

Supplementary Information

Synthesis and spectroscopic behaviour of metal complexes of *meso*-alkylidenyl carbaporphyrinoids and their expanded analogue

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Synthetic Scheme

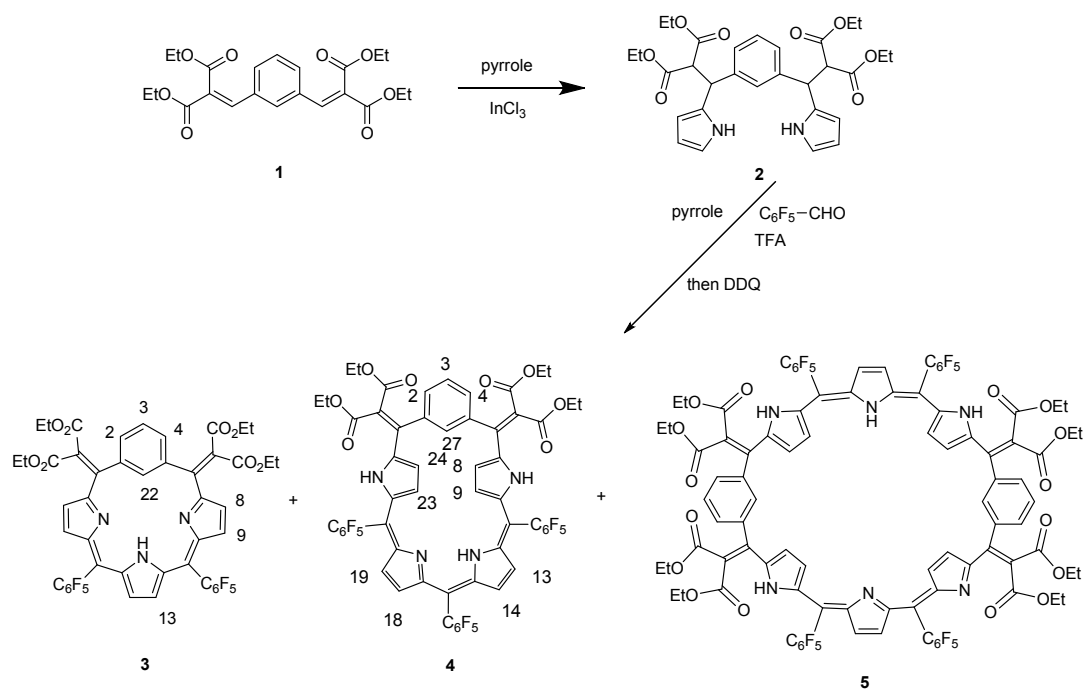


Fig. 1S: ^1H NMR spectrum of compound **5** in CDCl_3

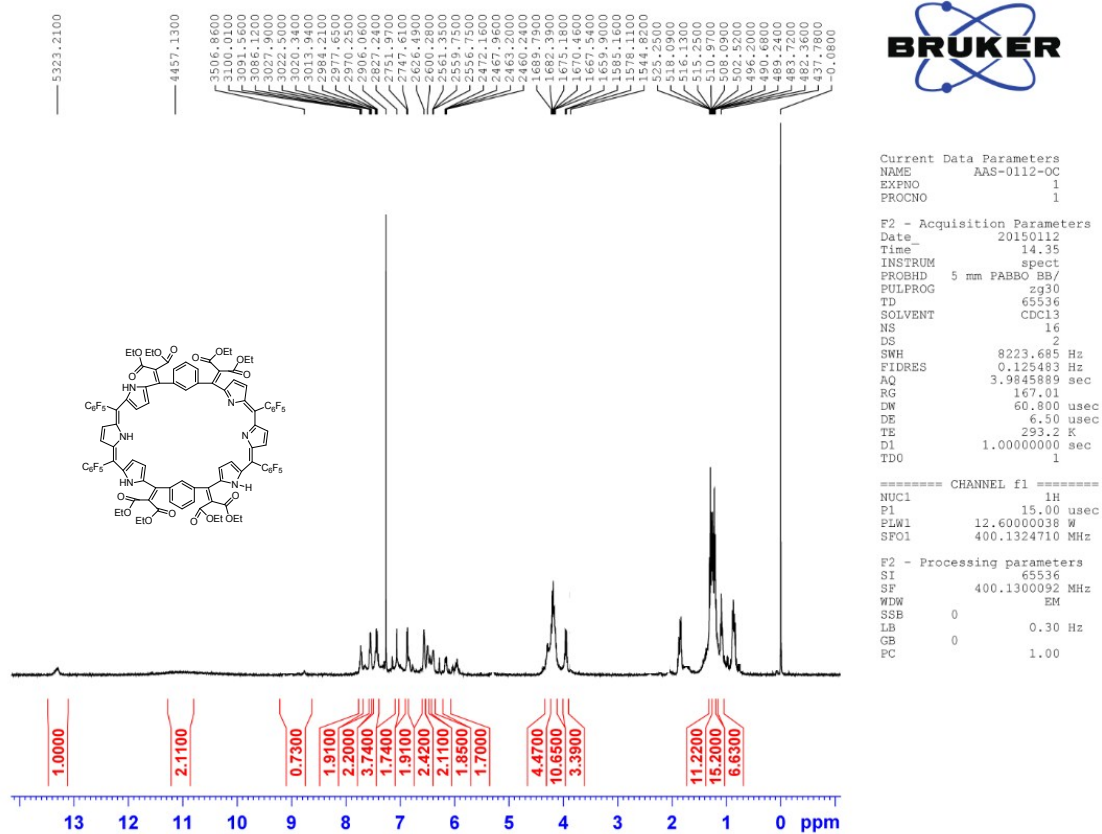


Fig. 2S: ^{13}C NMR spectrum of compound **5** in CDCl_3

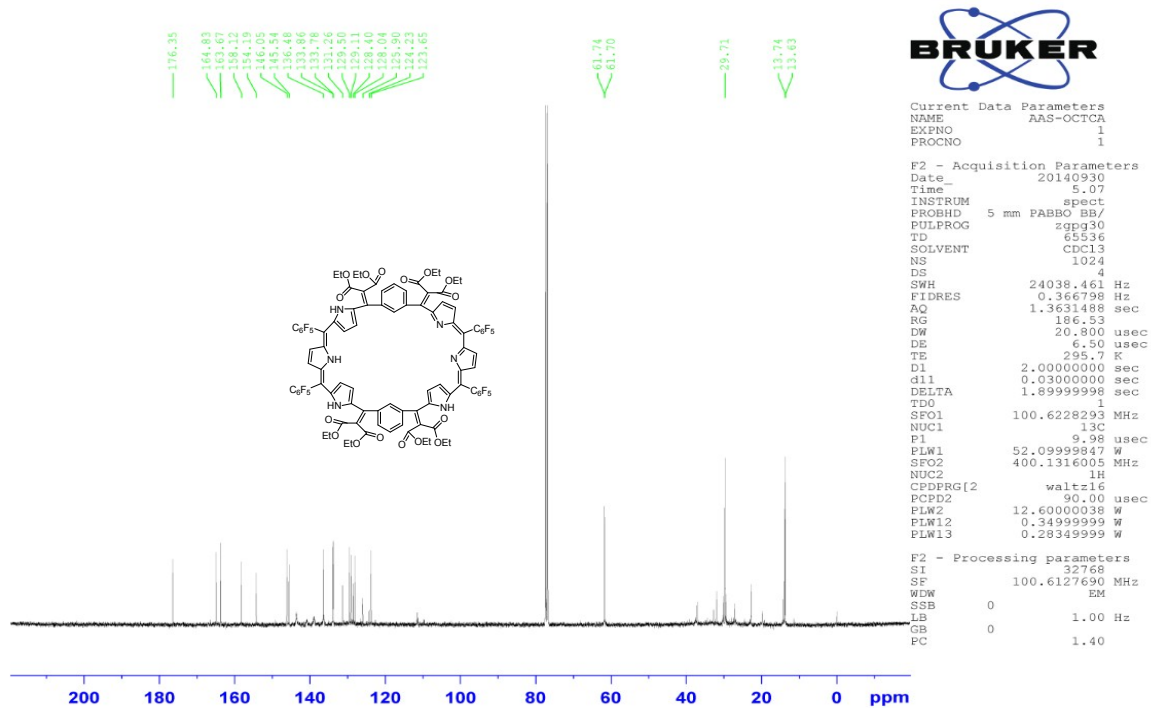


Fig. 3S: MALDI-TOF of compound 5

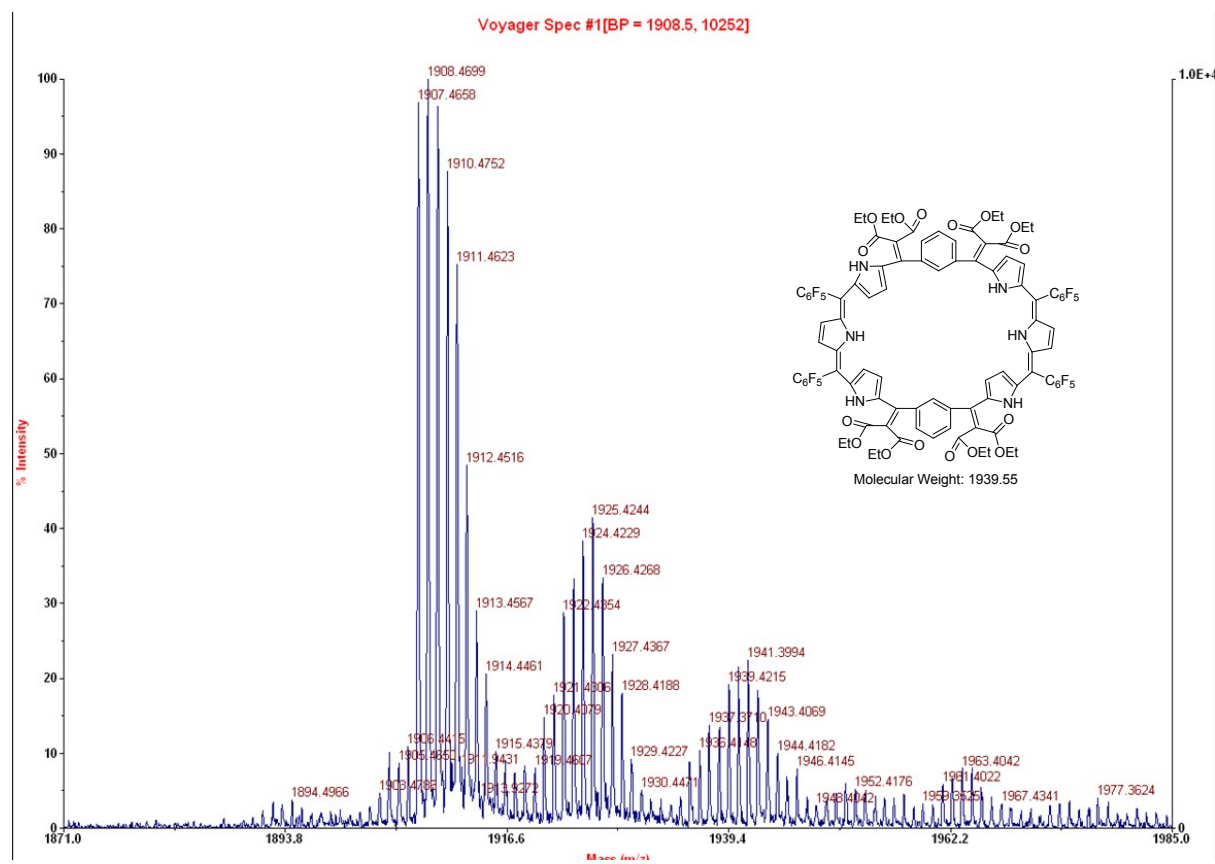


Fig. 4S: UV-Vis absorption spectral changes of *m*-benziotaphyrin **5** (2.06×10^{-5} M, in CH_3CN) observed upon titration with TFA. The black line corresponds to the spectrum of the free base, while the remaining spectra were recorded at increment of 0.25-100 molar equiv. of TFA.

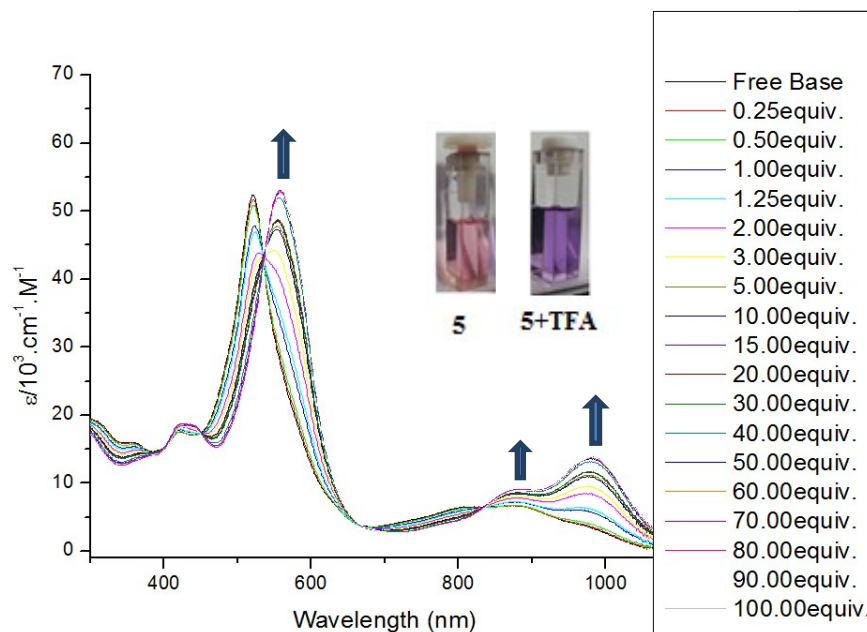


Fig. 5S: UV-Vis absorption spectra of *m*-benziotaphyrin **5** (green) ($20.6 \mu\text{M}$), *m*-benzipentaphyrin **4** (red) ($33.0 \mu\text{M}$), *m*-benziporphyrin **3** (black) ($40.9 \mu\text{M}$) in acetonitrile

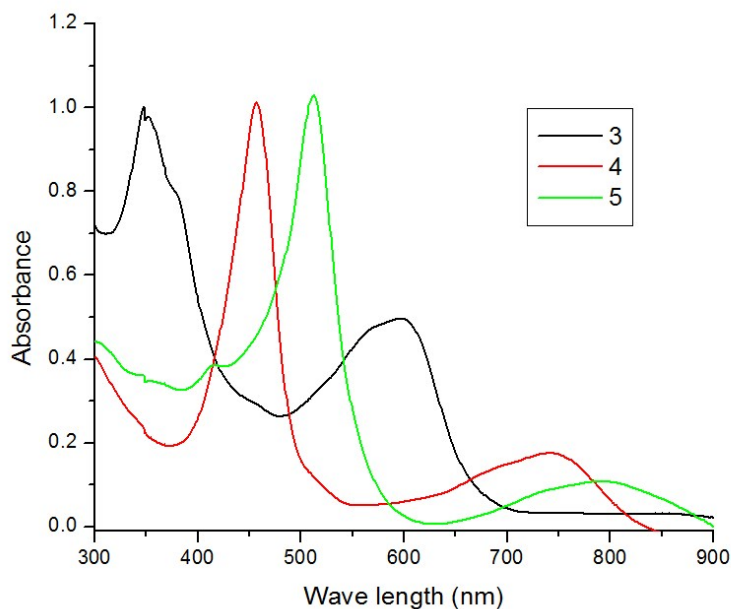


Fig. 6S: ^1H NMR spectrum of complex **7a** in CDCl_3

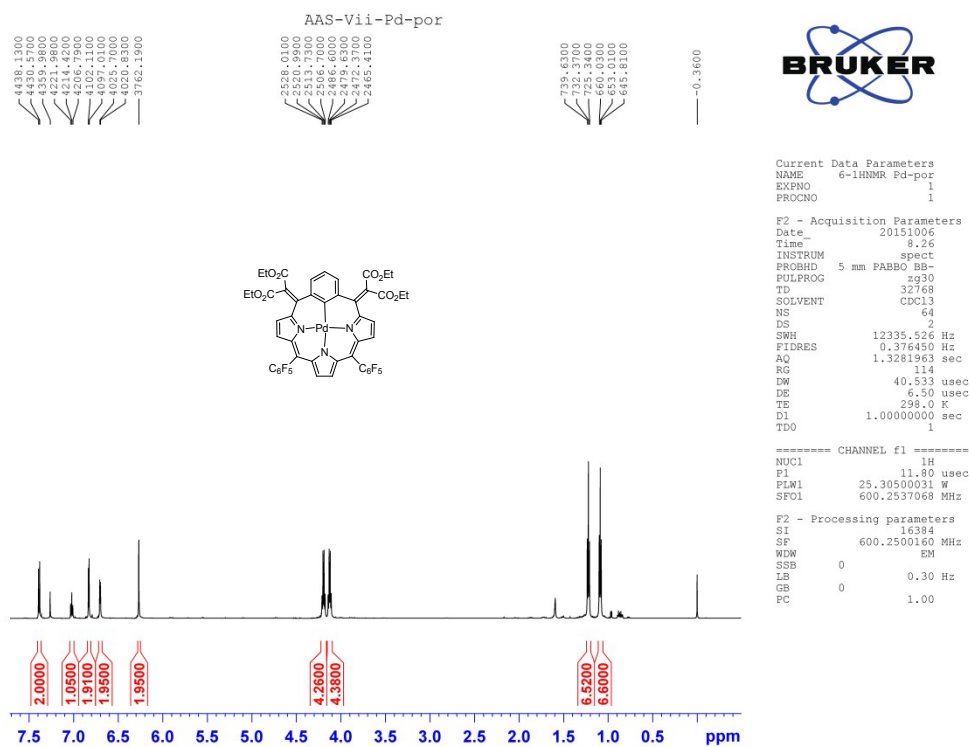


Fig. 7S: ^1H NMR spectrum of complex **7a** after addition of 30 equiv. TFA in CDCl_3

