)-C(74)	2.355(7)	C(26)-H(26)	0.9300
C(70)-C(78)	1.417(11)	C(31)-C(32)	1.375(10)
C(70)-C(71)	1.418(11)	C(31)-C(36)	1.382(10)
C(70)-C(74)	1.422(10)	C(32)-C(33)	1.385(11)
C(71)-C(72)	1.381(11)	C(32)-H(32)	0.9300
C(71)-C(710)	1.520(11)	C(33)-C(34)	1.355(12)
C(72)-C(73)	1.433(10)	C(33)-H(33)	0.9300
C(72)-C(720)	1.508(11)	C(34)-C(35)	1.363(12)
C(73)-C(74)	1.422(11)	C(34)-H(34)	0.9300
C(73)-C(730)	1.513(10)	C(35)-C(36)	1.363(11)
C(74)-C(75)	1.405(11)	C(35)-H(35)	0.9300
C(75)-C(76)	1.366(14)	C(36)-H(36)	0.9300
C(75)-H(75)	0.9300	P(2)-C(61)	1.788(7)
C(76)-C(77)	1.388(14)	P(2)-C(41)	1.792(7)
C(76)-H(76)	0.9300	P(2)-C(51)	1.804(7)
C(77)-C(78)	1.365(13)	C(41)-C(42)	1.392(9)
C(77)-H(77)	0.9300	C(41)-C(46)	1.397(10)
C(78)-H(78)	0.9300	C(42)-C(43)	1.354(11)
C(710)-H(711)	0.9600	C(42)-H(42)	0.9300
C(710)-H(712)	0.9600	C(43)-C(44)	1.398(12)
C(710)-H(713)	0.9600	C(43)-H(43)	0.9300
C(720)-H(721)	0.9600	C(44)-C(45)	1.363(11)
C(720)-H(722)	0.9600	C(44)-H(44)	0.9300
C(720)-H(723)	0.9600	C(45)-C(46)	1.393(10)
C(730)-H(731)	0.9600	C(45)-H(45)	0.9300
C(730)-H(732)	0.9600	C(46)-H(46)	0.9300
C(730)-H(733)	0.9600	C(51)-C(52)	1.372(10)
C(1)-C(2)	1.344(10)	C(51)-C(56)	1.382(10)
C(1)-H(1)	0.8782	C(52)-C(53)	1.417(10)
C(2)-C(81)	1.513(10)	C(52)-H(52)	0.9300
C(2)-P(2)	1.801(7)	C(53)-C(54)	1.380(11)
C(3)-O(3)	1.170(9)	C(53)-H(53)	0.9300
P(1)-C(11)	1.813(8)	C(54)-C(55)	1.366(12)
P(1)-C(21)	1.819(7)	C(54)-H(54)	0.9300
P(1)-C(31)	1.821(7)	C(55)-C(56)	1.372(11)
C(11)-C(12)	1.381(10)	C(55)-H(55)	0.9300
C(11)-C(16)	1.401(11)	C(56)-H(56)	0.9300
C(12)-C(13)	1.396(11)	C(61)-C(66)	1.381(10)
C(12)-H(12)	0.9300	C(61)-C(62)	1.401(10)
C(13)-C(14)	1.352(13)	C(62)-C(63)	1.401(11)
C(13)-H(13)	0.9300	C(62)-H(62)	0.9300
C(14)-C(15)	1.387(13)	C(63)-C(64)	1.344(12)
C(14)-H(14)	0.9300	C(63)-H(63)	0.9300
C(15)-C(16)	1.380(11)	C(64)-C(65)	1.390(12)
C(15)-H(15)	0.9300	C(64)-H(64)	0.9300
C(16)-H(16)	0.9300	C(65)-C(66)	1.382(11)
C(21)-C(26)	1.377(10)	C(65)-H(65)	0.9300
C(21)-C(22)	1.388(10)	C(66)-H(66)	0.9300
C(22)-C(23)	1.384(11)	C(81)-C(82)	1.372(10)

C(81)-C(86)	1.373(10)	C(85)-C(86)	1.391(11)
C(82)-C(83)	1.381(11)	C(85)-H(85)	0.9300
C(82)-H(82)	0.9300	C(86)-H(86)	0.9300
C(83)-C(84)	1.370(12)	B(1)-F(3)	1.366(12)
C(83)-H(83)	0.9300	B(1)-F(2)	1.370(11)
C(84)-C(85)	1.362(12)	B(1)-F(4)	1.376(11)
C(84)-H(84)	0.9300	B(1)-F(1)	1.387(12)
C(3)-Ru(1)-C(1)	97.8(3)	C(730)-C(73)-Ru(1)	132.9(6)
C(3)-Ru(1)-C(71)	91.7(4)	C(75)-C(74)-C(73)	131.7(8)
C(1)-Ru(1)-C(71)	117.8(3)	C(75)-C(74)-C(70)	120.2(9)
C(3)-Ru(1)-C(72)	119.5(3)	C(73)-C(74)-C(70)	107.9(7)
C(1)-Ru(1)-C(72)	90.4(3)	C(75)-C(74)-Ru(1)	129.4(6)
C(71)-Ru(1)-C(72)	35.6(3)	C(73)-C(74)-Ru(1)	69.4(4)
C(3)-Ru(1)-C(73)	152.5(3)	C(70)-C(74)-Ru(1)	71.1(4)
C(1)-Ru(1)-C(73)	96.0(3)	C(76)-C(75)-C(74)	118.3(10)
C(71)-Ru(1)-C(73)	60.8(3)	C(76)-C(75)-H(75)	120.8
C(72)-Ru(1)-C(73)	36.7(3)	C(74)-C(75)-H(75)	120.8
C(3)-Ru(1)-C(70)	98.1(3)	C(75)-C(76)-C(77)	122.2(10)
C(1)-Ru(1)-C(70)	149.6(3)	C(75)-C(76)-H(76)	118.9
C(71)-Ru(1)-C(70)	36.2(3)	C(77)-C(76)-H(76)	118.9
C(72)-Ru(1)-C(70)	59.3(3)	C(78)-C(77)-C(76)	121.1(10)
C(73)-Ru(1)-C(70)	59.9(3)	C(78)-C(77)-H(77)	119.5
C(3)-Ru(1)-P(1)	92.0(3)	C(76)-C(77)-H(77)	119.5
C(1)-Ru(1)-P(1)	86.7(2)	C(77)-C(78)-C(70)	119.0(10)
C(71)-Ru(1)-P(1)	154.5(2)	C(77)-C(78)-H(78)	120.5
C(72)-Ru(1)-P(1)	148.5(2)	C(70)-C(78)-H(78)	120.5
C(73)-Ru(1)-P(1)	112.5(2)	C(71)-C(710)-H(711)	109.5
C(70)-Ru(1)-P(1)	118.4(2)	C(71)-C(710)-H(712)	109.5
C(3)-Ru(1)-C(74)	131.2(3)	H(711)-C(710)-H(712)	109.5
C(1)-Ru(1)-C(74)	129.8(3)	C(71)-C(710)-H(713)	109.5
C(71)-Ru(1)-C(74)	59.8(3)	H(711)-C(710)-H(713)	109.5
C(72)-Ru(1)-C(74)	59.3(3)	H(712)-C(710)-H(713)	109.5
C(73)-Ru(1)-C(74)	35.7(3)	C(72)-C(720)-H(721)	109.5
C(70)-Ru(1)-C(74)	35.4(2)	C(72)-C(720)-H(722)	109.5
P(1)-Ru(1)-C(74)	99.7(2)	H(721)-C(720)-H(722)	109.5
C(78)-C(70)-C(71)	132.9(8)	C(72)-C(720)-H(723)	109.5
C(78)-C(70)-C(74)	119.2(8)	H(721)-C(720)-H(723)	109.5
C(71)-C(70)-C(74)	107.7(7)	H(722)-C(720)-H(723)	109.5
C(78)-C(70)-Ru(1)	127.9(6)	C(73)-C(730)-H(731)	109.5
C(71)-C(70)-Ru(1)	68.7(4)	C(73)-C(730)-H(732)	109.5
C(74)-C(70)-Ru(1)	73.5(4)	H(731)-C(730)-H(732)	109.5
C(72)-C(71)-C(70)	108.5(7)	C(73)-C(730)-H(733)	109.5
C(72)-C(71)-C(710)	126.8(9)	H(731)-C(730)-H(733)	109.5
C(70)-C(71)-C(710)	123.9(8)	H(732)-C(730)-H(733)	109.5
C(72)-C(71)-Ru(1)	73.4(5)	C(2)-C(1)-Ru(1)	135.6(6)
C(70)-C(71)-Ru(1)	75.1(5)	C(2)-C(1)-H(1)	111.2
C(710)-C(71)-Ru(1)	126.1(6)	Ru(1)-C(1)-H(1)	113.1
C(71)-C(72)-C(73)	109.0(7)	C(1)-C(2)-C(81)	124.9(7)
C(71)-C(72)-C(720)	126.3(8)	C(1)-C(2)-P(2)	120.5(6)
C(73)-C(72)-C(720)	124.4(8)	C(81)-C(2)-P(2)	114.5(5)
C(71)-C(72)-Ru(1)	70.9(5)	O(3)-C(3)-Ru(1)	174.9(8)
C(73)-C(72)-Ru(1)	72.1(4)	C(11)-P(1)-C(21)	101.3(4)
C(720)-C(72)-Ru(1)	128.6(6)	C(11)-P(1)-C(31)	102.8(3)
C(74)-C(73)-C(72)	106.7(7)	C(21)-P(1)-C(31)	103.8(3)
C(74)-C(73)-C(730)	127.1(8)	C(11)-P(1)-Ru(1)	117.2(3)
C(72)-C(73)-C(730)	123.8(8)	C(21)-P(1)-Ru(1)	114.2(3)
C(74)-C(73)-Ru(1)	74.9(4)	C(31)-P(1)-Ru(1)	115.5(2)
C(72)-C(73)-Ru(1)	71.2(4)	C(12)-C(11)-C(16)	116.6(8)

C(12)-C(11)-P(1)	120.8(7)	C(42)-C(41)-C(46)	117.8(7)
C(16)-C(11)-P(1)	122.6(6)	C(42)-C(41)-P(2)	124.0(6)
C(11)-C(12)-C(13)	121.9(9)	C(46)-C(41)-P(2)	118.1(5)
C(11)-C(12)-H(12)	119.0	C(43)-C(42)-C(41)	121.7(8)
C(13)-C(12)-H(12)	119.0	C(43)-C(42)-H(42)	119.1
C(14)-C(13)-C(12)	119.9(9)	C(41)-C(42)-H(42)	119.1
C(14)-C(13)-H(13)	120.0	C(42)-C(43)-C(44)	120.6(8)
C(12)-C(13)-H(13)	120.0	C(42)-C(43)-H(43)	119.7
C(13)-C(14)-C(15)	120.2(9)	C(44)-C(43)-H(43)	119.7
C(13)-C(14)-H(14)	119.9	C(45)-C(44)-C(43)	118.7(9)
C(15)-C(14)-H(14)	119.9	C(45)-C(44)-H(44)	120.7
C(16)-C(15)-C(14)	119.5(9)	C(43)-C(44)-H(44)	120.7
C(16)-C(15)-H(15)	120.2	C(44)-C(45)-C(46)	121.1(9)
C(14)-C(15)-H(15)	120.2	C(44)-C(45)-H(45)	119.4
C(15)-C(16)-C(11)	121.7(9)	C(46)-C(45)-H(45)	119.4
C(15)-C(16)-H(16)	119.1	C(45)-C(46)-C(41)	120.0(8)
C(11)-C(16)-H(16)	119.1	C(45)-C(46)-H(46)	120.0
C(26)-C(21)-C(22)	117.9(7)	C(41)-C(46)-H(46)	120.0
C(26)-C(21)-P(1)	117.3(6)	C(52)-C(51)-C(56)	120.0(8)
C(22)-C(21)-P(1)	124.7(6)	C(52)-C(51)-P(2)	120.0(6)
C(23)-C(22)-C(21)	120.1(8)	C(56)-C(51)-P(2)	120.0(6)
C(23)-C(22)-H(22)	120.0	C(51)-C(52)-C(53)	119.7(9)
C(21)-C(22)-H(22)	120.0	C(51)-C(52)-H(52)	120.1
C(24)-C(23)-C(22)	121.6(9)	C(53)-C(52)-H(52)	120.1
C(24)-C(23)-H(23)	119.2	C(54)-C(53)-C(52)	118.6(8)
C(22)-C(23)-H(23)	119.2	C(54)-C(53)-H(53)	120.7
C(23)-C(24)-C(25)	119.4(9)	C(52)-C(53)-H(53)	120.7
C(23)-C(24)-H(24)	120.3	C(55)-C(54)-C(53)	121.2(8)
C(25)-C(24)-H(24)	120.3	C(55)-C(54)-H(54)	119.4
C(24)-C(25)-C(26)	119.0(9)	C(53)-C(54)-H(54)	119.4
C(24)-C(25)-H(25)	120.5	C(54)-C(55)-C(56)	119.8(9)
C(26)-C(25)-H(25)	120.5	C(54)-C(55)-H(55)	120.1
C(21)-C(26)-C(25)	122.0(8)	C(56)-C(55)-H(55)	120.1
C(21)-C(26)-H(26)	119.0	C(55)-C(56)-C(51)	120.7(8)
C(25)-C(26)-H(26)	119.0	C(55)-C(56)-H(56)	119.7
C(32)-C(31)-C(36)	117.5(8)	C(51)-C(56)-H(56)	119.7
C(32)-C(31)-P(1)	123.7(6)	C(66)-C(61)-C(62)	118.9(7)
C(36)-C(31)-P(1)	118.7(6)	C(66)-C(61)-P(2)	121.1(6)
C(31)-C(32)-C(33)	120.3(8)	C(62)-C(61)-P(2)	120.0(6)
C(31)-C(32)-H(32)	119.9	C(63)-C(62)-C(61)	119.9(8)
C(33)-C(32)-H(32)	119.9	C(63)-C(62)-H(62)	120.0
C(34)-C(33)-C(32)	121.3(10)	C(61)-C(62)-H(62)	120.0
C(34)-C(33)-H(33)	119.4	C(64)-C(63)-C(62)	119.7(8)
C(32)-C(33)-H(33)	119.4	C(64)-C(63)-H(63)	120.1
C(33)-C(34)-C(35)	118.7(9)	C(62)-C(63)-H(63)	120.1
C(33)-C(34)-H(34)	120.7	C(63)-C(64)-C(65)	121.5(9)
C(35)-C(34)-H(34)	120.7	C(63)-C(64)-H(64)	119.2
C(34)-C(35)-C(36)	120.8(8)	C(65)-C(64)-H(64)	119.2
C(34)-C(35)-H(35)	119.6	C(66)-C(65)-C(64)	119.2(9)
C(36)-C(35)-H(35)	119.6	C(66)-C(65)-H(65)	120.4
C(35)-C(36)-C(31)	121.5(8)	C(64)-C(65)-H(65)	120.4
C(35)-C(36)-H(36)	119.3	C(61)-C(66)-C(65)	120.8(8)
C(31)-C(36)-H(36)	119.3	C(61)-C(66)-H(66)	119.6
C(61)-P(2)-C(41)	108.5(3)	C(65)-C(66)-H(66)	119.6
C(61)-P(2)-C(2)	109.9(4)	C(82)-C(81)-C(86)	117.5(7)
C(41)-P(2)-C(2)	111.6(4)	C(82)-C(81)-C(2)	120.3(7)
C(61)-P(2)-C(51)	109.6(3)	C(86)-C(81)-C(2)	122.1(7)
C(41)-P(2)-C(51)	105.6(3)	C(81)-C(82)-C(83)	121.2(8)
C(2)-P(2)-C(51)	111.5(3)	C(81)-C(82)-H(82)	119.4

C(83)-C(82)-H(82)	119.4	C(81)-C(86)-C(85)	121.0(8)
C(84)-C(83)-C(82)	121.3(9)	C(81)-C(86)-H(86)	119.5
C(84)-C(83)-H(83)	119.3	C(85)-C(86)-H(86)	119.5
C(82)-C(83)-H(83)	119.3	F(3)-B(1)-F(2)	110.1(9)
C(85)-C(84)-C(83)	117.8(9)	F(3)-B(1)-F(4)	109.4(8)
C(85)-C(84)-H(84)	121.1	F(2)-B(1)-F(4)	110.1(9)
C(83)-C(84)-H(84)	121.1	F(3)-B(1)-F(1)	110.4(9)
C(84)-C(85)-C(86)	121.3(9)	F(2)-B(1)-F(1)	108.4(8)
C(84)-C(85)-H(85)	119.4	F(4)-B(1)-F(1)	108.5(9)
C(86)-C(85)-H(85)	119.4		