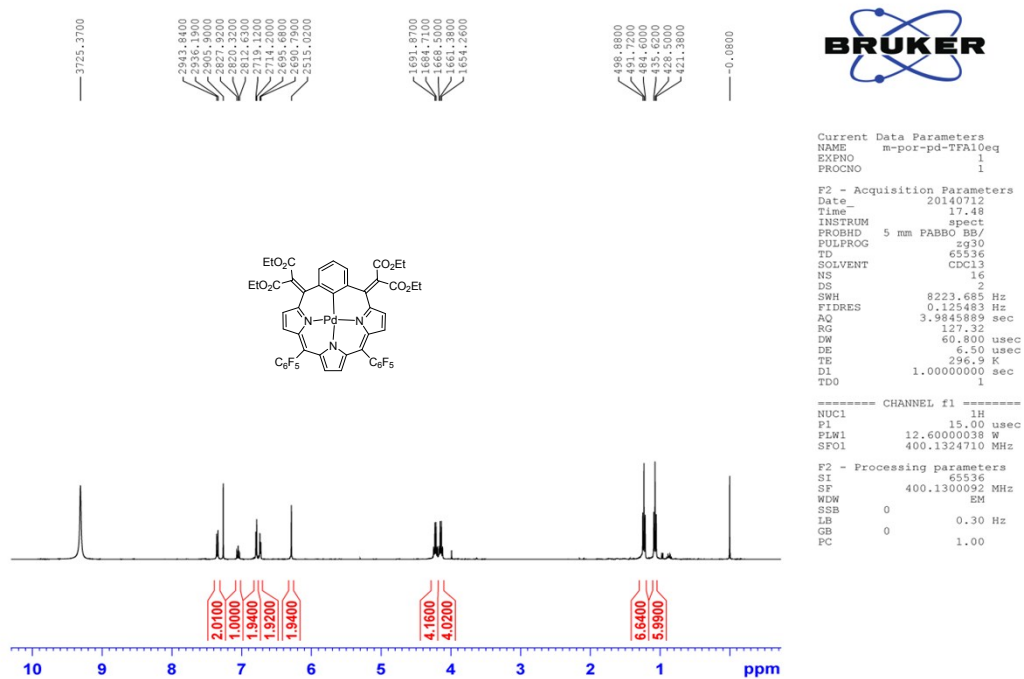


Fig. 8S: ^{13}C NMR spectrum of complex **7a** in CDCl_3

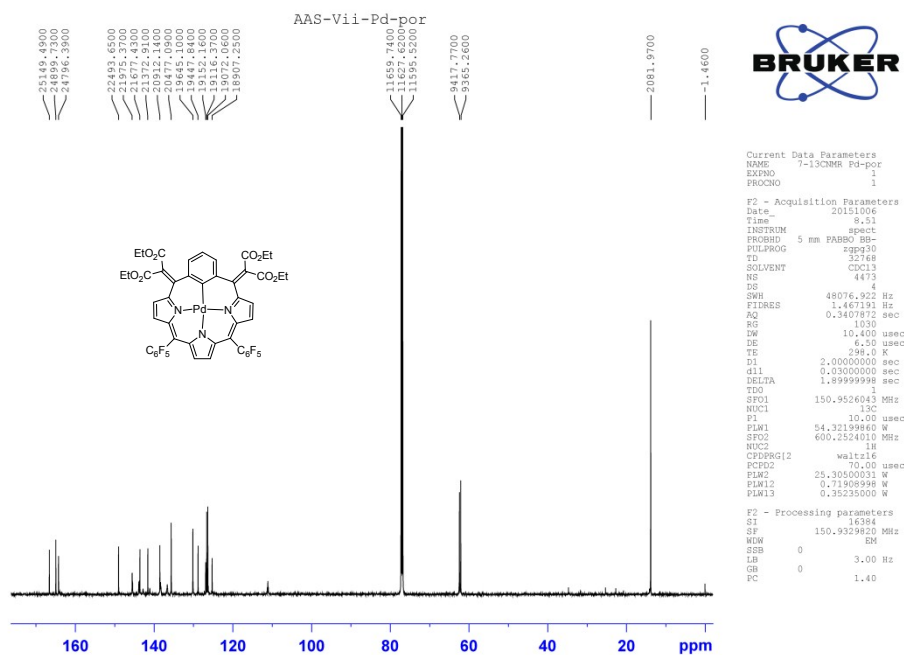


Fig. 9S: MALDI-TOF spectrum of complex **7a**

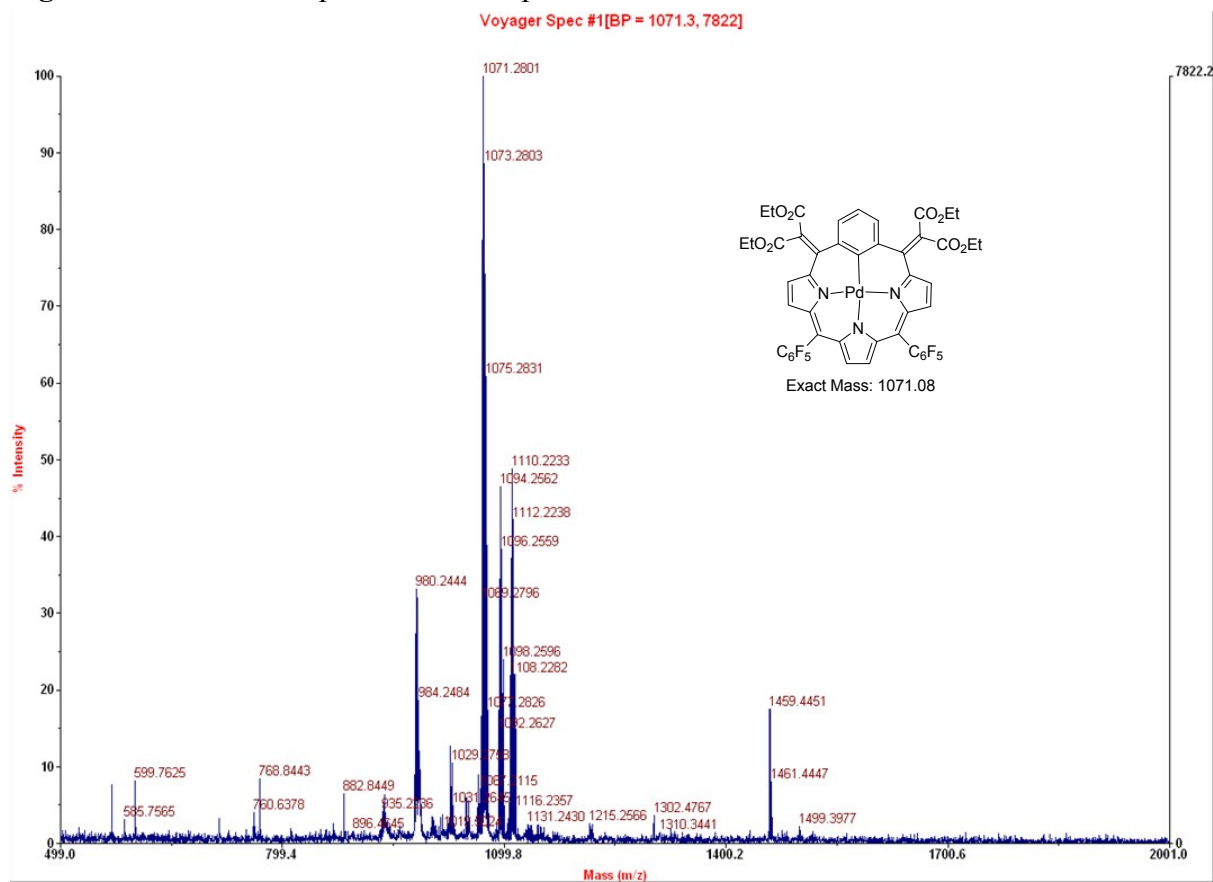


Fig. 10S: ^1H - ^1H COSY spectrum of **7a** in CDCl_3

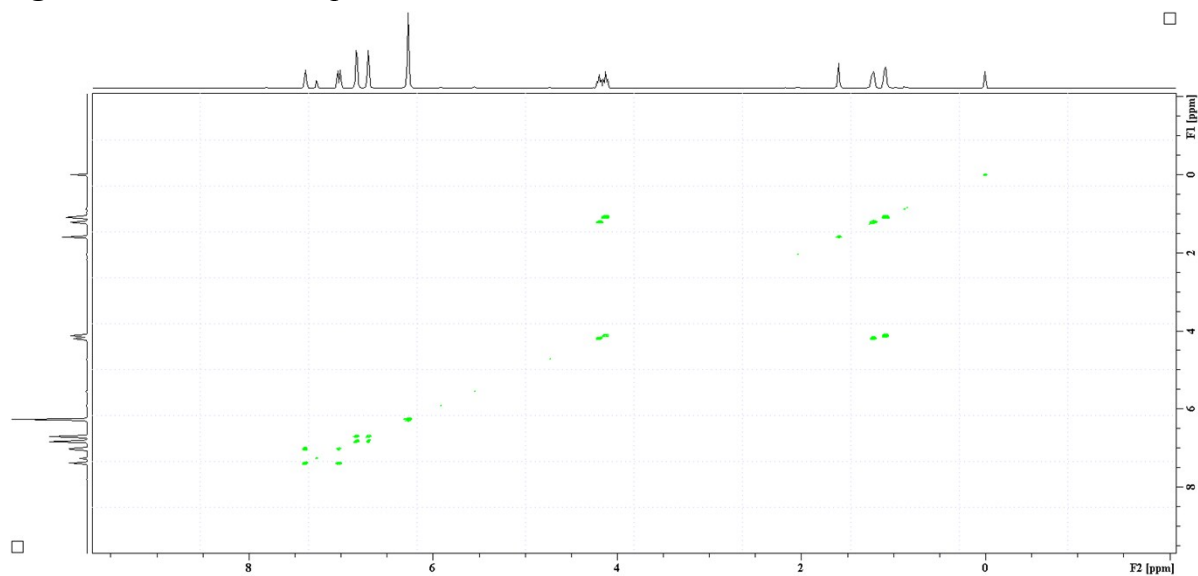


Fig. 11S: Partial region of ^1H - ^1H COSY spectrum of **7a** in CDCl_3 .

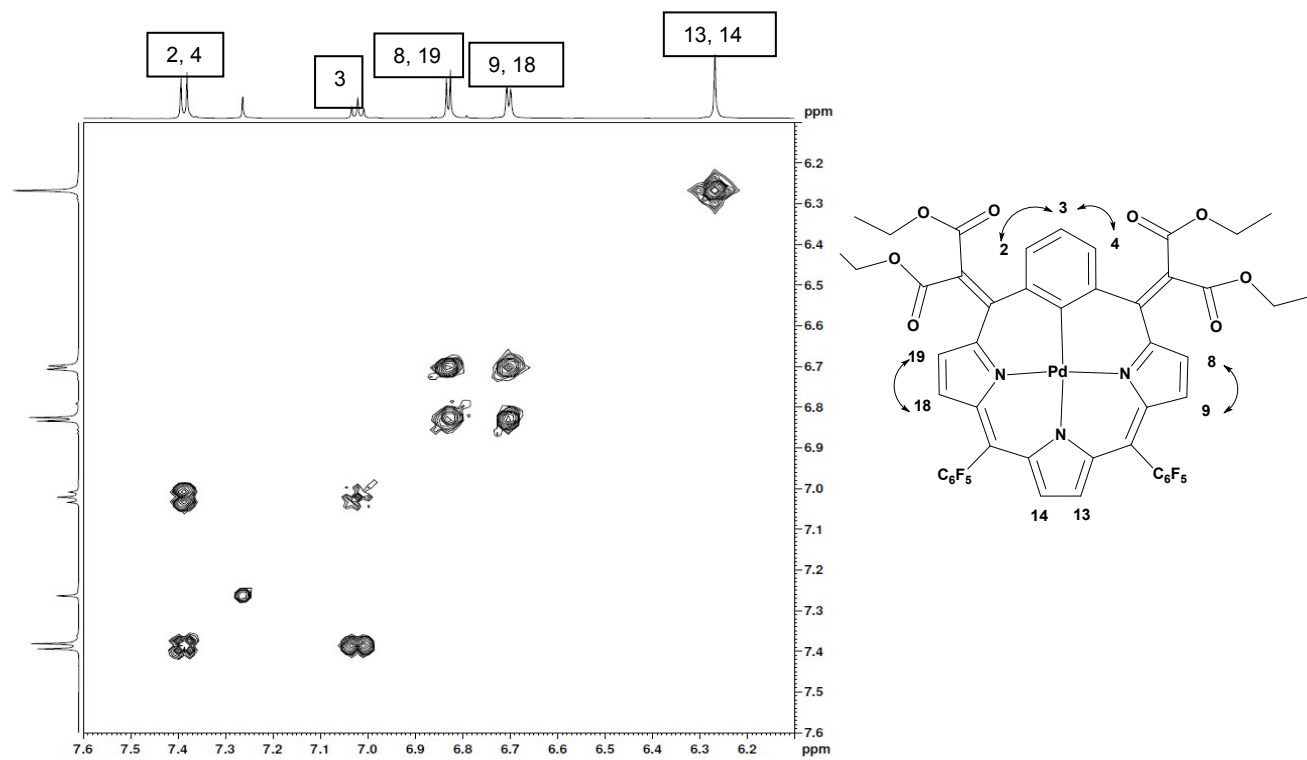


Fig. 12S: ^1H - ^{13}C HSQC spectrum of **7a** in CDCl_3 .

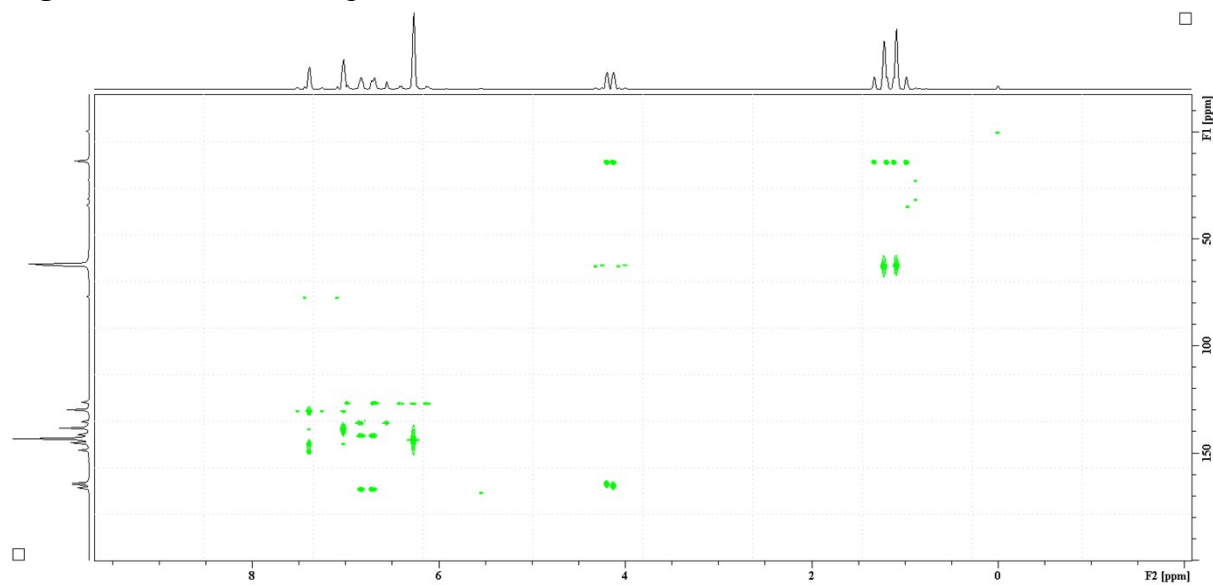


Fig. 13S: Selected region of ^1H - ^{13}C HSQC spectrum of **7a** in CDCl_3 .

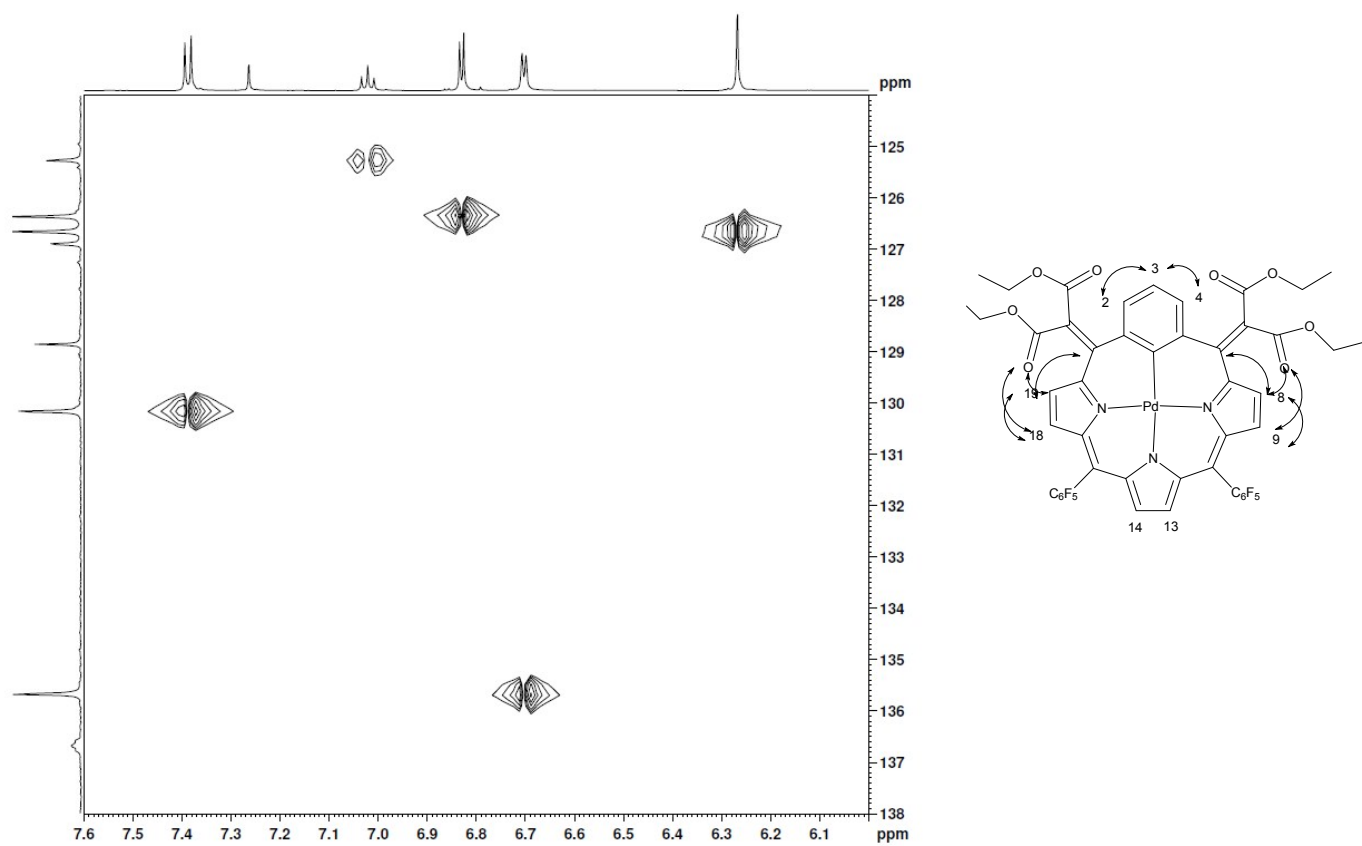


Fig. 14S: ^1H - ^{13}C HMBC spectrum of **7a** in CDCl_3 .

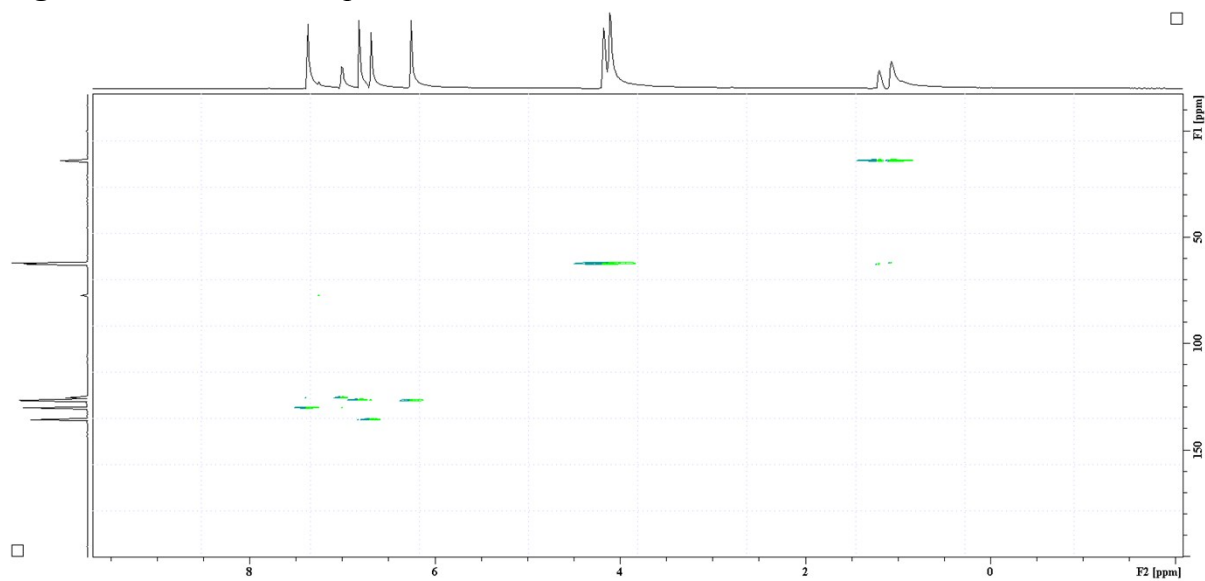


Fig. 15S: Partial region of ^1H - ^{13}C HMBC spectrum of **7a** in CDCl_3 .

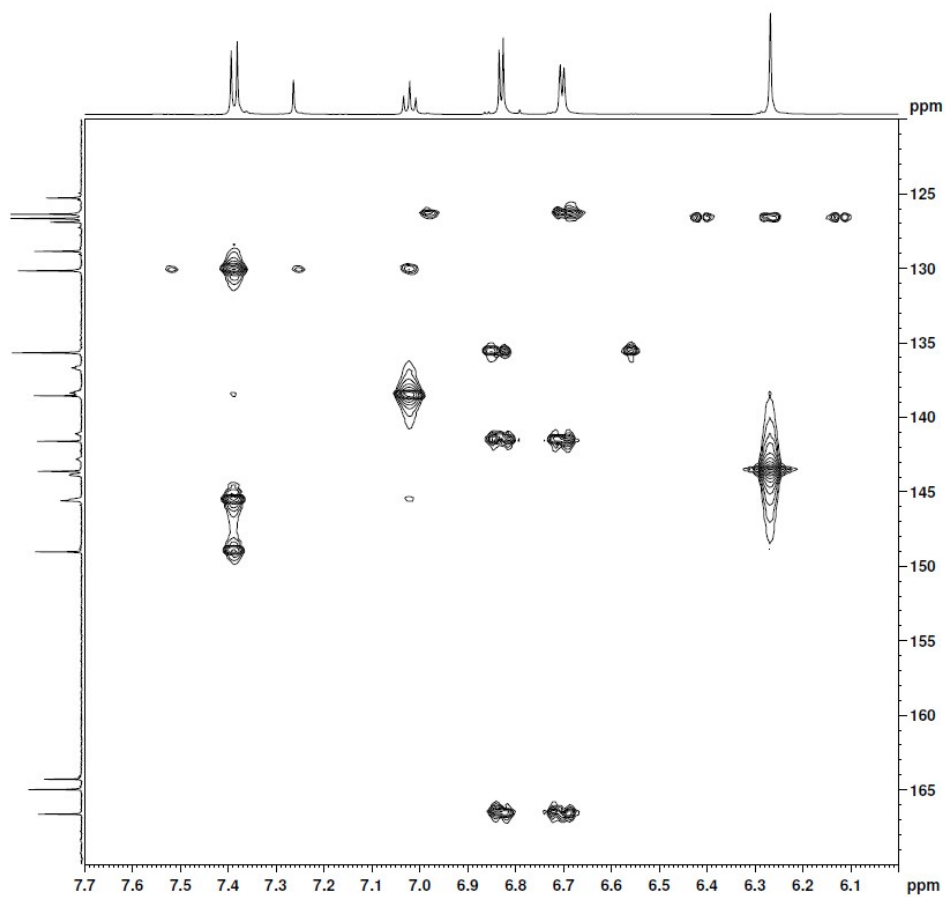


Fig. 16S: Solid state structure of Pd-(*m*-benzi) porphyrin **7a** from X-ray diffraction analysis:

A) top view and B) side view

A)

B)

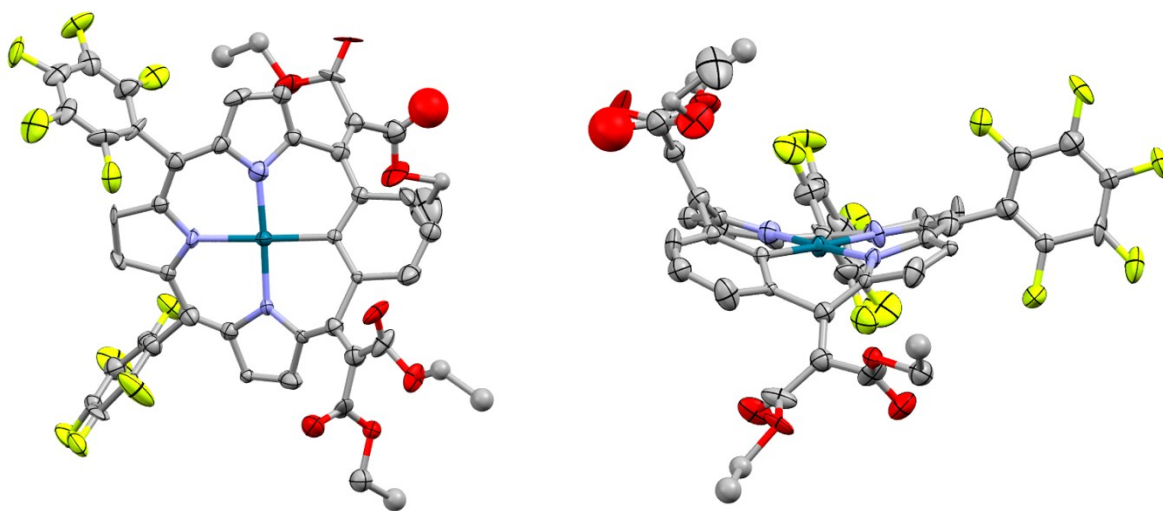


Fig. 17S: ¹H NMR spectrum of complex **7c** in CDCl₃

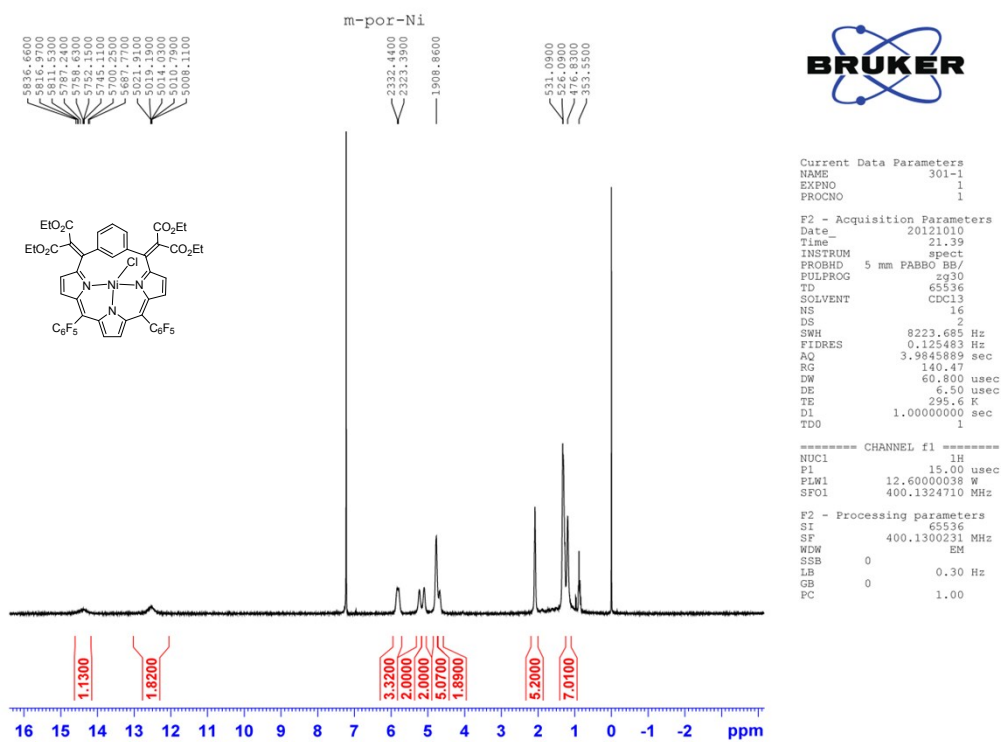


Fig. 18S: MALDI-TOF spectrum of complex 7c

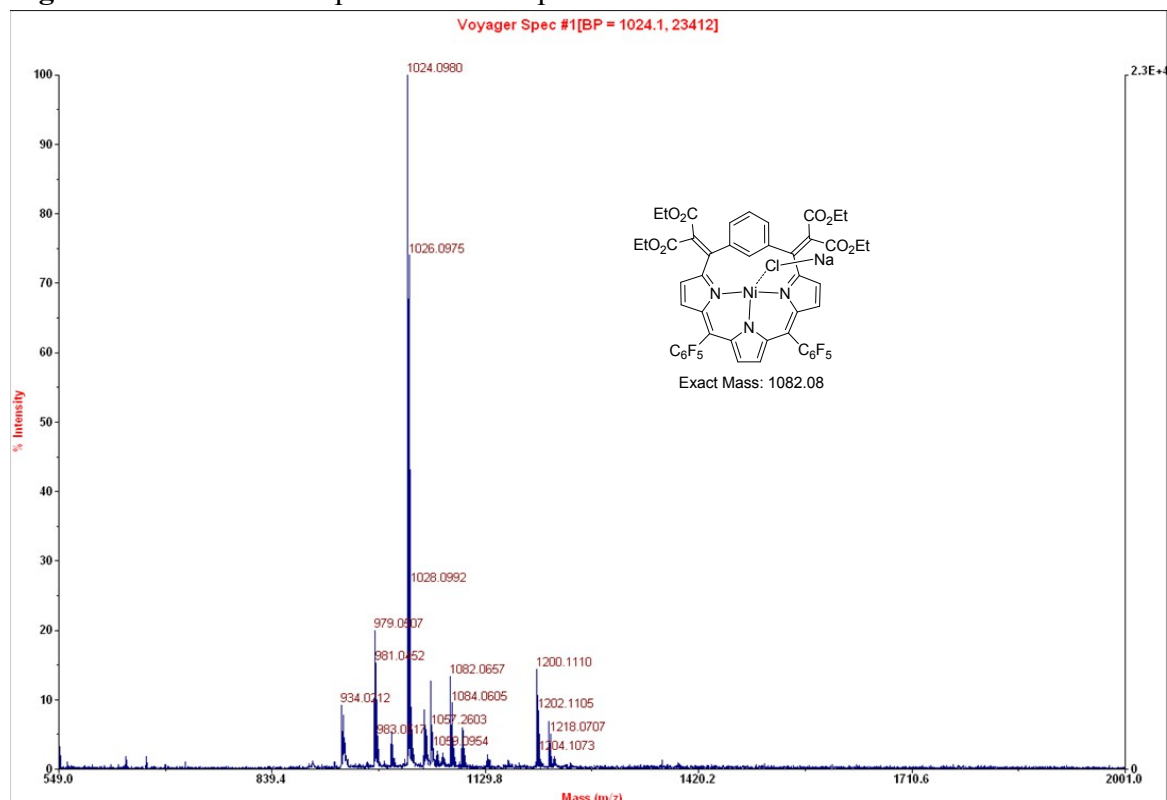


Fig. 19S: ¹H NMR spectrum of complex 7d in CDCl₃

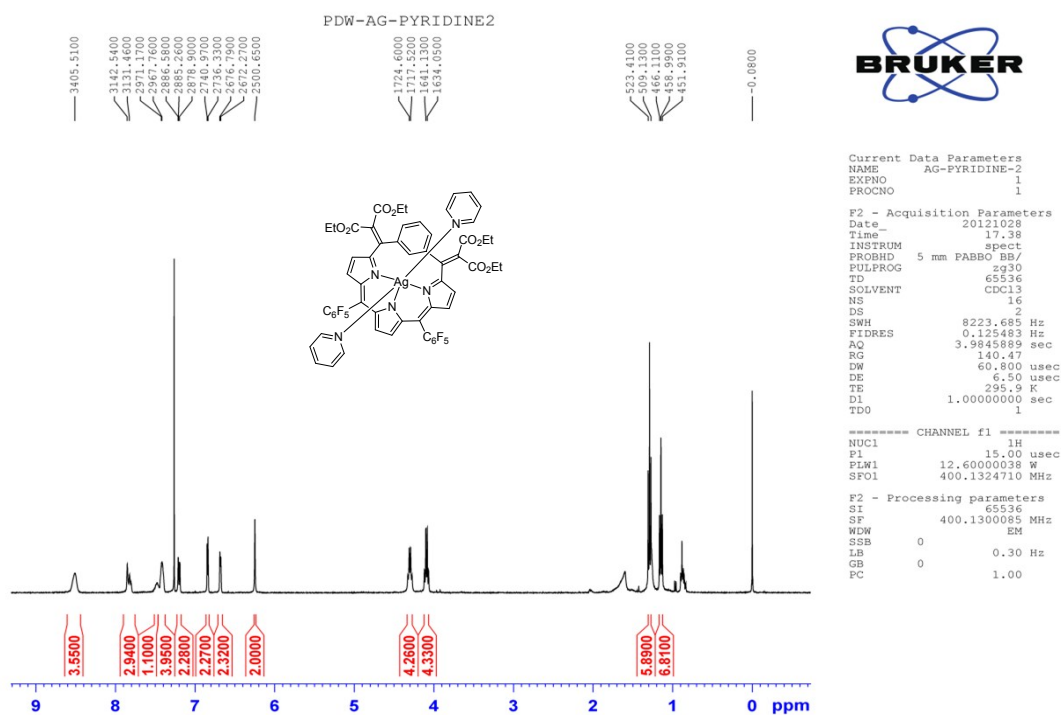


Fig. 20S: MALDI-TOF spectrum of complex **7d**

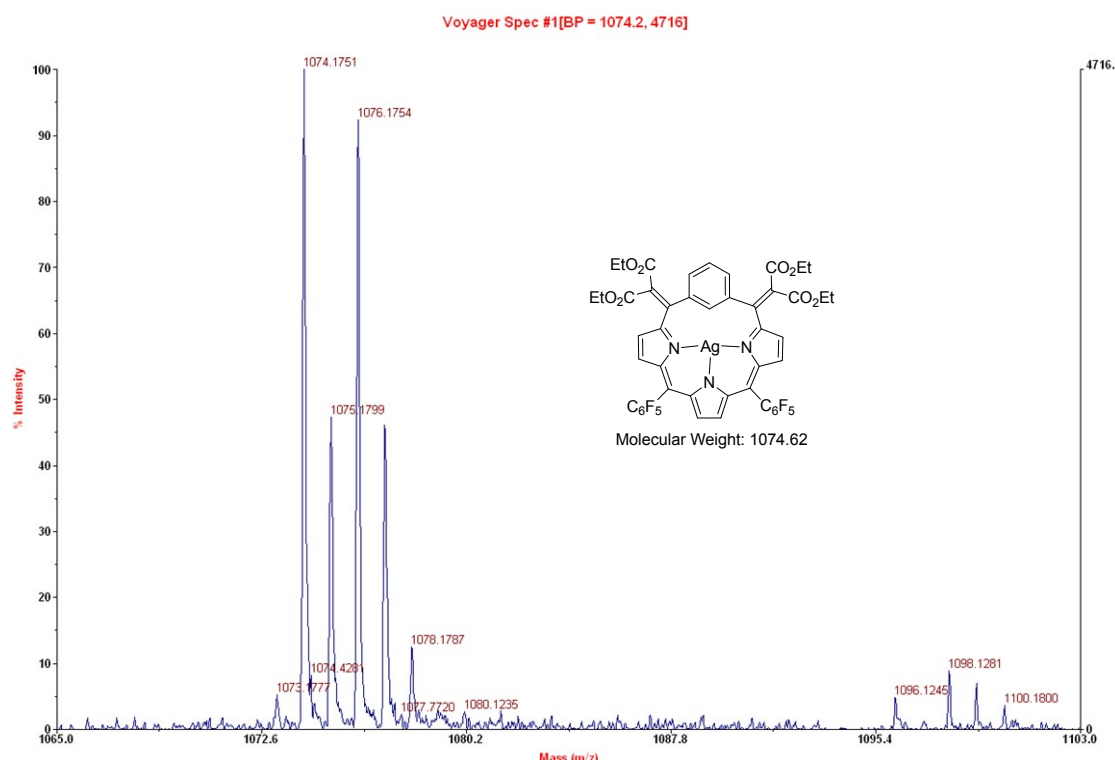


Fig. 21S: ^1H NMR spectrum of complex **8** in CDCl_3

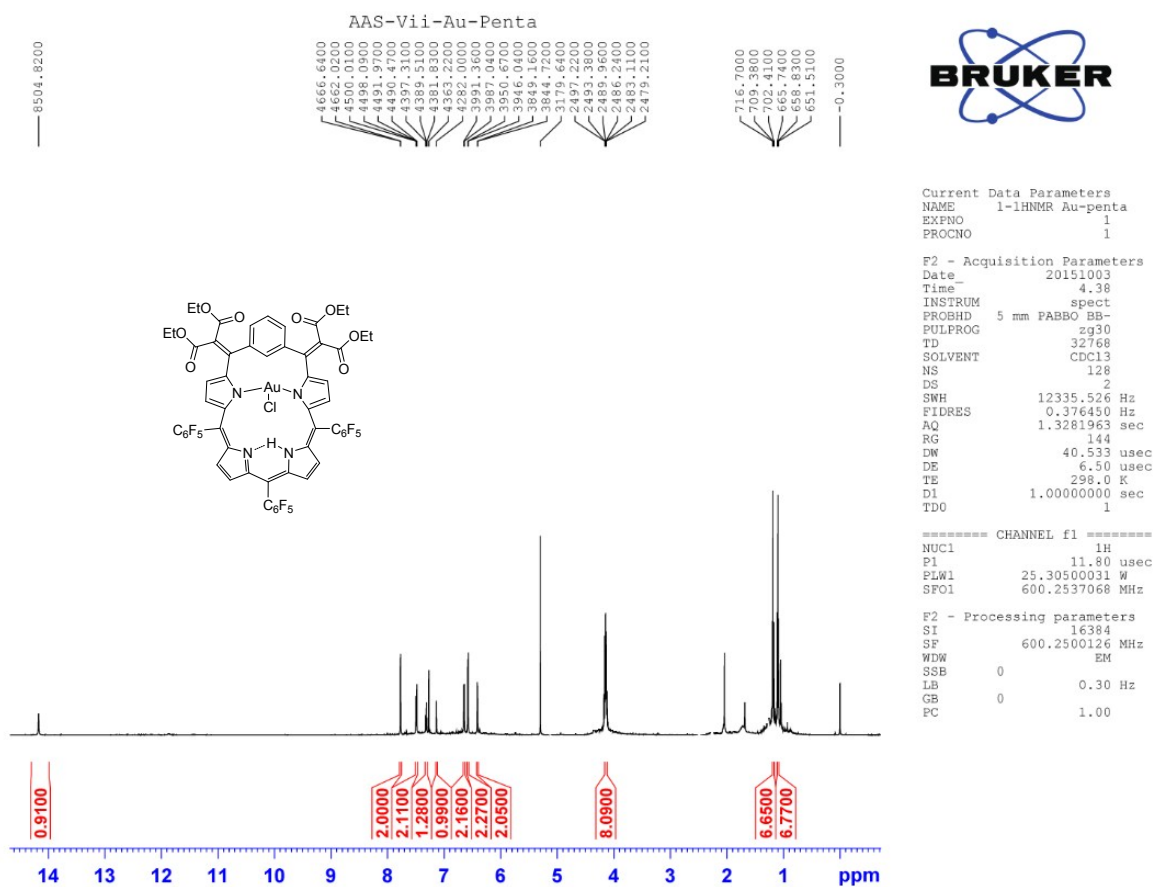


Fig. 22S: ^{13}C NMR spectrum of complex **8** in CDCl_3

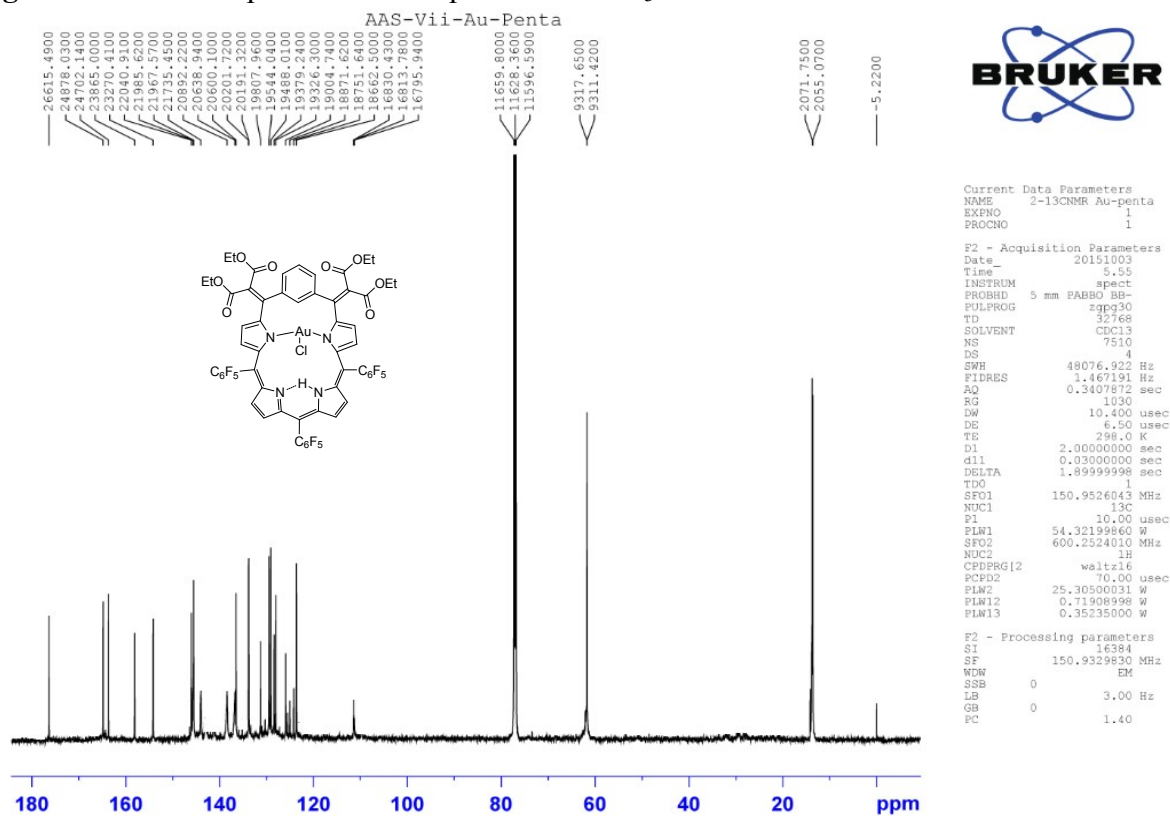


Fig. 23S: MALDI-TOF spectrum of complex **8**

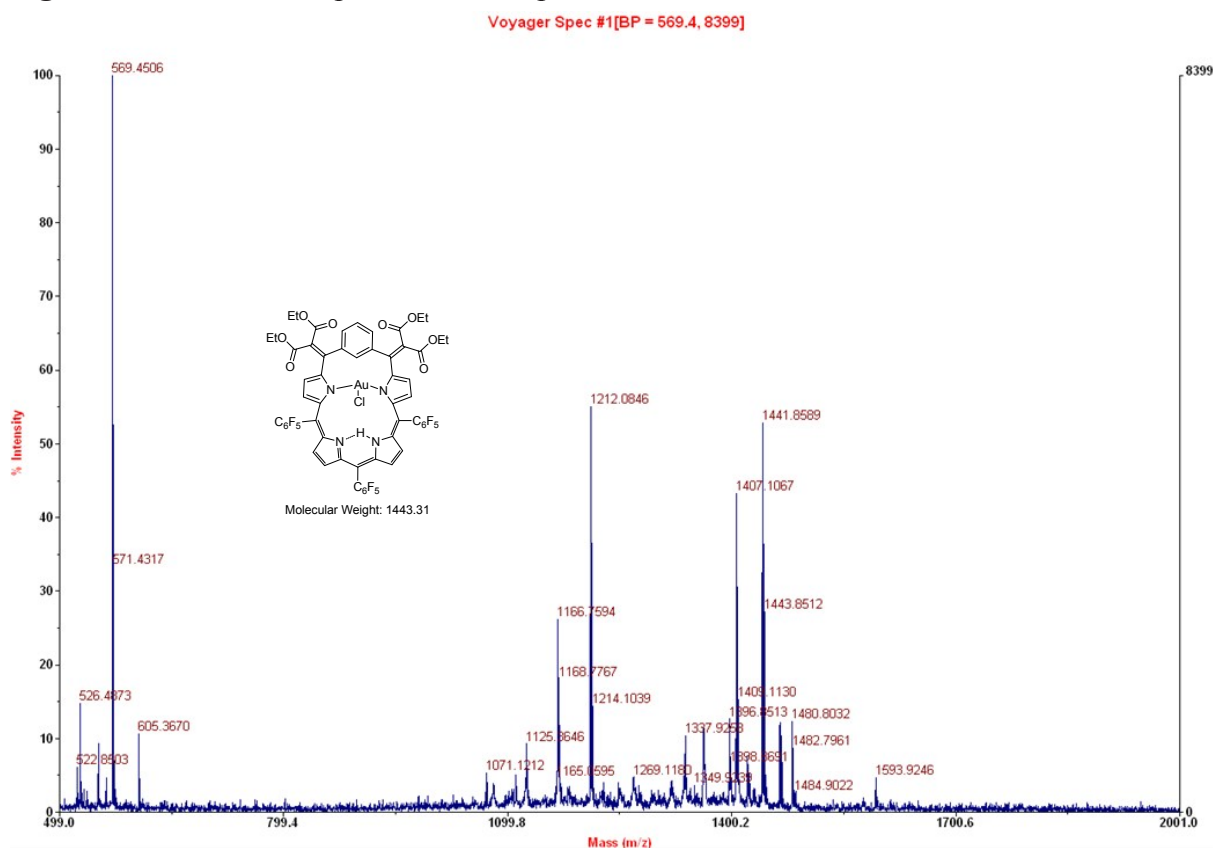


Fig. 24S: ^1H - ^1H COSY spectrum of **8** in CDCl_3 .

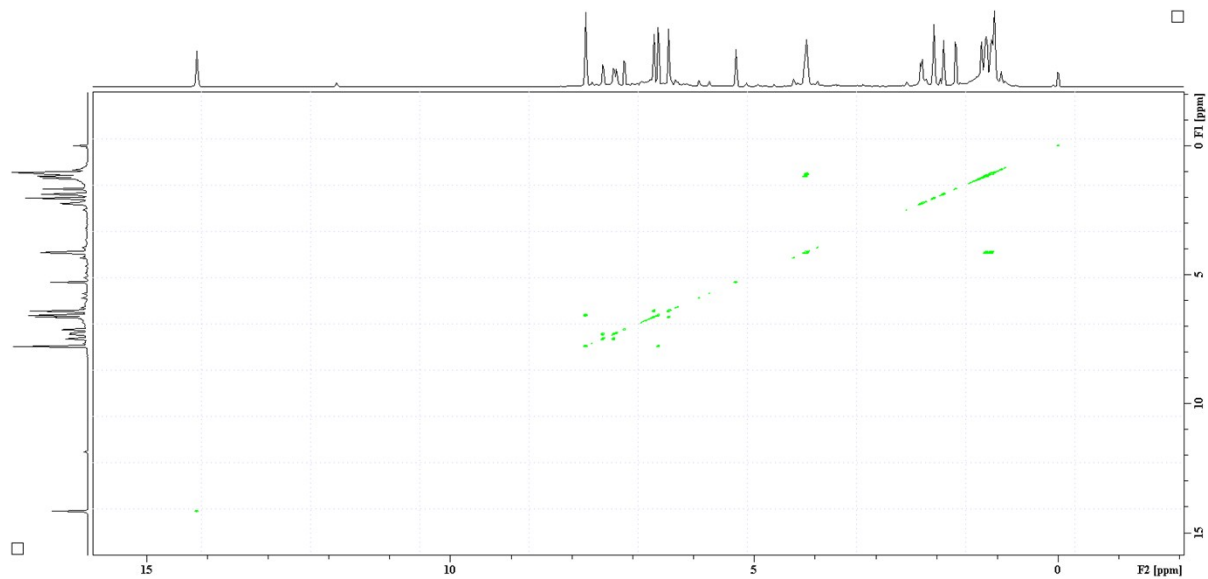


Fig. 25S: Selected region of ^1H - ^1H COSY spectrum of **8** in CDCl_3 .