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (E)-7. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	38(1)	35(1)	36(1)	0(1)	8(1)	-3(1)
C(70)	64(6)	31(4)	54(5)	2(4)	17(4)	-10(4)
C(71)	71(7)	46(6)	59(6)	9(5)	18(5)	9(5)
C(72)	39(5)	57(6)	50(5)	13(4)	-3(4)	7(4)
C(73)	76(6)	40(5)	38(4)	3(4)	2(4)	6(5)
C(74)	72(6)	45(5)	31(4)	8(4)	17(4)	5(5)
C(75)	99(8)	82(8)	55(6)	13(5)	34(6)	16(7)
C(76)	84(9)	125(11)	78(8)	40(8)	45(7)	22(8)
C(77)	72(8)	84(9)	112(10)	20(7)	21(7)	-22(7)
C(78)	106(9)	51(6)	93(8)	1(5)	29(7)	-13(6)
C(710)	130(10)	53(6)	102(8)	7(6)	44(7)	34(6)
C(720)	40(6)	109(8)	92(7)	18(6)	-16(5)	15(6)
C(730)	117(9)	59(6)	47(5)	-14(5)	-21(5)	-10(6)
C(1)	44(5)	37(5)	34(4)	1(3)	-3(4)	1(4)
C(2)	40(5)	36(5)	51(5)	7(4)	6(4)	-4(4)
C(3)	55(6)	64(6)	51(5)	-8(5)	18(5)	-5(5)
O(3)	102(6)	96(5)	68(4)	-44(4)	11(4)	-22(4)
P(1)	35(1)	42(1)	40(1)	-2(1)	0(1)	-4(1)
C(11)	57(6)	39(5)	41(4)	-7(4)	-2(4)	-10(4)
C(12)	64(7)	81(7)	45(5)	6(5)	2(5)	-18(5)
C(13)	119(10)	86(8)	30(5)	10(5)	4(5)	-22(7)
C(14)	90(9)	61(7)	65(7)	12(5)	-39(6)	-20(6)
C(15)	53(7)	66(7)	76(7)	12(6)	-28(6)	-9(5)
C(16)	62(7)	52(6)	53(5)	2(4)	-16(5)	1(5)
C(21)	21(4)	48(5)	58(5)	-2(4)	-2(4)	-5(4)
C(22)	36(5)	61(6)	62(5)	2(5)	-2(4)	2(4)
C(23)	41(6)	92(8)	62(6)	-5(5)	13(5)	10(5)
C(24)	39(6)	103(9)	75(7)	-4(6)	14(5)	-5(6)
C(25)	40(6)	87(8)	102(8)	-14(6)	17(5)	-17(5)
C(26)	40(5)	79(6)	65(5)	-21(5)	10(4)	-17(5)
C(31)	29(4)	40(5)	50(5)	-4(4)	-8(3)	8(3)
C(32)	100(8)	43(6)	57(6)	-1(5)	-8(5)	-5(5)
C(33)	111(10)	39(6)	93(8)	6(6)	-3(7)	2(6)
C(34)	63(7)	54(6)	85(7)	-26(6)	7(6)	-12(5)
C(35)	60(7)	63(7)	72(6)	-27(6)	-31(5)	10(5)
C(36)	75(6)	49(5)	57(5)	-10(5)	-11(4)	9(6)
P(2)	36(1)	40(1)	41(1)	-1(1)	4(1)	-6(1)
C(41)	45(5)	37(5)	33(4)	-2(3)	0(3)	-4(4)
C(42)	59(6)	52(5)	56(5)	8(4)	14(4)	-14(5)
C(43)	90(8)	62(6)	52(6)	18(5)	12(6)	-13(6)
C(44)	105(9)	49(6)	53(6)	13(5)	-2(6)	-6(6)
C(45)	61(7)	66(7)	72(7)	11(5)	-8(5)	3(5)
C(46)	45(6)	58(5)	51(5)	15(4)	-7(4)	0(4)
C(51)	34(5)	50(5)	34(4)	2(4)	3(3)	-1(4)
C(52)	41(5)	56(5)	56(5)	-7(5)	7(4)	-8(5)
C(53)	51(6)	71(7)	46(5)	-16(5)	-1(4)	-9(5)
C(54)	55(6)	62(7)	75(7)	-34(5)	10(5)	-20(5)
C(55)	52(6)	60(6)	80(7)	-13(5)	10(5)	-6(5)
C(56)	37(5)	51(6)	61(6)	-5(4)	6(4)	-5(4)
C(61)	29(5)	46(5)	46(5)	-1(4)	-1(4)	0(4)
C(62)	60(6)	56(5)	43(5)	-3(4)	10(4)	-1(5)
C(63)	61(7)	74(7)	67(6)	-9(5)	20(5)	14(5)

					18(6)	23(6)
			89(8)	-17(7)		12(6)
C(64)	44(6)	107(9)	89(8)	-23(7)	-3(5)	9(5)
C(65)	33(6)	136(10)	63(6)	-22(5)	1(4)	-10(4)
C(66)	29(5)	102(8)	39(4)	-9(3)	5(4)	10(5)
C(81)	50(5)	41(5)	50(5)	-8(5)	9(5)	7(5)
C(82)	71(7)	59(6)	90(8)	-10(6)	26(6)	-11(6)
C(83)	71(7)	52(6)	71(7)	-27(6)	29(6)	-14(6)
C(84)	85(8)	70(7)	43(6)	-5(5)	10(5)	-13(5)
C(85)	91(8)	81(7)	44(5)	-12(4)	6(5)	9(7)
C(86)	77(7)	55(6)	52(6)	15(6)	22(6)	6(3)
B(1)	62(8)	80(9)	83(4)	21(3)	-6(3)	25(4)
F(1)	69(4)	103(5)	83(4)	5(4)	29(4)	-27(4)
F(2)	89(5)	143(6)	82(4)	-27(4)	25(3)	-14(4)
F(3)	98(5)	107(5)	90(4)	29(3)	6(4)	
F(4)	117(5)	79(4)				

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (E)-7.

	x	y	z	U(eq)
H(75)	990	1699	2736	96(5)
H(76)	-122	672	2717	96(5)
H(77)	-134	-591	2119	96(5)
H(78)	1005	-903	1552	96(5)
H(711)	2409	-1044	1152	96(5)
H(712)	3367	-933	1551	96(5)
H(713)	3121	-461	883	96(5)
H(721)	4264	1546	2024	96(5)
H(722)	4188	979	1394	96(5)
H(723)	4405	527	2071	96(5)
H(731)	3507	2353	2494	96(5)
H(732)	3003	2013	3044	96(5)
H(733)	2534	2680	2530	96(5)
H(1)	2752	2753	1019	96(5)
H(12)	1383	2217	-350	96(5)
H(13)	784	2349	-1430	96(5)
H(14)	-698	2654	-1725	96(5)
H(15)	-1625	2759	-947	96(5)
H(16)	-1030	2644	128	96(5)
H(22)	-366	3207	1720	96(5)
H(23)	-1638	2808	2122	96(5)
H(24)	-2276	1461	1908	96(5)
H(25)	-1678	499	1225	96(5)
H(26)	-404	900	817	96(5)
H(32)	537	4070	251	96(5)
H(33)	963	5471	581	96(5)
H(34)	1648	5737	1613	96(5)
H(35)	1951	4580	2315	96(5)
H(36)	1578	3183	1991	96(5)
H(42)	4499	4299	-797	96(5)
H(43)	3842	5227	-1575	96(5)
H(44)	2300	5451	-1728	96(5)
H(45)	1455	4725	-1079	96(5)
H(46)	2110	3750	-300	96(5)
H(52)	4410	3051	1574	96(5)
H(53)	4527	3982	2482	96(5)
H(54)	4102	5434	2336	96(5)
H(55)	3614	5979	1326	96(5)
H(56)	3536	5078	440	96(5)
H(62)	4629	2599	-843	96(5)
H(63)	6048	2130	-994	96(5)
H(64)	7198	2182	-163	96(5)
H(65)	6998	2719	837	96(5)
H(66)	5604	3216	990	96(5)
H(82)	3949	752	462	96(5)
H(83)	4101	-354	-255	96(5)
H(84)	3585	-187	-1342	96(5)
H(85)	2875	1100	-1688	96(5)
H(86)	2696	2206	-969	96(5)

Table 7. Torsion angles [°] for (E)-7.

C(3)-Ru(1)-C(70)-C(78)	-46.9(8)	C(1)-Ru(1)-C(72)-C(71)	-142.2(5)
C(1)-Ru(1)-C(70)-C(78)	-167.9(7)	C(73)-Ru(1)-C(72)-C(71)	118.2(7)
C(71)-Ru(1)-C(70)-C(78)	-128.5(10)	C(70)-Ru(1)-C(72)-C(71)	38.5(5)
C(72)-Ru(1)-C(70)-C(78)	-166.4(9)	P(1)-Ru(1)-C(72)-C(71)	133.5(5)
C(73)-Ru(1)-C(70)-C(78)	150.8(9)	C(74)-Ru(1)-C(72)-C(71)	79.9(5)
P(1)-Ru(1)-C(70)-C(78)	49.8(8)	C(3)-Ru(1)-C(72)-C(73)	-161.3(5)
C(74)-Ru(1)-C(70)-C(78)	114.5(10)	C(1)-Ru(1)-C(72)-C(73)	99.5(5)
C(3)-Ru(1)-C(70)-C(71)	81.6(6)	C(71)-Ru(1)-C(72)-C(73)	-118.2(7)
C(1)-Ru(1)-C(70)-C(71)	-39.4(8)	C(70)-Ru(1)-C(72)-C(73)	-79.7(5)
C(72)-Ru(1)-C(70)-C(71)	-37.9(5)	P(1)-Ru(1)-C(72)-C(73)	15.3(7)
C(73)-Ru(1)-C(70)-C(71)	-80.7(5)	C(74)-Ru(1)-C(72)-C(73)	-38.3(4)
P(1)-Ru(1)-C(70)-C(71)	178.3(4)	C(3)-Ru(1)-C(72)-C(720)	78.6(9)
C(74)-Ru(1)-C(70)-C(71)	-117.1(8)	C(1)-Ru(1)-C(72)-C(720)	-20.6(8)
C(3)-Ru(1)-C(70)-C(74)	-161.3(5)	C(71)-Ru(1)-C(72)-C(720)	121.6(10)
C(1)-Ru(1)-C(70)-C(74)	77.6(7)	C(73)-Ru(1)-C(72)-C(720)	-120.1(10)
C(71)-Ru(1)-C(70)-C(74)	117.1(8)	C(70)-Ru(1)-C(72)-C(720)	160.2(9)
C(72)-Ru(1)-C(70)-C(74)	79.1(5)	P(1)-Ru(1)-C(72)-C(720)	-104.8(8)
C(73)-Ru(1)-C(70)-C(74)	36.3(5)	C(74)-Ru(1)-C(72)-C(720)	-158.4(9)
P(1)-Ru(1)-C(70)-C(74)	-64.6(5)	C(71)-C(72)-C(73)-C(74)	5.5(9)
C(78)-C(70)-C(71)-C(72)	-171.0(9)	C(720)-C(72)-C(73)-C(74)	-167.8(7)
C(74)-C(70)-C(71)-C(72)	2.7(9)	Ru(1)-C(72)-C(73)-C(74)	67.2(5)
Ru(1)-C(70)-C(71)-C(72)	66.4(6)	C(71)-C(72)-C(73)-C(730)	168.6(7)
C(78)-C(70)-C(71)-C(710)	-1.1(16)	C(720)-C(72)-C(73)-C(730)	-4.6(12)
C(74)-C(70)-C(71)-C(710)	172.6(8)	Ru(1)-C(72)-C(73)-C(730)	-129.7(7)
Ru(1)-C(70)-C(71)-C(710)	-123.7(9)	C(71)-C(72)-C(73)-Ru(1)	-61.7(6)
C(78)-C(70)-C(71)-Ru(1)	122.6(10)	C(720)-C(72)-C(73)-Ru(1)	125.0(8)
C(74)-C(70)-C(71)-Ru(1)	-63.7(6)	C(3)-Ru(1)-C(73)-C(74)	-76.6(8)
C(3)-Ru(1)-C(71)-C(72)	143.5(5)	C(1)-Ru(1)-C(73)-C(74)	163.6(5)
C(1)-Ru(1)-C(71)-C(72)	43.8(6)	C(71)-Ru(1)-C(73)-C(74)	-77.9(5)
C(73)-Ru(1)-C(71)-C(72)	-37.0(5)	C(72)-Ru(1)-C(73)-C(74)	-113.9(7)
C(70)-Ru(1)-C(71)-C(72)	-114.9(7)	C(70)-Ru(1)-C(73)-C(74)	-36.1(5)
P(1)-Ru(1)-C(71)-C(72)	-118.3(6)	P(1)-Ru(1)-C(73)-C(74)	74.7(5)
C(74)-Ru(1)-C(71)-C(72)	-78.3(5)	C(3)-Ru(1)-C(73)-C(72)	37.3(9)
C(3)-Ru(1)-C(71)-C(70)	-101.5(5)	C(1)-Ru(1)-C(73)-C(72)	-82.6(5)
C(1)-Ru(1)-C(71)-C(70)	158.7(5)	C(71)-Ru(1)-C(73)-C(72)	36.0(5)
C(72)-Ru(1)-C(71)-C(70)	114.9(7)	C(70)-Ru(1)-C(73)-C(72)	77.8(5)
C(73)-Ru(1)-C(71)-C(70)	77.9(5)	P(1)-Ru(1)-C(73)-C(72)	-171.4(4)
P(1)-Ru(1)-C(71)-C(70)	-3.4(9)	C(74)-Ru(1)-C(73)-C(72)	113.9(7)
C(74)-Ru(1)-C(71)-C(70)	36.6(5)	C(3)-Ru(1)-C(73)-C(730)	156.3(8)
C(3)-Ru(1)-C(71)-C(710)	19.8(9)	C(1)-Ru(1)-C(73)-C(730)	36.5(9)
C(1)-Ru(1)-C(71)-C(710)	-80.0(9)	C(71)-Ru(1)-C(73)-C(730)	155.1(10)
C(72)-Ru(1)-C(71)-C(710)	-123.8(10)	C(72)-Ru(1)-C(73)-C(730)	119.1(11)
C(73)-Ru(1)-C(71)-C(710)	-160.8(10)	C(70)-Ru(1)-C(73)-C(730)	-163.1(10)
C(70)-Ru(1)-C(71)-C(710)	121.3(11)	P(1)-Ru(1)-C(73)-C(730)	-52.3(9)
P(1)-Ru(1)-C(71)-C(710)	117.9(7)	C(74)-Ru(1)-C(73)-C(730)	-127.0(11)
C(74)-Ru(1)-C(71)-C(710)	157.9(10)	C(72)-C(73)-C(74)-C(75)	170.4(8)
C(70)-C(71)-C(72)-C(73)	-5.1(9)	C(730)-C(73)-C(74)-C(75)	7.9(14)
C(710)-C(71)-C(72)-C(73)	-174.6(8)	Ru(1)-C(73)-C(74)-C(75)	-125.0(9)
Ru(1)-C(71)-C(72)-C(73)	62.4(5)	C(72)-C(73)-C(74)-C(70)	-3.7(8)
C(70)-C(71)-C(72)-C(720)	168.0(8)	C(730)-C(73)-C(74)-C(70)	-166.2(8)
C(710)-C(71)-C(72)-C(720)	-1.4(14)	Ru(1)-C(73)-C(74)-C(70)	60.9(5)
Ru(1)-C(71)-C(72)-C(720)	-124.4(8)	C(72)-C(73)-C(74)-Ru(1)	-64.6(5)
C(70)-C(71)-C(72)-Ru(1)	-67.5(6)	C(730)-C(73)-C(74)-Ru(1)	132.9(8)
C(710)-C(71)-C(72)-Ru(1)	123.0(9)	C(78)-C(70)-C(74)-C(75)	0.5(12)
C(3)-Ru(1)-C(72)-C(71)	-43.0(6)	C(71)-C(70)-C(74)-C(75)	-174.2(7)

Ru(1)-C(70)-C(74)-C(75)	125.2(7)	C(71)-Ru(1)-P(1)-C(21)	0.6(6)
C(78)-C(70)-C(74)-C(73)	175.4(8)	C(72)-Ru(1)-P(1)-C(21)	-78.3(5)
C(71)-C(70)-C(74)-C(73)	0.7(9)	C(73)-Ru(1)-P(1)-C(21)	-68.5(4)
Ru(1)-C(70)-C(74)-C(73)	-59.9(5)	C(70)-Ru(1)-P(1)-C(21)	-1.7(4)
C(78)-C(70)-C(74)-Ru(1)	-124.7(8)	C(74)-Ru(1)-P(1)-C(21)	-33.8(4)
C(71)-C(70)-C(74)-Ru(1)	60.6(6)	C(3)-Ru(1)-P(1)-C(31)	-141.1(4)
C(3)-Ru(1)-C(74)-C(75)	-89.0(9)	C(1)-Ru(1)-P(1)-C(31)	-43.3(3)
C(1)-Ru(1)-C(74)-C(75)	106.1(9)	C(71)-Ru(1)-P(1)-C(31)	120.9(6)
C(71)-Ru(1)-C(74)-C(75)	-151.4(10)	C(72)-Ru(1)-P(1)-C(31)	41.9(5)
C(72)-Ru(1)-C(74)-C(75)	167.0(10)	C(73)-Ru(1)-P(1)-C(31)	51.8(4)
C(73)-Ru(1)-C(74)-C(75)	127.6(11)	C(70)-Ru(1)-P(1)-C(31)	118.6(3)
C(70)-Ru(1)-C(74)-C(75)	-113.9(11)	C(74)-Ru(1)-P(1)-C(31)	86.5(3)
P(1)-Ru(1)-C(74)-C(75)	12.3(9)	C(21)-P(1)-C(11)-C(12)	-159.6(7)
C(3)-Ru(1)-C(74)-C(73)	143.4(5)	C(31)-P(1)-C(11)-C(12)	93.2(7)
C(1)-Ru(1)-C(74)-C(73)	-21.5(6)	Ru(1)-P(1)-C(11)-C(12)	-34.7(8)
C(71)-Ru(1)-C(74)-C(73)	81.0(5)	C(21)-P(1)-C(11)-C(16)	20.8(7)
C(72)-Ru(1)-C(74)-C(73)	39.4(5)	C(31)-P(1)-C(11)-C(16)	-86.4(7)
C(70)-Ru(1)-C(74)-C(73)	118.4(7)	Ru(1)-P(1)-C(11)-C(16)	145.7(6)
P(1)-Ru(1)-C(74)-C(73)	-115.3(5)	C(16)-C(11)-C(12)-C(13)	0.7(12)
C(3)-Ru(1)-C(74)-C(70)	24.9(7)	P(1)-C(11)-C(12)-C(13)	-178.9(7)
C(1)-Ru(1)-C(74)-C(70)	-140.0(5)	C(11)-C(12)-C(13)-C(14)	0.3(14)
C(71)-Ru(1)-C(74)-C(70)	-37.4(5)	C(12)-C(13)-C(14)-C(15)	-1.7(15)
C(72)-Ru(1)-C(74)-C(70)	-79.0(5)	C(13)-C(14)-C(15)-C(16)	2.1(15)
C(73)-Ru(1)-C(74)-C(70)	-118.4(7)	C(14)-C(15)-C(16)-C(11)	-1.0(14)
P(1)-Ru(1)-C(74)-C(70)	126.2(5)	C(12)-C(11)-C(16)-C(15)	-0.3(12)
C(73)-C(74)-C(75)-C(76)	-171.7(9)	P(1)-C(11)-C(16)-C(15)	179.3(7)
C(70)-C(74)-C(75)-C(76)	1.8(13)	C(11)-P(1)-C(21)-C(26)	66.9(7)
Ru(1)-C(74)-C(75)-C(76)	91.3(11)	C(31)-P(1)-C(21)-C(26)	173.3(6)
C(74)-C(75)-C(76)-C(77)	-2.8(16)	Ru(1)-P(1)-C(21)-C(26)	-60.1(7)
C(75)-C(76)-C(77)-C(78)	1.4(18)	C(11)-P(1)-C(21)-C(22)	-109.6(7)
C(76)-C(77)-C(78)-C(70)	1.0(16)	C(31)-P(1)-C(21)-C(22)	-3.2(8)
C(71)-C(70)-C(78)-C(77)	171.2(10)	Ru(1)-P(1)-C(21)-C(22)	123.5(6)
C(74)-C(70)-C(78)-C(77)	-1.9(14)	C(26)-C(21)-C(22)-C(23)	1.4(12)
Ru(1)-C(70)-C(78)-C(77)	-93.2(11)	P(1)-C(21)-C(22)-C(23)	177.9(6)
C(3)-Ru(1)-C(1)-C(2)	-26.0(9)	C(21)-C(22)-C(23)-C(24)	0.3(13)
C(71)-Ru(1)-C(1)-C(2)	70.1(9)	C(22)-C(23)-C(24)-C(25)	-1.8(15)
C(72)-Ru(1)-C(1)-C(2)	93.9(8)	C(23)-C(24)-C(25)-C(26)	1.7(15)
C(73)-Ru(1)-C(1)-C(2)	130.2(8)	C(22)-C(21)-C(26)-C(25)	-1.6(13)
C(70)-Ru(1)-C(1)-C(2)	95.2(9)	P(1)-C(21)-C(26)-C(25)	-178.3(7)
P(1)-Ru(1)-C(1)-C(2)	-117.5(8)	C(24)-C(25)-C(26)-C(21)	0.0(14)
C(74)-Ru(1)-C(1)-C(2)	142.6(8)	C(11)-P(1)-C(31)-C(32)	0.1(8)
Ru(1)-C(1)-C(2)-C(81)	0.5(13)	C(21)-P(1)-C(31)-C(32)	-105.2(7)
Ru(1)-C(1)-C(2)-P(2)	-176.0(5)	Ru(1)-P(1)-C(31)-C(32)	129.0(7)
C(1)-Ru(1)-C(3)-O(3)	153(9)	C(11)-P(1)-C(31)-C(36)	-176.3(6)
C(71)-Ru(1)-C(3)-O(3)	35(9)	C(21)-P(1)-C(31)-C(36)	78.4(7)
C(72)-Ru(1)-C(3)-O(3)	59(9)	Ru(1)-P(1)-C(31)-C(36)	-47.4(7)
C(73)-Ru(1)-C(3)-O(3)	34(9)	C(36)-C(31)-C(32)-C(33)	-0.5(13)
C(70)-Ru(1)-C(3)-O(3)	-1(9)	P(1)-C(31)-C(32)-C(33)	-177.0(7)
P(1)-Ru(1)-C(3)-O(3)	-120(9)	C(31)-C(32)-C(33)-C(34)	-0.9(16)
C(74)-Ru(1)-C(3)-O(3)	-15(9)	C(32)-C(33)-C(34)-C(35)	1.1(16)
C(3)-Ru(1)-P(1)-C(11)	-19.6(4)	C(33)-C(34)-C(35)-C(36)	-0.1(15)
C(1)-Ru(1)-P(1)-C(11)	78.1(4)	C(34)-C(35)-C(36)-C(31)	-1.3(14)
C(71)-Ru(1)-P(1)-C(11)	-117.7(6)	C(32)-C(31)-C(36)-C(35)	1.6(13)
C(72)-Ru(1)-P(1)-C(11)	163.4(5)	P(1)-C(31)-C(36)-C(35)	178.2(7)
C(73)-Ru(1)-P(1)-C(11)	173.2(4)	C(1)-C(2)-P(2)-C(61)	133.2(7)
C(70)-Ru(1)-P(1)-C(11)	-119.9(4)	C(81)-C(2)-P(2)-C(61)	-43.7(7)
C(74)-Ru(1)-P(1)-C(11)	-152.0(4)	C(1)-C(2)-P(2)-C(41)	-106.4(7)
C(3)-Ru(1)-P(1)-C(21)	98.7(4)	C(81)-C(2)-P(2)-C(41)	76.7(6)
C(1)-Ru(1)-P(1)-C(21)	-163.6(3)	C(1)-C(2)-P(2)-C(51)	11.4(8)

C(81)-C(2)-P(2)-C(51)	-165.4(5)	P(2)-C(51)-C(56)-C(55)	179.3(6)
C(61)-P(2)-C(41)-C(42)	-21.8(7)	C(41)-P(2)-C(61)-C(66)	134.8(7)
C(2)-P(2)-C(41)-C(42)	-143.0(6)	C(2)-P(2)-C(61)-C(66)	-103.0(8)
C(51)-P(2)-C(41)-C(42)	95.7(7)	C(51)-P(2)-C(61)-C(66)	19.9(8)
C(61)-P(2)-C(41)-C(46)	161.8(6)	C(41)-P(2)-C(61)-C(62)	-46.1(7)
C(2)-P(2)-C(41)-C(46)	40.5(7)	C(2)-P(2)-C(61)-C(62)	76.2(7)
C(51)-P(2)-C(41)-C(46)	-80.7(6)	C(51)-P(2)-C(61)-C(62)	-161.0(6)
C(46)-C(41)-C(42)-C(43)	2.0(12)	C(66)-C(61)-C(62)-C(63)	1.2(12)
P(2)-C(41)-C(42)-C(43)	-174.5(7)	P(2)-C(61)-C(62)-C(63)	-178.0(6)
C(41)-C(42)-C(43)-C(44)	-0.5(14)	C(61)-C(62)-C(63)-C(64)	0.2(13)
C(42)-C(43)-C(44)-C(45)	-0.1(14)	C(62)-C(63)-C(64)-C(65)	-0.8(16)
C(43)-C(44)-C(45)-C(46)	-0.7(14)	C(63)-C(64)-C(65)-C(66)	0.0(17)
C(44)-C(45)-C(46)-C(41)	2.2(13)	C(62)-C(61)-C(66)-C(65)	-1.9(14)
C(42)-C(41)-C(46)-C(45)	-2.7(12)	P(2)-C(61)-C(66)-C(65)	177.2(8)
P(2)-C(41)-C(46)-C(45)	173.9(6)	C(64)-C(65)-C(66)-C(61)	1.4(16)
C(61)-P(2)-C(51)-C(52)	-67.3(7)	C(1)-C(2)-C(81)-C(82)	-67.7(11)
C(41)-P(2)-C(51)-C(52)	176.0(6)	P(2)-C(2)-C(81)-C(82)	109.0(7)
C(2)-P(2)-C(51)-C(52)	54.7(7)	C(1)-C(2)-C(81)-C(86)	116.1(9)
C(61)-P(2)-C(51)-C(56)	112.2(6)	P(2)-C(2)-C(81)-C(86)	-67.2(9)
C(41)-P(2)-C(51)-C(56)	-4.5(7)	C(86)-C(81)-C(82)-C(83)	-2.2(13)
C(2)-P(2)-C(51)-C(56)	-125.8(6)	C(2)-C(81)-C(82)-C(83)	-178.6(8)
C(56)-C(51)-C(52)-C(53)	0.3(11)	C(81)-C(82)-C(83)-C(84)	1.9(14)
P(2)-C(51)-C(52)-C(53)	179.8(6)	C(82)-C(83)-C(84)-C(85)	-0.7(14)
C(51)-C(52)-C(53)-C(54)	0.8(12)	C(83)-C(84)-C(85)-C(86)	0.1(15)
C(52)-C(53)-C(54)-C(55)	-1.0(13)	C(82)-C(81)-C(86)-C(85)	1.6(12)
C(53)-C(54)-C(55)-C(56)	0.2(13)	C(2)-C(81)-C(86)-C(85)	177.9(8)
C(54)-C(55)-C(56)-C(51)	1.0(13)	C(84)-C(85)-C(86)-C(81)	-0.6(14)
C(52)-C(51)-C(56)-C(55)	-1.2(12)		

Table 8. Crystal data and structure refinement for complex (*EE*)-12b.

Identification code	(<i>EE</i>)-12b
Empirical formula	C ₇₉ H ₆₈ Cl ₄ B F ₄ Fe P ₃ Ru
Formula weight	1495.86
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 2 ₁ /n
Unit cell dimensions	a = 16.212(10) Å b = 23.551(16) Å c = 18.143(9) Å β = 94.39(6)°
Volume	6907(7) Å ³
Z	4
Density (calculated)	1.436 Mg/m ³
Absorption coefficient	0.708 mm ⁻¹
F(000)	3052
Crystal size	0.36 x 0.33 x 0.2 mm ³
Theta range for data collection	1.42 to 25.97°
Index ranges	-19 ≤ h ≤ 19, 0 ≤ k ≤ 29, 0 ≤ l ≤ 22
Reflections collected	13961
Independent reflections	13526 [R(int) = 0.0522]
Completeness to theta = 25.97°	99.9 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	13526 / 3 / 778
Goodness-of-fit on F ²	1.023
Final R indices [I > 2σ(I)]	R1 = 0.0873, wR2 = 0.2114
R indices (all data)	R1 = 0.1799, wR2 = 0.2661
Largest diff. peak and hole	0.986 and -0.962 e.Å ⁻³

Table 9. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for complex (EE)-12b. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	388(1)	1227(1)	3287(1)	32(1)
Fe(1)	-2297(1)	3739(1)	3646(1)	49(1)
C(70)	-354(6)	514(4)	3956(5)	43(2)
C(71)	51(5)	965(4)	4399(5)	41(2)
C(72)	-361(5)	1481(4)	4207(4)	39(2)
C(73)	-934(5)	1379(4)	3594(5)	44(2)
C(74)	-962(5)	776(4)	3455(5)	42(2)
C(75)	-1515(6)	441(4)	3015(5)	50(2)
C(76)	-1466(7)	-127(5)	3099(6)	63(3)
C(77)	-833(7)	-401(4)	3564(6)	56(3)
C(78)	-294(6)	-72(4)	3978(5)	49(2)
C(1)	891(5)	2019(3)	3248(4)	35(2)
C(2)	568(5)	2549(3)	3245(4)	35(2)
C(3)	-322(5)	2686(4)	3259(5)	42(2)
C(4)	-742(6)	3149(4)	3036(5)	45(2)
C(81)	-1642(6)	3185(4)	3056(5)	46(2)
C(82)	-2181(6)	3517(4)	2586(6)	53(2)
C(83)	-2996(7)	3419(5)	2768(7)	65(3)
C(84)	-2982(6)	3035(5)	3357(7)	69(3)
C(85)	-2155(6)	2884(4)	3542(6)	54(3)
C(91)	-1464(9)	4275(7)	4166(9)	93(5)
C(92)	-2068(10)	4583(5)	3768(7)	77(4)
C(93)	-2828(9)	4455(6)	4018(9)	90(4)
C(94)	-2732(15)	4059(8)	4570(11)	126(7)
C(95)	-1876(17)	3945(8)	4679(9)	128(7)
P(1)	249(1)	1195(1)	1993(1)	38(1)
C(11)	804(6)	1676(4)	1396(5)	43(2)
C(12)	1608(6)	1838(4)	1599(6)	48(2)
C(13)	2056(7)	2161(5)	1119(6)	60(3)
C(14)	1689(7)	2325(5)	444(6)	65(3)
C(15)	891(8)	2187(5)	253(6)	76(4)
C(16)	444(7)	1853(5)	713(5)	63(3)
C(21)	-822(5)	1340(4)	1645(5)	41(2)
C(22)	-1179(6)	1845(4)	1841(5)	50(2)
C(23)	-1970(7)	1976(5)	1601(6)	63(3)
C(24)	-2448(7)	1603(5)	1167(6)	67(3)
C(25)	-2104(7)	1118(5)	951(6)	70(3)
C(26)	-1294(6)	972(4)	1182(5)	53(2)
C(31)	446(6)	506(4)	1558(5)	41(2)
C(32)	113(7)	31(4)	1869(6)	63(3)
C(33)	253(8)	-515(5)	1585(7)	77(3)
C(34)	714(9)	-556(5)	981(7)	85(4)
C(35)	1022(10)	-93(5)	671(7)	100(5)
C(36)	911(8)	439(4)	965(6)	68(3)
P(2)	1704(1)	866(1)	3561(1)	37(1)
C(41)	2285(6)	1190(4)	4349(5)	45(2)
C(42)	3094(6)	1020(5)	4545(6)	55(3)
C(43)	3545(8)	1236(5)	5163(6)	75(3)
C(44)	3166(8)	1612(6)	5614(6)	77(4)
C(45)	2358(7)	1792(5)	5444(6)	65(3)
C(46)	1924(6)	1573(4)	4815(5)	49(2)
C(51)	1708(5)	117(4)	3858(5)	44(2)
C(52)	1916(6)	-40(4)	4579(5)	53(3)

C(53)	1867(7)	-608(6)	4804(7)	70(3)
C(54)	1614(8)	-1013(5)	4304(8)	79(4)
C(55)	1372(8)	-866(5)	3580(7)	71(3)
C(56)	1433(6)	-302(4)	3376(6)	52(2)
C(61)	2504(6)	897(4)	2879(5)	45(2)
C(62)	2489(7)	514(5)	2299(6)	60(3)
C(63)	3024(8)	574(5)	1752(6)	73(3)
C(64)	3597(7)	1019(6)	1781(7)	76(4)
C(65)	3624(7)	1399(6)	2363(7)	74(3)
C(66)	3064(6)	1338(4)	2890(6)	54(3)
P(3)	1229(2)	3155(1)	3241(1)	40(1)
C(101)	2304(6)	2987(4)	3416(5)	48(2)
C(102)	2628(7)	2894(5)	4140(6)	68(3)
C(103)	3460(8)	2780(6)	4281(7)	82(4)
C(104)	3968(8)	2763(6)	3704(10)	91(4)
C(105)	3660(8)	2858(5)	2993(9)	83(4)
C(106)	2819(6)	2959(5)	2845(6)	57(3)
C(111)	1131(6)	3502(4)	2347(6)	51(2)
C(112)	1581(7)	3987(5)	2208(6)	67(3)
C(113)	1500(8)	4218(6)	1506(7)	83(4)
C(114)	1027(8)	3970(6)	942(7)	78(4)
C(115)	604(7)	3481(6)	1072(6)	72(3)
C(116)	652(7)	3237(4)	1773(5)	55(3)
C(121)	973(6)	3624(4)	3963(5)	47(2)
C(122)	685(6)	3393(4)	4596(5)	53(2)
C(123)	525(7)	3728(5)	5208(6)	66(3)
C(124)	668(7)	4301(5)	5181(7)	67(3)
C(125)	929(9)	4536(5)	4551(7)	86(4)
C(126)	1072(9)	4216(4)	3940(7)	83(4)
B(1)	96(5)	2306(3)	6265(5)	157(10)
F(1)	132(8)	1871(4)	6742(6)	215(6)
F(2)	-736(6)	2411(6)	6035(8)	291(9)
F(3)	413(8)	2272(5)	5644(5)	184(9)
F(4)	119(10)	2800(4)	6605(7)	194(10)
F(5)	913(7)	2595(6)	6364(8)	147(16)
C(20)	6204(7)	1698(3)	2863(4)	201(11)
Cl(21)	6187(7)	1064(4)	2384(4)	304(5)
Cl(22)	6082(8)	1670(3)	3770(4)	143(3)
Cl(23)	6763(7)	1503(5)	3698(5)	143(3)
Cl(24)	5344(8)	1623(4)	3798(5)	143(3)
C(30)	5040(20)	-291(11)	6845(10)	308(19)
Cl(31)	4672(9)	-179(6)	5861(7)	362(7)
Cl(32)	4573(10)	213(9)	7394(10)	181(4)
Cl(33)	4395(10)	349(6)	7067(11)	181(4)
Cl(34)	3919(6)	16(11)	6401(11)	181(4)

Table 10. Selected bond lengths [Å] and angles [°] for complex (EE)-12b.

Ru(1)-C*	1.986(1)
Δ	0.205(1)
C(1)-Ru(1)-C*	123.7(2)
P(1)-Ru(1)-C*	123.78(6)
P(2)-Ru(1)-C*	119.47(8)
FA	14.8(6)
HA	7.4(7)
DA	100.7(6)
CA	144.0(1)

^a $\Delta = d[\text{Ru}(1)-\text{C}(74), \text{C}(70)] - d[\text{Ru}(1)-\text{C}(71), \text{C}(73)]$.

^bFA(fold angle) = angle between normals to least-squares planes defined by C(71), C(72), C(73) and C(70), C(74), C(75), C(76), C(77), C(78).

^cHA(hinge angle) = angle between normals to least-squares planes defined by C(71), C(72), C(73) and C(71), C(74), C(70), C(73).

^dDA(dihedral angle) = angle between normals to least-squares planes defined by C*, Ru(1), C(1) and Ru(1), C(1), C(2), C(3).

^eCA(conformational angle) = angle between normals to least-squares planes defined by C**, C*, Ru(1) and C*, Ru(1), C(1).

C* = centroid of C(70), C(71), C(72), C(73), C(74).

C** = centroid of C(70), C(74), C(75), C(76), C(77), C(78).

Table 11. Bond lengths [Å] and angles [°] for complex (EE)-12b.

Ru(1)-C(1)	2.039(8)	C(93)-C(94)	1.37(2)
Ru(1)-C(71)	2.219(9)	C(93)-H(93)	0.9300
Ru(1)-C(72)	2.220(8)	C(94)-C(95)	1.41(2)
Ru(1)-C(73)	2.283(9)	C(94)-H(94)	0.9300
Ru(1)-P(2)	2.315(3)	C(95)-H(95)	0.9300
Ru(1)-P(1)	2.341(2)	P(1)-C(21)	1.833(9)
Ru(1)-C(70)	2.441(8)	P(1)-C(31)	1.844(9)
Ru(1)-C(74)	2.472(9)	P(1)-C(11)	1.848(9)
Fe(1)-C(95)	2.004(14)	C(11)-C(12)	1.381(13)
Fe(1)-C(94)	2.014(13)	C(11)-C(16)	1.392(12)
Fe(1)-C(82)	2.015(10)	C(12)-C(13)	1.403(13)
Fe(1)-C(91)	2.026(13)	C(12)-H(12)	0.9300
Fe(1)-C(83)	2.029(11)	C(13)-C(14)	1.376(14)
Fe(1)-C(92)	2.031(12)	C(13)-H(13)	0.9300
Fe(1)-C(93)	2.031(12)	C(14)-C(15)	1.353(15)
Fe(1)-C(81)	2.037(9)	C(14)-H(14)	0.9300
Fe(1)-C(85)	2.038(9)	C(15)-C(16)	1.388(14)
Fe(1)-C(84)	2.042(11)	C(15)-H(15)	0.9300
C(70)-C(78)	1.384(12)	C(16)-H(16)	0.9300
C(70)-C(74)	1.429(12)	C(21)-C(22)	1.383(12)
C(70)-C(71)	1.457(12)	C(21)-C(26)	1.395(12)
C(71)-C(72)	1.416(12)	C(22)-C(23)	1.357(13)
C(71)-H(71)	0.9300	C(22)-H(22)	0.9300
C(72)-C(73)	1.415(12)	C(23)-C(24)	1.379(15)
C(72)-H(72)	0.9300	C(23)-H(23)	0.9300
C(73)-C(74)	1.441(12)	C(24)-C(25)	1.343(15)
C(73)-H(73)	0.9300	C(24)-H(24)	0.9300
C(74)-C(75)	1.398(12)	C(25)-C(26)	1.392(14)
C(75)-C(76)	1.348(14)	C(25)-H(25)	0.9300
C(75)-H(75)	0.9300	C(26)-H(26)	0.9300
C(76)-C(77)	1.431(14)	C(31)-C(36)	1.369(13)
C(76)-H(76)	0.9300	C(31)-C(32)	1.381(13)
C(77)-C(78)	1.352(13)	C(32)-C(33)	1.410(15)
C(77)-H(77)	0.9300	C(32)-H(32)	0.9300
C(78)-H(78)	0.9300	C(33)-C(34)	1.376(16)
C(1)-C(2)	1.354(11)	C(33)-H(33)	0.9300
C(1)-H(1)	0.9300	C(34)-C(35)	1.341(17)
C(2)-C(3)	1.481(11)	C(34)-H(34)	0.9300
C(2)-P(3)	1.783(8)	C(35)-C(36)	1.379(15)
C(3)-C(4)	1.334(12)	C(35)-H(35)	0.9300
C(3)-H(3)	0.9300	C(36)-H(36)	0.9300
C(4)-C(81)	1.465(13)	P(2)-C(41)	1.818(9)
C(4)-H(4)	0.9300	P(2)-C(51)	1.845(9)
C(81)-C(82)	1.409(13)	P(2)-C(61)	1.861(9)
C(81)-C(85)	1.443(13)	C(41)-C(42)	1.391(13)
C(82)-C(83)	1.407(14)	C(41)-C(46)	1.397(13)
C(82)-H(82)	0.9300	C(42)-C(43)	1.386(14)
C(83)-C(84)	1.398(16)	C(42)-H(42)	0.9300
C(83)-H(83)	0.9300	C(43)-C(44)	1.382(16)
C(84)-C(85)	1.403(14)	C(43)-H(43)	0.9300
C(84)-H(84)	0.9300	C(44)-C(45)	1.388(15)
C(85)-H(85)	0.9300	C(44)-H(44)	0.9300
C(91)-C(92)	1.378(18)	C(45)-C(46)	1.392(13)
C(91)-C(95)	1.42(2)	C(45)-H(45)	0.9300
C(91)-H(91)	0.9300	C(46)-H(46)	0.9300
C(92)-C(93)	1.378(18)	C(51)-C(56)	1.370(13)
C(92)-H(92)	0.9300	C(51)-C(52)	1.377(13)