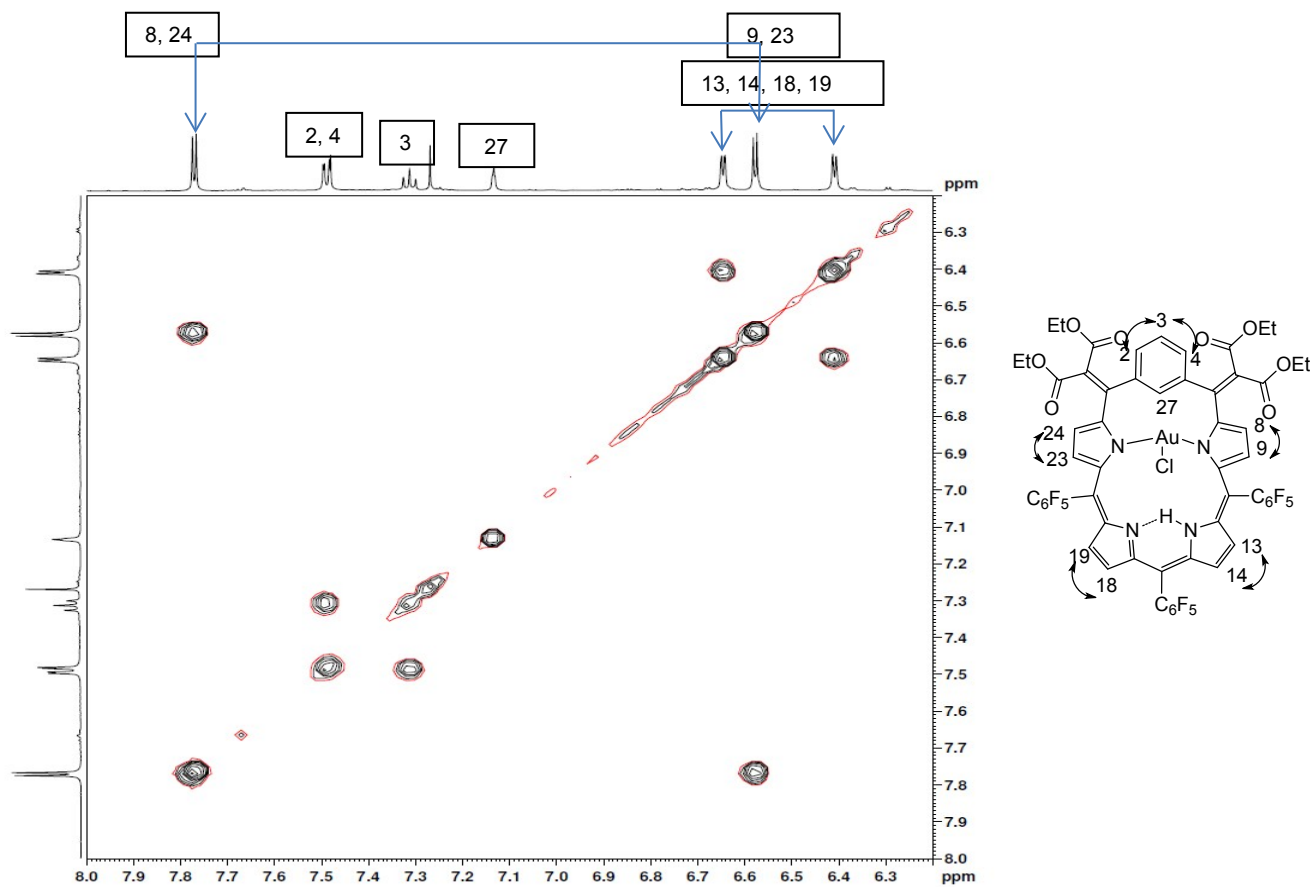


Fig. 26S: ^1H - ^{13}C HSQC NMR spectrum of **8** in CDCl_3 .

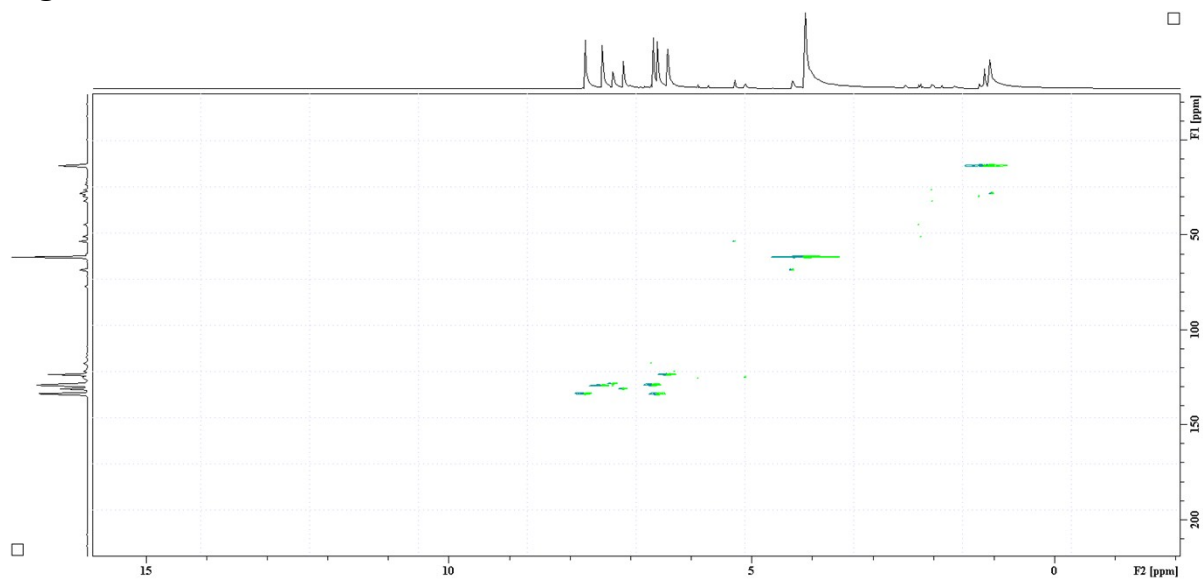


Fig. 27S: Partial region of ^1H - ^{13}C HSQC spectrum of **8** in CDCl_3 .

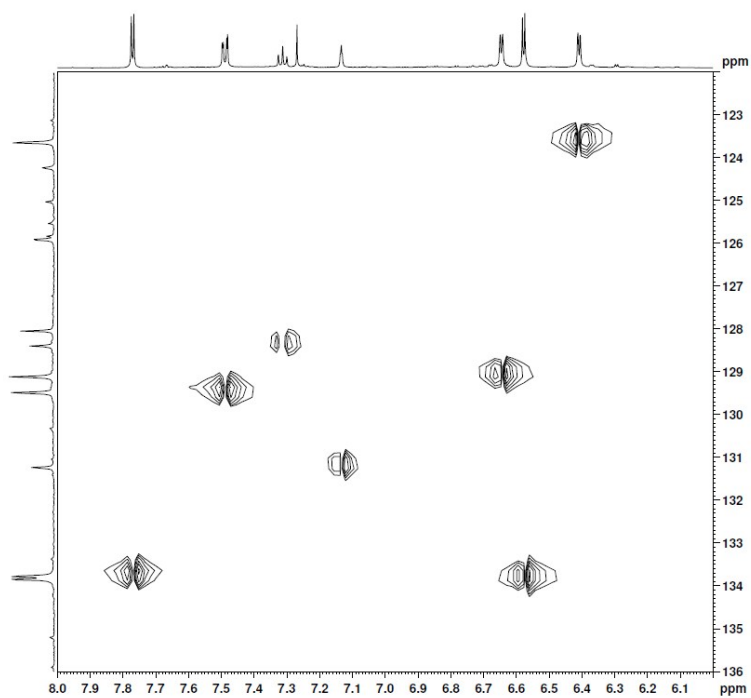


Fig. 28S: ^1H - ^{13}C HMBC spectrum of **8** in CDCl_3 .

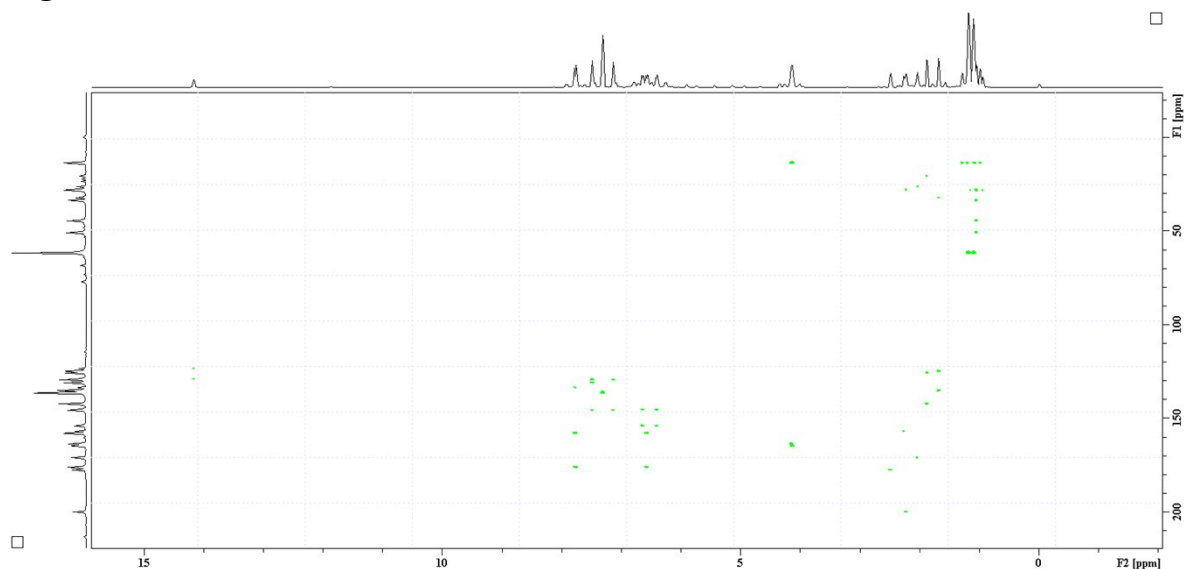


Fig. 29S: Selected region of ^1H - ^{13}C HMBC spectrum of **8** in CDCl_3 .

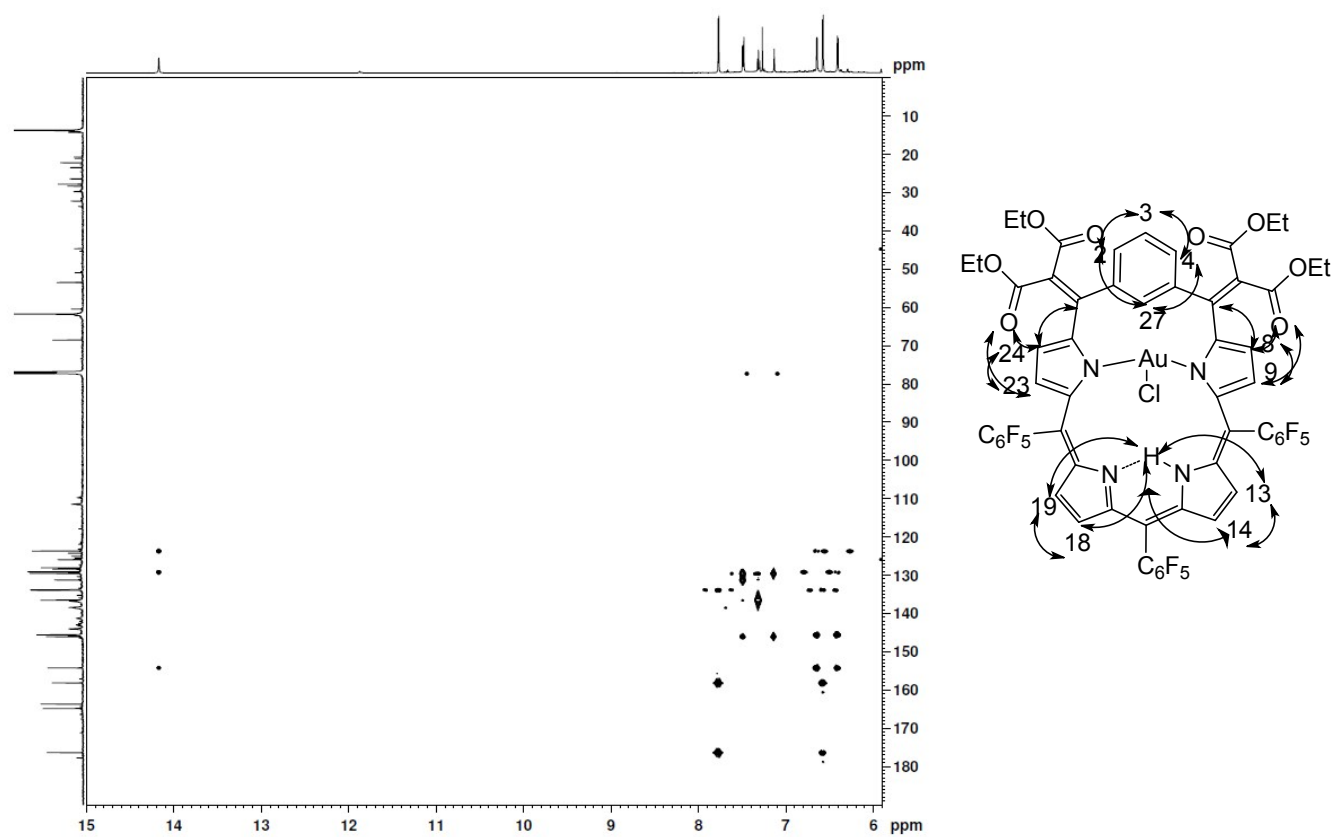
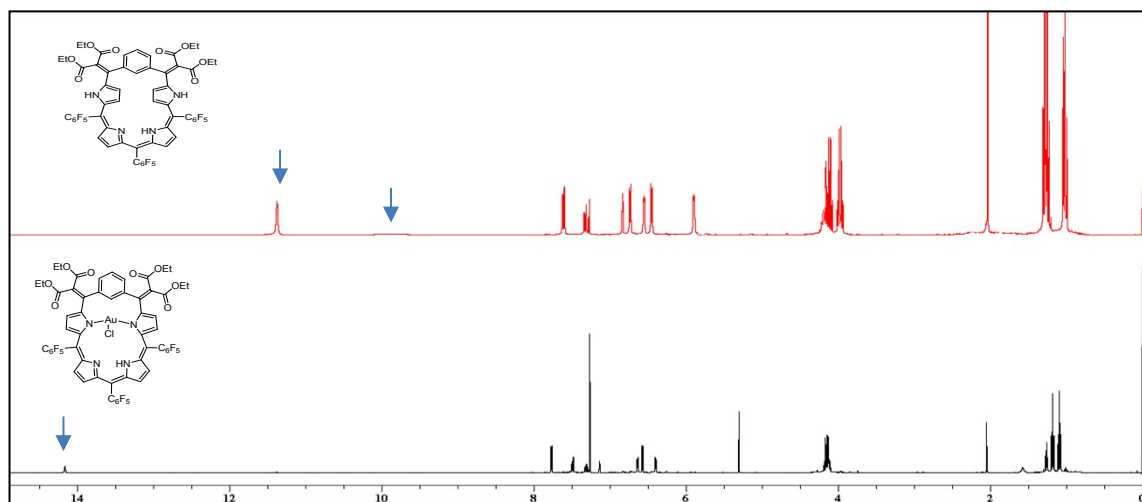
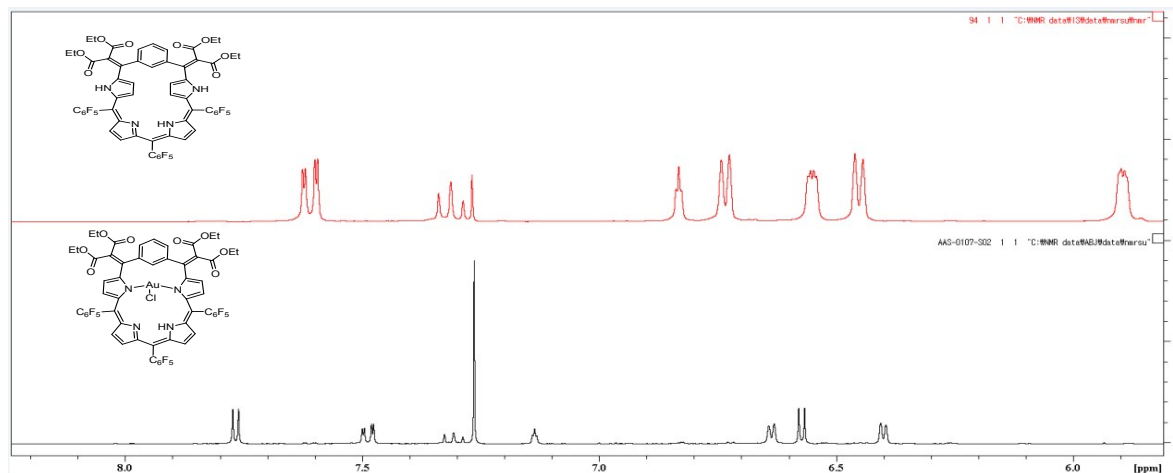


Fig. 30S: Comparative ^1H NMR spectra of **4** (top) and Au(III) complex **8** (bottom, CDCl_3 , 300 K)