C(52)-C(53)	1.402(15)	C(113)-H(113)	0.9300
C(52)-H(52)	0.9300	C(114)-C(115)	1.371(17)
C(53)-C(54)	1.360(17)	C(114)-H(114)	0.9300
C(53)-H(53)	0.9300	C(115)-C(116)	1.392(14)
C(54)-C(55)	1.385(17)	C(115)-H(115)	0.9300
C(54)-H(54)	0.9300	C(116)-H(116)	0.9300
C(55)-C(56)	1.386(14)	C(121)-C(122)	1.384(13)
C(55)-H(55)	0.9300	C(121)-C(126)	1.406(13)
C(56)-H(56)	0.9300	C(122)-C(123)	1.402(13)
C(61)-C(66)	1.381(13)	C(122)-H(122)	0.9300
C(61)-C(62)	1.385(13)	C(123)-C(124)	1.370(15)
C(62)-C(63)	1.373(14)	C(123)-H(123)	0.9300
C(62)-H(62)	0.9300	C(124)-C(125)	1.365(16)
C(63)-C(64)	1.397(17)	C(124)-H(124)	0.9300
C(63)-H(63)	0.9300	C(125)-C(126)	1.375(15)
C(64)-C(65)	1.383(17)	C(125)-H(125)	0.9300
C(64)-H(64)	0.9300	C(126)-H(126)	0.9300
C(65)-C(66)	1.374(14)	B(1)-F(3)	1.2768
C(65)-H(65)	0.9300	B(1)-F(4)	1.3163
C(66)-H(66)	0.9300	B(1)-F(1)	1.3392
P(3)-C(121)	1.787(9)	B(1)-F(2)	1.4034
P(3)-C(101)	1.792(10)	B(1)-F(5)	1.4881
P(3)-C(111)	1.812(10)	F(3)-F(5)	1.6663
C(101)-C(106)	1.382(13)	F(4)-F(5)	1.4715
C(101)-C(102)	1.394(13)	C(20)-Cl(22)	1.6742
C(102)-C(103)	1.380(16)	C(20)-Cl(21)	1.7271
C(102)-H(102)	0.9300	C(20)-Cl(23)	1.7666
C(103)-C(104)	1.381(18)	Cl(22)-Cl(23)	1.1880
C(103)-H(103)	0.9300	Cl(22)-Cl(24)	1.2070
C(104)-C(105)	1.366(18)	Cl(23)-Cl(24)	2.3385
C(104)-H(104)	0.9300	C(30)-Cl(32)	1.76(3)
C(105)-C(106)	1.390(15)	C(30)-Cl(31)	1.86(2)
C(105)-H(105)	0.9300	C(30)-Cl(33)	1.89(3)
C(106)-H(106)	0.9300	C(30)-Cl(34)	2.06(4)
C(111)-C(112)	1.390(14)	Cl(31)-Cl(34)	1.6845
C(111)-C(116)	1.396(14)	Cl(32)-Cl(33)	0.7149
C(112)-C(113)	1.382(15)	Cl(32)-Cl(34)	2.0715
C(112)-H(112)	0.9300	Cl(33)-Cl(34)	1.5903
C(113)-C(114)	1.363(17)		
C(1)-Ru(1)-C(71)	114.4(3)	P(2)-Ru(1)-C(70)	97.0(2)
C(1)-Ru(1)-C(72)	91.3(3)	P(1)-Ru(1)-C(70)	117.6(2)
C(71)-Ru(1)-C(72)	37.2(3)	C(1)-Ru(1)-C(74)	139.2(3)
C(1)-Ru(1)-C(73)	104.5(3)	C(71)-Ru(1)-C(74)	59.1(3)
C(71)-Ru(1)-C(73)	61.4(3)	C(72)-Ru(1)-C(74)	58.8(3)
C(72)-Ru(1)-C(73)	36.6(3)	C(73)-Ru(1)-C(74)	35.0(3)
C(1)-Ru(1)-P(2)	88.8(3)	P(2)-Ru(1)-C(74)	128.7(2)
C(71)-Ru(1)-P(2)	89.4(2)	P(1)-Ru(1)-C(74)	95.3(2)
C(72)-Ru(1)-P(2)	119.0(2)	C(70)-Ru(1)-C(74)	33.8(3)
C(73)-Ru(1)-P(2)	150.7(2)	C(95)-Fe(1)-C(94)	41.2(7)
C(1)-Ru(1)-P(1)	90.1(2)	C(95)-Fe(1)-C(82)	154.8(8)
C(71)-Ru(1)-P(1)	153.1(2)	C(94)-Fe(1)-C(82)	162.8(8)
C(72)-Ru(1)-P(1)	138.3(2)	C(95)-Fe(1)-C(91)	41.2(7)
C(73)-Ru(1)-P(1)	103.3(2)	C(94)-Fe(1)-C(91)	69.1(7)
P(2)-Ru(1)-P(1)	102.70(10)	C(82)-Fe(1)-C(91)	119.9(6)
C(1)-Ru(1)-C(70)	149.3(3)	C(95)-Fe(1)-C(83)	162.5(9)
C(71)-Ru(1)-C(70)	36.0(3)	C(94)-Fe(1)-C(83)	125.6(8)
C(72)-Ru(1)-C(70)	59.5(3)	C(82)-Fe(1)-C(83)	40.7(4)
C(73)-Ru(1)-C(70)	58.6(3)	C(91)-Fe(1)-C(83)	155.4(7)

C(95)-Fe(1)-C(92)	67.4(7)	C(75)-C(74)-C(70)	120.0(8)
C(94)-Fe(1)-C(92)	67.4(6)	C(75)-C(74)-C(73)	131.8(9)
C(82)-Fe(1)-C(92)	109.2(5)	C(70)-C(74)-C(73)	107.7(8)
C(91)-Fe(1)-C(92)	39.7(5)	C(75)-C(74)-Ru(1)	135.0(6)
C(83)-Fe(1)-C(92)	122.4(5)	C(70)-C(74)-Ru(1)	71.9(5)
C(95)-Fe(1)-C(93)	67.1(7)	C(73)-C(74)-Ru(1)	65.3(5)
C(94)-Fe(1)-C(93)	39.5(6)	C(76)-C(75)-C(74)	117.9(10)
C(82)-Fe(1)-C(93)	127.2(6)	C(76)-C(75)-H(75)	121.1
C(91)-Fe(1)-C(93)	67.2(6)	C(74)-C(75)-H(75)	121.1
C(83)-Fe(1)-C(93)	110.1(5)	C(75)-C(76)-C(77)	123.1(10)
C(92)-Fe(1)-C(93)	39.7(5)	C(75)-C(76)-H(76)	118.5
C(95)-Fe(1)-C(81)	119.5(7)	C(77)-C(76)-H(76)	118.5
C(94)-Fe(1)-C(81)	155.1(8)	C(78)-C(77)-C(76)	118.3(9)
C(82)-Fe(1)-C(81)	40.7(4)	C(78)-C(77)-H(77)	120.9
C(91)-Fe(1)-C(81)	106.8(5)	C(76)-C(77)-H(77)	120.9
C(83)-Fe(1)-C(81)	68.4(4)	C(77)-C(78)-C(70)	120.9(10)
C(92)-Fe(1)-C(81)	125.9(5)	C(77)-C(78)-H(78)	119.5
C(93)-Fe(1)-C(81)	163.2(6)	C(70)-C(78)-H(78)	119.5
C(95)-Fe(1)-C(85)	107.0(6)	C(2)-C(1)-Ru(1)	133.5(7)
C(94)-Fe(1)-C(85)	119.8(7)	C(2)-C(1)-H(1)	113.2
C(82)-Fe(1)-C(85)	68.7(4)	Ru(1)-C(1)-H(1)	113.2
C(91)-Fe(1)-C(85)	125.6(6)	C(1)-C(2)-C(3)	125.2(7)
C(83)-Fe(1)-C(85)	67.6(4)	C(1)-C(2)-P(3)	120.4(6)
C(92)-Fe(1)-C(85)	163.1(5)	C(3)-C(2)-P(3)	114.4(6)
C(93)-Fe(1)-C(85)	154.8(6)	C(4)-C(3)-C(2)	130.4(8)
C(81)-Fe(1)-C(85)	41.5(4)	C(4)-C(3)-H(3)	114.8
C(95)-Fe(1)-C(84)	125.1(8)	C(2)-C(3)-H(3)	114.8
C(94)-Fe(1)-C(84)	107.4(6)	C(3)-C(4)-C(81)	121.7(9)
C(82)-Fe(1)-C(84)	68.5(5)	C(3)-C(4)-H(4)	119.2
C(91)-Fe(1)-C(84)	162.7(7)	C(81)-C(4)-H(4)	119.2
C(83)-Fe(1)-C(84)	40.2(5)	C(82)-C(81)-C(85)	106.5(9)
C(92)-Fe(1)-C(84)	156.0(6)	C(82)-C(81)-C(4)	126.0(9)
C(93)-Fe(1)-C(84)	121.5(5)	C(85)-C(81)-C(4)	127.4(9)
C(81)-Fe(1)-C(84)	68.9(4)	C(82)-C(81)-Fe(1)	68.8(5)
C(85)-Fe(1)-C(84)	40.2(4)	C(85)-C(81)-Fe(1)	69.3(5)
C(78)-C(70)-C(74)	119.5(9)	C(4)-C(81)-Fe(1)	127.6(7)
C(78)-C(70)-C(71)	133.1(9)	C(83)-C(82)-C(81)	108.4(10)
C(74)-C(70)-C(71)	107.2(8)	C(83)-C(82)-Fe(1)	70.2(6)
C(78)-C(70)-Ru(1)	131.6(7)	C(81)-C(82)-Fe(1)	70.5(5)
C(74)-C(70)-Ru(1)	74.3(5)	C(83)-C(82)-H(82)	125.8
C(71)-C(70)-Ru(1)	63.6(5)	C(81)-C(82)-H(82)	125.8
C(72)-C(71)-C(70)	107.7(8)	Fe(1)-C(82)-H(82)	125.1
C(72)-C(71)-Ru(1)	71.4(5)	C(84)-C(83)-C(82)	109.0(10)
C(70)-C(71)-Ru(1)	80.3(5)	C(84)-C(83)-Fe(1)	70.4(7)
C(72)-C(71)-H(71)	126.1	C(82)-C(83)-Fe(1)	69.1(6)
C(70)-C(71)-H(71)	126.1	C(84)-C(83)-H(83)	125.5
Ru(1)-C(71)-H(71)	114.4	C(82)-C(83)-H(83)	125.5
C(73)-C(72)-C(71)	108.5(8)	Fe(1)-C(83)-H(83)	126.5
C(73)-C(72)-Ru(1)	74.1(5)	C(83)-C(84)-C(85)	107.8(9)
C(71)-C(72)-Ru(1)	71.4(5)	C(83)-C(84)-Fe(1)	69.4(6)
C(73)-C(72)-H(72)	125.8	C(85)-C(84)-Fe(1)	69.7(6)
C(71)-C(72)-H(72)	125.8	C(83)-C(84)-H(84)	126.1
Ru(1)-C(72)-H(72)	120.5	C(85)-C(84)-H(84)	126.1
C(72)-C(73)-C(74)	108.3(8)	Fe(1)-C(84)-H(84)	126.4
C(72)-C(73)-Ru(1)	69.3(5)	C(84)-C(85)-C(81)	108.3(9)
C(74)-C(73)-Ru(1)	79.7(5)	C(84)-C(85)-Fe(1)	70.0(6)
C(72)-C(73)-H(73)	125.8	C(81)-C(85)-Fe(1)	69.2(5)
C(74)-C(73)-H(73)	125.8	C(84)-C(85)-H(85)	125.9
Ru(1)-C(73)-H(73)	117.1	C(81)-C(85)-H(85)	125.9

Fe(1)-C(85)-H(85)	126.5	C(23)-C(22)-H(22)	119.4
C(92)-C(91)-C(95)	106.3(15)	C(21)-C(22)-H(22)	119.4
C(92)-C(91)-Fe(1)	70.3(8)	C(22)-C(23)-C(24)	121.0(11)
C(95)-C(91)-Fe(1)	68.6(9)	C(22)-C(23)-H(23)	119.5
C(92)-C(91)-H(91)	126.8	C(24)-C(23)-H(23)	119.5
C(95)-C(91)-H(91)	126.8	C(25)-C(24)-C(23)	118.7(10)
Fe(1)-C(91)-H(91)	125.9	C(25)-C(24)-H(24)	120.6
C(93)-C(92)-C(91)	109.2(14)	C(23)-C(24)-H(24)	120.6
C(93)-C(92)-Fe(1)	70.2(7)	C(24)-C(25)-C(26)	121.8(10)
C(91)-C(92)-Fe(1)	70.0(7)	C(24)-C(25)-H(25)	119.1
C(93)-C(92)-H(92)	125.4	C(26)-C(25)-H(25)	119.1
C(91)-C(92)-H(92)	125.4	C(25)-C(26)-C(21)	119.3(10)
Fe(1)-C(92)-H(92)	126.0	C(25)-C(26)-H(26)	120.3
C(94)-C(93)-C(92)	109.7(15)	C(21)-C(26)-H(26)	120.3
C(94)-C(93)-Fe(1)	69.6(8)	C(36)-C(31)-C(32)	118.9(9)
C(92)-C(93)-Fe(1)	70.2(7)	C(36)-C(31)-P(1)	124.2(7)
C(94)-C(93)-H(93)	125.2	C(32)-C(31)-P(1)	116.9(7)
C(92)-C(93)-H(93)	125.2	C(31)-C(32)-C(33)	120.6(10)
Fe(1)-C(93)-H(93)	126.7	C(31)-C(32)-H(32)	119.7
C(93)-C(94)-C(95)	106.7(17)	C(33)-C(32)-H(32)	119.7
C(93)-C(94)-Fe(1)	70.9(8)	C(34)-C(33)-C(32)	117.9(11)
C(95)-C(94)-Fe(1)	69.0(8)	C(34)-C(33)-H(33)	121.1
C(93)-C(94)-H(94)	126.7	C(32)-C(33)-H(33)	121.1
C(95)-C(94)-H(94)	126.7	C(35)-C(34)-C(33)	121.3(12)
Fe(1)-C(94)-H(94)	125.0	C(35)-C(34)-H(34)	119.3
C(94)-C(95)-C(91)	108.1(17)	C(33)-C(34)-H(34)	119.3
C(94)-C(95)-Fe(1)	69.8(9)	C(34)-C(35)-C(36)	120.7(12)
C(91)-C(95)-Fe(1)	70.3(8)	C(34)-C(35)-H(35)	119.6
C(94)-C(95)-H(95)	125.9	C(36)-C(35)-H(35)	119.6
C(91)-C(95)-H(95)	125.9	C(31)-C(36)-C(35)	120.4(10)
Fe(1)-C(95)-H(95)	125.6	C(31)-C(36)-H(36)	119.8
C(21)-P(1)-C(31)	101.9(4)	C(35)-C(36)-H(36)	119.8
C(21)-P(1)-C(11)	100.1(4)	C(41)-P(2)-C(51)	100.4(4)
C(31)-P(1)-C(11)	100.4(4)	C(41)-P(2)-C(61)	99.3(4)
C(21)-P(1)-Ru(1)	110.8(3)	C(51)-P(2)-C(61)	104.1(4)
C(31)-P(1)-Ru(1)	116.8(3)	C(41)-P(2)-Ru(1)	115.4(3)
C(11)-P(1)-Ru(1)	123.7(3)	C(51)-P(2)-Ru(1)	113.4(3)
C(12)-C(11)-C(16)	118.6(9)	C(61)-P(2)-Ru(1)	121.4(3)
C(12)-C(11)-P(1)	120.2(7)	C(42)-C(41)-C(46)	117.5(9)
C(16)-C(11)-P(1)	121.1(7)	C(42)-C(41)-P(2)	120.2(7)
C(11)-C(12)-C(13)	120.4(9)	C(46)-C(41)-P(2)	122.1(7)
C(11)-C(12)-H(12)	119.8	C(43)-C(42)-C(41)	121.9(10)
C(13)-C(12)-H(12)	119.8	C(43)-C(42)-H(42)	119.0
C(14)-C(13)-C(12)	119.7(10)	C(41)-C(42)-H(42)	119.0
C(14)-C(13)-H(13)	120.1	C(44)-C(43)-C(42)	118.9(11)
C(12)-C(13)-H(13)	120.1	C(44)-C(43)-H(43)	120.6
C(15)-C(14)-C(13)	120.0(10)	C(42)-C(43)-H(43)	120.6
C(15)-C(14)-H(14)	120.0	C(43)-C(44)-C(45)	121.3(11)
C(13)-C(14)-H(14)	120.0	C(43)-C(44)-H(44)	119.3
C(14)-C(15)-C(16)	121.0(10)	C(45)-C(44)-H(44)	119.3
C(14)-C(15)-H(15)	119.5	C(44)-C(45)-C(46)	118.5(11)
C(16)-C(15)-H(15)	119.5	C(44)-C(45)-H(45)	120.7
C(15)-C(16)-C(11)	120.1(10)	C(46)-C(45)-H(45)	120.7
C(15)-C(16)-H(16)	119.9	C(45)-C(46)-C(41)	121.8(9)
C(11)-C(16)-H(16)	119.9	C(45)-C(46)-H(46)	119.1
C(22)-C(21)-C(26)	118.0(9)	C(41)-C(46)-H(46)	119.1
C(22)-C(21)-P(1)	118.4(7)	C(56)-C(51)-C(52)	117.2(9)
C(26)-C(21)-P(1)	123.6(7)	C(56)-C(51)-P(2)	120.6(7)
C(23)-C(22)-C(21)	121.1(9)	C(52)-C(51)-P(2)	122.0(8)