Expanded aromatic region of comparative ^1H NMR spectra



Expanded aliphatic region of comparative ^1H NMR spectra

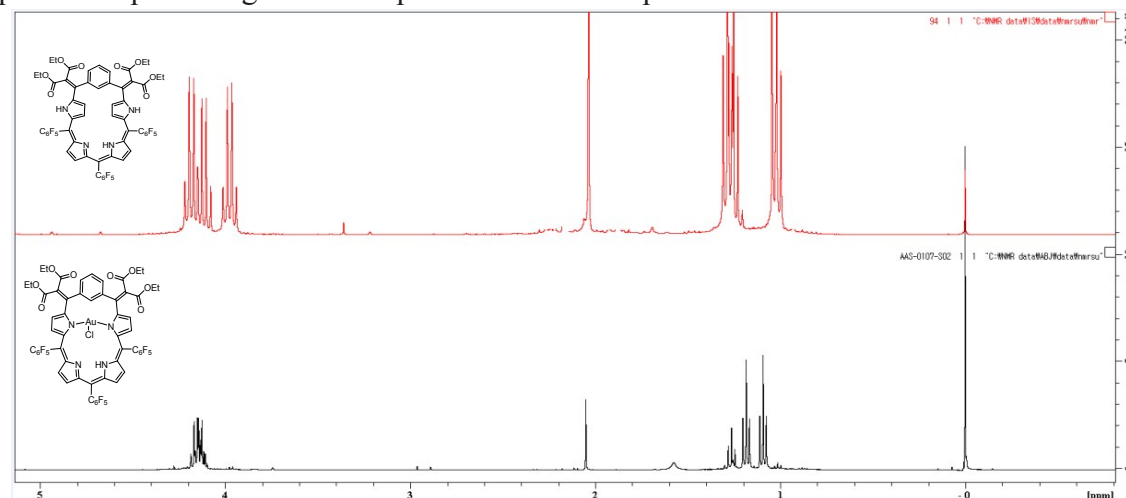


Fig. 31S: ^1H NMR spectrum of complex **9** in CDCl_3

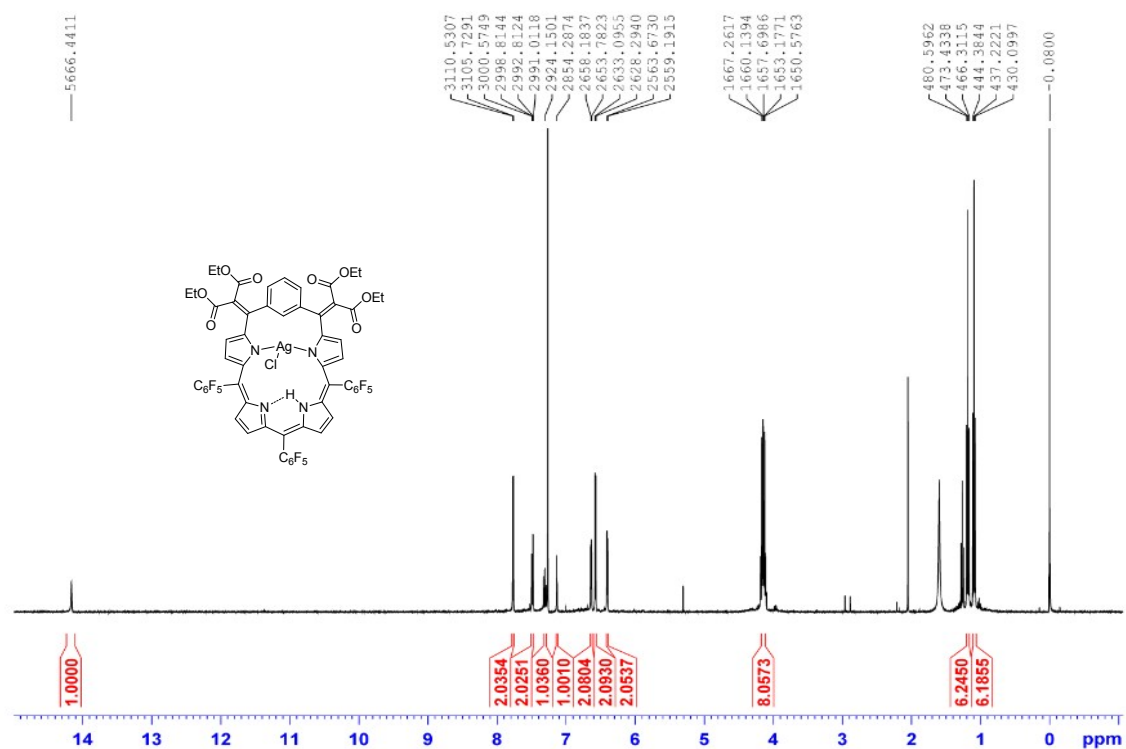


Fig. 32S: ^{13}C NMR spectrum of complex **9** in CDCl_3

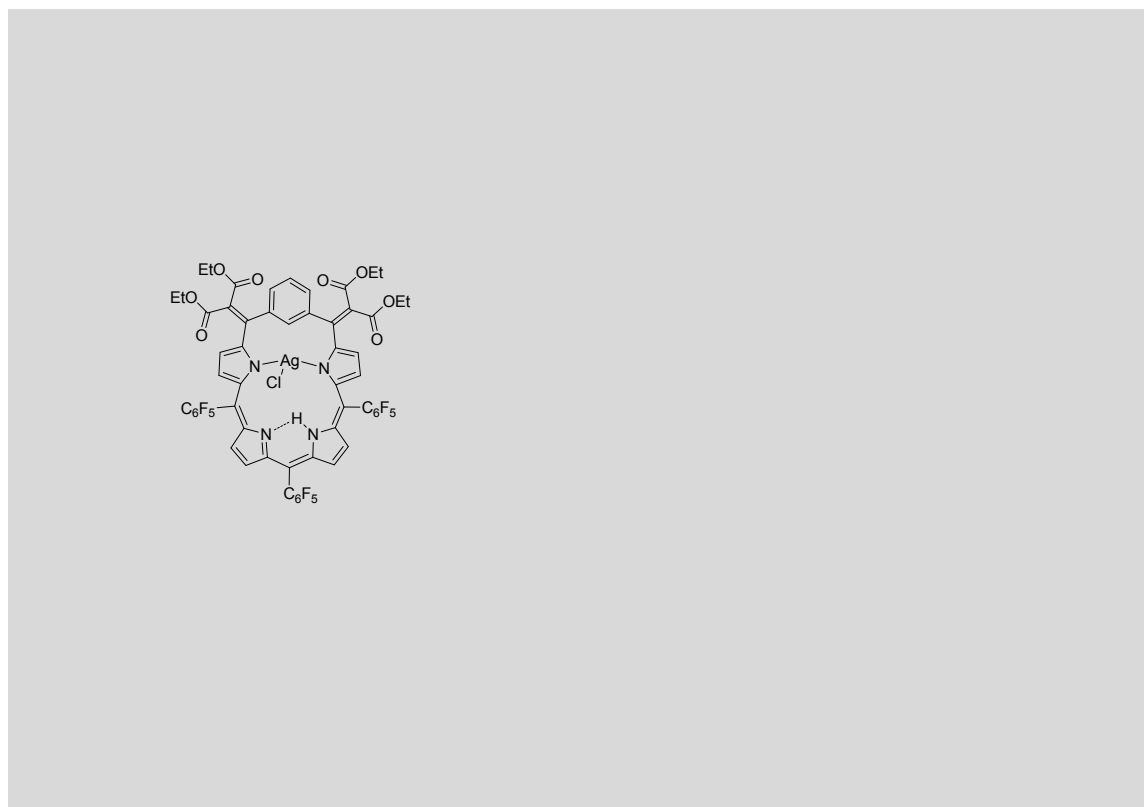


Fig. 33S: MALDI-TOF spectrum of complex **9**

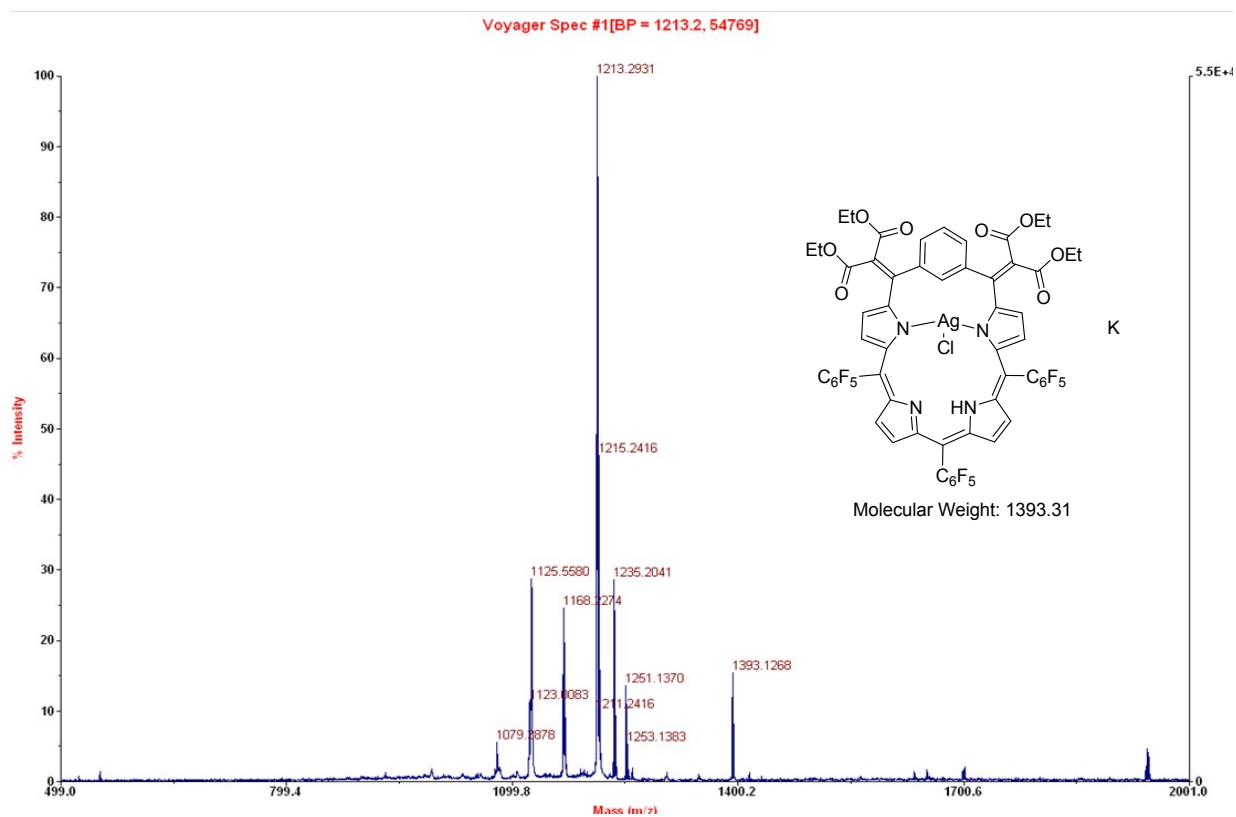


Fig. 34S: Comparative ^1H NMR spectra of **4** (top) and Ag(III) complex **9** (bottom) in CDCl_3 at 300 K.

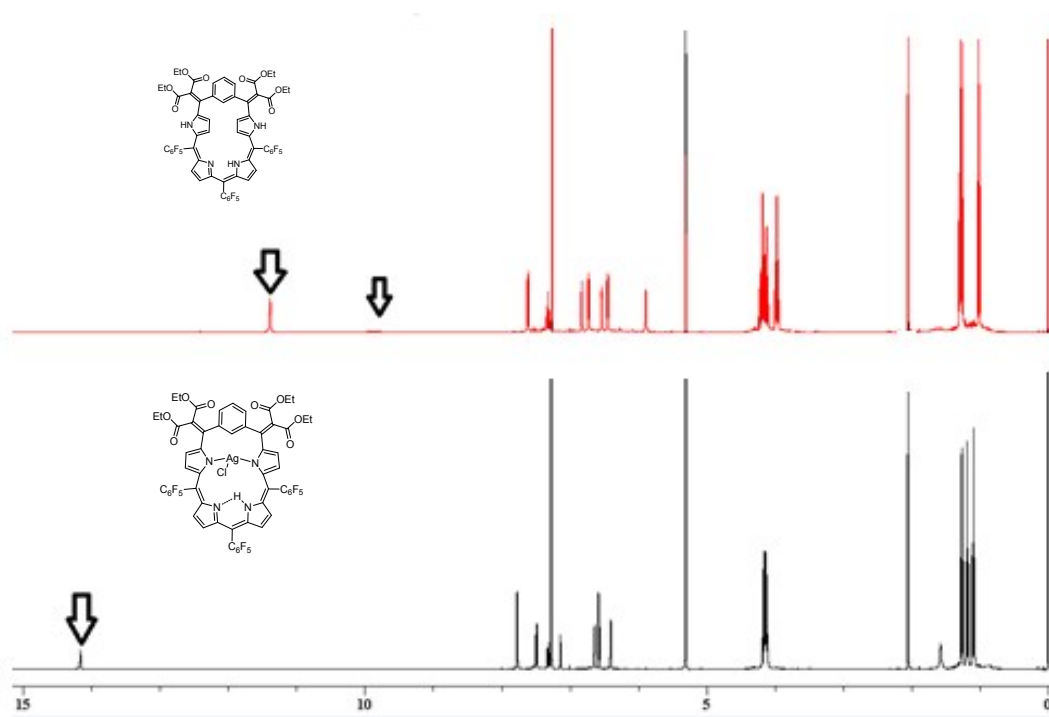


Fig. 35S: UV-Vis absorption spectra of *m*-benzipentaphyrin **4** (green) (33.0 μM), Au-complex **8** (red) (27.7 μM), Ag-complex **9** (black) (28.7 μM) in acetonitrile.

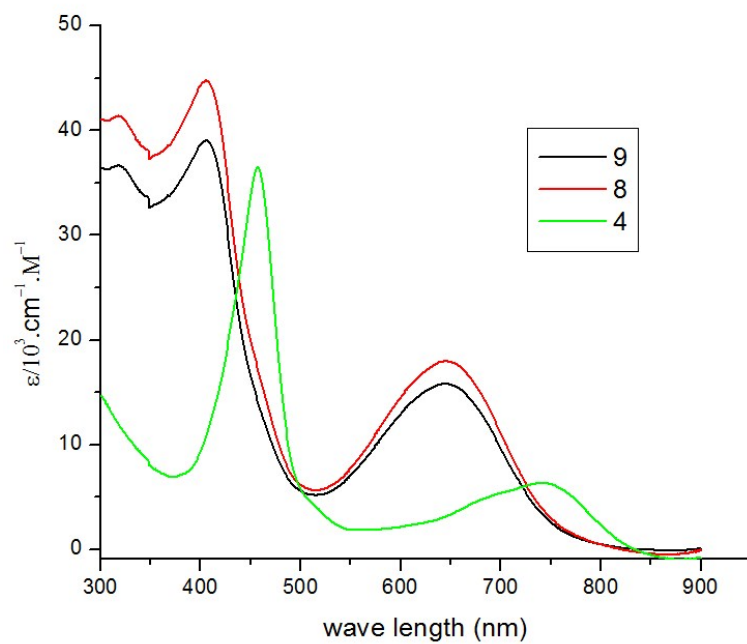


Table 1S: Crystal data and structure refinement for complex **7a**.

Empirical formula	$C_{96}H_{23}F_{20}N_6O_{17.5}Pd_2$	
Formula weight	2133.00	
Temperature	170(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	$a = 17.137(3)$ Å	$\alpha = 90.00^\circ$
	$b = 24.199(5)$ Å	$\beta = 94.81(3)^\circ$
	$c = 23.303(5)$ Å	$\gamma = 90.00^\circ$
Volume	$9630(3)$ Å ³	
Z	4	
Density (calculated)	1.471 Mg/m ³	
Absorption coefficient	0.480 mm ⁻¹	
F(000)	4212	
Crystal size	0.15 x 0.03 x 0.03 mm ³	
Theta range for data collection	1.65 to 26.00°	
Index ranges	-11 ≤ h ≤ 21, -29 ≤ k ≤ 29, -28 ≤ l ≤ 26	
Reflections collected	26742	
Independent reflections	12070 [R(int) = 0.0983]	
Completeness to theta = 26.00°	99.0 %	
Absorption correction	multi-scan	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	12070 / 332 / 1278	
Goodness-of-fit on F ²	0.984	
Final R indices [I > 2σ(I)]	R ₁ = 0.0712, wR ₂ = 0.1728	
R indices (all data)	R ₁ = 0.1210, wR ₂ = 0.2045	
Absolute structure parameter	0.15(9)	
Largest diff. peak and hole	1.196 and -0.690 e·Å ⁻³	

Table 2. Atomic coordinates (Å x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for Pd. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	8376(2)	2457(1)	3254(1)	27(1)
Pd(2)	1165(2)	2458(1)	5098(1)	25(1)
F(11)	5876(8)	1231(5)	2844(7)	58(4)
F(12)	4950(7)	371(6)	2488(7)	80(5)
F(13)	5612(7)	-541(6)	2019(7)	62(4)
F(14)	7204(8)	-579(5)	2031(6)	62(4)
F(15)	8104(8)	293(6)	2353(8)	88(6)
F(16)	9875(7)	1140(5)	4932(6)	56(4)
F(17)	10000(9)	625(7)	5948(6)	81(5)
F(18)	9076(8)	887(6)	6771(6)	65(4)
F(19)	8003(8)	1731(7)	6607(6)	67(5)
F(21)	-301(8)	1150(6)	3426(6)	66(4)
F(22)	-458(8)	629(6)	2400(7)	82(5)

F(23)	513(8)	902(6)	1546(6)	67(4)
F(24)	1544(9)	1710(6)	1746(6)	67(4)
F(25)	1729(7)	2232(5)	2768(5)	48(3)
F(26)	3739(7)	1233(6)	5511(6)	57(4)
F(27)	4634(8)	383(10)	5990(10)	42(5)
F(37)	4584(9)	330(14)	5775(13)	69(9)
F(28)	3901(8)	-557(6)	6270(7)	68(4)
F(29)	2368(8)	-582(6)	6399(7)	72(4)
F(110)	7840(8)	2243(7)	5584(6)	61(4)
F(210)	1474(8)	257(6)	5951(7)	67(4)
N(11)	8117(9)	2117(6)	2478(7)	23(4)
N(12)	8139(10)	1729(6)	3651(7)	30(4)
N(13)	8598(10)	2765(7)	4030(8)	37(4)
N(21)	947(8)	2808(6)	4309(6)	20(3)
N(22)	1401(10)	1716(7)	4693(8)	32(4)
N(23)	1395(10)	2095(7)	5872(8)	31(4)
O(11)	7572(11)	4490(7)	4832(6)	75(6)
O(12)	7123(8)	3632(8)	4655(6)	52(4)
O(13)	7460(30)	4945(10)	3620(30)	140(20)
O(33)	7290(20)	4981(6)	3602(12)	39(7)
O(14)	6861(10)	4260(7)	3048(6)	68(5)
O(15)	10595(9)	3097(8)	1999(7)	52(4)
O(16)	10387(7)	3138(6)	1055(7)	46(4)
O(17)	9721(10)	1851(6)	1066(7)	53(4)
O(18)	8951(8)	2480(4)	615(6)	28(3)
O(21)	-137(11)	1804(7)	7290(8)	62(5)
O(22)	657(12)	2449(6)	7763(6)	59(5)
O(23)	-1045(9)	3043(8)	6327(8)	64(5)
O(24)	-830(8)	3144(6)	7309(6)	48(4)
O(25)	2008(9)	4492(7)	3539(7)	57(4)
O(26)	2480(9)	3658(7)	3697(5)	49(4)
O(27)	2607(11)	4896(7)	4716(8)	48(5)
O(37)	2085(12)	5013(5)	4800(8)	24(5)
O(28)	2721(9)	4231(7)	5209(8)	73(5)
C(11)	8298(10)	2307(7)	1971(8)	18(4)
C(12)	7873(14)	1964(9)	1533(10)	46(6)
C(13)	7489(9)	1555(7)	1797(8)	17(4)
C(14)	7613(11)	1614(8)	2391(9)	28(5)
C(15)	7458(12)	1291(9)	2789(10)	39(5)
C(16)	7747(10)	1293(7)	3389(8)	22(4)
C(17)	7613(14)	861(8)	3807(10)	43(6)
C(18)	8046(11)	1040(7)	4348(8)	32(5)
C(19)	8320(12)	1571(8)	4223(9)	27(5)
C(110)	8679(12)	1952(9)	4625(10)	33(5)
C(111)	8850(15)	2517(8)	4562(11)	33(6)
C(112)	9039(12)	2941(10)	4989(9)	43(6)
C(113)	8888(12)	3421(9)	4749(10)	33(5)
C(114)	8592(11)	3318(8)	4191(9)	27(5)
C(115)	8233(12)	3741(8)	3729(9)	34(5)
C(116)	8527(11)	3692(8)	3169(9)	26(4)
C(117)	8706(13)	4177(8)	2884(10)	44(6)
C(118)	8896(12)	4201(9)	2401(10)	40(5)

C(119)	8992(14)	3737(10)	2070(10)	51(6)
C(120)	8857(10)	3188(7)	2332(8)	14(3)
C(121)	8580(10)	3190(7)	2880(8)	20(4)
C(122)	8899(10)	2669(7)	1938(8)	31(4)
C(123)	6995(12)	762(9)	2628(9)	36(5)
C(124)	7310(11)	320(7)	2417(7)	26(4)
C(125)	6856(13)	-168(8)	2214(9)	43(6)
C(126)	6103(10)	-131(6)	2280(7)	28(4)
C(127)	5771(11)	309(10)	2495(10)	46(5)
C(128)	6215(13)	777(10)	2625(10)	40(6)
C(129)	8856(11)	1711(9)	5222(8)	35(6)
C(130)	9393(13)	1297(10)	5365(10)	52(7)
C(131)	9511(14)	1053(11)	5874(10)	50(6)
C(132)	9037(13)	1192(11)	6284(9)	52(7)
C(133)	8461(13)	1621(9)	6170(11)	45(6)
C(134)	8425(14)	1862(11)	5670(11)	48(6)
C(135)	7677(12)	4084(8)	3910(9)	32(5)
C(136)	7480(13)	4118(9)	4525(9)	41(5)
C(137)	7045(16)	3568(12)	5279(6)	36(7)
C(337)	6738(13)	3701(10)	5195(8)	28(6)
C(138)	6420(20)	3148(14)	5283(18)	44(10)
C(438)	6150(20)	3253(14)	5180(20)	77(13)
C(139)	7174(10)	4474(5)	3534(8)	49(5)
C(140)	6536(11)	4713(7)	2672(10)	27(6)
C(340)	6643(16)	4610(20)	2540(19)	140(30)
C(141)	5817(12)	4441(10)	2414(12)	107(9)
C(142)	9476(13)	2693(10)	1553(10)	38(5)
C(143)	10188(12)	3021(10)	1592(10)	47(6)
C(144)	11154(15)	3419(19)	1055(17)	36(12)
C(145)	11350(20)	3676(15)	509(15)	48(9)
C(344)	11130(30)	3430(40)	972(18)	110(30)
C(345)	11140(20)	3551(17)	350(17)	44(9)
C(146)	9339(14)	2284(10)	1047(9)	45(6)
C(147)	8861(9)	2086(6)	127(5)	44(4)
C(148)	8330(20)	2357(15)	-324(13)	46(9)
C(448)	8110(19)	2230(20)	-200(20)	120(20)
C(21)	998(12)	3320(8)	4212(9)	34(5)
C(22)	680(12)	3415(10)	3582(10)	40(6)
C(23)	501(12)	2898(7)	3349(10)	33(5)
C(24)	740(14)	2494(7)	3802(11)	27(5)
C(25)	864(12)	1970(9)	3714(9)	34(5)
C(26)	1245(13)	1615(8)	4143(9)	35(5)
C(27)	1578(12)	1077(9)	4039(10)	42(5)
C(28)	1884(13)	890(9)	4512(10)	41(6)
C(29)	1827(14)	1284(10)	4941(12)	52(6)
C(210)	2049(10)	1250(8)	5529(8)	23(4)
C(211)	1852(10)	1655(6)	5980(8)	20(4)
C(212)	2023(14)	1589(8)	6592(10)	49(6)
C(213)	1643(9)	1966(7)	6844(8)	17(4)
C(214)	1229(13)	2259(10)	6392(10)	39(5)
C(215)	666(9)	2752(6)	6435(6)	17(3)
C(216)	709(12)	3249(8)	6055(9)	35(5)

C(217)	519(9)	3717(6)	6287(7)	15(3)
C(218)	576(10)	4216(7)	6027(8)	29(4)
C(219)	887(11)	4212(8)	5433(8)	27(4)
C(220)	1079(12)	3677(8)	5228(9)	33(5)
C(221)	928(11)	3163(9)	5477(10)	40(6)
C(222)	1345(12)	3697(7)	4590(8)	30(5)
C(223)	694(13)	1713(8)	3120(9)	42(6)
C(224)	138(11)	1302(7)	3029(9)	39(6)
C(225)	95(13)	1020(9)	2494(12)	52(7)
C(226)	564(13)	1156(8)	2051(10)	48(6)
C(227)	1058(15)	1546(11)	2146(9)	51(6)
C(228)	1173(11)	1849(8)	2677(9)	28(5)
C(229)	2561(12)	790(7)	5732(8)	27(5)
C(230)	3354(13)	782(8)	5693(9)	33(5)
C(231)	3856(8)	368(8)	5928(9)	44(5)
C(232)	3535(12)	-93(8)	6151(9)	50(6)
C(233)	2694(13)	-113(8)	6147(10)	45(6)
C(234)	2228(15)	293(9)	5968(12)	64(8)
C(235)	147(11)	2661(8)	6826(8)	25(4)
C(236)	141(12)	2254(10)	7308(9)	35(5)
C(237)	775(11)	2190(6)	8268(5)	59(5)
C(238)	1332(19)	2505(12)	8663(12)	39(8)
C(338)	1032(19)	2564(10)	8749(10)	41(7)
C(239)	-641(13)	2986(7)	6781(9)	34(5)
C(240)	-1616(10)	3381(10)	7307(8)	50(7)
C(241)	-1588(14)	3657(12)	7903(11)	101(11)
C(242)	1847(14)	4073(8)	4456(9)	47(6)
C(243)	2118(14)	4083(11)	3851(11)	51(6)
C(244)	2705(11)	3556(7)	3103(8)	56(6)
C(245)	3220(30)	3073(13)	3050(20)	38(12)
C(445)	3100(30)	3011(12)	3110(20)	70(20)
C(246)	2187(9)	4503(5)	4853(7)	47(5)
C(247)	3256(12)	4535(10)	5630(8)	106(7)
C(248)	3960(20)	4430(20)	6031(19)	86(14)
C(348)	2780(17)	4805(13)	6051(12)	65(8)
O(1W)	9537(13)	4784(9)	4273(11)	85(7)
O(2W)	268(17)	5586(12)	4063(14)	117(9)
O(3W)	10430(20)	9374(15)	4285(16)	148(12)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for Pd.

Pd(1)-N(13)	1.962(17)
Pd(1)-N(11)	2.004(15)
Pd(1)-C(121)	2.020(17)
Pd(1)-N(12)	2.045(15)
Pd(2)-C(221)	1.98(2)
Pd(2)-N(23)	2.015(17)
Pd(2)-N(21)	2.030(14)
Pd(2)-N(22)	2.084(17)
F(11)-C(128)	1.36(3)
F(12)-C(127)	1.414(17)
F(13)-C(126)	1.405(18)
F(14)-C(125)	1.25(2)
F(15)-C(124)	1.38(2)
F(16)-C(130)	1.41(2)
F(17)-C(131)	1.33(3)
F(18)-C(132)	1.35(2)
F(19)-C(133)	1.36(3)
F(21)-C(224)	1.29(3)
F(22)-C(225)	1.34(2)
F(23)-C(226)	1.33(2)
F(24)-C(227)	1.36(3)
F(25)-C(228)	1.33(2)
F(26)-C(230)	1.36(2)
F(27)-C(231)	1.330(2)
F(37)-C(231)	1.330(2)
F(28)-C(232)	1.30(2)
F(29)-C(233)	1.42(2)
F(110)-C(134)	1.36(3)
F(210)-C(234)	1.29(3)
N(11)-C(11)	1.33(2)
N(11)-C(14)	1.50(2)
N(12)-C(16)	1.37(2)
N(12)-C(19)	1.40(2)
N(13)-C(114)	1.39(2)
N(13)-C(111)	1.41(3)
N(21)-C(21)	1.26(2)
N(21)-C(24)	1.42(3)
N(22)-C(26)	1.31(3)
N(22)-C(29)	1.37(3)
N(23)-C(214)	1.33(3)
N(23)-C(211)	1.33(2)
O(11)-C(136)	1.15(2)
O(12)-C(136)	1.37(3)
O(12)-C(337)	1.480(2)
O(12)-C(137)	1.481(2)
O(13)-C(139)	1.251(2)
O(33)-C(139)	1.250(2)
O(14)-C(139)	1.32(2)
O(14)-C(340)	1.481(2)
O(14)-C(140)	1.481(2)

O(15)-C(143)	1.14(2)
O(16)-C(143)	1.35(3)
O(16)-C(344)	1.480(2)
O(16)-C(144)	1.480(2)
O(17)-C(146)	1.23(3)
O(18)-C(146)	1.25(3)
O(18)-C(147)	1.483(2)
O(21)-C(236)	1.19(3)
O(22)-C(237)	1.333(2)
O(22)-C(236)	1.41(3)
O(23)-C(239)	1.22(2)
O(24)-C(239)	1.35(2)
O(24)-C(240)	1.463(15)
O(25)-C(243)	1.23(3)
O(26)-C(243)	1.27(3)
O(26)-C(244)	1.488(17)
O(27)-C(246)	1.249(2)
O(37)-C(246)	1.250(2)
O(28)-C(246)	1.35(2)
O(28)-C(247)	1.481(2)
C(11)-C(122)	1.36(3)
C(11)-C(12)	1.46(3)
C(12)-C(13)	1.36(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.39(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.26(3)
C(15)-C(16)	1.44(3)
C(15)-C(123)	1.54(3)
C(16)-C(17)	1.46(3)
C(17)-C(18)	1.47(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.41(3)
C(18)-H(18)	0.9500
C(19)-C(110)	1.42(3)
C(110)-C(111)	1.41(3)
C(110)-C(129)	1.52(3)
C(111)-C(112)	1.45(3)
C(112)-C(113)	1.31(3)
C(112)-H(112)	0.9500
C(113)-C(114)	1.38(3)
C(113)-H(113)	0.9500
C(114)-C(115)	1.57(3)
C(115)-C(135)	1.36(3)
C(115)-C(116)	1.44(3)
C(116)-C(117)	1.39(3)
C(116)-C(121)	1.40(3)
C(117)-C(118)	1.20(3)
C(117)-H(117)	0.9500
C(118)-C(119)	1.38(3)
C(118)-H(118)	0.9500
C(119)-C(120)	1.49(3)

C(119)-H(119)	0.9500
C(120)-C(121)	1.40(2)
C(120)-C(122)	1.56(2)
C(122)-C(142)	1.39(3)
C(123)-C(124)	1.31(3)
C(123)-C(128)	1.34(3)
C(124)-C(125)	1.47(3)
C(125)-C(126)	1.32(2)
C(126)-C(127)	1.32(3)
C(127)-C(128)	1.38(3)
C(129)-C(130)	1.38(3)
C(129)-C(134)	1.38(3)
C(130)-C(131)	1.33(3)
C(131)-C(132)	1.35(3)
C(132)-C(133)	1.44(3)
C(133)-C(134)	1.30(3)
C(135)-C(136)	1.50(3)
C(135)-C(139)	1.510(17)
C(137)-C(337)	0.63(3)
C(137)-C(138)	1.480(2)
C(137)-C(438)	1.71(4)
C(337)-C(138)	1.47(4)
C(337)-C(438)	1.481(2)
C(138)-C(438)	0.56(6)
C(140)-C(141)	1.479(2)
C(340)-C(141)	1.480(2)
C(142)-C(143)	1.45(3)
C(142)-C(146)	1.54(3)
C(144)-C(145)	1.480(2)
C(344)-C(345)	1.480(2)
C(147)-C(448)	1.480(2)
C(147)-C(148)	1.480(2)
C(148)-C(448)	0.59(7)
C(21)-C(222)	1.37(3)
C(21)-C(22)	1.54(3)
C(22)-C(23)	1.39(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.47(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.30(3)
C(25)-C(26)	1.43(3)
C(25)-C(223)	1.52(3)
C(26)-C(27)	1.45(3)
C(27)-C(28)	1.26(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.39(3)
C(28)-H(28)	0.9500
C(29)-C(210)	1.39(3)
C(210)-C(229)	1.47(2)
C(210)-C(211)	1.49(2)
C(211)-C(212)	1.44(3)
C(212)-C(213)	1.29(3)

C(212)-H(212)	0.9500
C(213)-C(214)	1.41(3)
C(213)-H(213)	0.9500
C(214)-C(215)	1.54(3)
C(215)-C(235)	1.35(2)
C(215)-C(216)	1.50(2)
C(216)-C(217)	1.31(3)
C(216)-C(221)	1.44(3)
C(217)-C(218)	1.36(2)
C(217)-H(217)	0.9500
C(218)-C(219)	1.53(2)
C(218)-H(218)	0.9500
C(219)-C(220)	1.43(3)
C(219)-H(219)	0.9500
C(220)-C(221)	1.41(3)
C(220)-C(222)	1.59(3)
C(222)-C(242)	1.31(3)
C(223)-C(224)	1.38(3)
C(223)-C(228)	1.41(3)
C(224)-C(225)	1.42(3)
C(225)-C(226)	1.40(3)
C(226)-C(227)	1.27(3)
C(227)-C(228)	1.44(3)
C(229)-C(230)	1.37(3)
C(229)-C(234)	1.46(3)
C(230)-C(231)	1.40(3)
C(231)-C(232)	1.37(3)
C(232)-C(233)	1.44(3)
C(233)-C(234)	1.31(3)
C(235)-C(236)	1.49(3)
C(235)-C(239)	1.56(3)
C(237)-C(238)	1.480(2)
C(237)-C(338)	1.481(2)
C(240)-C(241)	1.54(3)
C(240)-H(24A)	0.9900
C(240)-H(24B)	0.9900
C(241)-H(24C)	0.9800
C(241)-H(24D)	0.9800
C(241)-H(24E)	0.9800
C(242)-C(246)	1.480(2)
C(242)-C(243)	1.52(3)
C(244)-C(245)	1.480(2)
C(244)-C(445)	1.480(2)
C(247)-C(248)	1.480(2)
C(247)-C(348)	1.480(2)
N(13)-Pd(1)-N(11)	177.3(7)
N(13)-Pd(1)-C(121)	92.2(7)
N(11)-Pd(1)-C(121)	90.3(6)
N(13)-Pd(1)-N(12)	86.6(7)
N(11)-Pd(1)-N(12)	90.9(6)
C(121)-Pd(1)-N(12)	177.9(8)

C(221)-Pd(2)-N(23)	90.5(8)
C(221)-Pd(2)-N(21)	90.9(7)
N(23)-Pd(2)-N(21)	178.6(7)
C(221)-Pd(2)-N(22)	179.4(8)
N(23)-Pd(2)-N(22)	90.0(7)
N(21)-Pd(2)-N(22)	88.7(6)
C(11)-N(11)-C(14)	109.6(15)
C(11)-N(11)-Pd(1)	127.6(12)
C(14)-N(11)-Pd(1)	122.6(12)
C(16)-N(12)-C(19)	106.0(15)
C(16)-N(12)-Pd(1)	124.9(13)
C(19)-N(12)-Pd(1)	129.1(13)
C(114)-N(13)-C(111)	100.4(16)
C(114)-N(13)-Pd(1)	127.4(14)
C(111)-N(13)-Pd(1)	132.0(14)
C(21)-N(21)-C(24)	113.0(16)
C(21)-N(21)-Pd(2)	124.2(13)
C(24)-N(21)-Pd(2)	122.8(12)
C(26)-N(22)-C(29)	109.0(19)
C(26)-N(22)-Pd(2)	124.9(13)
C(29)-N(22)-Pd(2)	125.6(15)
C(214)-N(23)-C(211)	103.6(17)
C(214)-N(23)-Pd(2)	130.2(15)
C(211)-N(23)-Pd(2)	125.7(14)
C(136)-O(12)-C(337)	109.3(16)
C(136)-O(12)-C(137)	112.7(17)
C(337)-O(12)-C(137)	24.7(13)
C(139)-O(14)-C(340)	121(3)
C(139)-O(14)-C(140)	108.8(15)
C(340)-O(14)-C(140)	17(3)
C(143)-O(16)-C(344)	120(2)
C(143)-O(16)-C(144)	113.0(19)
C(344)-O(16)-C(144)	8(2)
C(146)-O(18)-C(147)	112.8(14)
C(237)-O(22)-C(236)	123.2(16)
C(239)-O(24)-C(240)	113.4(15)
C(243)-O(26)-C(244)	124.7(17)
C(246)-O(28)-C(247)	120.9(16)
N(11)-C(11)-C(122)	120.5(15)
N(11)-C(11)-C(12)	106.5(17)
C(122)-C(11)-C(12)	131.5(19)
C(13)-C(12)-C(11)	109.2(19)
C(13)-C(12)-H(12)	125.4
C(11)-C(12)-H(12)	125.4
C(12)-C(13)-C(14)	109.6(17)
C(12)-C(13)-H(13)	125.2
C(14)-C(13)-H(13)	125.2
C(15)-C(14)-C(13)	130.2(19)
C(15)-C(14)-N(11)	124.0(19)
C(13)-C(14)-N(11)	104.9(16)
C(14)-C(15)-C(16)	129(2)
C(14)-C(15)-C(123)	118(2)

C(16)-C(15)-C(123)	111.5(18)
N(12)-C(16)-C(15)	123.4(17)
N(12)-C(16)-C(17)	110.8(15)
C(15)-C(16)-C(17)	125.6(17)
C(16)-C(17)-C(18)	105.3(15)
C(16)-C(17)-H(17)	127.4
C(18)-C(17)-H(17)	127.4
C(19)-C(18)-C(17)	104.2(16)
C(19)-C(18)-H(18)	127.9
C(17)-C(18)-H(18)	127.9
N(12)-C(19)-C(18)	113.4(17)
N(12)-C(19)-C(110)	120.1(18)
C(18)-C(19)-C(110)	126.3(19)
C(111)-C(110)-C(19)	130(2)
C(111)-C(110)-C(129)	116.2(19)
C(19)-C(110)-C(129)	113.5(18)
C(110)-C(111)-N(13)	116.9(19)
C(110)-C(111)-C(112)	131(2)
N(13)-C(111)-C(112)	109.7(17)
C(113)-C(112)-C(111)	108(2)
C(113)-C(112)-H(112)	125.9
C(111)-C(112)-H(112)	125.9
C(112)-C(113)-C(114)	107(2)
C(112)-C(113)-H(113)	126.7
C(114)-C(113)-H(113)	126.7
C(113)-C(114)-N(13)	114.7(18)
C(113)-C(114)-C(115)	128.3(18)
N(13)-C(114)-C(115)	116.9(17)
C(135)-C(115)-C(116)	129.7(19)
C(135)-C(115)-C(114)	115.4(18)
C(116)-C(115)-C(114)	114.8(17)
C(117)-C(116)-C(121)	118.5(19)
C(117)-C(116)-C(115)	118.0(19)
C(121)-C(116)-C(115)	123.3(18)
C(118)-C(117)-C(116)	125(2)
C(118)-C(117)-H(117)	117.4
C(116)-C(117)-H(117)	117.4
C(117)-C(118)-C(119)	123(2)
C(117)-C(118)-H(118)	118.7
C(119)-C(118)-H(118)	118.7
C(118)-C(119)-C(120)	118(2)
C(118)-C(119)-H(119)	121.1
C(120)-C(119)-H(119)	121.1
C(121)-C(120)-C(119)	116.6(17)
C(121)-C(120)-C(122)	125.1(16)
C(119)-C(120)-C(122)	117.5(16)
C(116)-C(121)-C(120)	119.0(17)
C(116)-C(121)-Pd(1)	122.4(14)
C(120)-C(121)-Pd(1)	118.4(13)
C(11)-C(122)-C(142)	130.3(18)
C(11)-C(122)-C(120)	114.4(16)
C(142)-C(122)-C(120)	114.5(16)

C(124)-C(123)-C(128)	118(2)
C(124)-C(123)-C(15)	123.4(19)
C(128)-C(123)-C(15)	118(2)
C(123)-C(124)-F(15)	121.2(17)
C(123)-C(124)-C(125)	123.5(18)
F(15)-C(124)-C(125)	115.3(16)
F(14)-C(125)-C(126)	126.4(17)
F(14)-C(125)-C(124)	119.6(19)
C(126)-C(125)-C(124)	113.9(18)
C(125)-C(126)-C(127)	123.8(16)
C(125)-C(126)-F(13)	117.3(15)
C(127)-C(126)-F(13)	118.1(16)
C(126)-C(127)-C(128)	119.7(18)
C(126)-C(127)-F(12)	122.7(19)
C(128)-C(127)-F(12)	116.3(19)
C(123)-C(128)-F(11)	119(2)
C(123)-C(128)-C(127)	121(2)
F(11)-C(128)-C(127)	119.9(19)
C(130)-C(129)-C(134)	113.4(19)
C(130)-C(129)-C(110)	125(2)
C(134)-C(129)-C(110)	121(2)
C(131)-C(130)-C(129)	126(2)
C(131)-C(130)-F(16)	118(2)
C(129)-C(130)-F(16)	116(2)
C(130)-C(131)-F(17)	120(2)
C(130)-C(131)-C(132)	118(2)
F(17)-C(131)-C(132)	121(2)
C(131)-C(132)-F(18)	118(2)
C(131)-C(132)-C(133)	120(2)
F(18)-C(132)-C(133)	122(2)
C(134)-C(133)-F(19)	126(2)
C(134)-C(133)-C(132)	118(3)
F(19)-C(133)-C(132)	116(2)
C(133)-C(134)-F(110)	115(2)
C(133)-C(134)-C(129)	125(2)
F(110)-C(134)-C(129)	120(2)
C(115)-C(135)-C(136)	123.5(15)
C(115)-C(135)-C(139)	125.7(19)
C(136)-C(135)-C(139)	110.8(17)
O(11)-C(136)-O(12)	125(2)
O(11)-C(136)-C(135)	127(2)
O(12)-C(136)-C(135)	107.6(15)
C(337)-C(137)-O(12)	77.6(7)
C(337)-C(137)-C(138)	76(4)
O(12)-C(137)-C(138)	102(2)
C(337)-C(137)-C(438)	58(3)
O(12)-C(137)-C(438)	94(2)
C(138)-C(137)-C(438)	19(2)
C(137)-C(337)-C(138)	79(3)
C(137)-C(337)-O(12)	77.7(7)
C(138)-C(337)-O(12)	102(2)
C(137)-C(337)-C(438)	101(4)

C(138)-C(337)-C(438)	22(2)
O(12)-C(337)-C(438)	104(2)
C(438)-C(138)-C(337)	80(4)
C(438)-C(138)-C(137)	105(5)
C(337)-C(138)-C(137)	24.8(14)
C(138)-C(438)-C(337)	78(4)
C(138)-C(438)-C(137)	57(3)
C(337)-C(438)-C(137)	21.3(13)
O(33)-C(139)-O(13)	14(3)
O(33)-C(139)-O(14)	122.9(19)
O(13)-C(139)-O(14)	129(3)
O(33)-C(139)-C(135)	118(2)
O(13)-C(139)-C(135)	106(3)
O(14)-C(139)-C(135)	115.1(14)
C(141)-C(140)-O(14)	99.8(14)
C(141)-C(340)-O(14)	99.8(14)
C(140)-C(141)-C(340)	17(3)
C(122)-C(142)-C(143)	129(2)
C(122)-C(142)-C(146)	113.3(18)
C(143)-C(142)-C(146)	118(2)
O(15)-C(143)-O(16)	123(2)
O(15)-C(143)-C(142)	126(2)
O(16)-C(143)-C(142)	109.5(18)
C(145)-C(144)-O(16)	117(3)
O(16)-C(344)-C(345)	108(3)
O(17)-C(146)-O(18)	127(2)
O(17)-C(146)-C(142)	118(2)
O(18)-C(146)-C(142)	114(2)
C(448)-C(147)-C(148)	23(3)
C(448)-C(147)-O(18)	106(3)
C(148)-C(147)-O(18)	106.2(18)
C(448)-C(148)-C(147)	78.5(14)
C(148)-C(448)-C(147)	78.5(14)
N(21)-C(21)-C(222)	124.7(18)
N(21)-C(21)-C(22)	107.0(18)
C(222)-C(21)-C(22)	128.0(18)
C(23)-C(22)-C(21)	106.8(19)
C(23)-C(22)-H(22)	126.6
C(21)-C(22)-H(22)	126.6
C(22)-C(23)-C(24)	106.2(19)
C(22)-C(23)-H(23)	126.9
C(24)-C(23)-H(23)	126.9
C(25)-C(24)-N(21)	128(2)
C(25)-C(24)-C(23)	125(2)
N(21)-C(24)-C(23)	106.0(15)
C(24)-C(25)-C(26)	123(2)
C(24)-C(25)-C(223)	121.3(19)
C(26)-C(25)-C(223)	115.5(18)
N(22)-C(26)-C(25)	127.9(19)
N(22)-C(26)-C(27)	106.3(17)
C(25)-C(26)-C(27)	125.8(19)
C(28)-C(27)-C(26)	108(2)

C(28)-C(27)-H(27)	125.8
C(26)-C(27)-H(27)	125.8
C(27)-C(28)-C(29)	109(2)
C(27)-C(28)-H(28)	125.3
C(29)-C(28)-H(28)	125.3
N(22)-C(29)-C(28)	107(2)
N(22)-C(29)-C(210)	123(2)
C(28)-C(29)-C(210)	130(2)
C(29)-C(210)-C(229)	117.8(18)
C(29)-C(210)-C(211)	126.4(17)
C(229)-C(210)-C(211)	115.7(15)
N(23)-C(211)-C(212)	110.0(17)
N(23)-C(211)-C(210)	123.7(16)
C(212)-C(211)-C(210)	125.7(16)
C(213)-C(212)-C(211)	107.7(18)
C(213)-C(212)-H(212)	126.2
C(211)-C(212)-H(212)	126.1
C(212)-C(213)-C(214)	104.8(18)
C(212)-C(213)-H(213)	127.6
C(214)-C(213)-H(213)	127.6
N(23)-C(214)-C(213)	114(2)
N(23)-C(214)-C(215)	118.2(18)
C(213)-C(214)-C(215)	128.1(19)
C(235)-C(215)-C(216)	126.8(15)
C(235)-C(215)-C(214)	111.7(15)
C(216)-C(215)-C(214)	121.4(16)
C(217)-C(216)-C(221)	127.2(19)
C(217)-C(216)-C(215)	115.1(17)
C(221)-C(216)-C(215)	117.6(17)
C(216)-C(217)-C(218)	123.7(18)
C(216)-C(217)-H(217)	118.2
C(218)-C(217)-H(217)	118.1
C(217)-C(218)-C(219)	116.3(16)
C(217)-C(218)-H(218)	121.9
C(219)-C(218)-H(218)	121.9
C(220)-C(219)-C(218)	114.7(18)
C(220)-C(219)-H(219)	122.7
C(218)-C(219)-H(219)	122.6
C(221)-C(220)-C(219)	127(2)
C(221)-C(220)-C(222)	119.3(18)
C(219)-C(220)-C(222)	112.2(17)
C(220)-C(221)-C(216)	109(2)
C(220)-C(221)-Pd(2)	121.8(17)
C(216)-C(221)-Pd(2)	128.3(15)
C(242)-C(222)-C(21)	124.6(19)
C(242)-C(222)-C(220)	119.4(17)
C(21)-C(222)-C(220)	116.0(18)
C(224)-C(223)-C(228)	120(2)
C(224)-C(223)-C(25)	121(2)
C(228)-C(223)-C(25)	119.4(18)
F(21)-C(224)-C(223)	122.1(18)
F(21)-C(224)-C(225)	120.1(17)