C(51)-C(52)-C(53)	121.2(11)	C(116)-C(111)-P(3)	118.1(8)
C(51)-C(52)-H(52)	119.4	C(113)-C(112)-C(111)	118.5(11)
C(53)-C(52)-H(52)	119.4	C(113)-C(112)-H(112)	120.7
C(54)-C(53)-C(52)	119.8(11)	C(111)-C(112)-H(112)	120.7
C(54)-C(53)-H(53)	120.1	C(114)-C(113)-C(112)	122.1(12)
C(52)-C(53)-H(53)	120.1	C(114)-C(113)-H(113)	119.0
C(53)-C(54)-C(55)	120.4(11)	C(112)-C(113)-H(113)	119.0
C(53)-C(54)-H(54)	119.8	C(113)-C(114)-C(115)	119.5(12)
C(55)-C(54)-H(54)	119.8	C(113)-C(114)-H(114)	120.3
C(54)-C(55)-C(56)	118.2(12)	C(115)-C(114)-H(114)	120.3
C(54)-C(55)-H(55)	120.9	C(114)-C(115)-C(116)	120.7(12)
C(56)-C(55)-H(55)	120.9	C(114)-C(115)-H(115)	119.7
C(51)-C(56)-C(55)	123.1(10)	C(116)-C(115)-H(115)	119.7
C(51)-C(56)-H(56)	118.4	C(115)-C(116)-C(111)	119.1(10)
C(55)-C(56)-H(56)	118.4	C(115)-C(116)-H(116)	120.5
C(66)-C(61)-C(62)	118.3(9)	C(111)-C(116)-H(116)	120.5
C(66)-C(61)-P(2)	120.7(7)	C(122)-C(121)-C(126)	117.5(9)
C(62)-C(61)-P(2)	120.6(8)	C(122)-C(121)-P(3)	118.6(7)
C(63)-C(62)-C(61)	120.5(11)	C(126)-C(121)-P(3)	123.9(8)
C(63)-C(62)-H(62)	119.8	C(121)-C(122)-C(123)	122.0(10)
C(61)-C(62)-H(62)	119.8	C(121)-C(122)-H(122)	119.0
C(62)-C(63)-C(64)	120.3(12)	C(123)-C(122)-H(122)	119.0
C(62)-C(63)-H(63)	119.9	C(124)-C(123)-C(122)	118.9(10)
C(64)-C(63)-H(63)	119.9	C(124)-C(123)-H(123)	120.5
C(65)-C(64)-C(63)	119.7(11)	C(122)-C(123)-H(123)	120.5
C(65)-C(64)-H(64)	120.1	C(125)-C(124)-C(123)	119.6(10)
C(63)-C(64)-H(64)	120.1	C(125)-C(124)-H(124)	120.2
C(66)-C(65)-C(64)	118.7(11)	C(123)-C(124)-H(124)	120.2
C(66)-C(65)-H(65)	120.7	C(124)-C(125)-C(126)	122.3(11)
C(64)-C(65)-H(65)	120.7	C(124)-C(125)-H(125)	118.8
C(65)-C(66)-C(61)	122.5(11)	C(126)-C(125)-H(125)	118.8
C(65)-C(66)-H(66)	118.8	C(125)-C(126)-C(121)	119.5(11)
C(61)-C(66)-H(66)	118.8	C(125)-C(126)-H(126)	120.3
C(2)-P(3)-C(121)	108.5(4)	C(121)-C(126)-H(126)	120.3
C(2)-P(3)-C(101)	113.5(4)	F(3)-B(1)-F(4)	118.0
C(121)-P(3)-C(101)	106.5(5)	F(3)-B(1)-F(1)	121.5
C(2)-P(3)-C(111)	110.7(4)	F(4)-B(1)-F(1)	112.0
C(121)-P(3)-C(111)	111.6(5)	F(3)-B(1)-F(2)	101.1
C(101)-P(3)-C(111)	106.0(4)	F(4)-B(1)-F(2)	88.6
C(106)-C(101)-C(102)	119.6(10)	F(1)-B(1)-F(2)	108.7
C(106)-C(101)-P(3)	120.9(8)	F(3)-B(1)-F(5)	73.7
C(102)-C(101)-P(3)	119.5(8)	F(4)-B(1)-F(5)	62.9
C(103)-C(102)-C(101)	119.9(11)	F(1)-B(1)-F(5)	106.1
C(103)-C(102)-H(102)	120.1	F(2)-B(1)-F(5)	141.4
C(101)-C(102)-H(102)	120.1	B(1)-F(3)-F(5)	59.0
C(102)-C(103)-C(104)	119.7(12)	B(1)-F(4)-F(5)	64.2
C(102)-C(103)-H(103)	120.1	F(4)-F(5)-B(1)	52.8
C(104)-C(103)-H(103)	120.1	F(4)-F(5)-F(3)	90.0
C(105)-C(104)-C(103)	121.1(12)	B(1)-F(5)-F(3)	47.3
C(105)-C(104)-H(104)	119.5	Cl(22)-C(20)-Cl(21)	117.5
C(103)-C(104)-H(104)	119.5	Cl(22)-C(20)-Cl(23)	40.3
C(104)-C(105)-C(106)	119.5(13)	Cl(21)-C(20)-Cl(23)	101.2
C(104)-C(105)-H(105)	120.3	Cl(23)-Cl(22)-Cl(24)	155.1
C(106)-C(105)-H(105)	120.3	Cl(23)-Cl(22)-C(20)	74.0
C(101)-C(106)-C(105)	120.2(11)	Cl(24)-Cl(22)-C(20)	103.7
C(101)-C(106)-H(106)	119.9	Cl(22)-Cl(23)-C(20)	65.7
C(105)-C(106)-H(106)	119.9	Cl(22)-Cl(23)-Cl(24)	12.6
C(112)-C(111)-C(116)	120.1(10)	C(20)-Cl(23)-Cl(24)	65.9
C(112)-C(111)-P(3)	121.5(8)	Cl(22)-Cl(24)-Cl(23)	12.4

Cl(32)-C(30)-Cl(31)	109.3(16)	Cl(32)-Cl(33)-Cl(34)	123.4
Cl(32)-C(30)-Cl(33)	22.2(4)	Cl(32)-Cl(33)-C(30)	68.1(6)
Cl(31)-C(30)-Cl(33)	87.2(12)	Cl(34)-Cl(33)-C(30)	71.8(11)
Cl(32)-C(30)-Cl(34)	65.3(11)	Cl(33)-Cl(34)-Cl(31)	104.2
Cl(31)-C(30)-Cl(34)	50.7(8)	Cl(33)-Cl(34)-C(30)	61.0(9)
Cl(33)-C(30)-Cl(34)	47.3(8)	Cl(31)-Cl(34)-C(30)	58.5(6)
Cl(34)-Cl(31)-C(30)	70.8(11)	Cl(33)-Cl(34)-Cl(32)	16.7
Cl(33)-Cl(32)-C(30)	89.7(8)	Cl(31)-Cl(34)-Cl(32)	102.8
Cl(33)-Cl(32)-Cl(34)	39.9	C(30)-Cl(34)-Cl(32)	50.3(8)
C(30)-Cl(32)-Cl(34)	64.4(11)		

Symmetry transformations used to generate equivalent atoms:

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

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Ru(1)	33(1)	33(1)	32(1)	0(1)	2(1)	0(1)
Fe(1)	49(1)	47(1)	53(1)	-1(1)	8(1)	8(1)
C(70)	45(5)	44(5)	39(5)	6(4)	5(4)	-7(4)
C(71)	35(5)	47(5)	40(5)	-4(4)	3(4)	-6(4)
C(72)	39(5)	46(5)	33(5)	-6(4)	18(4)	-8(4)
C(73)	36(5)	47(5)	50(5)	3(4)	7(4)	-3(4)
C(74)	35(5)	45(5)	46(5)	6(4)	6(4)	-5(4)
C(75)	49(6)	52(6)	49(6)	4(5)	10(5)	-10(5)
C(76)	67(7)	61(7)	62(7)	-1(5)	-3(6)	-25(6)
C(77)	61(7)	37(5)	72(7)	0(5)	18(6)	-5(5)
C(78)	51(6)	45(5)	52(6)	7(4)	12(5)	2(5)
C(1)	40(5)	33(4)	33(4)	4(3)	4(4)	-1(4)
C(2)	35(5)	34(4)	36(5)	-4(4)	-3(4)	-9(3)
C(3)	40(5)	42(5)	44(5)	-11(4)	3(4)	-8(4)
C(4)	50(6)	38(5)	49(5)	-3(4)	13(4)	2(4)
C(81)	45(5)	44(5)	49(6)	-5(4)	5(4)	5(4)
C(82)	49(6)	58(6)	50(6)	-6(5)	-12(5)	10(5)
C(83)	50(7)	62(7)	79(8)	-15(6)	-15(6)	9(5)
C(84)	39(6)	62(7)	110(10)	-3(7)	27(6)	-10(5)
C(85)	45(6)	38(5)	81(8)	-1(5)	8(5)	-1(4)
C(91)	86(10)	90(10)	101(12)	-47(9)	-10(9)	-9(9)
C(92)	106(11)	51(7)	73(8)	-8(6)	2(8)	0(7)
C(93)	78(10)	68(9)	123(13)	-23(9)	3(9)	31(7)
C(94)	190(20)	97(13)	105(14)	-42(11)	86(15)	-13(14)
C(95)	220(20)	100(13)	58(9)	-35(9)	-22(13)	21(15)
P(1)	39(1)	40(1)	33(1)	1(1)	-2(1)	-1(1)
C(11)	48(6)	48(5)	32(5)	0(4)	0(4)	-2(4)
C(12)	48(6)	41(5)	57(6)	3(4)	5(5)	5(4)
C(13)	58(7)	68(7)	55(7)	2(5)	6(5)	-7(6)
C(14)	75(8)	74(7)	47(6)	16(5)	21(6)	-9(6)
C(15)	85(9)	102(10)	42(6)	35(6)	-3(6)	-17(7)
C(16)	62(7)	86(8)	39(5)	12(5)	-5(5)	-14(6)
C(21)	38(5)	44(5)	40(5)	2(4)	-1(4)	-6(4)
C(22)	50(6)	55(6)	43(5)	-1(4)	-10(4)	-4(5)
C(23)	59(7)	67(7)	62(7)	2(6)	-6(6)	15(6)
C(24)	45(6)	77(8)	76(8)	-5(6)	-18(6)	5(6)
C(25)	56(7)	83(9)	68(7)	-8(6)	-21(6)	-14(6)
C(26)	50(6)	51(6)	56(6)	-12(5)	-7(5)	-3(5)
C(31)	43(5)	39(5)	39(5)	-1(4)	-2(4)	1(4)
C(32)	77(8)	53(6)	59(7)	-3(5)	9(6)	4(6)
C(33)	84(9)	58(7)	90(9)	-2(6)	11(7)	-6(6)
C(34)	130(12)	62(8)	66(8)	-17(6)	26(8)	5(8)
C(35)	163(15)	65(8)	76(9)	-16(7)	48(10)	-9(9)
C(36)	105(10)	47(6)	55(7)	0(5)	31(6)	-10(6)
P(2)	37(1)	38(1)	37(1)	1(1)	3(1)	3(1)
C(41)	46(5)	51(5)	38(5)	5(4)	-4(4)	4(5)
C(42)	44(6)	70(7)	50(6)	-2(5)	-4(5)	4(5)
C(43)	67(7)	96(9)	59(7)	-1(7)	-21(6)	16(7)
C(44)	67(8)	113(10)	47(7)	-2(7)	-18(6)	-10(7)
C(45)	71(8)	72(8)	51(6)	-9(5)	-1(6)	-8(6)
C(46)	42(5)	58(6)	46(5)	-4(5)	-6(4)	1(5)
C(51)	36(5)	34(5)	62(6)	3(4)	2(4)	6(4)
C(52)	53(6)	58(6)	49(6)	14(5)	13(5)	9(5)

C(53)	57(7)	92(9)	65(7)	18(7)	23(6)	23(7)
C(54)	70(8)	57(7)	115(11)	36(7)	36(8)	25(6)
C(55)	101(10)	45(6)	72(8)	-3(6)	33(7)	7(6)
C(56)	51(6)	41(5)	65(7)	7(5)	10(5)	7(4)
C(61)	39(5)	52(5)	43(5)	1(4)	5(4)	10(4)
C(62)	60(7)	62(7)	60(7)	0(5)	21(5)	11(5)
C(63)	85(9)	78(8)	57(7)	2(6)	14(6)	31(7)
C(64)	58(7)	95(9)	79(9)	16(7)	30(7)	5(7)
C(65)	48(7)	93(9)	81(9)	18(7)	14(6)	-14(6)
C(66)	41(5)	67(7)	55(6)	5(5)	-1(5)	3(5)
P(3)	42(1)	37(1)	42(1)	0(1)	3(1)	-4(1)
C(101)	42(5)	43(5)	57(6)	6(4)	-6(5)	-4(4)
C(102)	64(7)	86(8)	52(7)	6(6)	-8(6)	-4(6)
C(103)	65(8)	104(10)	72(9)	10(7)	-21(7)	-4(7)
C(104)	49(8)	86(10)	136(14)	4(9)	-11(9)	-9(7)
C(105)	53(8)	78(9)	120(12)	-2(8)	23(8)	-1(7)
C(106)	45(6)	71(7)	55(6)	-4(5)	-2(5)	8(5)
C(111)	37(5)	55(6)	61(6)	10(5)	8(5)	5(5)
C(112)	69(8)	66(7)	66(7)	13(6)	-2(6)	-18(6)
C(113)	74(9)	89(9)	85(9)	29(8)	13(7)	-8(7)
C(114)	59(8)	107(10)	69(8)	33(7)	7(6)	-3(7)
C(115)	57(7)	102(10)	57(7)	2(7)	-1(6)	11(7)
C(116)	61(7)	55(6)	51(6)	1(5)	6(5)	4(5)
C(121)	49(6)	39(5)	52(6)	-8(4)	1(4)	-6(4)
C(122)	61(7)	50(6)	49(6)	-7(5)	3(5)	1(5)
C(123)	78(8)	76(8)	45(6)	-9(6)	5(5)	-2(7)
C(124)	69(8)	65(7)	64(7)	-29(6)	-6(6)	7(6)
C(125)	130(12)	44(6)	85(9)	-28(6)	21(9)	-13(7)
C(126)	133(12)	37(6)	81(9)	-13(6)	28(8)	-12(7)

Table 13. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for complex (EE)-12b.

	x	y	z	U(eq)
H(71)	499	922	4746	49
H(72)	-269	1828	4444	47
H(73)	-1241	1653	3326	53
H(75)	-1903	605	2676	60
H(76)	-1863	-352	2842	76
H(77)	-794	-794	3581	67
H(78)	124	-242	4281	59
H(1)	1462	2015	3228	42
H(3)	-640	2402	3456	51
H(4)	-456	3458	2862	54
H(82)	-2023	3761	2218	64
H(83)	-3469	3582	2535	78
H(84)	-3439	2903	3586	83
H(85)	-1968	2633	3914	65
H(91)	-899	4281	4110	112
H(92)	-1978	4837	3391	93
H(93)	-3329	4613	3839	108
H(94)	-3150	3897	4824	151
H(95)	-1626	3697	5026	153
H(12)	1854	1731	2059	58
H(13)	2600	2265	1256	72
H(14)	1989	2531	118	78
H(15)	638	2316	-192	92
H(16)	-96	1748	564	75
H(22)	-873	2101	2143	60
H(23)	-2193	2322	1732	76
H(24)	-2999	1686	1025	80
H(25)	-2416	873	639	85
H(26)	-1069	632	1029	63
H(32)	-208	71	2270	75
H(33)	41	-837	1799	92
H(34)	815	-912	785	102
H(35)	1315	-131	252	119
H(36)	1152	754	760	82
H(42)	3340	753	4254	66
H(43)	4093	1129	5272	90
H(44)	3457	1747	6039	92
H(45)	2113	2053	5744	78
H(46)	1379	1686	4703	59
H(52)	2092	235	4924	64
H(53)	2008	-707	5294	84
H(54)	1603	-1392	4448	95
H(55)	1175	-1139	3241	86
H(56)	1279	-203	2889	63
H(62)	2115	215	2279	72
H(63)	3005	318	1361	88
H(64)	3958	1058	1411	92
H(65)	4013	1690	2398	88
H(66)	3063	1605	3268	65
H(102)	2284	2910	4527	82
H(103)	3678	2714	4762	98
H(104)	4528	2685	3801	110

H(105)	4011	2856	2610	100
H(106)	2603	3008	2359	69
H(112)	1929	4153	2579	81
H(113)	1778	4553	1415	99
H(114)	991	4131	472	94
H(115)	281	3310	688	87
H(116)	370	2902	1858	66
H(122)	596	3003	4617	64
H(123)	324	3565	5625	80
H(124)	589	4528	5588	80
H(125)	1014	4926	4536	103
H(126)	1232	4391	3513	99

Table 14. Torsion angles [°] for complex (EE)-12b.

C(1)-Ru(1)-C(70)-C(78)	-145.6(9)	P(1)-Ru(1)-C(73)-C(72)	-165.6(5)
C(71)-Ru(1)-C(70)-C(78)	-125.4(12)	C(70)-Ru(1)-C(73)-C(72)	79.9(6)
C(72)-Ru(1)-C(70)-C(78)	-165.8(11)	C(74)-Ru(1)-C(73)-C(72)	114.2(8)
C(73)-Ru(1)-C(70)-C(78)	151.2(11)	C(1)-Ru(1)-C(73)-C(74)	173.8(5)
P(2)-Ru(1)-C(70)-C(78)	-46.2(9)	C(71)-Ru(1)-C(73)-C(74)	-76.1(6)
P(1)-Ru(1)-C(70)-C(78)	62.1(10)	C(72)-Ru(1)-C(73)-C(74)	-114.2(8)
C(74)-Ru(1)-C(70)-C(78)	115.7(11)	P(2)-Ru(1)-C(73)-C(74)	-71.7(7)
C(1)-Ru(1)-C(70)-C(74)	98.7(7)	P(1)-Ru(1)-C(73)-C(74)	80.1(5)
C(71)-Ru(1)-C(70)-C(74)	118.9(8)	C(70)-Ru(1)-C(73)-C(74)	-34.3(5)
C(72)-Ru(1)-C(70)-C(74)	78.5(6)	C(78)-C(70)-C(74)-C(75)	2.8(13)
C(73)-Ru(1)-C(70)-C(74)	35.5(5)	C(71)-C(70)-C(74)-C(75)	-172.7(8)
P(2)-Ru(1)-C(70)-C(74)	-161.9(5)	Ru(1)-C(70)-C(74)-C(75)	132.1(8)
P(1)-Ru(1)-C(70)-C(74)	-53.6(6)	C(78)-C(70)-C(74)-C(73)	175.1(8)
C(1)-Ru(1)-C(70)-C(71)	-20.2(9)	C(71)-C(70)-C(74)-C(73)	-0.4(10)
C(72)-Ru(1)-C(70)-C(71)	-40.4(5)	Ru(1)-C(70)-C(74)-C(73)	-55.6(6)
C(73)-Ru(1)-C(70)-C(71)	-83.3(6)	C(78)-C(70)-C(74)-Ru(1)	-129.2(8)
P(2)-Ru(1)-C(70)-C(71)	79.2(5)	C(71)-C(70)-C(74)-Ru(1)	55.2(6)
P(1)-Ru(1)-C(70)-C(71)	-172.5(4)	C(72)-C(73)-C(74)-C(75)	166.9(9)
C(74)-Ru(1)-C(70)-C(71)	-118.9(8)	Ru(1)-C(73)-C(74)-C(75)	-129.2(10)
C(78)-C(70)-C(71)-C(72)	-169.8(10)	C(72)-C(73)-C(74)-C(70)	-4.2(10)
C(74)-C(70)-C(71)-C(72)	4.9(9)	Ru(1)-C(73)-C(74)-C(70)	59.7(6)
Ru(1)-C(70)-C(71)-C(72)	66.8(6)	C(72)-C(73)-C(74)-Ru(1)	-63.9(6)
C(78)-C(70)-C(71)-Ru(1)	123.4(11)	C(1)-Ru(1)-C(74)-C(75)	116.0(10)
C(74)-C(70)-C(71)-Ru(1)	-61.9(6)	C(71)-Ru(1)-C(74)-C(75)	-151.6(11)
C(1)-Ru(1)-C(71)-C(72)	56.3(6)	C(72)-Ru(1)-C(74)-C(75)	164.7(11)
C(73)-Ru(1)-C(71)-C(72)	-37.5(5)	C(73)-Ru(1)-C(74)-C(75)	125.2(12)
P(2)-Ru(1)-C(71)-C(72)	144.7(5)	P(2)-Ru(1)-C(74)-C(75)	-91.4(10)
P(1)-Ru(1)-C(71)-C(72)	-97.7(7)	P(1)-Ru(1)-C(74)-C(75)	19.6(10)
C(70)-Ru(1)-C(71)-C(72)	-112.5(7)	C(70)-Ru(1)-C(74)-C(75)	-114.7(12)
C(74)-Ru(1)-C(71)-C(72)	-78.0(5)	C(1)-Ru(1)-C(74)-C(70)	-129.3(6)
C(1)-Ru(1)-C(71)-C(70)	168.8(5)	C(71)-Ru(1)-C(74)-C(70)	-36.9(5)
C(72)-Ru(1)-C(71)-C(70)	112.5(7)	C(72)-Ru(1)-C(74)-C(70)	-80.6(6)
C(73)-Ru(1)-C(71)-C(70)	75.0(5)	C(73)-Ru(1)-C(74)-C(70)	-120.1(8)
P(2)-Ru(1)-C(71)-C(70)	-102.8(5)	P(2)-Ru(1)-C(74)-C(70)	23.3(6)
P(1)-Ru(1)-C(71)-C(70)	14.9(9)	P(1)-Ru(1)-C(74)-C(70)	134.3(5)
C(74)-Ru(1)-C(71)-C(70)	34.6(5)	C(1)-Ru(1)-C(74)-C(73)	-9.2(8)
C(70)-C(71)-C(72)-C(73)	-7.6(9)	C(71)-Ru(1)-C(74)-C(73)	83.2(6)
Ru(1)-C(71)-C(72)-C(73)	65.4(6)	C(72)-Ru(1)-C(74)-C(73)	39.4(5)
C(70)-C(71)-C(72)-Ru(1)	-72.9(6)	P(2)-Ru(1)-C(74)-C(73)	143.4(5)
C(1)-Ru(1)-C(72)-C(73)	113.0(5)	P(1)-Ru(1)-C(74)-C(73)	-105.7(5)
C(71)-Ru(1)-C(72)-C(73)	-116.3(7)	C(70)-Ru(1)-C(74)-C(73)	120.1(8)
P(2)-Ru(1)-C(72)-C(73)	-157.7(4)	C(70)-C(74)-C(75)-C(76)	2.0(14)
P(1)-Ru(1)-C(72)-C(73)	21.3(7)	C(73)-C(74)-C(75)-C(76)	-168.2(10)
C(70)-Ru(1)-C(72)-C(73)	-77.2(5)	Ru(1)-C(74)-C(75)-C(76)	96.0(11)
C(74)-Ru(1)-C(72)-C(73)	-37.7(5)	C(74)-C(75)-C(76)-C(77)	-5.8(16)
C(1)-Ru(1)-C(72)-C(71)	-130.7(5)	C(75)-C(76)-C(77)-C(78)	4.8(16)
C(73)-Ru(1)-C(72)-C(71)	116.3(7)	C(76)-C(77)-C(78)-C(70)	0.4(15)
P(2)-Ru(1)-C(72)-C(71)	-41.4(5)	C(74)-C(70)-C(78)-C(77)	-4.0(14)
P(1)-Ru(1)-C(72)-C(71)	137.6(4)	C(71)-C(70)-C(78)-C(77)	170.2(9)
C(70)-Ru(1)-C(72)-C(71)	39.1(5)	Ru(1)-C(70)-C(78)-C(77)	-98.8(11)
C(74)-Ru(1)-C(72)-C(71)	78.7(5)	C(71)-Ru(1)-C(1)-C(2)	-77.2(9)
C(71)-C(72)-C(73)-C(74)	7.3(9)	C(72)-Ru(1)-C(1)-C(2)	-47.0(9)
Ru(1)-C(72)-C(73)-C(74)	70.9(6)	C(73)-Ru(1)-C(1)-C(2)	-12.5(9)
C(71)-C(72)-C(73)-Ru(1)	-63.6(6)	P(2)-Ru(1)-C(1)-C(2)	-166.0(8)
C(1)-Ru(1)-C(73)-C(72)	-72.0(6)	P(1)-Ru(1)-C(1)-C(2)	91.3(8)
C(71)-Ru(1)-C(73)-C(72)	38.1(5)	C(70)-Ru(1)-C(1)-C(2)	-64.4(11)
P(2)-Ru(1)-C(73)-C(72)	42.6(8)	C(74)-Ru(1)-C(1)-C(2)	-7.0(11)

Ru(1)-C(1)-C(2)-C(3)	-1.1(14)	C(82)-Fe(1)-C(83)-C(84)	120.4(9)
Ru(1)-C(1)-C(2)-P(3)	177.7(5)	C(91)-Fe(1)-C(83)-C(84)	165.5(12)
C(1)-C(2)-C(3)-C(4)	-156.6(9)	C(92)-Fe(1)-C(83)-C(84)	-157.8(7)
P(3)-C(2)-C(3)-C(4)	24.6(12)	C(93)-Fe(1)-C(83)-C(84)	-115.4(8)
C(2)-C(3)-C(4)-C(81)	176.0(8)	C(81)-Fe(1)-C(83)-C(84)	82.5(7)
C(3)-C(4)-C(81)-C(82)	-152.0(9)	C(85)-Fe(1)-C(83)-C(84)	37.6(6)
C(3)-C(4)-C(81)-C(85)	26.6(15)	C(95)-Fe(1)-C(83)-C(82)	-158(2)
C(3)-C(4)-C(81)-Fe(1)	118.2(9)	C(94)-Fe(1)-C(83)-C(82)	165.8(9)
C(95)-Fe(1)-C(81)-C(82)	-159.4(9)	C(91)-Fe(1)-C(83)-C(82)	45.2(15)
C(94)-Fe(1)-C(81)-C(82)	167.1(15)	C(92)-Fe(1)-C(83)-C(82)	81.8(8)
C(91)-Fe(1)-C(81)-C(82)	-116.6(8)	C(93)-Fe(1)-C(83)-C(82)	124.2(8)
C(83)-Fe(1)-C(81)-C(82)	37.9(6)	C(81)-Fe(1)-C(83)-C(82)	-37.9(6)
C(92)-Fe(1)-C(81)-C(82)	-77.2(8)	C(85)-Fe(1)-C(83)-C(82)	-82.8(7)
C(93)-Fe(1)-C(81)-C(82)	-50.1(19)	C(84)-Fe(1)-C(83)-C(82)	-120.4(9)
C(85)-Fe(1)-C(81)-C(82)	118.2(9)	C(82)-C(83)-C(84)-C(85)	-0.9(13)
C(84)-Fe(1)-C(81)-C(82)	81.2(7)	Fe(1)-C(83)-C(84)-C(85)	-59.4(8)
C(95)-Fe(1)-C(81)-C(85)	82.4(10)	C(82)-C(83)-C(84)-Fe(1)	58.5(7)
C(94)-Fe(1)-C(81)-C(85)	48.9(17)	C(95)-Fe(1)-C(84)-C(83)	167.0(10)
C(82)-Fe(1)-C(81)-C(85)	-118.2(9)	C(94)-Fe(1)-C(84)-C(83)	125.1(10)
C(91)-Fe(1)-C(81)-C(85)	125.3(8)	C(82)-Fe(1)-C(84)-C(83)	-37.2(6)
C(83)-Fe(1)-C(81)-C(85)	-80.3(7)	C(91)-Fe(1)-C(84)-C(83)	-159.6(17)
C(92)-Fe(1)-C(81)-C(85)	164.6(7)	C(92)-Fe(1)-C(84)-C(83)	51.8(15)
C(93)-Fe(1)-C(81)-C(85)	-168.3(16)	C(93)-Fe(1)-C(84)-C(83)	84.2(9)
C(84)-Fe(1)-C(81)-C(85)	-37.0(6)	C(81)-Fe(1)-C(84)-C(83)	-81.0(7)
C(95)-Fe(1)-C(81)-C(4)	-39.6(12)	C(85)-Fe(1)-C(84)-C(83)	-119.1(9)
C(94)-Fe(1)-C(81)-C(4)	-73.1(18)	C(95)-Fe(1)-C(84)-C(85)	-73.9(11)
C(82)-Fe(1)-C(81)-C(4)	119.9(11)	C(94)-Fe(1)-C(84)-C(85)	-115.8(10)
C(91)-Fe(1)-C(81)-C(4)	3.3(11)	C(82)-Fe(1)-C(84)-C(85)	81.9(7)
C(83)-Fe(1)-C(81)-C(4)	157.8(10)	C(91)-Fe(1)-C(84)-C(85)	-40(2)
C(92)-Fe(1)-C(81)-C(4)	42.6(11)	C(83)-Fe(1)-C(84)-C(85)	119.1(9)
C(93)-Fe(1)-C(81)-C(4)	70(2)	C(92)-Fe(1)-C(84)-C(85)	170.9(11)
C(85)-Fe(1)-C(81)-C(4)	-122.0(11)	C(93)-Fe(1)-C(84)-C(85)	-156.7(8)
C(84)-Fe(1)-C(81)-C(4)	-158.9(10)	C(81)-Fe(1)-C(84)-C(85)	38.1(6)
C(85)-C(81)-C(82)-C(83)	-0.8(11)	C(83)-C(84)-C(85)-C(81)	0.3(12)
C(4)-C(81)-C(82)-C(83)	178.1(9)	Fe(1)-C(84)-C(85)-C(81)	-58.8(7)
Fe(1)-C(81)-C(82)-C(83)	-60.2(7)	C(83)-C(84)-C(85)-Fe(1)	59.2(8)
C(85)-C(81)-C(82)-Fe(1)	59.3(6)	C(82)-C(81)-C(85)-C(84)	0.3(11)
C(4)-C(81)-C(82)-Fe(1)	-121.8(9)	C(4)-C(81)-C(85)-C(84)	-178.6(9)
C(95)-Fe(1)-C(82)-C(83)	164.8(15)	Fe(1)-C(81)-C(85)-C(84)	59.3(7)
C(94)-Fe(1)-C(82)-C(83)	-43(2)	C(82)-C(81)-C(85)-Fe(1)	-59.0(6)
C(91)-Fe(1)-C(82)-C(83)	-160.1(8)	C(4)-C(81)-C(85)-Fe(1)	122.1(10)
C(92)-Fe(1)-C(82)-C(83)	-117.8(8)	C(95)-Fe(1)-C(85)-C(84)	124.7(11)
C(93)-Fe(1)-C(82)-C(83)	-77.2(9)	C(94)-Fe(1)-C(85)-C(84)	81.8(11)
C(81)-Fe(1)-C(82)-C(83)	118.9(9)	C(82)-Fe(1)-C(85)-C(84)	-81.5(7)
C(85)-Fe(1)-C(82)-C(83)	80.1(7)	C(91)-Fe(1)-C(85)-C(84)	166.2(9)
C(84)-Fe(1)-C(82)-C(83)	36.7(6)	C(83)-Fe(1)-C(85)-C(84)	-37.5(7)
C(95)-Fe(1)-C(82)-C(81)	45.9(17)	C(92)-Fe(1)-C(85)-C(84)	-167.3(16)
C(94)-Fe(1)-C(82)-C(81)	-161(2)	C(93)-Fe(1)-C(85)-C(84)	52.4(15)
C(91)-Fe(1)-C(82)-C(81)	80.9(8)	C(81)-Fe(1)-C(85)-C(84)	-119.7(9)
C(83)-Fe(1)-C(82)-C(81)	-118.9(9)	C(95)-Fe(1)-C(85)-C(81)	-115.6(10)
C(92)-Fe(1)-C(82)-C(81)	123.3(7)	C(94)-Fe(1)-C(85)-C(81)	-158.6(10)
C(93)-Fe(1)-C(82)-C(81)	163.8(7)	C(82)-Fe(1)-C(85)-C(81)	38.1(6)
C(85)-Fe(1)-C(82)-C(81)	-38.8(6)	C(91)-Fe(1)-C(85)-C(81)	-74.1(9)
C(84)-Fe(1)-C(82)-C(81)	-82.2(6)	C(83)-Fe(1)-C(85)-C(81)	82.1(7)
C(81)-C(82)-C(83)-C(84)	1.1(12)	C(92)-Fe(1)-C(85)-C(81)	-47.6(19)
Fe(1)-C(82)-C(83)-C(84)	-59.3(8)	C(93)-Fe(1)-C(85)-C(81)	172.1(12)
C(81)-C(82)-C(83)-Fe(1)	60.4(7)	C(84)-Fe(1)-C(85)-C(81)	119.7(9)
C(95)-Fe(1)-C(83)-C(84)	-38(2)	C(95)-Fe(1)-C(91)-C(92)	-117.5(14)
C(94)-Fe(1)-C(83)-C(84)	-73.9(10)	C(94)-Fe(1)-C(91)-C(92)	-79.4(10)

C(82)-Fe(1)-C(91)-C(92)	84.3(10)	C(92)-Fe(1)-C(94)-C(93)	36.3(10)
C(83)-Fe(1)-C(91)-C(92)	52.1(16)	C(81)-Fe(1)-C(94)-C(93)	164.1(11)
C(93)-Fe(1)-C(91)-C(92)	-36.7(9)	C(85)-Fe(1)-C(94)-C(93)	-160.8(9)
C(81)-Fe(1)-C(91)-C(92)	126.6(9)	C(84)-Fe(1)-C(94)-C(93)	-118.8(11)
C(85)-Fe(1)-C(91)-C(92)	168.3(8)	C(82)-Fe(1)-C(94)-C(95)	-162.7(18)
C(84)-Fe(1)-C(91)-C(92)	-160.7(15)	C(91)-Fe(1)-C(94)-C(95)	-38.1(11)
C(94)-Fe(1)-C(91)-C(95)	38.1(11)	C(83)-Fe(1)-C(94)-C(95)	164.4(11)
C(82)-Fe(1)-C(91)-C(95)	-158.2(11)	C(92)-Fe(1)-C(94)-C(95)	-81.0(12)
C(83)-Fe(1)-C(91)-C(95)	169.5(13)	C(93)-Fe(1)-C(94)-C(95)	-117.2(17)
C(92)-Fe(1)-C(91)-C(95)	117.5(14)	C(81)-Fe(1)-C(94)-C(95)	47(2)
C(93)-Fe(1)-C(91)-C(95)	80.8(11)	C(85)-Fe(1)-C(94)-C(95)	81.9(13)
C(81)-Fe(1)-C(91)-C(95)	-115.9(11)	C(84)-Fe(1)-C(94)-C(95)	124.0(12)
C(85)-Fe(1)-C(91)-C(95)	-74.2(12)	C(93)-C(94)-C(95)-C(91)	-1.2(18)
C(84)-Fe(1)-C(91)-C(95)	-43(2)	Fe(1)-C(94)-C(95)-C(91)	60.1(10)
C(95)-C(91)-C(92)-C(93)	0.1(15)	C(93)-C(94)-C(95)-Fe(1)	-61.3(11)
Fe(1)-C(91)-C(92)-C(93)	59.4(9)	C(92)-C(91)-C(95)-C(94)	0.7(16)
C(95)-C(91)-C(92)-Fe(1)	-59.4(9)	Fe(1)-C(91)-C(95)-C(94)	-59.8(11)
C(95)-Fe(1)-C(92)-C(93)	-81.0(11)	C(92)-C(91)-C(95)-Fe(1)	60.5(9)
C(94)-Fe(1)-C(92)-C(93)	-36.2(10)	C(82)-Fe(1)-C(95)-C(94)	168.1(12)
C(82)-Fe(1)-C(92)-C(93)	125.8(9)	C(91)-Fe(1)-C(95)-C(94)	118.9(16)
C(91)-Fe(1)-C(92)-C(93)	-120.2(13)	C(83)-Fe(1)-C(95)-C(94)	-47(3)
C(83)-Fe(1)-C(92)-C(93)	82.6(10)	C(92)-Fe(1)-C(95)-C(94)	81.0(12)
C(81)-Fe(1)-C(92)-C(93)	168.1(8)	C(93)-Fe(1)-C(95)-C(94)	37.9(11)
C(85)-Fe(1)-C(92)-C(93)	-154.7(16)	C(81)-Fe(1)-C(95)-C(94)	-159.3(10)
C(84)-Fe(1)-C(92)-C(93)	45.7(17)	C(85)-Fe(1)-C(95)-C(94)	-116.0(11)
C(95)-Fe(1)-C(92)-C(91)	39.3(10)	C(84)-Fe(1)-C(95)-C(94)	-75.5(13)
C(94)-Fe(1)-C(92)-C(91)	84.0(11)	C(94)-Fe(1)-C(95)-C(91)	-118.9(16)
C(82)-Fe(1)-C(92)-C(91)	-114.0(9)	C(82)-Fe(1)-C(95)-C(91)	49.1(19)
C(83)-Fe(1)-C(92)-C(91)	-157.1(9)	C(83)-Fe(1)-C(95)-C(91)	-165.5(17)
C(93)-Fe(1)-C(92)-C(91)	120.2(13)	C(92)-Fe(1)-C(95)-C(91)	-37.9(9)
C(81)-Fe(1)-C(92)-C(91)	-71.7(10)	C(93)-Fe(1)-C(95)-C(91)	-81.1(10)
C(85)-Fe(1)-C(92)-C(91)	-35(2)	C(81)-Fe(1)-C(95)-C(91)	81.7(11)
C(84)-Fe(1)-C(92)-C(91)	166.0(12)	C(85)-Fe(1)-C(95)-C(91)	125.1(10)
C(91)-C(92)-C(93)-C(94)	-0.8(16)	C(84)-Fe(1)-C(95)-C(91)	165.6(8)
Fe(1)-C(92)-C(93)-C(94)	58.5(10)	C(1)-Ru(1)-P(1)-C(21)	-101.6(4)
C(91)-C(92)-C(93)-Fe(1)	-59.3(9)	C(71)-Ru(1)-P(1)-C(21)	54.8(6)
C(95)-Fe(1)-C(93)-C(94)	-39.4(12)	C(72)-Ru(1)-P(1)-C(21)	-9.5(5)
C(82)-Fe(1)-C(93)-C(94)	164.6(12)	C(73)-Ru(1)-P(1)-C(21)	3.4(4)
C(91)-Fe(1)-C(93)-C(94)	-84.3(12)	P(2)-Ru(1)-P(1)-C(21)	169.6(3)
C(83)-Fe(1)-C(93)-C(94)	122.0(13)	C(70)-Ru(1)-P(1)-C(21)	64.6(4)
C(92)-Fe(1)-C(93)-C(94)	-121.1(15)	C(74)-Ru(1)-P(1)-C(21)	37.9(4)
C(81)-Fe(1)-C(93)-C(94)	-156.4(17)	C(1)-Ru(1)-P(1)-C(31)	142.4(4)
C(85)-Fe(1)-C(93)-C(94)	42.0(19)	C(71)-Ru(1)-P(1)-C(31)	-61.2(6)
C(84)-Fe(1)-C(93)-C(94)	78.9(13)	C(72)-Ru(1)-P(1)-C(31)	-125.5(5)
C(95)-Fe(1)-C(93)-C(92)	81.6(11)	C(73)-Ru(1)-P(1)-C(31)	-112.7(4)
C(94)-Fe(1)-C(93)-C(92)	121.1(15)	P(2)-Ru(1)-P(1)-C(31)	53.6(3)
C(82)-Fe(1)-C(93)-C(92)	-74.3(10)	C(70)-Ru(1)-P(1)-C(31)	-51.4(4)
C(91)-Fe(1)-C(93)-C(92)	36.8(9)	C(74)-Ru(1)-P(1)-C(31)	-78.1(4)
C(83)-Fe(1)-C(93)-C(92)	-116.9(9)	C(1)-Ru(1)-P(1)-C(11)	16.9(4)
C(81)-Fe(1)-C(93)-C(92)	-35(2)	C(71)-Ru(1)-P(1)-C(11)	173.4(6)
C(85)-Fe(1)-C(93)-C(92)	163.0(11)	C(72)-Ru(1)-P(1)-C(11)	109.0(5)
C(84)-Fe(1)-C(93)-C(92)	-160.1(8)	C(73)-Ru(1)-P(1)-C(11)	121.9(4)
C(92)-C(93)-C(94)-C(95)	1.2(17)	P(2)-Ru(1)-P(1)-C(11)	-71.9(4)
Fe(1)-C(93)-C(94)-C(95)	60.1(10)	C(70)-Ru(1)-P(1)-C(11)	-176.8(4)
C(92)-C(93)-C(94)-Fe(1)	-58.8(10)	C(74)-Ru(1)-P(1)-C(11)	156.4(4)
C(95)-Fe(1)-C(94)-C(93)	117.2(17)	C(21)-P(1)-C(11)-C(12)	160.7(8)
C(82)-Fe(1)-C(94)-C(93)	-45(3)	C(31)-P(1)-C(11)-C(12)	-95.1(8)
C(91)-Fe(1)-C(94)-C(93)	79.2(11)	Ru(1)-P(1)-C(11)-C(12)	37.2(9)
C(83)-Fe(1)-C(94)-C(93)	-78.3(12)	C(21)-P(1)-C(11)-C(16)	-23.5(9)

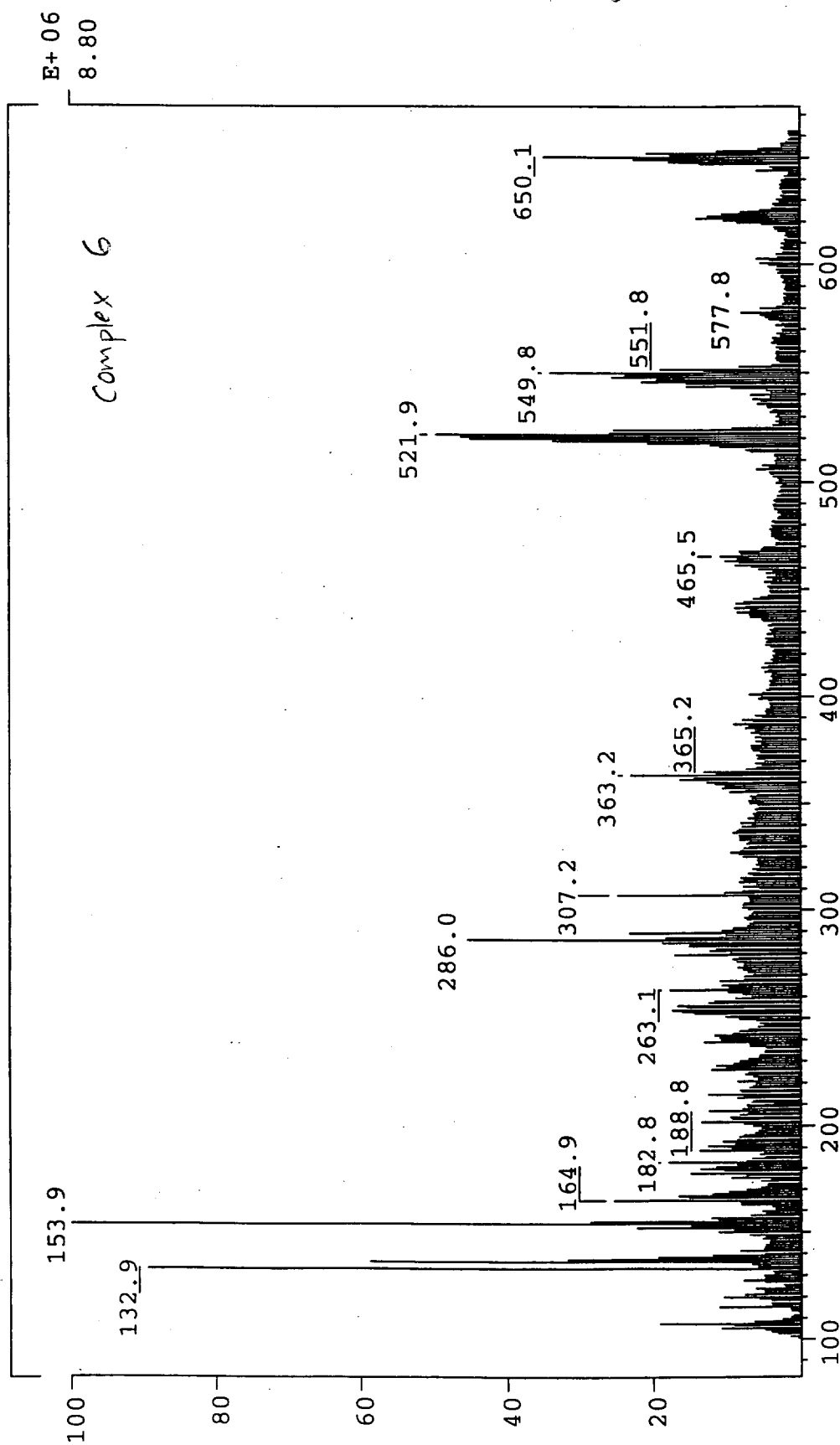
C(31)-P(1)-C(11)-C(16)	80.7(9)	C(51)-P(2)-C(41)-C(42)	60.1(9)
Ru(1)-P(1)-C(11)-C(16)	-147.0(7)	C(61)-P(2)-C(41)-C(42)	-46.2(9)
C(16)-C(11)-C(12)-C(13)	-1.6(14)	Ru(1)-P(2)-C(41)-C(42)	-177.6(7)
P(1)-C(11)-C(12)-C(13)	174.3(7)	C(51)-P(2)-C(41)-C(46)	-114.0(8)
C(11)-C(12)-C(13)-C(14)	0.8(15)	C(61)-P(2)-C(41)-C(46)	139.7(8)
C(12)-C(13)-C(14)-C(15)	1.7(18)	Ru(1)-P(2)-C(41)-C(46)	8.3(9)
C(13)-C(14)-C(15)-C(16)	-4(2)	C(46)-C(41)-C(42)-C(43)	-2.4(15)
C(14)-C(15)-C(16)-C(11)	2.8(19)	P(2)-C(41)-C(42)-C(43)	-176.8(9)
C(12)-C(11)-C(16)-C(15)	-0.2(16)	C(41)-C(42)-C(43)-C(44)	2.9(18)
P(1)-C(11)-C(16)-C(15)	-176.1(9)	C(42)-C(43)-C(44)-C(45)	-2.5(19)
C(31)-P(1)-C(21)-C(22)	-177.7(7)	C(43)-C(44)-C(45)-C(46)	1.7(18)
C(11)-P(1)-C(21)-C(22)	-74.7(8)	C(44)-C(45)-C(46)-C(41)	-1.3(16)
Ru(1)-P(1)-C(21)-C(22)	57.3(8)	C(42)-C(41)-C(46)-C(45)	1.6(15)
C(31)-P(1)-C(21)-C(26)	1.1(9)	P(2)-C(41)-C(46)-C(45)	175.9(8)
C(11)-P(1)-C(21)-C(26)	104.1(8)	C(41)-P(2)-C(51)-C(56)	-170.6(8)
Ru(1)-P(1)-C(21)-C(26)	-123.8(8)	C(61)-P(2)-C(51)-C(56)	-68.2(8)
C(26)-C(21)-C(22)-C(23)	1.1(14)	Ru(1)-P(2)-C(51)-C(56)	65.7(8)
P(1)-C(21)-C(22)-C(23)	-180.0(8)	C(41)-P(2)-C(51)-C(52)	15.2(9)
C(21)-C(22)-C(23)-C(24)	1.4(16)	C(61)-P(2)-C(51)-C(52)	117.6(8)
C(22)-C(23)-C(24)-C(25)	-3.4(18)	Ru(1)-P(2)-C(51)-C(52)	-108.5(7)
C(23)-C(24)-C(25)-C(26)	3.0(19)	C(56)-C(51)-C(52)-C(53)	1.6(14)
C(24)-C(25)-C(26)-C(21)	-0.5(18)	P(2)-C(51)-C(52)-C(53)	176.0(7)
C(22)-C(21)-C(26)-C(25)	-1.6(14)	C(51)-C(52)-C(53)-C(54)	0.3(16)
P(1)-C(21)-C(26)-C(25)	179.6(8)	C(52)-C(53)-C(54)-C(55)	-2.6(17)
C(21)-P(1)-C(31)-C(36)	104.2(9)	C(53)-C(54)-C(55)-C(56)	3.0(17)
C(11)-P(1)-C(31)-C(36)	1.5(10)	C(52)-C(51)-C(56)-C(55)	-1.3(15)
Ru(1)-P(1)-C(31)-C(36)	-134.9(9)	P(2)-C(51)-C(56)-C(55)	-175.7(8)
C(21)-P(1)-C(31)-C(32)	-77.3(8)	C(54)-C(55)-C(56)-C(51)	-1.0(17)
C(11)-P(1)-C(31)-C(32)	180.0(8)	C(41)-P(2)-C(61)-C(66)	-33.2(9)
Ru(1)-P(1)-C(31)-C(32)	43.5(9)	C(51)-P(2)-C(61)-C(66)	-136.5(8)
C(36)-C(31)-C(32)-C(33)	0.5(17)	Ru(1)-P(2)-C(61)-C(66)	94.3(8)
P(1)-C(31)-C(32)-C(33)	-178.1(9)	C(41)-P(2)-C(61)-C(62)	154.4(8)
C(31)-C(32)-C(33)-C(34)	-1.4(19)	C(51)-P(2)-C(61)-C(62)	51.1(9)
C(32)-C(33)-C(34)-C(35)	0(2)	Ru(1)-P(2)-C(61)-C(62)	-78.1(9)
C(33)-C(34)-C(35)-C(36)	2(3)	C(66)-C(61)-C(62)-C(63)	0.4(15)
C(32)-C(31)-C(36)-C(35)	1.9(18)	P(2)-C(61)-C(62)-C(63)	173.0(8)
P(1)-C(31)-C(36)-C(35)	-179.6(11)	C(61)-C(62)-C(63)-C(64)	0.8(17)
C(34)-C(35)-C(36)-C(31)	-3(2)	C(62)-C(63)-C(64)-C(65)	0.0(18)
C(1)-Ru(1)-P(2)-C(41)	53.9(4)	C(63)-C(64)-C(65)-C(66)	-1.9(18)
C(71)-Ru(1)-P(2)-C(41)	-60.4(4)	C(64)-C(65)-C(66)-C(61)	3.2(17)
C(72)-Ru(1)-P(2)-C(41)	-36.9(4)	C(62)-C(61)-C(66)-C(65)	-2.4(15)
C(73)-Ru(1)-P(2)-C(41)	-64.3(6)	P(2)-C(61)-C(66)-C(65)	-175.0(8)
P(1)-Ru(1)-P(2)-C(41)	143.8(3)	C(1)-C(2)-P(3)-C(121)	-129.3(7)
C(70)-Ru(1)-P(2)-C(41)	-95.8(4)	C(3)-C(2)-P(3)-C(121)	49.6(7)
C(74)-Ru(1)-P(2)-C(41)	-108.6(4)	C(1)-C(2)-P(3)-C(101)	-11.1(9)
C(1)-Ru(1)-P(2)-C(51)	169.0(4)	C(3)-C(2)-P(3)-C(101)	167.8(6)
C(71)-Ru(1)-P(2)-C(51)	54.6(4)	C(1)-C(2)-P(3)-C(111)	107.9(7)
C(72)-Ru(1)-P(2)-C(51)	78.2(4)	C(3)-C(2)-P(3)-C(111)	-73.2(7)
C(73)-Ru(1)-P(2)-C(51)	50.8(6)	C(2)-P(3)-C(101)-C(106)	101.6(9)
P(1)-Ru(1)-P(2)-C(51)	-101.1(3)	C(121)-P(3)-C(101)-C(106)	-139.1(8)
C(70)-Ru(1)-P(2)-C(51)	19.3(4)	C(111)-P(3)-C(101)-C(106)	-20.1(10)
C(74)-Ru(1)-P(2)-C(51)	6.5(4)	C(2)-P(3)-C(101)-C(102)	-79.7(9)
C(1)-Ru(1)-P(2)-C(61)	-66.0(4)	C(121)-P(3)-C(101)-C(102)	39.7(9)
C(71)-Ru(1)-P(2)-C(61)	179.7(4)	C(111)-P(3)-C(101)-C(102)	158.7(8)
C(72)-Ru(1)-P(2)-C(61)	-156.8(4)	C(106)-C(101)-C(102)-C(103)	0.5(17)
C(73)-Ru(1)-P(2)-C(61)	175.8(6)	P(3)-C(101)-C(102)-C(103)	-178.3(9)
P(1)-Ru(1)-P(2)-C(61)	23.9(4)	C(101)-C(102)-C(103)-C(104)	1(2)
C(70)-Ru(1)-P(2)-C(61)	144.3(4)	C(102)-C(103)-C(104)-C(105)	0(2)
C(74)-Ru(1)-P(2)-C(61)	131.5(5)	C(103)-C(104)-C(105)-C(106)	-2(2)

C(102)-C(101)-C(106)-C(105)	-2.2(16)	F(1)-B(1)-F(5)-F(3)	118.8
P(3)-C(101)-C(106)-C(105)	176.6(9)	F(2)-B(1)-F(5)-F(3)	-87.4
C(104)-C(105)-C(106)-C(101)	2.8(19)	B(1)-F(3)-F(5)-F(4)	-34.8
C(2)-P(3)-C(111)-C(112)	179.6(8)	Cl(21)-C(20)-Cl(22)-Cl(23)	73.9
C(121)-P(3)-C(111)-C(112)	58.6(10)	Cl(21)-C(20)-Cl(22)-Cl(24)	-80.4
C(101)-P(3)-C(111)-C(112)	-56.9(10)	Cl(23)-C(20)-Cl(22)-Cl(24)	-154.3
C(2)-P(3)-C(111)-C(116)	-6.8(9)	Cl(24)-Cl(22)-Cl(23)-C(20)	88.3
C(121)-P(3)-C(111)-C(116)	-127.7(8)	C(20)-Cl(22)-Cl(23)-Cl(24)	-88.3
C(101)-P(3)-C(111)-C(116)	116.8(8)	Cl(21)-C(20)-Cl(23)-Cl(22)	-119.7
C(116)-C(111)-C(112)-C(113)	4.1(17)	Cl(22)-C(20)-Cl(23)-Cl(24)	13.8
P(3)-C(111)-C(112)-C(113)	177.6(9)	Cl(21)-C(20)-Cl(23)-Cl(24)	-105.9
C(111)-C(112)-C(113)-C(114)	-3(2)	C(20)-Cl(22)-Cl(24)-Cl(23)	81.6
C(112)-C(113)-C(114)-C(115)	1(2)	C(20)-Cl(23)-Cl(24)-Cl(22)	-86.0
C(113)-C(114)-C(115)-C(116)	0.1(19)	Cl(32)-C(30)-Cl(31)-Cl(34)	-30.9(17)
C(114)-C(115)-C(116)-C(111)	0.8(17)	Cl(33)-C(30)-Cl(31)-Cl(34)	-33.1(9)
C(112)-C(111)-C(116)-C(115)	-2.9(15)	Cl(31)-C(30)-Cl(32)-Cl(33)	-6(2)
P(3)-C(111)-C(116)-C(115)	-176.7(8)	Cl(34)-C(30)-Cl(32)-Cl(33)	-31.9(6)
C(2)-P(3)-C(121)-C(122)	31.5(9)	Cl(31)-C(30)-Cl(32)-Cl(34)	25.9(15)
C(101)-P(3)-C(121)-C(122)	-91.1(9)	Cl(33)-C(30)-Cl(32)-Cl(34)	31.9(6)
C(111)-P(3)-C(121)-C(122)	153.8(8)	C(30)-Cl(32)-Cl(33)-Cl(34)	48.0(15)
C(2)-P(3)-C(121)-C(126)	-150.7(10)	Cl(34)-Cl(32)-Cl(33)-C(30)	-48.0(15)
C(101)-P(3)-C(121)-C(126)	86.7(11)	Cl(31)-C(30)-Cl(33)-Cl(32)	174.4(19)
C(111)-P(3)-C(121)-C(126)	-28.5(11)	Cl(34)-C(30)-Cl(33)-Cl(32)	139.2(9)
C(126)-C(121)-C(122)-C(123)	-2.3(16)	Cl(32)-C(30)-Cl(33)-Cl(34)	-139.2(9)
P(3)-C(121)-C(122)-C(123)	175.6(8)	Cl(31)-C(30)-Cl(33)-Cl(34)	35.2(10)
C(121)-C(122)-C(123)-C(124)	-1.0(17)	Cl(32)-Cl(33)-Cl(34)-Cl(31)	-87.3
C(122)-C(123)-C(124)-C(125)	2.8(18)	C(30)-Cl(33)-Cl(34)-Cl(31)	-40.8(11)
C(123)-C(124)-C(125)-C(126)	-1(2)	Cl(32)-Cl(33)-Cl(34)-C(30)	-46.5(11)
C(124)-C(125)-C(126)-C(121)	-2(2)	C(30)-Cl(33)-Cl(34)-Cl(32)	46.5(11)
C(122)-C(121)-C(126)-C(125)	3.8(19)	C(30)-Cl(31)-Cl(34)-Cl(33)	42.1(14)
P(3)-C(121)-C(126)-C(125)	-174.0(10)	C(30)-Cl(31)-Cl(34)-Cl(32)	24.9(14)
F(4)-B(1)-F(3)-F(5)	46.2	Cl(32)-C(30)-Cl(34)-Cl(33)	15.8(4)
F(1)-B(1)-F(3)-F(5)	-99.2	Cl(31)-C(30)-Cl(34)-Cl(33)	-132.0(12)
F(2)-B(1)-F(3)-F(5)	140.6	Cl(32)-C(30)-Cl(34)-Cl(31)	147.8(16)
F(3)-B(1)-F(4)-F(5)	-51.1	Cl(33)-C(30)-Cl(34)-Cl(31)	132.0(12)
F(1)-B(1)-F(4)-F(5)	97.4	Cl(31)-C(30)-Cl(34)-Cl(32)	-147.8(16)
F(2)-B(1)-F(4)-F(5)	-152.9	Cl(33)-C(30)-Cl(34)-Cl(32)	-15.8(4)
B(1)-F(4)-F(5)-F(3)	31.8	C(30)-Cl(32)-Cl(34)-Cl(33)	-124.5(15)
F(3)-B(1)-F(5)-F(4)	134.3	Cl(33)-Cl(32)-Cl(34)-Cl(31)	96.7
F(1)-B(1)-F(5)-F(4)	-106.9	C(30)-Cl(32)-Cl(34)-Cl(31)	-27.8(15)
F(2)-B(1)-F(5)-F(4)	46.9	Cl(33)-Cl(32)-Cl(34)-C(30)	124.5(15)
F(4)-B(1)-F(5)-F(3)	-134.3		

Symmetry transformations used to generate equivalent atoms:

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Mode: FAB +VE +HMR
Oper: Client: covadonga glez
Base: 153.9 Inten: 8800301
Norm: 153.9 RIC: 394200755
Peak: 1000.00 mmu

16-Dec-96

Elapse: 06:33.0
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OC152170.C1
DATE 16-10-31

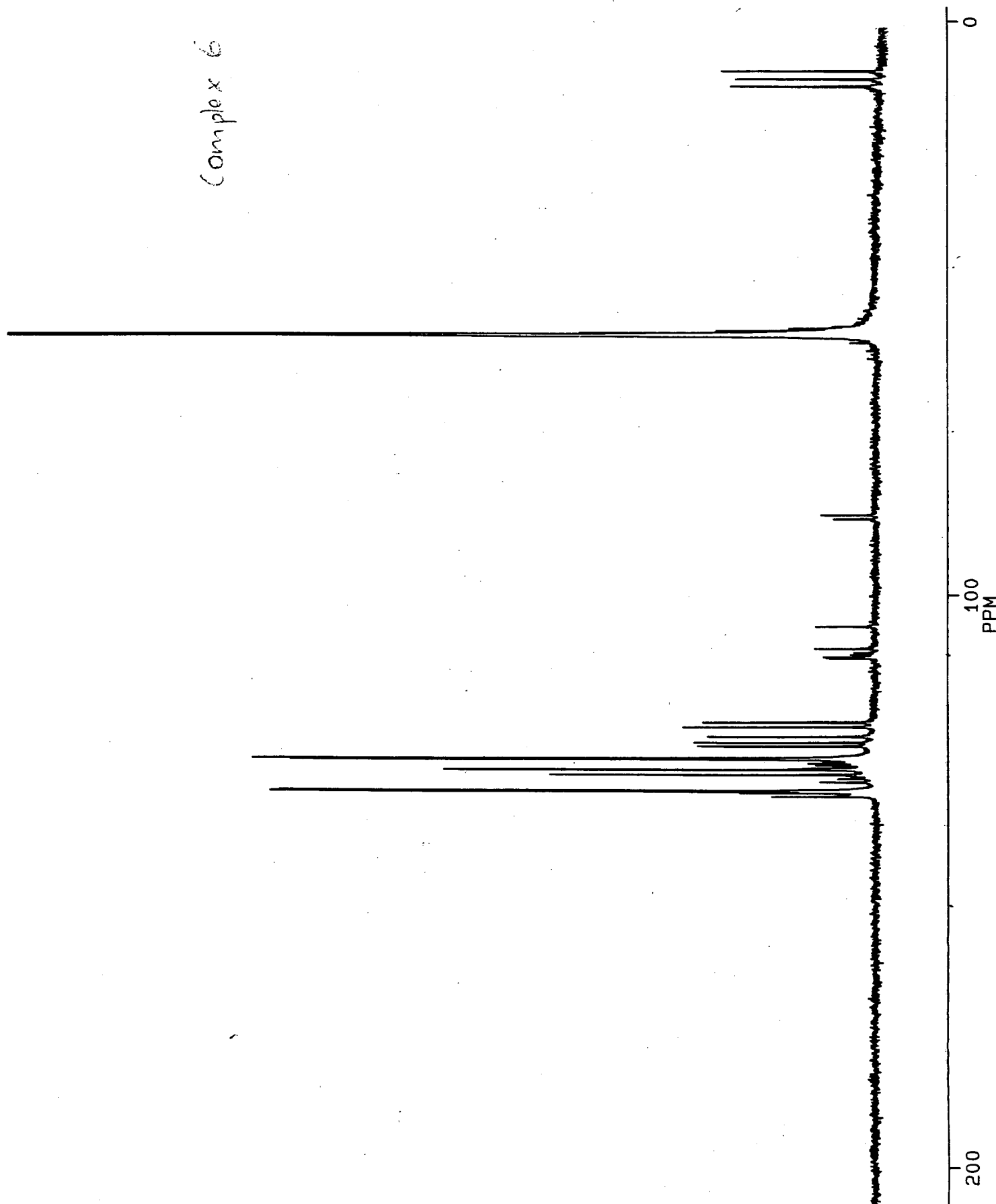
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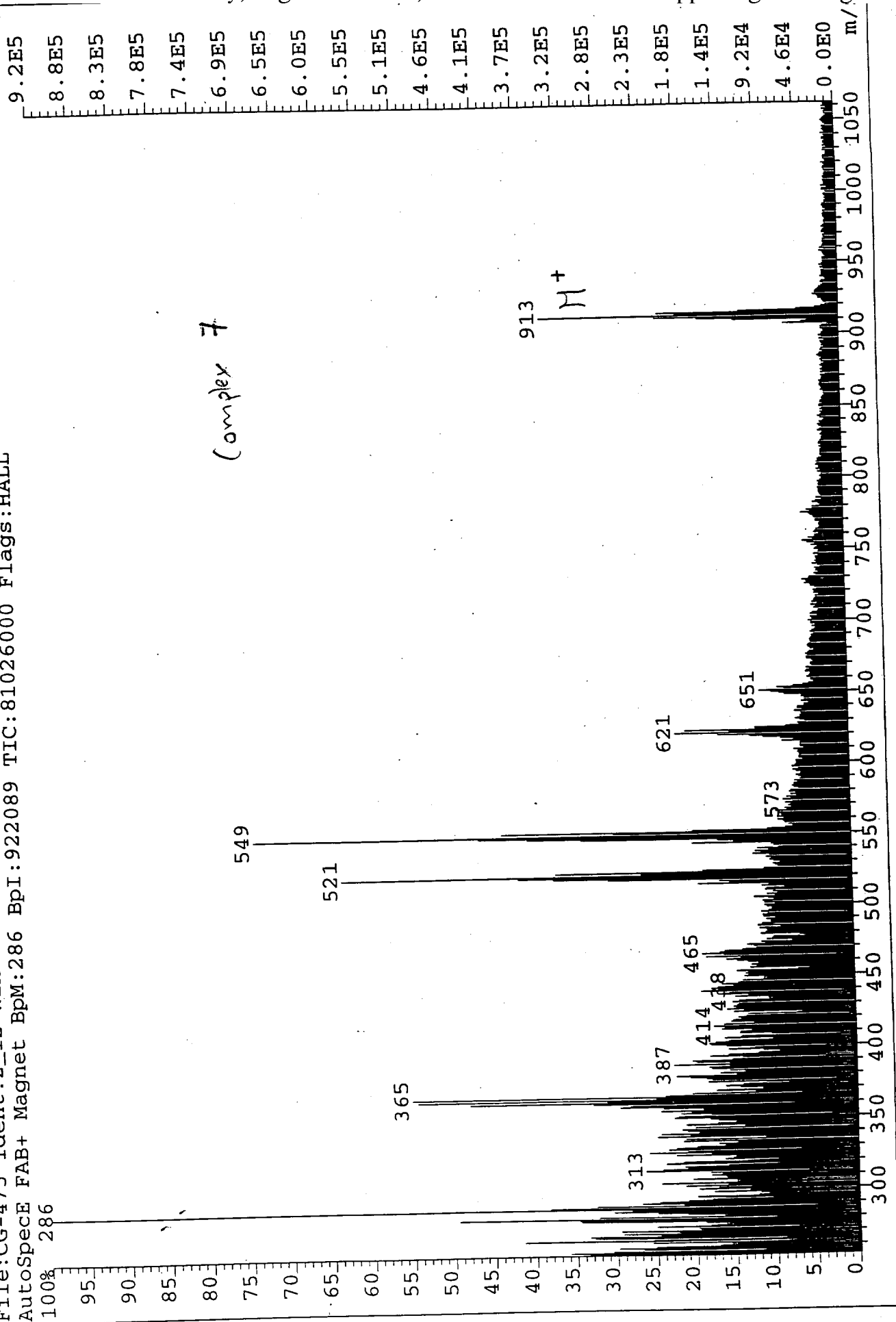
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Complex 6



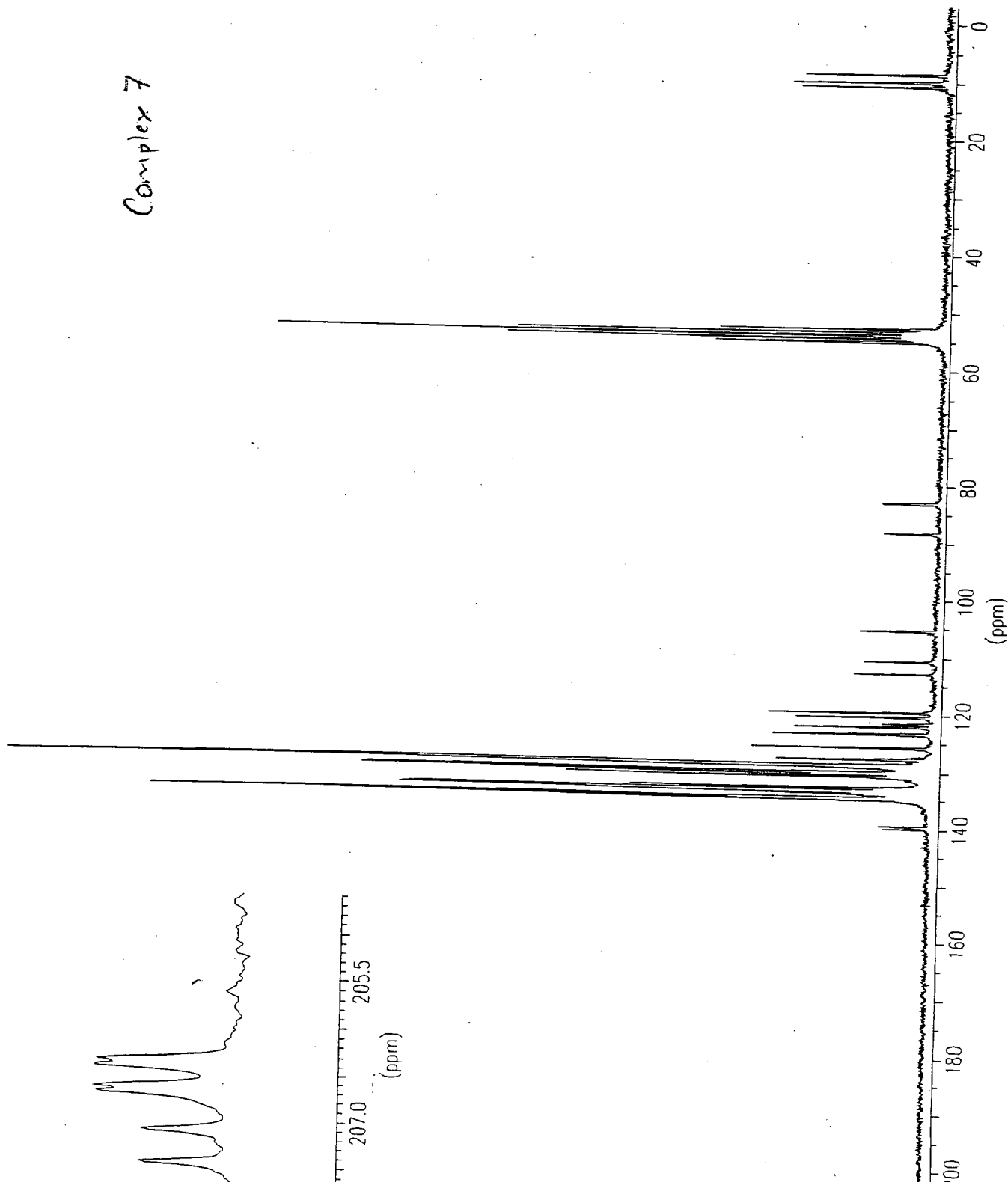
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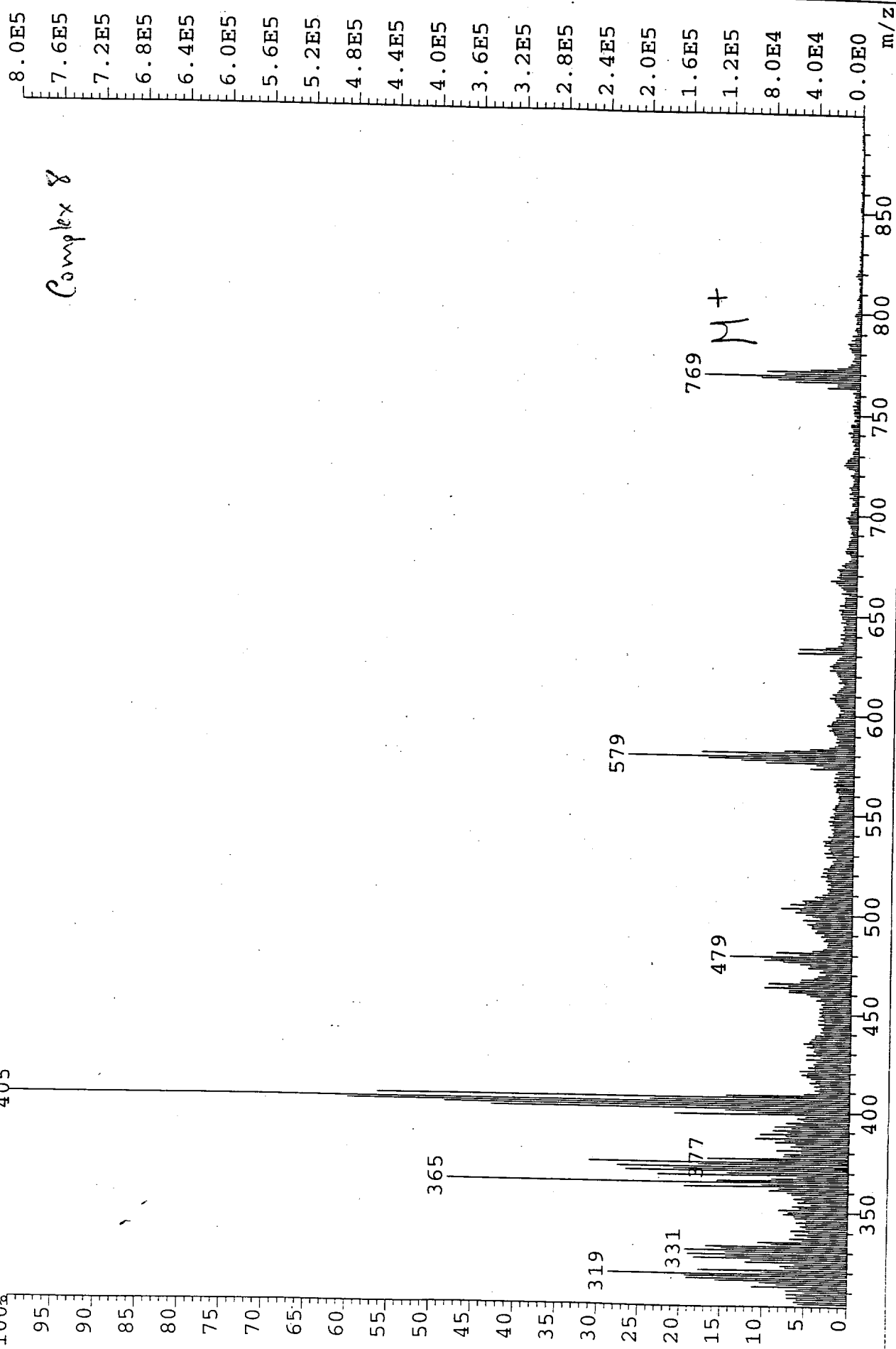
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BaseInt : 26827
AQtime : 1.0811630 sec
*** Aspect 3000 Parameters ***
O1 : 10745.47 Hz

Complex 7



-475 cd2c12 200mhz

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Complex 8

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