C(223)-C(224)-C(225)	118(2)
F(22)-C(225)-C(226)	119(2)
F(22)-C(225)-C(224)	118(2)
C(226)-C(225)-C(224)	123.0(18)
C(227)-C(226)-F(23)	119(2)
C(227)-C(226)-C(225)	117(2)
F(23)-C(226)-C(225)	123.1(18)
C(226)-C(227)-F(24)	122(2)
C(226)-C(227)-C(228)	125(2)
F(24)-C(227)-C(228)	113(2)
F(25)-C(228)-C(223)	119.8(17)
F(25)-C(228)-C(227)	122(2)
C(223)-C(228)-C(227)	118(2)
C(230)-C(229)-C(234)	115.8(17)
C(230)-C(229)-C(210)	123.9(18)
C(234)-C(229)-C(210)	120.3(19)
F(26)-C(230)-C(229)	121.3(17)
F(26)-C(230)-C(231)	113.4(18)
C(229)-C(230)-C(231)	124.4(18)
F(37)-C(231)-F(27)	22.4(16)
F(37)-C(231)-C(232)	118(2)
F(27)-C(231)-C(232)	114.3(18)
F(37)-C(231)-C(230)	120(2)
F(27)-C(231)-C(230)	127(2)
C(232)-C(231)-C(230)	118.6(15)
F(28)-C(232)-C(231)	125.6(19)
F(28)-C(232)-C(233)	115.9(18)
C(231)-C(232)-C(233)	117.3(17)
C(234)-C(233)-F(29)	119(2)
C(234)-C(233)-C(232)	124(2)
F(29)-C(233)-C(232)	116.9(17)
F(210)-C(234)-C(233)	123(2)
F(210)-C(234)-C(229)	117.8(18)
C(233)-C(234)-C(229)	119(2)
C(215)-C(235)-C(236)	131.6(17)
C(215)-C(235)-C(239)	119.4(15)
C(236)-C(235)-C(239)	108.9(16)
O(21)-C(236)-O(22)	124(2)
O(21)-C(236)-C(235)	127(2)
O(22)-C(236)-C(235)	107.7(17)
O(22)-C(237)-C(238)	110.4(18)
O(22)-C(237)-C(338)	113.1(18)
C(238)-C(237)-C(338)	22.8(16)
O(23)-C(239)-O(24)	126.4(19)
O(23)-C(239)-C(235)	122.6(19)
O(24)-C(239)-C(235)	110.7(16)
O(24)-C(240)-C(241)	102.0(15)
O(24)-C(240)-H(24A)	111.4
C(241)-C(240)-H(24A)	111.4
O(24)-C(240)-H(24B)	111.4
C(241)-C(240)-H(24B)	111.4
H(24A)-C(240)-H(24B)	109.2

C(240)-C(241)-H(24C)	109.5
C(240)-C(241)-H(24D)	109.5
H(24C)-C(241)-H(24D)	109.5
C(240)-C(241)-H(24E)	109.5
H(24C)-C(241)-H(24E)	109.5
H(24D)-C(241)-H(24E)	109.5
C(222)-C(242)-C(246)	125(2)
C(222)-C(242)-C(243)	119.4(15)
C(246)-C(242)-C(243)	115.7(19)
O(25)-C(243)-O(26)	123(2)
O(25)-C(243)-C(242)	121(2)
O(26)-C(243)-C(242)	116(2)
C(245)-C(244)-C(445)	12(3)
C(245)-C(244)-O(26)	114(2)
C(445)-C(244)-O(26)	107(3)
O(27)-C(246)-O(37)	45.9(13)
O(27)-C(246)-O(28)	98.8(15)
O(37)-C(246)-O(28)	128.5(15)
O(27)-C(246)-C(242)	125.4(18)
O(37)-C(246)-C(242)	126.0(17)
O(28)-C(246)-C(242)	104.6(13)
C(248)-C(247)-C(348)	97(3)
C(248)-C(247)-O(28)	139(3)
C(348)-C(247)-O(28)	108(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Pd. 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
Pd(1)	33(1)	26(1)	21(1)	-3(1)	4(1)	-4(1)
Pd(2)	27(1)	23(1)	24(1)	1(1)	1(1)	3(1)
F(11)	53(8)	39(8)	83(11)	-19(7)	7(7)	-5(6)
F(12)	38(6)	80(8)	121(11)	-33(8)	6(5)	-38(5)
F(13)	52(8)	49(8)	85(10)	-23(7)	4(7)	-30(6)
F(14)	87(10)	23(6)	73(8)	-6(5)	-7(7)	-4(6)
F(15)	44(8)	51(8)	173(16)	-50(9)	26(9)	-1(6)
F(16)	53(8)	42(7)	75(10)	18(6)	10(7)	-6(6)
F(17)	80(11)	88(11)	70(10)	29(8)	-28(8)	29(9)
F(18)	90(9)	55(8)	50(8)	38(6)	1(6)	-6(7)
F(19)	51(9)	118(13)	36(9)	9(8)	20(7)	12(8)
F(21)	68(9)	87(10)	47(8)	-3(7)	25(7)	-46(7)
F(22)	70(10)	53(8)	126(13)	-52(9)	25(8)	-22(7)
F(23)	68(9)	81(10)	49(8)	-19(7)	-22(7)	26(7)
F(24)	91(12)	85(11)	27(8)	-11(7)	17(7)	14(8)
F(25)	58(8)	51(8)	38(7)	-14(6)	25(6)	-22(6)
F(26)	41(7)	58(9)	74(10)	17(8)	9(6)	11(6)
F(28)	78(10)	38(7)	87(11)	13(7)	-3(8)	28(7)
F(29)	58(8)	47(8)	111(12)	40(7)	6(7)	6(6)
F(110)	46(8)	85(10)	50(9)	-2(8)	-12(6)	-7(8)
F(210)	49(9)	45(7)	104(11)	21(7)	-5(7)	10(6)
N(11)	30(6)	15(5)	23(6)	2(4)	5(4)	-2(4)
N(12)	43(7)	24(6)	24(6)	9(4)	-1(4)	-15(4)
N(13)	37(4)	37(4)	37(4)	0(1)	3(1)	0(1)
N(21)	20(3)	19(3)	20(3)	0(1)	2(1)	1(1)
N(22)	32(4)	32(4)	32(4)	0(1)	3(1)	1(1)
N(23)	31(4)	31(4)	31(4)	0(1)	3(1)	0(1)
O(11)	148(13)	54(7)	26(6)	-33(5)	21(6)	9(7)
O(12)	48(9)	72(12)	40(9)	-5(8)	27(7)	-3(8)
O(14)	84(11)	86(12)	28(7)	14(7)	-25(6)	20(9)
O(15)	48(10)	86(12)	23(8)	14(7)	6(7)	-14(8)
O(16)	23(8)	63(10)	51(10)	19(8)	7(7)	-18(7)
O(17)	68(11)	41(8)	50(10)	-1(7)	14(8)	15(7)
O(18)	29(3)	28(3)	28(3)	0(1)	3(1)	0(1)
O(21)	71(12)	46(9)	69(13)	28(8)	12(9)	-5(8)
O(22)	96(12)	58(7)	24(6)	23(5)	8(5)	8(6)
O(23)	42(10)	105(14)	44(11)	3(9)	-7(8)	9(9)
O(24)	70(11)	60(10)	14(7)	3(7)	8(7)	1(8)
O(25)	58(5)	56(5)	56(5)	1(2)	4(2)	0(2)
O(26)	64(10)	56(10)	25(8)	12(7)	-1(7)	-5(8)
O(28)	53(10)	61(10)	103(13)	-16(9)	2(8)	-7(7)
C(11)	20(6)	14(5)	20(6)	-2(4)	1(4)	1(4)
C(12)	61(11)	39(9)	35(9)	-9(6)	-12(7)	4(7)
C(13)	17(4)	17(4)	17(4)	0(1)	2(1)	0(1)
C(14)	28(5)	28(5)	28(5)	0(1)	2(1)	0(1)
C(15)	39(9)	33(8)	43(9)	0(6)	-13(6)	1(6)
C(16)	23(4)	22(4)	22(4)	0(1)	2(1)	0(1)

C(17)	68(12)	17(6)	40(9)	-1(5)	-8(7)	-17(6)
C(18)	47(9)	15(6)	33(8)	17(5)	-4(6)	-9(5)
C(19)	27(5)	27(5)	27(5)	0(1)	2(1)	0(1)
C(110)	33(5)	33(5)	33(5)	0(1)	3(1)	0(1)
C(111)	33(9)	38(9)	26(8)	5(5)	3(5)	-10(5)
C(112)	32(12)	76(15)	20(11)	-7(10)	1(9)	-16(10)
C(113)	33(5)	33(5)	33(5)	-1(1)	2(1)	0(1)
C(114)	27(5)	27(5)	27(5)	0(1)	2(1)	0(1)
C(115)	34(5)	34(5)	34(5)	0(1)	3(1)	0(1)
C(116)	26(4)	26(4)	26(4)	0(1)	2(1)	0(1)
C(117)	65(12)	20(7)	46(10)	-6(6)	-8(7)	-6(6)
C(118)	40(5)	40(5)	40(5)	0(1)	3(1)	0(1)
C(119)	63(12)	58(11)	31(8)	0(7)	-2(7)	-20(8)
C(120)	14(3)	14(3)	14(3)	0(1)	1(1)	0(1)
C(121)	20(4)	19(4)	19(4)	0(1)	1(1)	0(1)
C(122)	31(5)	31(5)	30(4)	0(1)	2(1)	0(1)
C(123)	36(5)	36(5)	36(5)	0(1)	3(1)	0(1)
C(124)	26(4)	25(4)	26(4)	0(1)	2(1)	0(1)
C(125)	66(15)	24(10)	35(11)	-18(8)	-19(9)	-3(9)
C(126)	28(4)	27(4)	28(4)	0(1)	2(1)	-1(1)
C(127)	46(5)	46(5)	46(5)	0(1)	4(1)	0(1)
C(128)	40(6)	40(6)	40(6)	0(1)	3(1)	0(1)
C(129)	19(10)	71(14)	14(10)	18(9)	-5(8)	-23(9)
C(130)	39(14)	80(17)	39(13)	-24(11)	16(10)	-6(12)
C(131)	47(13)	65(15)	34(12)	18(11)	-20(10)	-14(11)
C(132)	41(13)	81(17)	32(13)	0(11)	-10(10)	-25(11)
C(133)	33(11)	41(10)	57(15)	3(9)	-13(10)	-6(8)
C(134)	49(15)	60(16)	33(15)	3(12)	1(11)	13(12)
C(135)	32(5)	32(5)	32(5)	0(1)	3(1)	0(1)
C(136)	50(10)	33(8)	39(9)	-28(6)	5(6)	3(6)
C(139)	49(5)	49(5)	49(5)	0(1)	4(1)	1(1)
C(141)	86(16)	89(15)	130(20)	15(13)	-56(16)	5(12)
C(142)	38(5)	38(5)	38(5)	0(1)	3(1)	0(1)
C(143)	26(11)	80(15)	36(14)	26(11)	1(10)	3(10)
C(146)	67(12)	42(9)	31(8)	6(6)	35(7)	8(7)
C(147)	45(4)	45(4)	44(4)	-1(1)	4(1)	0(1)
C(21)	44(9)	34(8)	27(8)	14(6)	14(6)	13(6)
C(22)	40(6)	40(6)	40(6)	1(1)	3(1)	0(1)
C(23)	44(12)	15(7)	40(13)	2(8)	-3(9)	-4(7)
C(24)	27(5)	27(5)	26(5)	0(1)	2(1)	0(1)
C(25)	29(8)	44(9)	27(8)	-10(5)	-7(5)	10(5)
C(26)	51(10)	25(7)	27(8)	-4(5)	-4(6)	12(6)
C(27)	42(5)	42(5)	42(5)	0(1)	4(1)	0(1)
C(28)	41(6)	40(6)	41(6)	0(1)	3(1)	0(1)
C(29)	54(11)	35(8)	68(12)	-4(7)	9(7)	11(6)
C(210)	23(4)	23(4)	23(4)	0(1)	2(1)	0(1)
C(211)	20(7)	15(6)	24(7)	7(4)	1(5)	9(4)
C(212)	71(12)	25(7)	50(11)	3(6)	-11(8)	5(6)
C(213)	17(4)	17(4)	17(4)	0(1)	2(1)	0(1)
C(214)	40(5)	40(5)	39(5)	0(1)	3(1)	0(1)
C(215)	18(3)	18(3)	17(3)	0(1)	1(1)	0(1)
C(216)	40(9)	37(9)	31(8)	2(6)	9(6)	8(6)

C(217)	15(4)	15(4)	15(4)	0(1)	1(1)	0(1)
C(218)	38(9)	30(7)	19(7)	-2(5)	2(6)	20(5)
C(219)	27(4)	27(4)	27(4)	0(1)	2(1)	0(1)
C(220)	32(8)	29(7)	34(9)	-4(5)	-10(6)	9(5)
C(221)	25(8)	39(8)	57(10)	24(7)	10(6)	17(6)
C(222)	54(10)	18(6)	16(7)	7(5)	-11(5)	10(5)
C(223)	60(15)	24(10)	38(14)	9(9)	-10(11)	-4(9)
C(224)	36(12)	25(9)	53(13)	-23(9)	-11(10)	5(8)
C(225)	40(13)	33(10)	82(18)	-12(11)	-2(12)	-14(9)
C(226)	58(14)	33(10)	53(14)	-37(9)	6(11)	-13(9)
C(227)	65(15)	73(16)	18(10)	-6(10)	11(9)	18(12)
C(228)	25(10)	36(11)	23(11)	-5(9)	1(8)	7(8)
C(229)	46(9)	18(6)	15(6)	-6(4)	-8(5)	16(5)
C(230)	42(9)	21(6)	37(8)	2(5)	6(6)	10(5)
C(231)	39(9)	44(9)	48(10)	-11(7)	-7(7)	20(7)
C(232)	50(6)	50(6)	50(6)	0(1)	4(1)	1(1)
C(233)	57(14)	22(9)	60(14)	2(9)	34(10)	6(8)
C(234)	52(11)	37(9)	104(17)	24(8)	2(9)	18(7)
C(235)	34(8)	29(7)	11(6)	1(4)	-6(5)	3(5)
C(236)	35(5)	35(5)	35(5)	0(1)	3(1)	0(1)
C(237)	60(6)	59(6)	59(6)	0(1)	5(1)	0(1)
C(239)	54(13)	19(8)	33(12)	13(8)	15(10)	3(8)
C(240)	36(9)	84(13)	34(9)	2(8)	27(6)	36(8)
C(241)	65(16)	150(30)	94(19)	-4(16)	48(13)	65(16)
C(242)	79(13)	32(8)	31(8)	9(6)	16(7)	7(7)
C(243)	51(6)	51(6)	51(6)	0(1)	4(1)	0(1)
C(244)	56(6)	57(6)	56(6)	0(1)	5(1)	0(1)
C(246)	47(5)	47(5)	47(5)	0(1)	4(1)	-1(1)
C(247)	106(8)	106(8)	106(8)	0(1)	9(1)	0(1)
O(1W)	85(7)	85(7)	85(7)	3(2)	5(2)	-3(2)
O(2W)	118(10)	117(10)	116(10)	-1(2)	11(2)	-2(2)
O(3W)	147(12)	148(12)	148(12)	1(2)	11(2)	1(2)

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

	x	y	z	U(eq)
H(12)	7866	2017	1129	55
H(13)	7183	1273	1604	20
H(17)	7311	534	3743	51
H(18)	8123	842	4700	39
H(112)	9239	2881	5376	51
H(113)	8967	3773	4925	40
H(117)	8676	4514	3089	53
H(118)	8983	4554	2239	48
H(119)	9140	3767	1688	61
H(22)	617	3761	3391	48
H(23)	271	2821	2972	40
H(27)	1569	897	3677	51
H(28)	2115	535	4566	49
H(212)	2355	1317	6777	59
H(213)	1641	2032	7246	21
H(217)	330	3707	6659	18
H(218)	431	4549	6206	35
H(219)	948	4539	5216	32
H(24A)	-2024	3091	7265	60
H(24B)	-1713	3655	6994	60
H(24C)	-1708	3383	8192	152
H(24D)	-1975	3956	7895	152
H(24E)	-1064	3809	8002	152

Table 6. Torsion angles [°] for Pd.

N(13)-Pd(1)-N(11)-C(11)	173(14)
C(121)-Pd(1)-N(11)-C(11)	18.1(16)
N(12)-Pd(1)-N(11)-C(11)	-163.7(16)
N(13)-Pd(1)-N(11)-C(14)	-2(16)
C(121)-Pd(1)-N(11)-C(14)	-156.3(14)
N(12)-Pd(1)-N(11)-C(14)	21.9(14)
N(13)-Pd(1)-N(12)-C(16)	164.1(17)
N(11)-Pd(1)-N(12)-C(16)	-14.8(17)
C(121)-Pd(1)-N(12)-C(16)	109(19)
N(13)-Pd(1)-N(12)-C(19)	-14.9(18)
N(11)-Pd(1)-N(12)-C(19)	166.2(18)
C(121)-Pd(1)-N(12)-C(19)	-70(19)
N(11)-Pd(1)-N(13)-C(114)	-135(14)
C(121)-Pd(1)-N(13)-C(114)	19.7(18)
N(12)-Pd(1)-N(13)-C(114)	-158.5(17)
N(11)-Pd(1)-N(13)-C(111)	50(16)
C(121)-Pd(1)-N(13)-C(111)	-155(2)
N(12)-Pd(1)-N(13)-C(111)	26(2)
C(221)-Pd(2)-N(21)-C(21)	24.4(17)
N(23)-Pd(2)-N(21)-C(21)	-138(28)
N(22)-Pd(2)-N(21)-C(21)	-156.1(16)
C(221)-Pd(2)-N(21)-C(24)	-157.5(16)
N(23)-Pd(2)-N(21)-C(24)	41(29)
N(22)-Pd(2)-N(21)-C(24)	22.0(16)
C(221)-Pd(2)-N(22)-C(26)	38(86)
N(23)-Pd(2)-N(22)-C(26)	168.5(19)
N(21)-Pd(2)-N(22)-C(26)	-12.0(19)
C(221)-Pd(2)-N(22)-C(29)	-150(85)
N(23)-Pd(2)-N(22)-C(29)	-19.9(19)
N(21)-Pd(2)-N(22)-C(29)	159.6(19)
C(221)-Pd(2)-N(23)-C(214)	15(2)
N(21)-Pd(2)-N(23)-C(214)	177(100)
N(22)-Pd(2)-N(23)-C(214)	-164.4(19)
C(221)-Pd(2)-N(23)-C(211)	-155.6(17)
N(21)-Pd(2)-N(23)-C(211)	6(29)
N(22)-Pd(2)-N(23)-C(211)	24.9(16)
C(14)-N(11)-C(11)-C(122)	-163.4(16)
Pd(1)-N(11)-C(11)-C(122)	22(2)
C(14)-N(11)-C(11)-C(12)	4(2)
Pd(1)-N(11)-C(11)-C(12)	-170.9(13)
N(11)-C(11)-C(12)-C(13)	-4(2)
C(122)-C(11)-C(12)-C(13)	161.8(19)
C(11)-C(12)-C(13)-C(14)	2(2)
C(12)-C(13)-C(14)-C(15)	-169(2)
C(12)-C(13)-C(14)-N(11)	1(2)
C(11)-N(11)-C(14)-C(15)	168(2)
Pd(1)-N(11)-C(14)-C(15)	-17(3)
C(11)-N(11)-C(14)-C(13)	-3(2)
Pd(1)-N(11)-C(14)-C(13)	172.2(12)
C(13)-C(14)-C(15)-C(16)	164(2)

N(11)-C(14)-C(15)-C(16)	-5(4)
C(13)-C(14)-C(15)-C(123)	-6(3)
N(11)-C(14)-C(15)-C(123)	-174.4(18)
C(19)-N(12)-C(16)-C(15)	-179.8(18)
Pd(1)-N(12)-C(16)-C(15)	1(3)
C(19)-N(12)-C(16)-C(17)	5(2)
Pd(1)-N(12)-C(16)-C(17)	-174.5(15)
C(14)-C(15)-C(16)-N(12)	13(4)
C(123)-C(15)-C(16)-N(12)	-176.2(18)
C(14)-C(15)-C(16)-C(17)	-172(2)
C(123)-C(15)-C(16)-C(17)	-1(3)
N(12)-C(16)-C(17)-C(18)	-7(2)
C(15)-C(16)-C(17)-C(18)	177.9(19)
C(16)-C(17)-C(18)-C(19)	6(2)
C(16)-N(12)-C(19)-C(18)	-1(2)
Pd(1)-N(12)-C(19)-C(18)	178.4(14)
C(16)-N(12)-C(19)-C(110)	-175.2(18)
Pd(1)-N(12)-C(19)-C(110)	4(3)
C(17)-C(18)-C(19)-N(12)	-3(2)
C(17)-C(18)-C(19)-C(110)	171(2)
N(12)-C(19)-C(110)-C(111)	6(4)
C(18)-C(19)-C(110)-C(111)	-168(2)
N(12)-C(19)-C(110)-C(129)	-178.3(18)
C(18)-C(19)-C(110)-C(129)	8(3)
C(19)-C(110)-C(111)-N(13)	4(4)
C(129)-C(110)-C(111)-N(13)	-172.1(19)
C(19)-C(110)-C(111)-C(112)	163(2)
C(129)-C(110)-C(111)-C(112)	-13(4)
C(114)-N(13)-C(111)-C(110)	159(2)
Pd(1)-N(13)-C(111)-C(110)	-25(3)
C(114)-N(13)-C(111)-C(112)	-5(2)
Pd(1)-N(13)-C(111)-C(112)	171.4(14)
C(110)-C(111)-C(112)-C(113)	-158(2)
N(13)-C(111)-C(112)-C(113)	2(3)
C(111)-C(112)-C(113)-C(114)	2(3)
C(112)-C(113)-C(114)-N(13)	-5(3)
C(112)-C(113)-C(114)-C(115)	173(2)
C(111)-N(13)-C(114)-C(113)	6(2)
Pd(1)-N(13)-C(114)-C(113)	-170.4(14)
C(111)-N(13)-C(114)-C(115)	-172.3(18)
Pd(1)-N(13)-C(114)-C(115)	11(3)
C(113)-C(114)-C(115)-C(135)	-50(3)
N(13)-C(114)-C(115)-C(135)	128(2)
C(113)-C(114)-C(115)-C(116)	132(2)
N(13)-C(114)-C(115)-C(116)	-50(2)
C(135)-C(115)-C(116)-C(117)	45(3)
C(114)-C(115)-C(116)-C(117)	-137.0(19)
C(135)-C(115)-C(116)-C(121)	-129(2)
C(114)-C(115)-C(116)-C(121)	48(3)
C(121)-C(116)-C(117)-C(118)	1(3)
C(115)-C(116)-C(117)-C(118)	-174(2)
C(116)-C(117)-C(118)-C(119)	-3(4)

C(117)-C(118)-C(119)-C(120)	0(3)
C(118)-C(119)-C(120)-C(121)	5(3)
C(118)-C(119)-C(120)-C(122)	175.0(17)
C(117)-C(116)-C(121)-C(120)	4(3)
C(115)-C(116)-C(121)-C(120)	178.6(17)
C(117)-C(116)-C(121)-Pd(1)	177.6(14)
C(115)-C(116)-C(121)-Pd(1)	-8(3)
C(119)-C(120)-C(121)-C(116)	-7(2)
C(122)-C(120)-C(121)-C(116)	-175.7(16)
C(119)-C(120)-C(121)-Pd(1)	179.4(13)
C(122)-C(120)-C(121)-Pd(1)	10(2)
N(13)-Pd(1)-C(121)-C(116)	-22.7(15)
N(11)-Pd(1)-C(121)-C(116)	156.2(15)
N(12)-Pd(1)-C(121)-C(116)	32(20)
N(13)-Pd(1)-C(121)-C(120)	151.1(13)
N(11)-Pd(1)-C(121)-C(120)	-30.1(13)
N(12)-Pd(1)-C(121)-C(120)	-154(18)
N(11)-C(11)-C(122)-C(142)	138(2)
C(12)-C(11)-C(122)-C(142)	-26(3)
N(11)-C(11)-C(122)-C(120)	-52(2)
C(12)-C(11)-C(122)-C(120)	143.7(19)
C(121)-C(120)-C(122)-C(11)	36(2)
C(119)-C(120)-C(122)-C(11)	-133.1(17)
C(121)-C(120)-C(122)-C(142)	-153.1(17)
C(119)-C(120)-C(122)-C(142)	38(2)
C(14)-C(15)-C(123)-C(124)	78(3)
C(16)-C(15)-C(123)-C(124)	-93(3)
C(14)-C(15)-C(123)-C(128)	-92(3)
C(16)-C(15)-C(123)-C(128)	97(2)
C(128)-C(123)-C(124)-F(15)	173.7(19)
C(15)-C(123)-C(124)-F(15)	4(3)
C(128)-C(123)-C(124)-C(125)	-4(3)
C(15)-C(123)-C(124)-C(125)	-174.3(18)
C(123)-C(124)-C(125)-F(14)	-178(2)
F(15)-C(124)-C(125)-F(14)	4(3)
C(123)-C(124)-C(125)-C(126)	-2(3)
F(15)-C(124)-C(125)-C(126)	-180.0(17)
F(14)-C(125)-C(126)-C(127)	178(2)
C(124)-C(125)-C(126)-C(127)	2(3)
F(14)-C(125)-C(126)-F(13)	-13(3)
C(124)-C(125)-C(126)-F(13)	170.6(15)
C(125)-C(126)-C(127)-C(128)	5(3)
F(13)-C(126)-C(127)-C(128)	-164.2(18)
C(125)-C(126)-C(127)-F(12)	171.1(19)
F(13)-C(126)-C(127)-F(12)	2(3)
C(124)-C(123)-C(128)-F(11)	179.8(19)
C(15)-C(123)-C(128)-F(11)	-10(3)
C(124)-C(123)-C(128)-C(127)	11(3)
C(15)-C(123)-C(128)-C(127)	-179(2)
C(126)-C(127)-C(128)-C(123)	-11(3)
F(12)-C(127)-C(128)-C(123)	-178.4(19)
C(126)-C(127)-C(128)-F(11)	179.8(18)

F(12)-C(127)-C(128)-F(11)	13(3)
C(111)-C(110)-C(129)-C(130)	-117(3)
C(19)-C(110)-C(129)-C(130)	66(3)
C(111)-C(110)-C(129)-C(134)	69(3)
C(19)-C(110)-C(129)-C(134)	-108(2)
C(134)-C(129)-C(130)-C(131)	0(3)
C(110)-C(129)-C(130)-C(131)	-174(2)
C(134)-C(129)-C(130)-F(16)	-177.4(18)
C(110)-C(129)-C(130)-F(16)	8(3)
C(129)-C(130)-C(131)-F(17)	174(2)
F(16)-C(130)-C(131)-F(17)	-8(3)
C(129)-C(130)-C(131)-C(132)	4(4)
F(16)-C(130)-C(131)-C(132)	-178.2(19)
C(130)-C(131)-C(132)-F(18)	170.2(19)
F(17)-C(131)-C(132)-F(18)	0(3)
C(130)-C(131)-C(132)-C(133)	-4(3)
F(17)-C(131)-C(132)-C(133)	-174(2)
C(131)-C(132)-C(133)-C(134)	0(3)
F(18)-C(132)-C(133)-C(134)	-175(2)
C(131)-C(132)-C(133)-F(19)	179.5(19)
F(18)-C(132)-C(133)-F(19)	5(3)
F(19)-C(133)-C(134)-F(110)	-3(4)
C(132)-C(133)-C(134)-F(110)	176.7(19)
F(19)-C(133)-C(134)-C(129)	-175(2)
C(132)-C(133)-C(134)-C(129)	5(4)
C(130)-C(129)-C(134)-C(133)	-5(3)
C(110)-C(129)-C(134)-C(133)	170(2)
C(130)-C(129)-C(134)-F(110)	-176(2)
C(110)-C(129)-C(134)-F(110)	-1(3)
C(116)-C(115)-C(135)-C(136)	-175(2)
C(114)-C(115)-C(135)-C(136)	8(3)
C(116)-C(115)-C(135)-C(139)	6(4)
C(114)-C(115)-C(135)-C(139)	-172.0(17)
C(337)-O(12)-C(136)-O(11)	11(3)
C(137)-O(12)-C(136)-O(11)	-15(3)
C(337)-O(12)-C(136)-C(135)	-165.4(16)
C(137)-O(12)-C(136)-C(135)	168.4(18)
C(115)-C(135)-C(136)-O(11)	114(3)
C(139)-C(135)-C(136)-O(11)	-66(3)
C(115)-C(135)-C(136)-O(12)	-69(3)
C(139)-C(135)-C(136)-O(12)	110.8(18)
C(136)-O(12)-C(137)-C(337)	87(4)
C(136)-O(12)-C(137)-C(138)	160(2)
C(337)-O(12)-C(137)-C(138)	73(4)
C(136)-O(12)-C(137)-C(438)	143(2)
C(337)-O(12)-C(137)-C(438)	56(3)
O(12)-C(137)-C(337)-C(138)	105(2)
C(438)-C(137)-C(337)-C(138)	3(3)
C(138)-C(137)-C(337)-O(12)	-105(2)
C(438)-C(137)-C(337)-O(12)	-102(2)
O(12)-C(137)-C(337)-C(438)	102(2)
C(138)-C(137)-C(337)-C(438)	-3(3)

C(136)-O(12)-C(337)-C(137)	-103(3)
C(136)-O(12)-C(337)-C(138)	-178(2)
C(137)-O(12)-C(337)-C(138)	-75(3)
C(136)-O(12)-C(337)-C(438)	159(2)
C(137)-O(12)-C(337)-C(438)	-98(4)
C(137)-C(337)-C(138)-C(438)	-172(8)
O(12)-C(337)-C(138)-C(438)	-98(8)
O(12)-C(337)-C(138)-C(137)	74.6(12)
C(438)-C(337)-C(138)-C(137)	172(8)
C(337)-C(137)-C(138)-C(438)	8(8)
O(12)-C(137)-C(138)-C(438)	-66(8)
O(12)-C(137)-C(138)-C(337)	-74.0(12)
C(438)-C(137)-C(138)-C(337)	-8(8)
C(137)-C(138)-C(438)-C(337)	-3(3)
C(337)-C(138)-C(438)-C(137)	3(3)
C(137)-C(337)-C(438)-C(138)	8(8)
O(12)-C(337)-C(438)-C(138)	88(8)
C(138)-C(337)-C(438)-C(137)	-8(8)
O(12)-C(337)-C(438)-C(137)	79.8(14)
C(337)-C(137)-C(438)-C(138)	-171(9)
O(12)-C(137)-C(438)-C(138)	116(8)
O(12)-C(137)-C(438)-C(337)	-72.9(14)
C(138)-C(137)-C(438)-C(337)	171(9)
C(340)-O(14)-C(139)-O(33)	2(4)
C(140)-O(14)-C(139)-O(33)	-11(3)
C(340)-O(14)-C(139)-O(13)	-14(5)
C(140)-O(14)-C(139)-O(13)	-27(4)
C(340)-O(14)-C(139)-C(135)	-154(3)
C(140)-O(14)-C(139)-C(135)	-167.7(18)
C(115)-C(135)-C(139)-O(33)	-111(3)
C(136)-C(135)-C(139)-O(33)	69(3)
C(115)-C(135)-C(139)-O(13)	-103(4)
C(136)-C(135)-C(139)-O(13)	78(4)
C(115)-C(135)-C(139)-O(14)	46(3)
C(136)-C(135)-C(139)-O(14)	-133.5(19)
C(139)-O(14)-C(140)-C(141)	-142(2)
C(340)-O(14)-C(140)-C(141)	79.7(19)
C(139)-O(14)-C(340)-C(141)	-127(3)
C(140)-O(14)-C(340)-C(141)	-79.6(19)
O(14)-C(140)-C(141)-C(340)	-79.6(19)
O(14)-C(340)-C(141)-C(140)	79.7(19)
C(11)-C(122)-C(142)-C(143)	-168(2)
C(120)-C(122)-C(142)-C(143)	23(3)
C(11)-C(122)-C(142)-C(146)	8(3)
C(120)-C(122)-C(142)-C(146)	-161.1(17)
C(344)-O(16)-C(143)-O(15)	-6(6)
C(144)-O(16)-C(143)-O(15)	-5(4)
C(344)-O(16)-C(143)-C(142)	-175(5)
C(144)-O(16)-C(143)-C(142)	-174(3)
C(122)-C(142)-C(143)-O(15)	41(4)
C(146)-C(142)-C(143)-O(15)	-135(3)
C(122)-C(142)-C(143)-O(16)	-151(2)

C(146)-C(142)-C(143)-O(16)	33(3)
C(143)-O(16)-C(144)-C(145)	-167(3)
C(344)-O(16)-C(144)-C(145)	5(39)
C(143)-O(16)-C(344)-C(345)	-174(4)
C(144)-O(16)-C(344)-C(345)	177(46)
C(147)-O(18)-C(146)-O(17)	11(3)
C(147)-O(18)-C(146)-C(142)	177.3(16)
C(122)-C(142)-C(146)-O(17)	-101(2)
C(143)-C(142)-C(146)-O(17)	75(3)
C(122)-C(142)-C(146)-O(18)	91(2)
C(143)-C(142)-C(146)-O(18)	-93(2)
C(146)-O(18)-C(147)-C(448)	151(3)
C(146)-O(18)-C(147)-C(148)	175(2)
O(18)-C(147)-C(148)-C(448)	-93(8)
O(18)-C(147)-C(448)-C(148)	94(8)
C(24)-N(21)-C(21)-C(222)	-165(2)
Pd(2)-N(21)-C(21)-C(222)	13(3)
C(24)-N(21)-C(21)-C(22)	9(2)
Pd(2)-N(21)-C(21)-C(22)	-172.5(12)
N(21)-C(21)-C(22)-C(23)	-4(2)
C(222)-C(21)-C(22)-C(23)	171(2)
C(21)-C(22)-C(23)-C(24)	-3(2)
C(21)-N(21)-C(24)-C(25)	157(3)
Pd(2)-N(21)-C(24)-C(25)	-21(3)
C(21)-N(21)-C(24)-C(23)	-11(3)
Pd(2)-N(21)-C(24)-C(23)	170.5(13)
C(22)-C(23)-C(24)-C(25)	-161(2)
C(22)-C(23)-C(24)-N(21)	8(3)
N(21)-C(24)-C(25)-C(26)	0(4)
C(23)-C(24)-C(25)-C(26)	167(2)
N(21)-C(24)-C(25)-C(223)	-172(2)
C(23)-C(24)-C(25)-C(223)	-6(4)
C(29)-N(22)-C(26)-C(25)	-175(2)
Pd(2)-N(22)-C(26)-C(25)	-2(3)
C(29)-N(22)-C(26)-C(27)	1(2)
Pd(2)-N(22)-C(26)-C(27)	174.2(13)
C(24)-C(25)-C(26)-N(22)	13(4)
C(223)-C(25)-C(26)-N(22)	-174(2)
C(24)-C(25)-C(26)-C(27)	-163(2)
C(223)-C(25)-C(26)-C(27)	10(3)
N(22)-C(26)-C(27)-C(28)	2(3)
C(25)-C(26)-C(27)-C(28)	178(2)
C(26)-C(27)-C(28)-C(29)	-4(3)
C(26)-N(22)-C(29)-C(28)	-4(3)
Pd(2)-N(22)-C(29)-C(28)	-176.3(15)
C(26)-N(22)-C(29)-C(210)	-176(2)
Pd(2)-N(22)-C(29)-C(210)	11(3)
C(27)-C(28)-C(29)-N(22)	5(3)
C(27)-C(28)-C(29)-C(210)	177(2)
N(22)-C(29)-C(210)-C(229)	-175(2)
C(28)-C(29)-C(210)-C(229)	14(4)
N(22)-C(29)-C(210)-C(211)	2(4)

C(28)-C(29)-C(210)-C(211)	-169(2)
C(214)-N(23)-C(211)-C(212)	-6(2)
Pd(2)-N(23)-C(211)-C(212)	167.0(14)
C(214)-N(23)-C(211)-C(210)	165.9(18)
Pd(2)-N(23)-C(211)-C(210)	-21(3)
C(29)-C(210)-C(211)-N(23)	3(3)
C(229)-C(210)-C(211)-N(23)	-179.8(18)
C(29)-C(210)-C(211)-C(212)	174(2)
C(229)-C(210)-C(211)-C(212)	-10(3)
N(23)-C(211)-C(212)-C(213)	3(2)
C(210)-C(211)-C(212)-C(213)	-168.3(17)
C(211)-C(212)-C(213)-C(214)	1(2)
C(211)-N(23)-C(214)-C(213)	7(2)
Pd(2)-N(23)-C(214)-C(213)	-165.7(14)
C(211)-N(23)-C(214)-C(215)	-177.0(17)
Pd(2)-N(23)-C(214)-C(215)	11(3)
C(212)-C(213)-C(214)-N(23)	-5(2)
C(212)-C(213)-C(214)-C(215)	179(2)
N(23)-C(214)-C(215)-C(235)	137.1(19)
C(213)-C(214)-C(215)-C(235)	-47(3)
N(23)-C(214)-C(215)-C(216)	-41(3)
C(213)-C(214)-C(215)-C(216)	135(2)
C(235)-C(215)-C(216)-C(217)	35(3)
C(214)-C(215)-C(216)-C(217)	-147.8(17)
C(235)-C(215)-C(216)-C(221)	-143.5(18)
C(214)-C(215)-C(216)-C(221)	34(2)
C(221)-C(216)-C(217)-C(218)	-7(3)
C(215)-C(216)-C(217)-C(218)	175.0(16)
C(216)-C(217)-C(218)-C(219)	0(3)
C(217)-C(218)-C(219)-C(220)	0(2)
C(218)-C(219)-C(220)-C(221)	8(3)
C(218)-C(219)-C(220)-C(222)	176.2(14)
C(219)-C(220)-C(221)-C(216)	-14(3)
C(222)-C(220)-C(221)-C(216)	179.2(16)
C(219)-C(220)-C(221)-Pd(2)	175.1(15)
C(222)-C(220)-C(221)-Pd(2)	8(2)
C(217)-C(216)-C(221)-C(220)	13(3)
C(215)-C(216)-C(221)-C(220)	-169.1(16)
C(217)-C(216)-C(221)-Pd(2)	-176.4(16)
C(215)-C(216)-C(221)-Pd(2)	2(3)
N(23)-Pd(2)-C(221)-C(220)	148.2(16)
N(21)-Pd(2)-C(221)-C(220)	-31.4(16)
N(22)-Pd(2)-C(221)-C(220)	-81(86)
N(23)-Pd(2)-C(221)-C(216)	-21.4(18)
N(21)-Pd(2)-C(221)-C(216)	159.1(18)
N(22)-Pd(2)-C(221)-C(216)	109(85)
N(21)-C(21)-C(222)-C(242)	133(2)
C(22)-C(21)-C(222)-C(242)	-41(3)
N(21)-C(21)-C(222)-C(220)	-50(3)
C(22)-C(21)-C(222)-C(220)	137(2)
C(221)-C(220)-C(222)-C(242)	-145(2)
C(219)-C(220)-C(222)-C(242)	46(2)

C(221)-C(220)-C(222)-C(21)	37(2)
C(219)-C(220)-C(222)-C(21)	-131.7(18)
C(24)-C(25)-C(223)-C(224)	-118(3)
C(26)-C(25)-C(223)-C(224)	69(3)
C(24)-C(25)-C(223)-C(228)	70(3)
C(26)-C(25)-C(223)-C(228)	-103(2)
C(228)-C(223)-C(224)-F(21)	177.9(18)
C(25)-C(223)-C(224)-F(21)	6(3)
C(228)-C(223)-C(224)-C(225)	2(3)
C(25)-C(223)-C(224)-C(225)	-170.2(19)
F(21)-C(224)-C(225)-F(22)	6(3)
C(223)-C(224)-C(225)-F(22)	-178.4(18)
F(21)-C(224)-C(225)-C(226)	-179(2)
C(223)-C(224)-C(225)-C(226)	-3(3)
F(22)-C(225)-C(226)-C(227)	177(2)
C(224)-C(225)-C(226)-C(227)	1(4)
F(22)-C(225)-C(226)-F(23)	-3(3)
C(224)-C(225)-C(226)-F(23)	-178.4(19)
F(23)-C(226)-C(227)-F(24)	-1(4)
C(225)-C(226)-C(227)-F(24)	180(2)
F(23)-C(226)-C(227)-C(228)	-179.4(19)
C(225)-C(226)-C(227)-C(228)	1(4)
C(224)-C(223)-C(228)-F(25)	-177.7(17)
C(25)-C(223)-C(228)-F(25)	-5(3)
C(224)-C(223)-C(228)-C(227)	0(3)
C(25)-C(223)-C(228)-C(227)	172.2(18)
C(226)-C(227)-C(228)-F(25)	176(2)
F(24)-C(227)-C(228)-F(25)	-3(3)
C(226)-C(227)-C(228)-C(223)	-2(3)
F(24)-C(227)-C(228)-C(223)	179.6(18)
C(29)-C(210)-C(229)-C(230)	80(3)
C(211)-C(210)-C(229)-C(230)	-98(2)
C(29)-C(210)-C(229)-C(234)	-98(3)
C(211)-C(210)-C(229)-C(234)	85(2)
C(234)-C(229)-C(230)-F(26)	-176(2)
C(210)-C(229)-C(230)-F(26)	7(3)
C(234)-C(229)-C(230)-C(231)	-8(3)
C(210)-C(229)-C(230)-C(231)	174.4(19)
F(26)-C(230)-C(231)-F(37)	-25(3)
C(229)-C(230)-C(231)-F(37)	166(2)
F(26)-C(230)-C(231)-F(27)	1(3)
C(229)-C(230)-C(231)-F(27)	-168(2)
F(26)-C(230)-C(231)-C(232)	176.8(18)
C(229)-C(230)-C(231)-C(232)	8(3)
F(37)-C(231)-C(232)-F(28)	6(3)
F(27)-C(231)-C(232)-F(28)	-19(3)
C(230)-C(231)-C(232)-F(28)	164.5(19)
F(37)-C(231)-C(232)-C(233)	-161(2)
F(27)-C(231)-C(232)-C(233)	174.4(19)
C(230)-C(231)-C(232)-C(233)	-2(3)
F(28)-C(232)-C(233)-C(234)	-171(2)
C(231)-C(232)-C(233)-C(234)	-3(3)

F(28)-C(232)-C(233)-F(29)	15(3)
C(231)-C(232)-C(233)-F(29)	-177.6(19)
F(29)-C(233)-C(234)-F(210)	-8(4)
C(232)-C(233)-C(234)-F(210)	178(2)
F(29)-C(233)-C(234)-C(229)	177(2)
C(232)-C(233)-C(234)-C(229)	3(4)
C(230)-C(229)-C(234)-F(210)	-172(2)
C(210)-C(229)-C(234)-F(210)	5(3)
C(230)-C(229)-C(234)-C(233)	3(3)
C(210)-C(229)-C(234)-C(233)	180(2)
C(216)-C(215)-C(235)-C(236)	-165(2)
C(214)-C(215)-C(235)-C(236)	17(3)
C(216)-C(215)-C(235)-C(239)	20(3)
C(214)-C(215)-C(235)-C(239)	-157.3(16)
C(237)-O(22)-C(236)-O(21)	-13(4)
C(237)-O(22)-C(236)-C(235)	178.2(18)
C(215)-C(235)-C(236)-O(21)	-91(3)
C(239)-C(235)-C(236)-O(21)	84(3)
C(215)-C(235)-C(236)-O(22)	78(3)
C(239)-C(235)-C(236)-O(22)	-107.5(18)
C(236)-O(22)-C(237)-C(238)	-178(2)
C(236)-O(22)-C(237)-C(338)	-154(2)
C(240)-O(24)-C(239)-O(23)	3(3)
C(240)-O(24)-C(239)-C(235)	-171.8(16)
C(215)-C(235)-C(239)-O(23)	46(3)
C(236)-C(235)-C(239)-O(23)	-130(2)
C(215)-C(235)-C(239)-O(24)	-139.5(17)
C(236)-C(235)-C(239)-O(24)	45(2)
C(239)-O(24)-C(240)-C(241)	-165.6(18)
C(21)-C(222)-C(242)-C(246)	176.1(19)
C(220)-C(222)-C(242)-C(246)	-1(3)
C(21)-C(222)-C(242)-C(243)	-4(3)
C(220)-C(222)-C(242)-C(243)	178.4(19)
C(244)-O(26)-C(243)-O(25)	-10(4)
C(244)-O(26)-C(243)-C(242)	172.0(17)
C(222)-C(242)-C(243)-O(25)	120(3)
C(246)-C(242)-C(243)-O(25)	-60(3)
C(222)-C(242)-C(243)-O(26)	-62(3)
C(246)-C(242)-C(243)-O(26)	118(2)
C(243)-O(26)-C(244)-C(245)	171(3)
C(243)-O(26)-C(244)-C(445)	-179(3)
C(247)-O(28)-C(246)-O(27)	43(2)
C(247)-O(28)-C(246)-O(37)	4(3)
C(247)-O(28)-C(246)-C(242)	172.9(19)
C(222)-C(242)-C(246)-O(27)	-173(2)
C(243)-C(242)-C(246)-O(27)	8(3)
C(222)-C(242)-C(246)-O(37)	-115(3)
C(243)-C(242)-C(246)-O(37)	65(3)
C(222)-C(242)-C(246)-O(28)	75(3)
C(243)-C(242)-C(246)-O(28)	-105(2)
C(246)-O(28)-C(247)-C(248)	-170(4)
C(246)-O(28)-C(247)-C(348)	64(3)

Symmetry transformations used to generate equivalent atoms: