Electronic Supplementary Information

Substituent-controlled preference of carbonyl group–metal coordination in d^8 metal complexes with non-symmetric pentadentate ligands. Structural and stereochemical aspects

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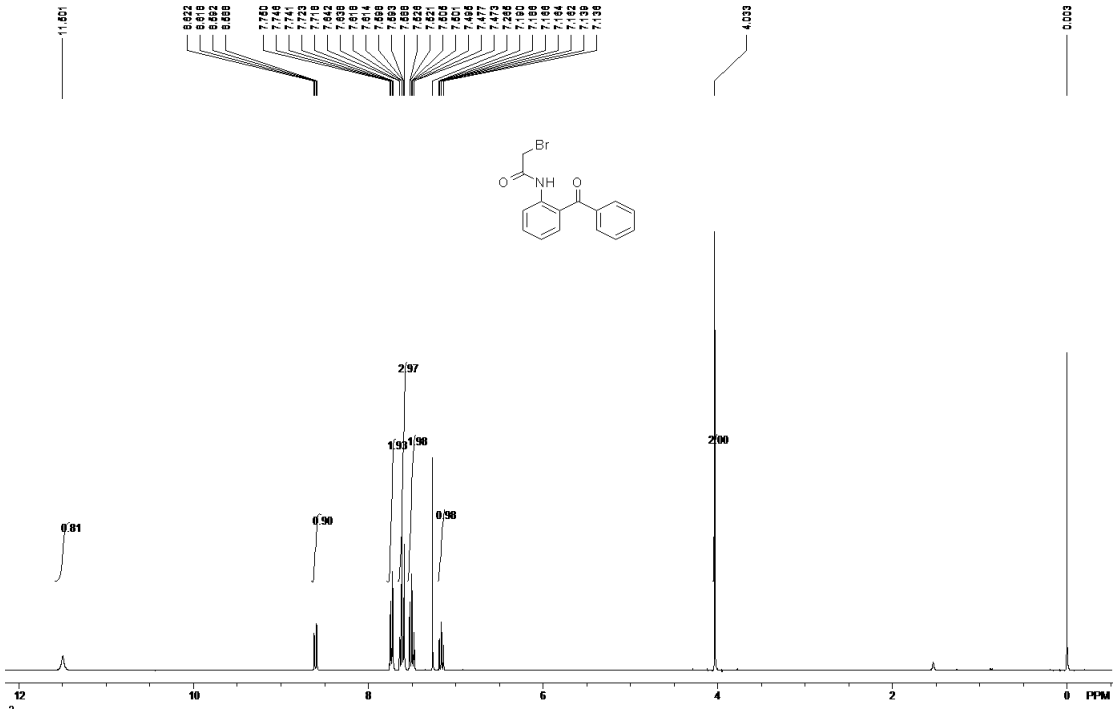

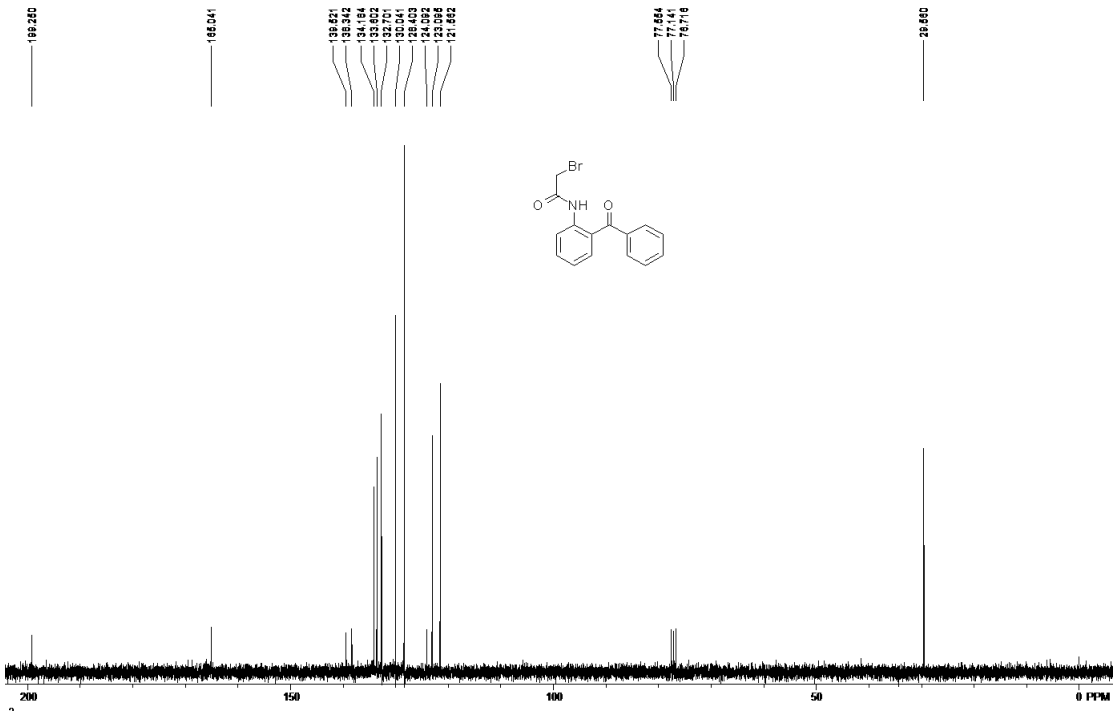

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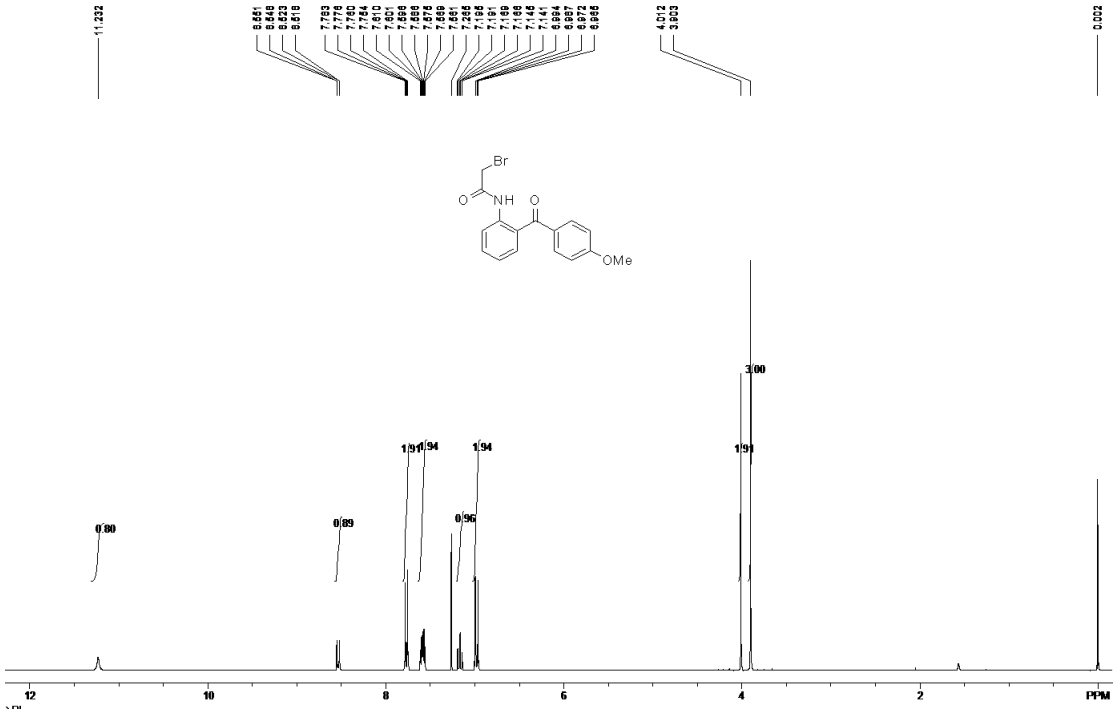
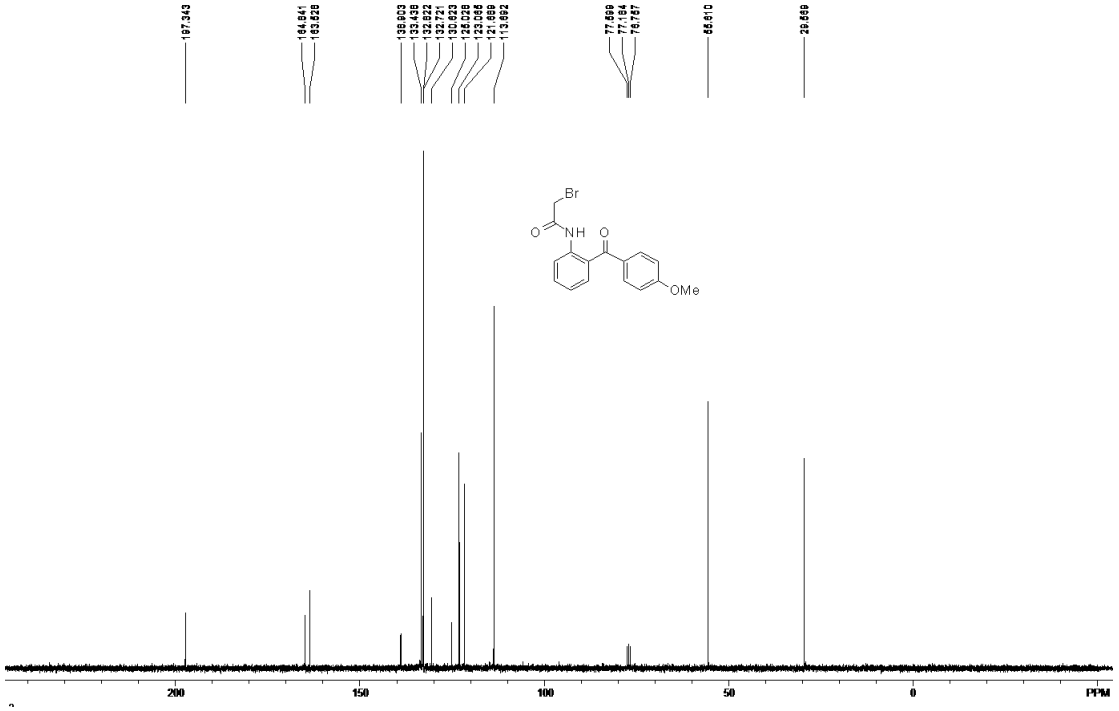
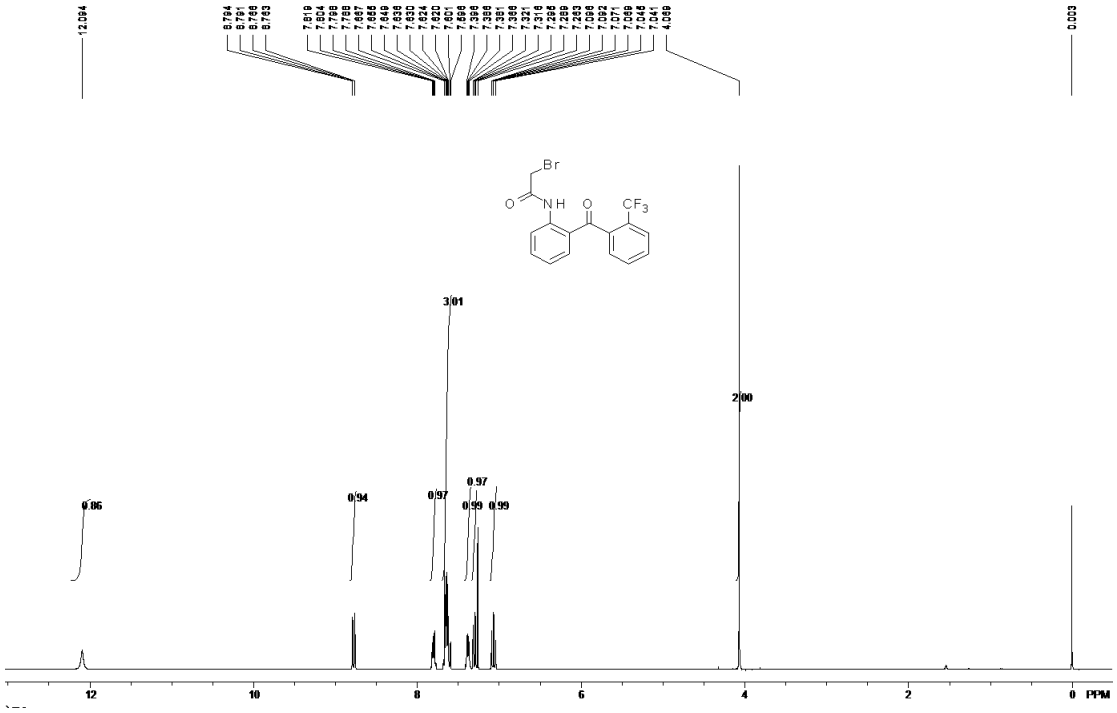
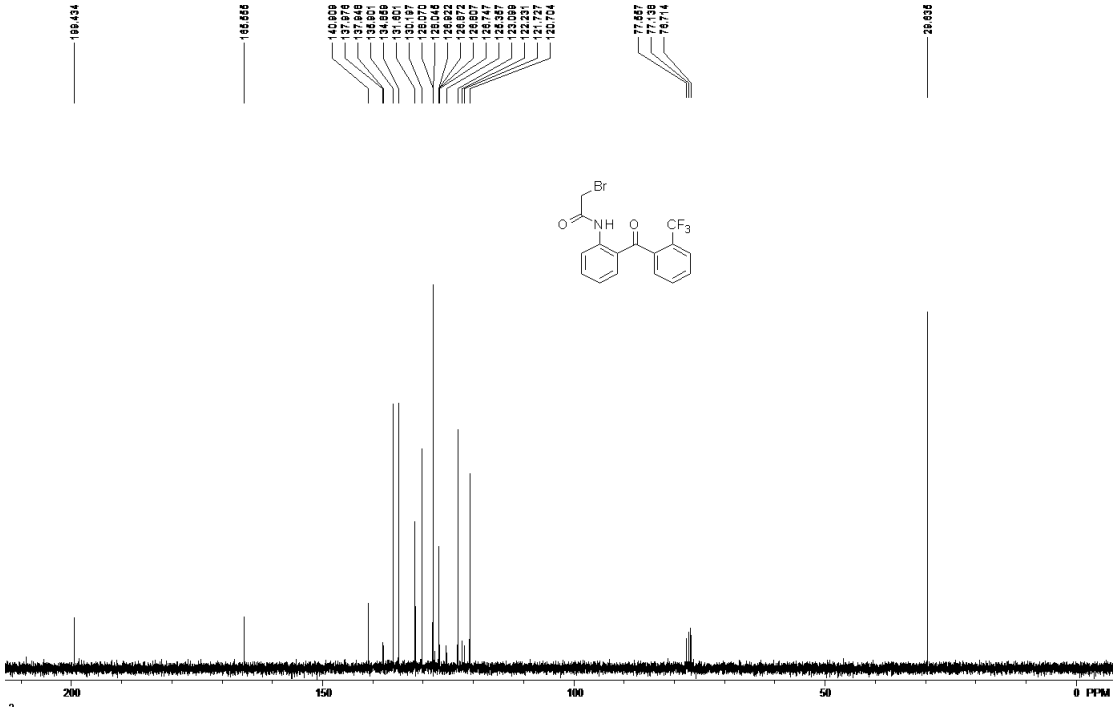


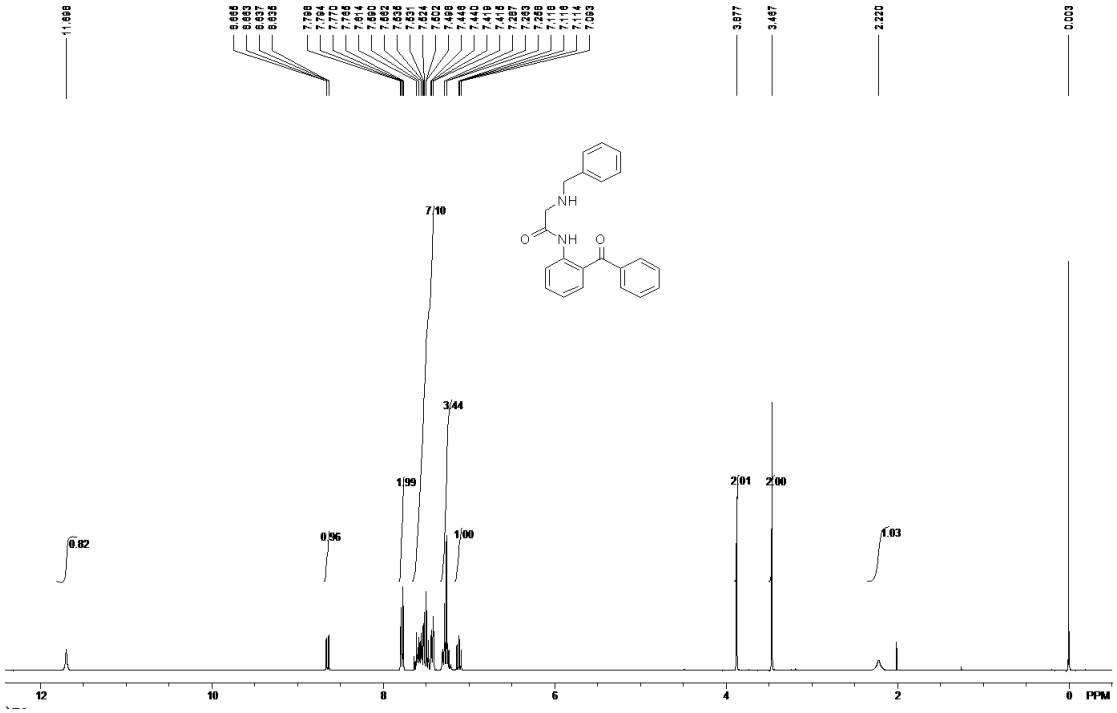


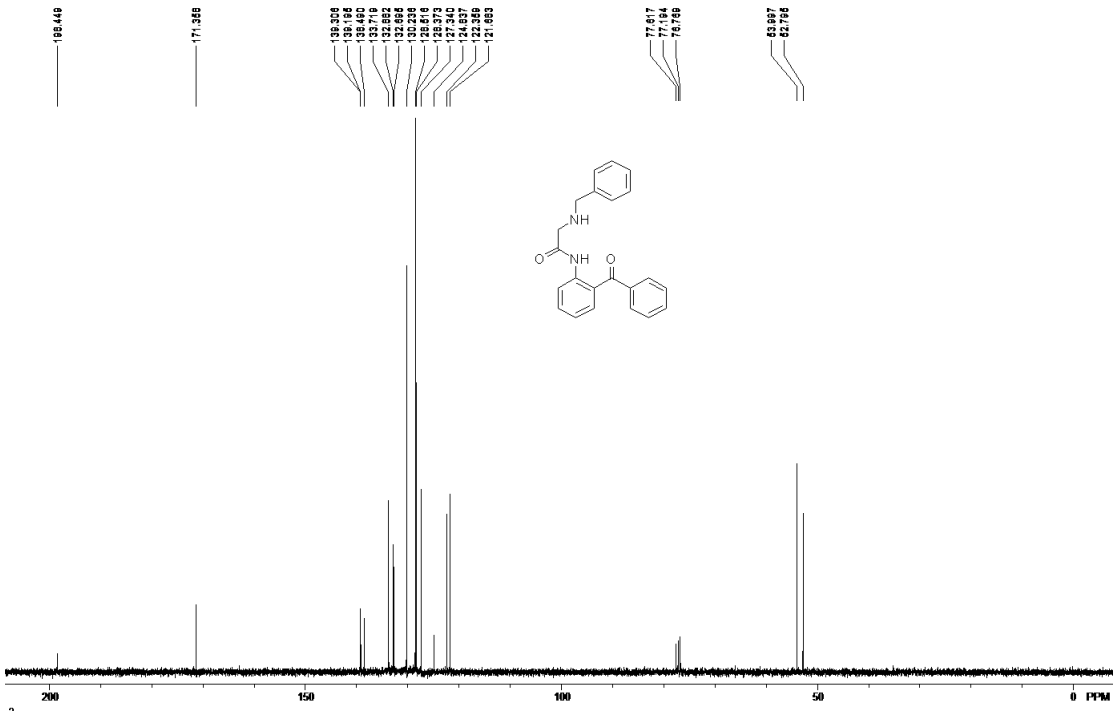
^{1}H and ^{13}C NMR spectra for compound 7



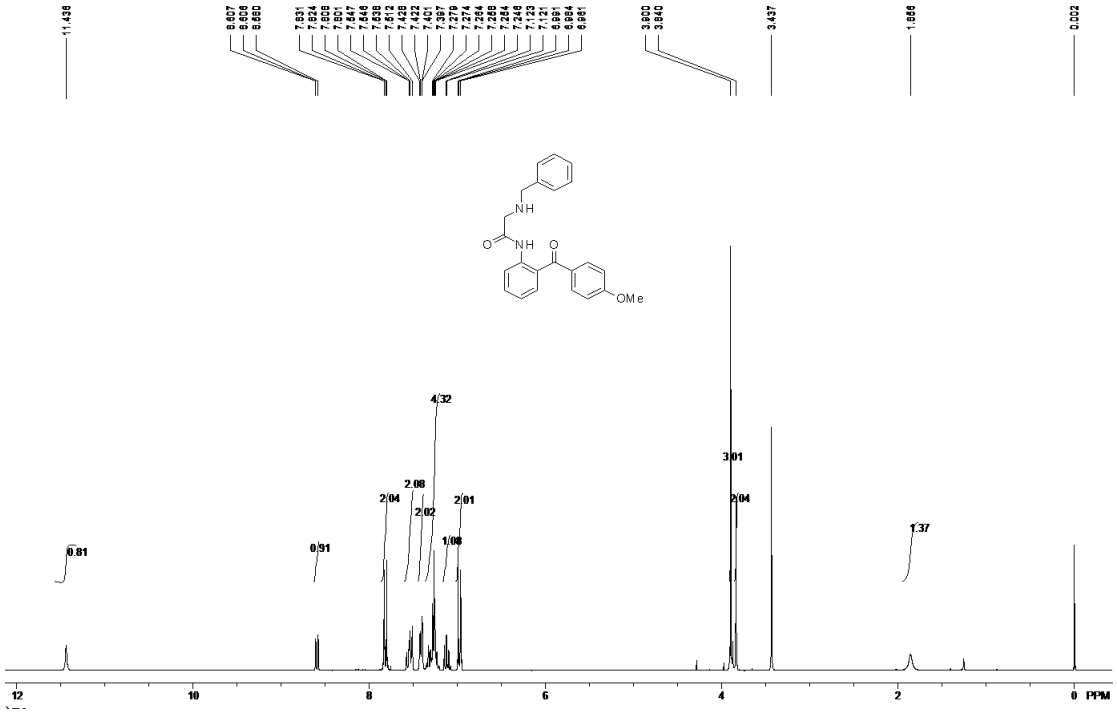


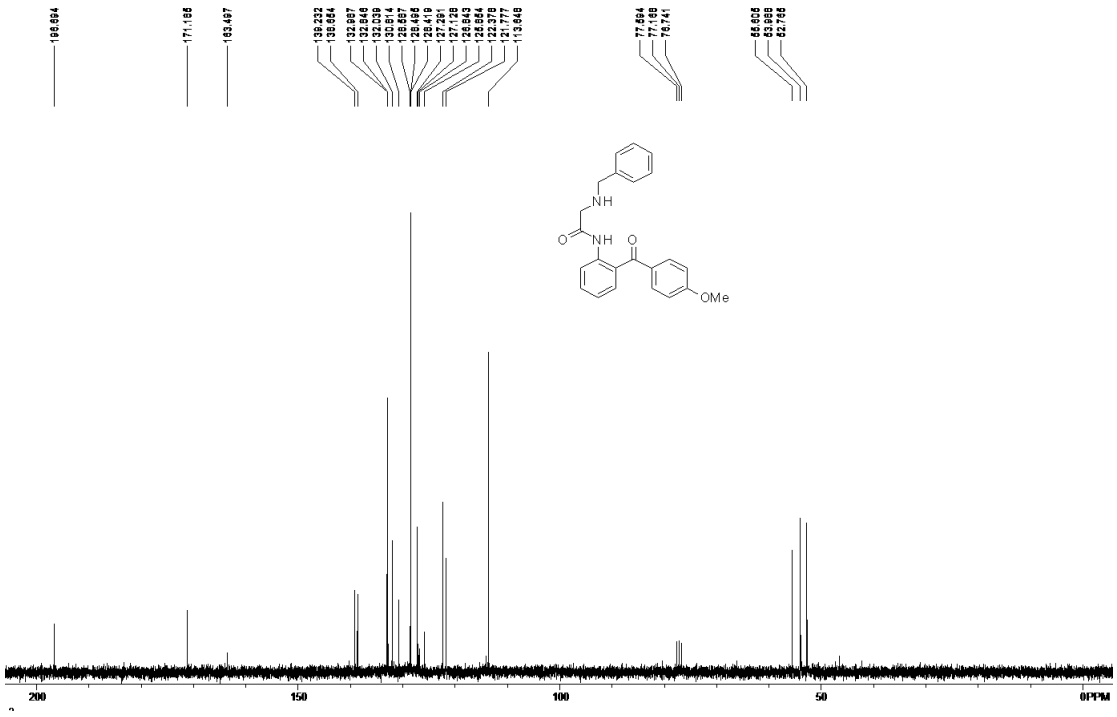
^{1}H and ^{13}C NMR spectra for compound 8





^{1}H and ^{13}C NMR spectra for compound 9





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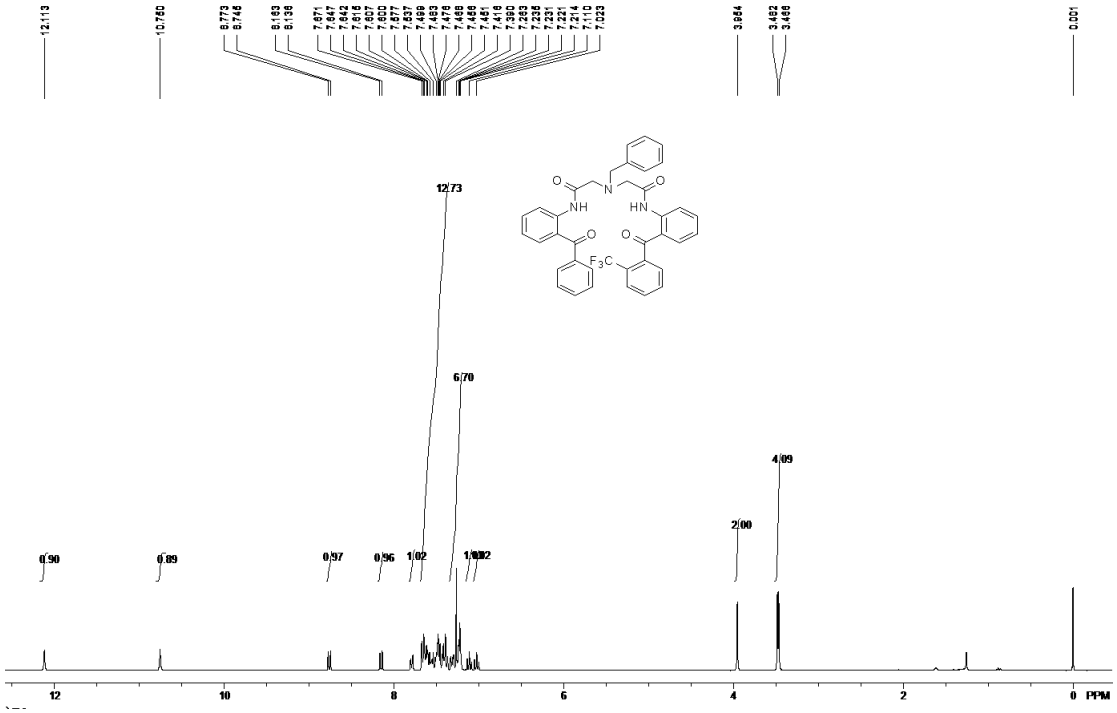
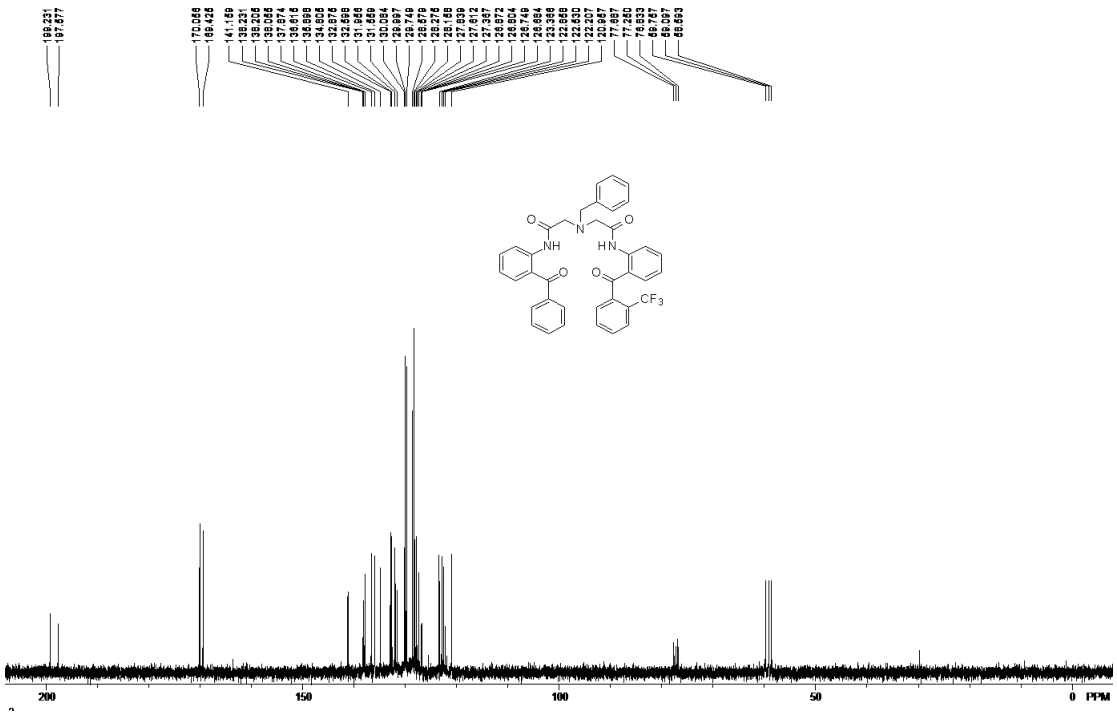
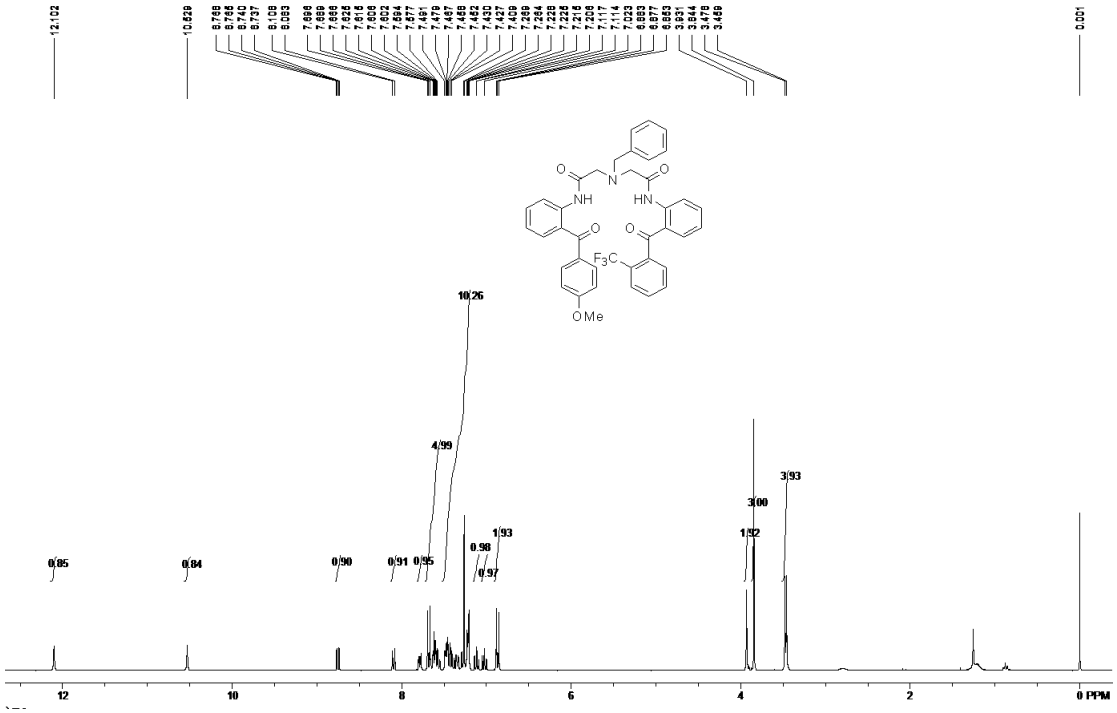
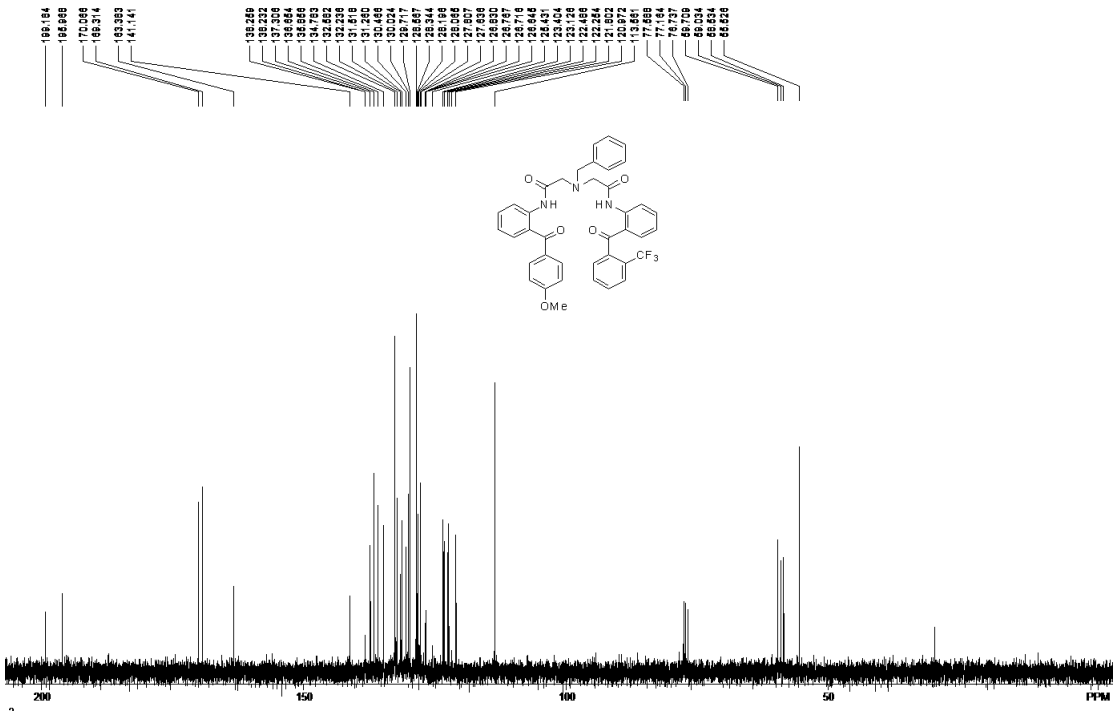


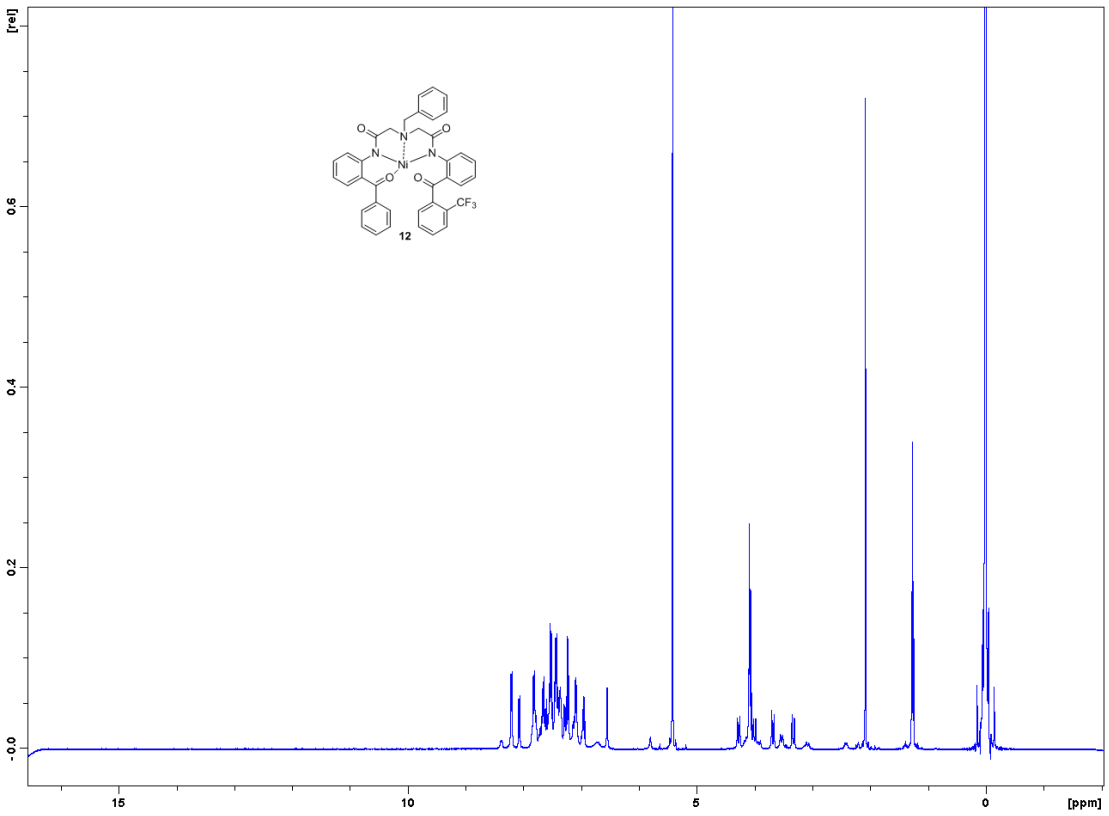


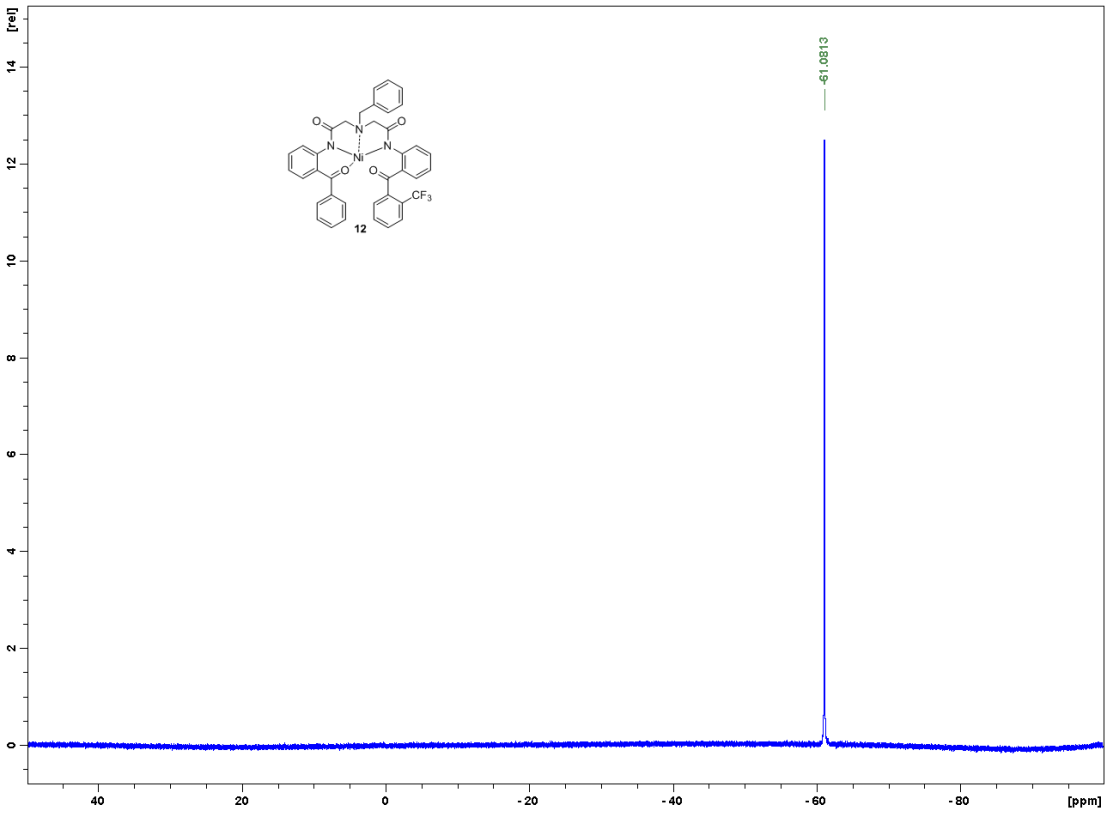
^{1}H and ^{13}C NMR spectra for compound 11



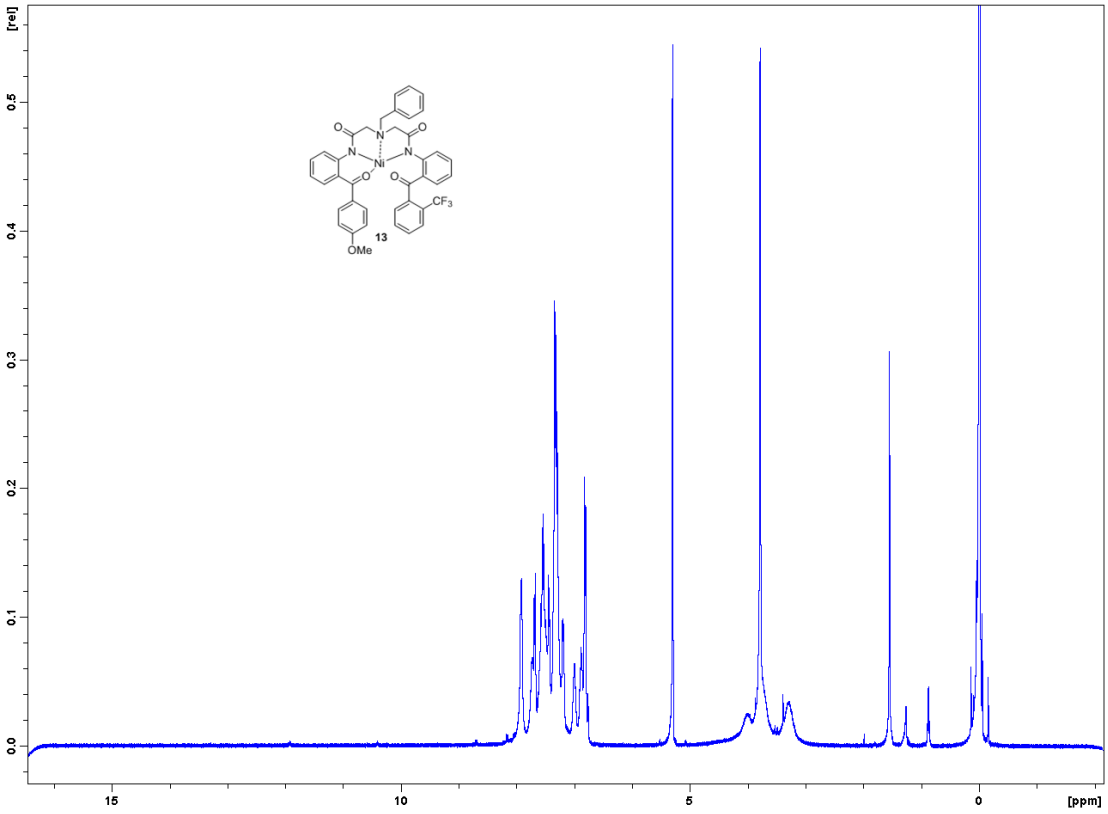


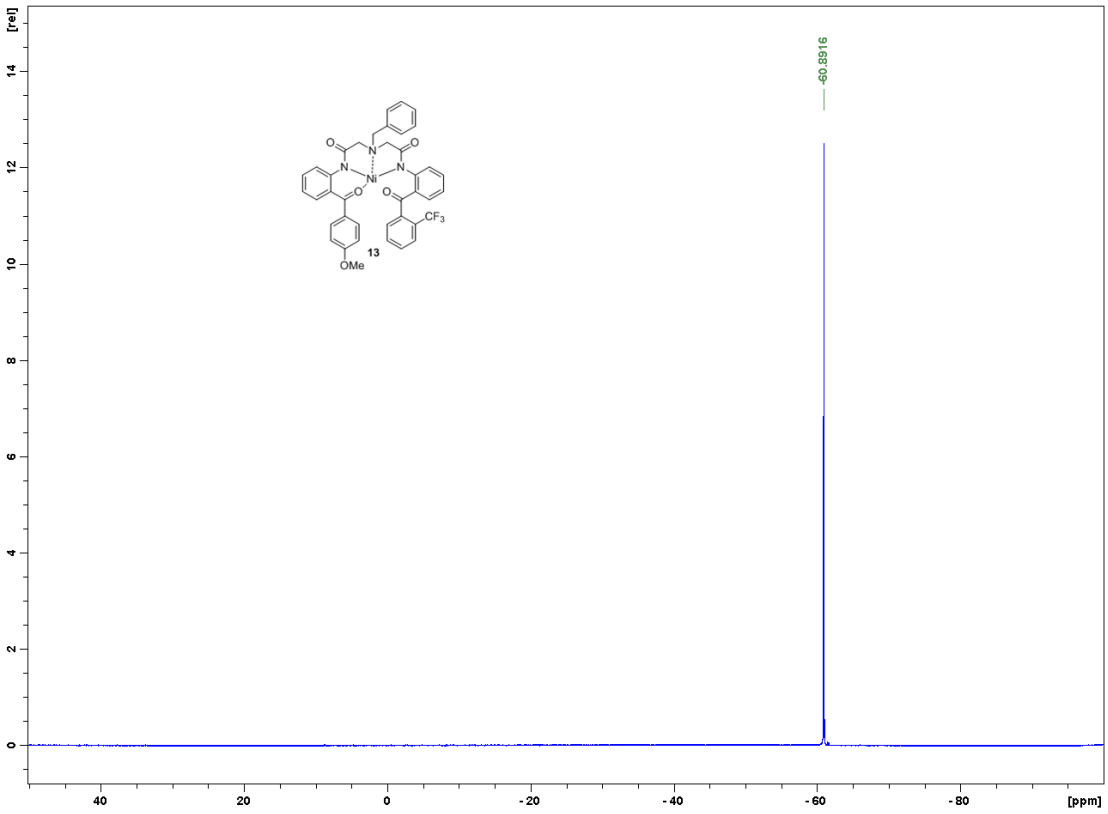
^{1}H and ^{19}F NMR spectra for compound 12



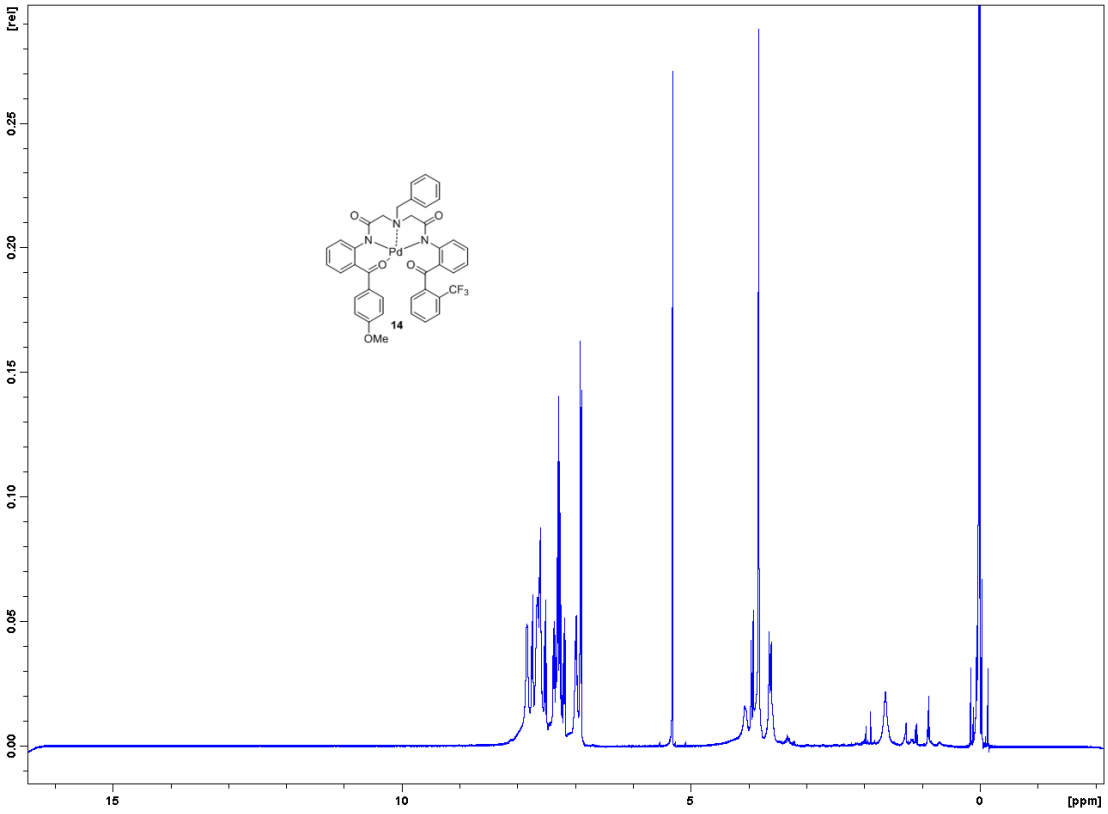


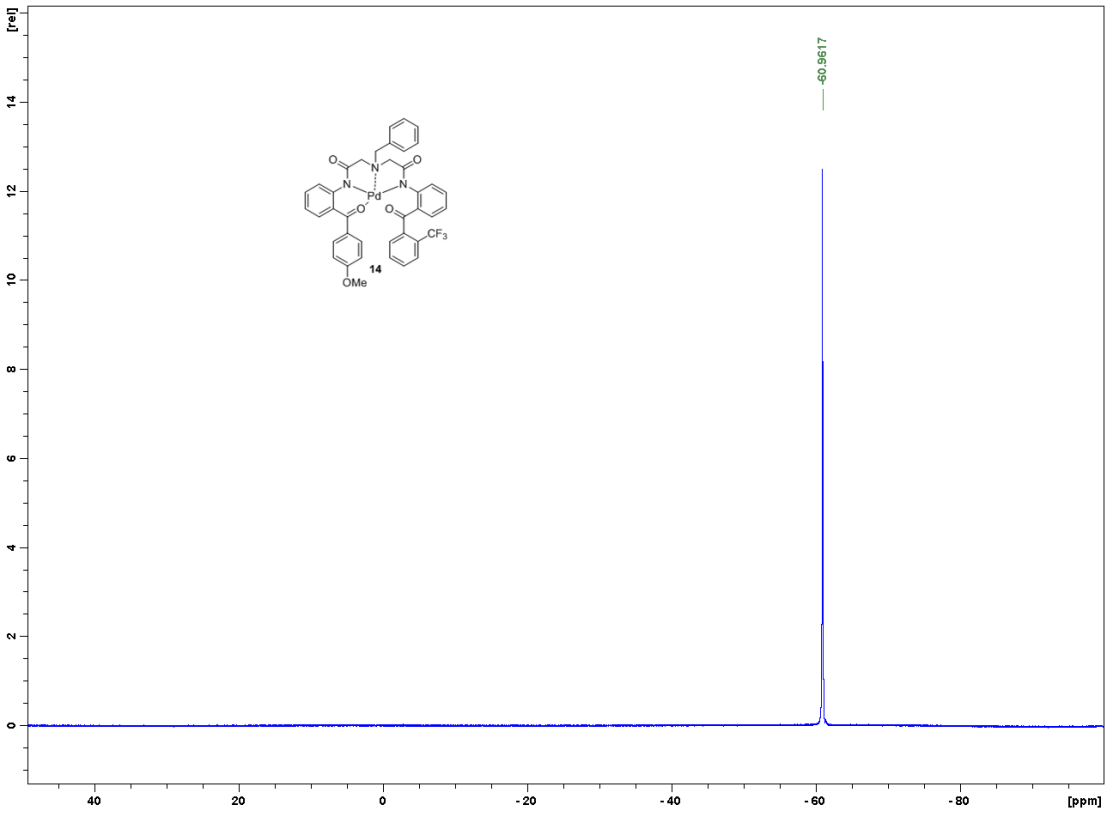
^{1}H and ^{19}F NMR spectra for compound 13



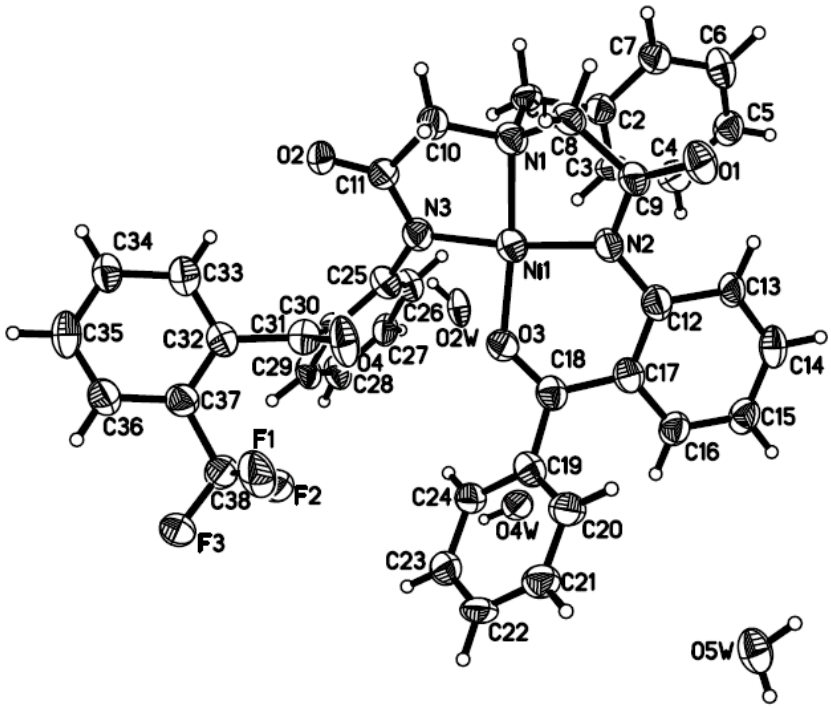


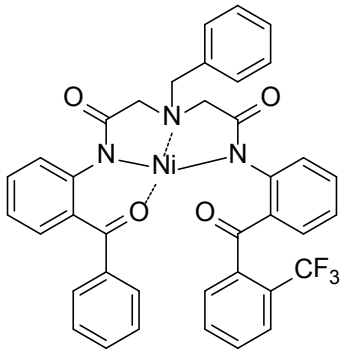
^{1}H and ^{19}F NMR spectra for compound 14





ORTEP drawing of compound 12. (CCDC number 951881)





Ni-o-CF3-p-H

Table 1. Crystal data and structure refinement for complex **12**.

Identification code	Ni-o-CF3-p-H
Empirical formula	C38 H28 F3 N3 Ni O4
Formula weight	706.34
Temperature	291(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 11.869(2) A alpha = 74.121(2) deg.
	b = 11.874(3) A beta = 78.329(3) deg.
	c = 14.3120(18) A gamma = 79.1460(10) deg.
Volume	1880.9(7) A^3
Z, Calculated density	2, 1.311 Mg/m^3
Absorption coefficient	0.578 mm^-1
F(000)	768
Crystal size	0.28 x 0.24 x 0.22 mm
Theta range for data collection	1.80 to 26.00 deg.
Limiting indices	-12<=h<=14, -14<=k<=14, -8<=l<=17
Reflections collected / unique	10366 / 7258 [R(int) = 0.0266]
Completeness to theta = 26.00	98.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8834 and 0.8549
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7258 / 0 / 484
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0572, wR2 = 0.1342
R indices (all data)	R1 = 0.0735, wR2 = 0.1395
Largest diff. peak and hole	0.325 and -0.270 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Ni-o-CF3-p-H. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	-2061(3)	4230(3)	1591(2)	35(1)
C(2)	-2835(3)	4836(3)	2362(2)	37(1)
C(3)	-2402(3)	5577(3)	2747(2)	38(1)
C(4)	-3103(3)	6118(3)	3446(3)	46(1)
C(5)	-4247(3)	5919(3)	3758(3)	43(1)
C(6)	-4691(3)	5201(3)	3368(3)	45(1)
C(7)	-3979(3)	4666(3)	2660(3)	40(1)
C(8)	-2018(3)	2259(3)	2744(2)	37(1)

C(9)	-2084(3)	2429(3)	3784(2)	37(1)
C(10)	-611(3)	2635(3)	1186(2)	36(1)
C(11)	453(3)	3263(3)	765(2)	33(1)
C(12)	-1081(3)	3189(3)	4730(2)	40(1)
C(13)	-2059(3)	3447(3)	5413(2)	38(1)
C(14)	-1923(3)	3804(3)	6237(3)	43(1)
C(15)	-820(3)	3817(3)	6432(2)	42(1)
C(16)	120(3)	3530(3)	5787(2)	40(1)
C(17)	33(3)	3204(3)	4939(2)	37(1)
C(18)	1098(3)	2941(3)	4258(2)	36(1)
C(19)	2210(3)	2430(3)	4655(3)	38(1)
C(20)	2221(3)	1513(3)	5495(3)	42(1)
C(21)	3271(3)	955(3)	5806(3)	43(1)
C(22)	4316(3)	1371(3)	5286(3)	42(1)
C(23)	4306(3)	2257(3)	4461(3)	41(1)
C(24)	3238(3)	2818(3)	4126(2)	38(1)
C(25)	1691(3)	4339(3)	1204(3)	40(1)
C(26)	1447(3)	5546(3)	1162(3)	39(1)
C(27)	2333(3)	6235(3)	999(2)	40(1)
C(28)	3478(3)	5709(3)	869(3)	43(1)
C(29)	3743(3)	4517(3)	862(2)	36(1)
C(30)	2865(3)	3818(3)	1057(2)	34(1)
C(31)	3207(3)	2530(3)	1191(2)	38(1)
C(32)	4125(3)	2127(3)	409(2)	36(1)
C(33)	3835(3)	2400(3)	-537(3)	45(1)
C(34)	4629(3)	2012(3)	-1291(3)	41(1)
C(35)	5712(3)	1350(3)	-1088(3)	48(1)
C(36)	5974(3)	1114(3)	-173(3)	44(1)
C(37)	5200(3)	1477(3)	584(3)	39(1)
C(38)	5562(3)	1226(3)	1572(3)	44(1)
F(1)	5046(2)	330(2)	2253(2)	57(1)
F(2)	5248(2)	2112(2)	2005(2)	46(1)
F(3)	6679(2)	938(2)	1555(2)	49(1)
N(1)	-1317(2)	3118(2)	2014(2)	37(1)
N(2)	-1172(2)	2912(2)	3856(2)	36(1)
N(3)	752(2)	3684(2)	1441(2)	39(1)
Ni(1)	-151(1)	3297(1)	2698(1)	37(1)
O(1)	-2863(2)	2035(2)	4448(2)	45(1)
O(2)	959(2)	3299(2)	-71(2)	38(1)
O(3)	1093(2)	3094(2)	3339(2)	39(1)
O(4)	2767(2)	1823(2)	1891(2)	53(1)
O(1W)	9867(5)	548(5)	7555(5)	47(2)
O(2W)	1089(5)	8975(5)	1055(5)	48(2)
O(3W)	10000	0	5000	46(1)

O(4W)	3131(6)	9255(6)	3544(5)	54(2)
O(5W)	1776(6)	1562(5)	8463(5)	51(2)

Table 3. Bond lengths [A] and angles [deg] for Ni-o-CF3-p-H.

C(1)-N(1)	1.493(4)
C(1)-C(2)	1.534(4)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(7)	1.374(5)
C(2)-C(3)	1.376(5)
C(3)-C(4)	1.385(5)
C(3)-H(3)	0.9300
C(4)-C(5)	1.383(5)
C(4)-H(4)	0.9300
C(5)-C(6)	1.365(5)
C(5)-H(5)	0.9300
C(6)-C(7)	1.395(5)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(8)-N(1)	1.487(4)
C(8)-C(9)	1.542(5)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-O(1)	1.241(4)
C(9)-N(2)	1.350(4)
C(10)-N(1)	1.492(4)
C(10)-C(11)	1.521(4)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-O(2)	1.219(4)
C(11)-N(3)	1.335(4)
C(12)-C(13)	1.402(4)
C(12)-N(2)	1.406(4)
C(12)-C(17)	1.419(5)
C(13)-C(14)	1.405(5)
C(13)-H(13)	0.9300
C(14)-C(15)	1.396(5)
C(14)-H(14)	0.9300
C(15)-C(16)	1.352(5)
C(15)-H(15)	0.9300
C(16)-C(17)	1.398(5)

C(16)-H(16)	0.9300
C(17)-C(18)	1.471(4)
C(18)-O(3)	1.279(4)
C(18)-C(19)	1.499(5)
C(19)-C(20)	1.384(5)
C(19)-C(24)	1.386(5)
C(20)-C(21)	1.394(5)
C(20)-H(20)	0.9300
C(21)-C(22)	1.412(5)
C(21)-H(21)	0.9300
C(22)-C(23)	1.350(5)
C(22)-H(22)	0.9300
C(23)-C(24)	1.426(5)
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(25)-C(26)	1.395(5)
C(25)-N(3)	1.411(4)
C(25)-C(30)	1.413(5)
C(26)-C(27)	1.397(5)
C(26)-H(26)	0.9300
C(27)-C(28)	1.383(5)
C(27)-H(27)	0.9300
C(28)-C(29)	1.394(5)
C(28)-H(28)	0.9300
C(29)-C(30)	1.390(4)
C(29)-H(29)	0.9300
C(30)-C(31)	1.476(4)
C(31)-O(4)	1.214(4)
C(31)-C(32)	1.507(5)
C(32)-C(37)	1.392(5)
C(32)-C(33)	1.402(5)
C(33)-C(34)	1.400(5)
C(33)-H(33)	0.9300
C(34)-C(35)	1.414(5)
C(34)-H(34)	0.9300
C(35)-C(36)	1.350(5)
C(35)-H(35)	0.9300
C(36)-C(37)	1.381(5)
C(36)-H(36)	0.9300
C(37)-C(38)	1.497(5)
C(38)-F(3)	1.302(4)
C(38)-F(2)	1.321(4)
C(38)-F(1)	1.376(4)
N(1)-Ni(1)	1.921(3)

N(2)-Ni(1)	1.846(3)
N(3)-Ni(1)	1.884(3)
Ni(1)-O(3)	1.836(2)
O(1W)-H(1WD)	0.8499
O(1W)-H(1WB)	0.8500
O(2W)-H(2WA)	0.8500
O(2W)-H(2WB)	0.8499
O(3W)-H(3WA)	0.8500
O(3W)-H(3WB)	0.8500
O(4W)-H(4WA)	0.8500
O(4W)-H(4WB)	0.8500
O(5W)-H(5WA)	0.8499
O(5W)-H(5WB)	0.8500
N(1)-C(1)-C(2)	114.3(3)
N(1)-C(1)-H(1A)	108.7
C(2)-C(1)-H(1A)	108.7
N(1)-C(1)-H(1B)	108.7
C(2)-C(1)-H(1B)	108.7
H(1A)-C(1)-H(1B)	107.6
C(7)-C(2)-C(3)	119.1(3)
C(7)-C(2)-C(1)	120.4(3)
C(3)-C(2)-C(1)	120.5(3)
C(2)-C(3)-C(4)	120.3(3)
C(2)-C(3)-H(3)	119.8
C(4)-C(3)-H(3)	119.8
C(5)-C(4)-C(3)	120.1(3)
C(5)-C(4)-H(4)	119.9
C(3)-C(4)-H(4)	119.9
C(6)-C(5)-C(4)	120.1(3)
C(6)-C(5)-H(5)	120.0
C(4)-C(5)-H(5)	120.0
C(5)-C(6)-C(7)	119.4(3)
C(5)-C(6)-H(6)	120.3
C(7)-C(6)-H(6)	120.3
C(2)-C(7)-C(6)	121.0(3)
C(2)-C(7)-H(7)	119.5
C(6)-C(7)-H(7)	119.5
N(1)-C(8)-C(9)	109.7(3)
N(1)-C(8)-H(8A)	109.7
C(9)-C(8)-H(8A)	109.7
N(1)-C(8)-H(8B)	109.7
C(9)-C(8)-H(8B)	109.7
H(8A)-C(8)-H(8B)	108.2
O(1)-C(9)-N(2)	128.5(3)

O(1)-C(9)-C(8)	119.1(3)
N(2)-C(9)-C(8)	112.1(3)
N(1)-C(10)-C(11)	109.9(2)
N(1)-C(10)-H(10A)	109.7
C(11)-C(10)-H(10A)	109.7
N(1)-C(10)-H(10B)	109.7
C(11)-C(10)-H(10B)	109.7
H(10A)-C(10)-H(10B)	108.2
O(2)-C(11)-N(3)	127.2(3)
O(2)-C(11)-C(10)	121.8(3)
N(3)-C(11)-C(10)	110.9(3)
C(13)-C(12)-N(2)	122.3(3)
C(13)-C(12)-C(17)	118.4(3)
N(2)-C(12)-C(17)	119.4(3)
C(12)-C(13)-C(14)	119.8(3)
C(12)-C(13)-H(13)	120.1
C(14)-C(13)-H(13)	120.1
C(15)-C(14)-C(13)	121.1(3)
C(15)-C(14)-H(14)	119.5
C(13)-C(14)-H(14)	119.5
C(16)-C(15)-C(14)	118.6(3)
C(16)-C(15)-H(15)	120.7
C(14)-C(15)-H(15)	120.7
C(15)-C(16)-C(17)	122.6(3)
C(15)-C(16)-H(16)	118.7
C(17)-C(16)-H(16)	118.7
C(16)-C(17)-C(12)	119.3(3)
C(16)-C(17)-C(18)	119.2(3)
C(12)-C(17)-C(18)	121.4(3)
O(3)-C(18)-C(17)	121.8(3)
O(3)-C(18)-C(19)	118.9(3)
C(17)-C(18)-C(19)	119.3(3)
C(20)-C(19)-C(24)	120.5(3)
C(20)-C(19)-C(18)	120.2(3)
C(24)-C(19)-C(18)	119.1(3)
C(19)-C(20)-C(21)	120.2(3)
C(19)-C(20)-H(20)	119.9
C(21)-C(20)-H(20)	119.9
C(20)-C(21)-C(22)	119.4(3)
C(20)-C(21)-H(21)	120.3
C(22)-C(21)-H(21)	120.3
C(23)-C(22)-C(21)	120.3(3)
C(23)-C(22)-H(22)	119.9
C(21)-C(22)-H(22)	119.9

C(22)-C(23)-C(24)	120.6(3)
C(22)-C(23)-H(23)	119.7
C(24)-C(23)-H(23)	119.7
C(19)-C(24)-C(23)	119.0(3)
C(19)-C(24)-H(24)	120.5
C(23)-C(24)-H(24)	120.5
C(26)-C(25)-N(3)	118.2(3)
C(26)-C(25)-C(30)	118.6(3)
N(3)-C(25)-C(30)	123.1(3)
C(25)-C(26)-C(27)	121.5(3)
C(25)-C(26)-H(26)	119.3
C(27)-C(26)-H(26)	119.3
C(28)-C(27)-C(26)	119.2(3)
C(28)-C(27)-H(27)	120.4
C(26)-C(27)-H(27)	120.4
C(27)-C(28)-C(29)	120.4(3)
C(27)-C(28)-H(28)	119.8
C(29)-C(28)-H(28)	119.8
C(30)-C(29)-C(28)	120.6(3)
C(30)-C(29)-H(29)	119.7
C(28)-C(29)-H(29)	119.7
C(29)-C(30)-C(25)	119.7(3)
C(29)-C(30)-C(31)	117.9(3)
C(25)-C(30)-C(31)	122.3(3)
O(4)-C(31)-C(30)	121.9(3)
O(4)-C(31)-C(32)	121.2(3)
C(30)-C(31)-C(32)	116.8(3)
C(37)-C(32)-C(33)	119.5(3)
C(37)-C(32)-C(31)	124.1(3)
C(33)-C(32)-C(31)	116.4(3)
C(34)-C(33)-C(32)	119.5(3)
C(34)-C(33)-H(33)	120.3
C(32)-C(33)-H(33)	120.3
C(33)-C(34)-C(35)	119.7(3)
C(33)-C(34)-H(34)	120.1
C(35)-C(34)-H(34)	120.1
C(36)-C(35)-C(34)	119.5(3)
C(36)-C(35)-H(35)	120.2
C(34)-C(35)-H(35)	120.2
C(35)-C(36)-C(37)	121.8(3)
C(35)-C(36)-H(36)	119.1
C(37)-C(36)-H(36)	119.1
C(36)-C(37)-C(32)	120.0(3)
C(36)-C(37)-C(38)	119.1(3)

C(32)-C(37)-C(38)	120.7(3)
F(3)-C(38)-F(2)	106.2(3)
F(3)-C(38)-F(1)	106.8(3)
F(2)-C(38)-F(1)	102.2(3)
F(3)-C(38)-C(37)	113.6(3)
F(2)-C(38)-C(37)	114.2(3)
F(1)-C(38)-C(37)	112.8(3)
C(8)-N(1)-C(10)	113.3(3)
C(8)-N(1)-C(1)	111.7(3)
C(10)-N(1)-C(1)	108.4(3)
C(8)-N(1)-Ni(1)	104.8(2)
C(10)-N(1)-Ni(1)	102.63(19)
C(1)-N(1)-Ni(1)	115.8(2)
C(9)-N(2)-C(12)	121.6(3)
C(9)-N(2)-Ni(1)	114.7(2)
C(12)-N(2)-Ni(1)	123.5(2)
C(11)-N(3)-C(25)	120.8(3)
C(11)-N(3)-Ni(1)	114.5(2)
C(25)-N(3)-Ni(1)	124.6(2)
O(3)-Ni(1)-N(2)	93.10(11)
O(3)-Ni(1)-N(3)	93.42(11)
N(2)-Ni(1)-N(3)	173.40(12)
O(3)-Ni(1)-N(1)	166.05(11)
N(2)-Ni(1)-N(1)	88.05(12)
N(3)-Ni(1)-N(1)	85.37(12)
C(18)-O(3)-Ni(1)	128.8(2)
H(1WD)-O(1W)-H(1WB)	109.5
H(2WA)-O(2W)-H(2WB)	109.5
H(3WA)-O(3W)-H(3WB)	109.5
H(4WA)-O(4W)-H(4WB)	109.5
H(5WA)-O(5W)-H(5WB)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for Ni-o-CF3-p-H.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	32(2)	41(2)	32(2)	-12(1)	-12(1)	3(1)
C(2)	33(2)	41(2)	34(2)	-7(1)	-6(1)	-1(1)
C(3)	36(2)	45(2)	40(2)	-15(2)	-16(1)	-3(1)

C(4)	43(2)	47(2)	49(2)	-19(2)	-13(2)	9(2)
C(5)	40(2)	46(2)	40(2)	-15(2)	-4(2)	5(2)
C(6)	36(2)	39(2)	53(2)	-14(2)	9(2)	-4(1)
C(7)	39(2)	43(2)	42(2)	-14(2)	-2(2)	-13(1)
C(8)	29(2)	45(2)	37(2)	-6(1)	-4(1)	-13(1)
C(9)	32(2)	45(2)	32(2)	-2(1)	-1(1)	-15(1)
C(10)	34(2)	40(2)	38(2)	-15(1)	-2(1)	-5(1)
C(11)	32(2)	34(2)	34(2)	-9(1)	-5(1)	-4(1)
C(12)	34(2)	42(2)	37(2)	-8(1)	-1(1)	-1(1)
C(13)	28(2)	49(2)	31(2)	-11(1)	0(1)	9(1)
C(14)	42(2)	39(2)	42(2)	-15(2)	11(2)	-1(1)
C(15)	46(2)	42(2)	35(2)	-14(2)	-3(2)	7(2)
C(16)	41(2)	44(2)	34(2)	-12(1)	-5(1)	3(2)
C(17)	36(2)	34(2)	40(2)	-11(1)	-2(1)	-3(1)
C(18)	35(2)	35(2)	40(2)	-10(1)	-1(1)	-10(1)
C(19)	33(2)	35(2)	46(2)	-13(1)	-2(1)	-4(1)
C(20)	38(2)	47(2)	42(2)	-6(2)	-10(2)	-8(2)
C(21)	44(2)	43(2)	42(2)	-10(2)	-14(2)	3(2)
C(22)	36(2)	49(2)	43(2)	-11(2)	-21(2)	8(2)
C(23)	40(2)	43(2)	39(2)	-13(2)	-6(1)	2(1)
C(24)	33(2)	44(2)	39(2)	-16(2)	-7(1)	-3(1)
C(25)	31(2)	41(2)	45(2)	-9(2)	-1(1)	-9(1)
C(26)	33(2)	38(2)	44(2)	-12(2)	0(1)	-3(1)
C(27)	40(2)	46(2)	34(2)	-14(2)	5(1)	-11(2)
C(28)	33(2)	48(2)	46(2)	-14(2)	5(1)	-12(2)
C(29)	30(2)	40(2)	38(2)	-12(1)	8(1)	-16(1)
C(30)	33(2)	38(2)	35(2)	-15(1)	2(1)	-10(1)
C(31)	41(2)	33(2)	39(2)	-9(1)	-4(1)	-7(1)
C(32)	32(2)	33(2)	42(2)	-11(1)	-1(1)	-5(1)
C(33)	42(2)	46(2)	42(2)	-11(2)	2(2)	-3(2)
C(34)	39(2)	42(2)	40(2)	-14(2)	6(2)	-9(1)
C(35)	51(2)	46(2)	39(2)	-11(2)	15(2)	-9(2)
C(36)	36(2)	45(2)	48(2)	-16(2)	-4(2)	0(1)
C(37)	36(2)	39(2)	45(2)	-15(2)	-10(2)	-2(1)
C(38)	46(2)	44(2)	39(2)	-14(2)	-14(2)	12(2)
F(1)	51(1)	48(1)	50(1)	1(1)	-1(1)	19(1)
F(2)	47(1)	48(1)	46(1)	-18(1)	-17(1)	8(1)
F(3)	45(1)	54(1)	45(1)	-13(1)	-17(1)	16(1)
N(1)	33(1)	38(1)	40(2)	-10(1)	-3(1)	-9(1)
N(2)	29(1)	42(2)	33(1)	-6(1)	0(1)	-4(1)
N(3)	35(1)	44(2)	40(2)	-13(1)	0(1)	-12(1)
Ni(1)	34(1)	38(1)	37(1)	-8(1)	-2(1)	-8(1)
O(1)	39(1)	42(1)	46(1)	-2(1)	4(1)	-14(1)
O(2)	33(1)	49(1)	32(1)	-13(1)	3(1)	-11(1)

O(3)	34(1)	46(1)	40(1)	-13(1)	-3(1)	-13(1)
O(4)	48(2)	47(1)	47(1)	-3(1)	21(1)	-5(1)
O(1W)	33(3)	34(3)	53(4)	5(3)	11(3)	6(2)
O(2W)	45(3)	40(3)	47(4)	-8(3)	18(3)	-11(3)
O(3W)	41(2)	45(2)	54(3)	-14(2)	-15(2)	-1(2)
O(4W)	58(4)	48(4)	51(4)	-14(3)	-16(3)	10(3)
O(5W)	44(3)	45(3)	57(4)	-8(3)	7(3)	-13(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Ni-o-CF3-p-H.

	x	y	z	U(eq)
H(1A)	-2551	4050	1201	42
H(1B)	-1563	4780	1153	42
H(3)	-1636	5716	2537	46
H(4)	-2805	6615	3706	55
H(5)	-4713	6275	4233	52
H(6)	-5460	5069	3573	54
H(7)	-4284	4188	2385	48
H(8A)	-1664	1459	2721	44
H(8B)	-2795	2378	2584	44
H(10A)	-1077	2746	675	44
H(10B)	-368	1793	1420	44
H(13)	-2796	3382	5320	46
H(14)	-2578	4035	6659	52
H(15)	-734	4020	6995	51
H(16)	854	3549	5912	49
H(20)	1526	1269	5853	51
H(21)	3283	314	6352	52
H(22)	5014	1034	5512	51
H(23)	5002	2504	4107	49
H(24)	3231	3434	3562	45
H(26)	677	5900	1245	47
H(27)	2156	7038	978	48
H(28)	4074	6153	785	51
H(29)	4515	4185	726	43
H(33)	3120	2834	-664	54
H(34)	4445	2190	-1921	49
H(35)	6240	1079	-1582	58
H(36)	6695	695	-49	52
H(1WD)	9280	729	7260	56

H(1WB)	10071	1174	7607	71
H(2WA)	1278	9668	873	72
H(2WB)	1103	8722	551	72
H(3WA)	10490	-492	4739	69
H(3WB)	10332	285	5339	69
H(4WA)	3813	9177	3221	80
H(4WB)	2836	9979	3413	80
H(5WA)	2123	1483	8946	76
H(5WB)	1052	1561	8667	76

Table 6. Torsion angles [deg] for Ni-o-CF3-p-H.

N(1)-C(1)-C(2)-C(7)	-97.9(4)
N(1)-C(1)-C(2)-C(3)	83.6(4)
C(7)-C(2)-C(3)-C(4)	1.8(5)
C(1)-C(2)-C(3)-C(4)	-179.7(3)
C(2)-C(3)-C(4)-C(5)	-0.3(5)
C(3)-C(4)-C(5)-C(6)	-0.8(5)
C(4)-C(5)-C(6)-C(7)	0.4(5)
C(3)-C(2)-C(7)-C(6)	-2.2(5)
C(1)-C(2)-C(7)-C(6)	179.3(3)
C(5)-C(6)-C(7)-C(2)	1.2(5)
N(1)-C(8)-C(9)-O(1)	160.8(3)
N(1)-C(8)-C(9)-N(2)	-25.3(4)
N(1)-C(10)-C(11)-O(2)	-157.2(3)
N(1)-C(10)-C(11)-N(3)	25.9(4)
N(2)-C(12)-C(13)-C(14)	-175.2(3)
C(17)-C(12)-C(13)-C(14)	5.1(5)
C(12)-C(13)-C(14)-C(15)	-5.1(5)
C(13)-C(14)-C(15)-C(16)	2.9(5)
C(14)-C(15)-C(16)-C(17)	-0.9(5)
C(15)-C(16)-C(17)-C(12)	1.0(5)
C(15)-C(16)-C(17)-C(18)	178.0(3)
C(13)-C(12)-C(17)-C(16)	-3.1(5)
N(2)-C(12)-C(17)-C(16)	177.2(3)
C(13)-C(12)-C(17)-C(18)	179.9(3)
N(2)-C(12)-C(17)-C(18)	0.3(5)
C(16)-C(17)-C(18)-O(3)	-152.1(3)
C(12)-C(17)-C(18)-O(3)	24.9(5)
C(16)-C(17)-C(18)-C(19)	30.7(4)
C(12)-C(17)-C(18)-C(19)	-152.3(3)
O(3)-C(18)-C(19)-C(20)	-132.2(3)

C(17)-C(18)-C(19)-C(20)	45.1(4)
O(3)-C(18)-C(19)-C(24)	42.3(4)
C(17)-C(18)-C(19)-C(24)	-140.4(3)
C(24)-C(19)-C(20)-C(21)	-1.3(5)
C(18)-C(19)-C(20)-C(21)	173.2(3)
C(19)-C(20)-C(21)-C(22)	3.1(5)
C(20)-C(21)-C(22)-C(23)	-3.8(5)
C(21)-C(22)-C(23)-C(24)	2.6(5)
C(20)-C(19)-C(24)-C(23)	0.0(5)
C(18)-C(19)-C(24)-C(23)	-174.6(3)
C(22)-C(23)-C(24)-C(19)	-0.7(5)
N(3)-C(25)-C(26)-C(27)	175.5(3)
C(30)-C(25)-C(26)-C(27)	-1.2(5)
C(25)-C(26)-C(27)-C(28)	0.5(5)
C(26)-C(27)-C(28)-C(29)	2.5(5)
C(27)-C(28)-C(29)-C(30)	-4.7(5)
C(28)-C(29)-C(30)-C(25)	3.9(5)
C(28)-C(29)-C(30)-C(31)	-170.8(3)
C(26)-C(25)-C(30)-C(29)	-1.0(5)
N(3)-C(25)-C(30)-C(29)	-177.6(3)
C(26)-C(25)-C(30)-C(31)	173.5(3)
N(3)-C(25)-C(30)-C(31)	-3.1(5)
C(29)-C(30)-C(31)-O(4)	130.1(4)
C(25)-C(30)-C(31)-O(4)	-44.4(5)
C(29)-C(30)-C(31)-C(32)	-50.3(4)
C(25)-C(30)-C(31)-C(32)	135.1(3)
O(4)-C(31)-C(32)-C(37)	-62.0(5)
C(30)-C(31)-C(32)-C(37)	118.4(4)
O(4)-C(31)-C(32)-C(33)	115.6(4)
C(30)-C(31)-C(32)-C(33)	-64.0(4)
C(37)-C(32)-C(33)-C(34)	0.1(5)
C(31)-C(32)-C(33)-C(34)	-177.5(3)
C(32)-C(33)-C(34)-C(35)	0.1(5)
C(33)-C(34)-C(35)-C(36)	-0.9(5)
C(34)-C(35)-C(36)-C(37)	1.6(6)
C(35)-C(36)-C(37)-C(32)	-1.3(6)
C(35)-C(36)-C(37)-C(38)	-177.7(3)
C(33)-C(32)-C(37)-C(36)	0.4(5)
C(31)-C(32)-C(37)-C(36)	177.9(3)
C(33)-C(32)-C(37)-C(38)	176.7(3)
C(31)-C(32)-C(37)-C(38)	-5.8(5)
C(36)-C(37)-C(38)-F(3)	15.8(5)
C(32)-C(37)-C(38)-F(3)	-160.5(3)
C(36)-C(37)-C(38)-F(2)	137.9(3)

C(32)-C(37)-C(38)-F(2)	-38.4(5)
C(36)-C(37)-C(38)-F(1)	-105.9(4)
C(32)-C(37)-C(38)-F(1)	77.8(4)
C(9)-C(8)-N(1)-C(10)	145.0(3)
C(9)-C(8)-N(1)-C(1)	-92.3(3)
C(9)-C(8)-N(1)-Ni(1)	33.9(3)
C(11)-C(10)-N(1)-C(8)	-153.4(3)
C(11)-C(10)-N(1)-C(1)	82.1(3)
C(11)-C(10)-N(1)-Ni(1)	-41.0(3)
C(2)-C(1)-N(1)-C(8)	54.9(3)
C(2)-C(1)-N(1)-C(10)	-179.6(3)
C(2)-C(1)-N(1)-Ni(1)	-65.0(3)
O(1)-C(9)-N(2)-C(12)	-9.4(5)
C(8)-C(9)-N(2)-C(12)	177.4(3)
O(1)-C(9)-N(2)-Ni(1)	176.0(3)
C(8)-C(9)-N(2)-Ni(1)	2.8(4)
C(13)-C(12)-N(2)-C(9)	-26.5(5)
C(17)-C(12)-N(2)-C(9)	153.2(3)
C(13)-C(12)-N(2)-Ni(1)	147.6(3)
C(17)-C(12)-N(2)-Ni(1)	-32.7(4)
O(2)-C(11)-N(3)-C(25)	5.7(5)
C(10)-C(11)-N(3)-C(25)	-177.7(3)
O(2)-C(11)-N(3)-Ni(1)	-173.0(3)
C(10)-C(11)-N(3)-Ni(1)	3.6(3)
C(26)-C(25)-N(3)-C(11)	110.1(4)
C(30)-C(25)-N(3)-C(11)	-73.3(5)
C(26)-C(25)-N(3)-Ni(1)	-71.4(4)
C(30)-C(25)-N(3)-Ni(1)	105.2(4)
C(9)-N(2)-Ni(1)-O(3)	-151.6(2)
C(12)-N(2)-Ni(1)-O(3)	34.0(3)
C(9)-N(2)-Ni(1)-N(3)	19.1(12)
C(12)-N(2)-Ni(1)-N(3)	-155.4(10)
C(9)-N(2)-Ni(1)-N(1)	14.5(2)
C(12)-N(2)-Ni(1)-N(1)	-160.0(3)
C(11)-N(3)-Ni(1)-O(3)	142.6(2)
C(25)-N(3)-Ni(1)-O(3)	-36.0(3)
C(11)-N(3)-Ni(1)-N(2)	-28.0(12)
C(25)-N(3)-Ni(1)-N(2)	153.3(10)
C(11)-N(3)-Ni(1)-N(1)	-23.4(2)
C(25)-N(3)-Ni(1)-N(1)	158.0(3)
C(8)-N(1)-Ni(1)-O(3)	67.8(5)
C(10)-N(1)-Ni(1)-O(3)	-50.8(5)
C(1)-N(1)-Ni(1)-O(3)	-168.6(4)
C(8)-N(1)-Ni(1)-N(2)	-27.2(2)

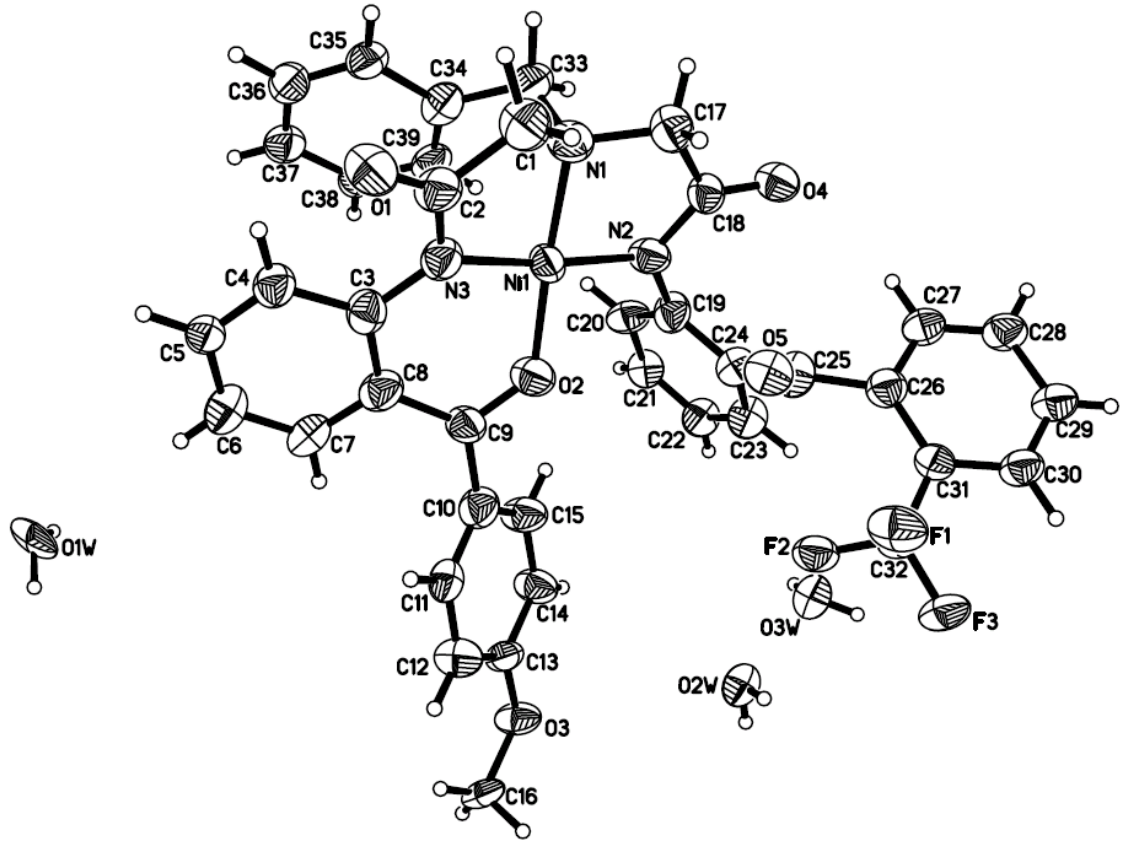
C(10)-N(1)-Ni(1)-N(2)	-145.8(2)
C(1)-N(1)-Ni(1)-N(2)	96.4(2)
C(8)-N(1)-Ni(1)-N(3)	153.3(2)
C(10)-N(1)-Ni(1)-N(3)	34.8(2)
C(1)-N(1)-Ni(1)-N(3)	-83.1(2)
C(17)-C(18)-O(3)-Ni(1)	-15.9(4)
C(19)-C(18)-O(3)-Ni(1)	161.4(2)
N(2)-Ni(1)-O(3)-C(18)	-10.0(3)
N(3)-Ni(1)-O(3)-C(18)	171.1(3)
N(1)-Ni(1)-O(3)-C(18)	-104.4(5)

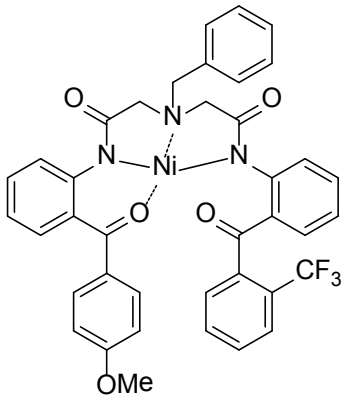
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for Ni-o-CF3-p-H [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

ORTEP drawing of compound 13. (CCDC number 951882)





Ni-o-CF3-p-OMe

Table 1. Crystal data and structure refinement for complex **13**.

Identification code	a
Empirical formula	C39 H30 F3 N3 Ni O5
Formula weight	736.36
Temperature	291(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 9.648(4) A alpha = 66.870(7) deg. b = 13.897(6) A beta = 74.393(7) deg. c = 16.270(7) A gamma = 87.648(8) deg.
Volume	1927.0(14) A^3
Z, Calculated density	2, 1.300 Mg/m^3
Absorption coefficient	0.565 mm^-1
F(000)	780
Crystal size	0.28 x 0.24 x 0.22 mm
Theta range for data collection	2.20 to 26.00 deg.
Limiting indices	-11<=h<=11, -9<=k<=17, -16<=l<=20
Reflections collected / unique	10590 / 7415 [R(int) = 0.0293]
Completeness to theta = 26.00	98.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8 and 0.7
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7415 / 1* / 488
	*Rigid bond restraint (DELU in Shelxl) was applied to anisotropic displacement parameters of N(2) and C(18) to treat asp's small elongation.
Goodness-of-fit on F^2	0.980
Final R indices [I>2sigma(I)]	R1 = 0.0552, wR2 = 0.0954
R indices (all data)	R1 = 0.0853, wR2 = 0.1010
Largest diff. peak and hole	0.559 and -0.421 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for No.1.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	491(4)	-529(3)	7456(2)	54(1)
C(2)	138(3)	239(2)	7921(2)	44(1)
C(3)	946(3)	1880(2)	7833(2)	42(1)
C(4)	593(3)	1637(2)	8786(2)	43(1)
C(5)	745(3)	2353(2)	9140(2)	40(1)

C(6)	1203(3)	3358(2)	8564(2)	47(1)
C(7)	1576(3)	3661(2)	7638(2)	44(1)
C(8)	1430(3)	2932(2)	7240(2)	47(1)
C(9)	1830(3)	3330(2)	6227(2)	42(1)
C(10)	1998(3)	4441(2)	5613(2)	47(1)
C(11)	1015(3)	5134(2)	5742(2)	38(1)
C(12)	1110(3)	6185(2)	5175(2)	48(1)
C(13)	2308(3)	6566(2)	4424(2)	40(1)
C(14)	3383(3)	5906(2)	4246(2)	51(1)
C(15)	3186(4)	4840(2)	4853(2)	55(1)
C(16)	1688(3)	8346(2)	3960(2)	44(1)
C(17)	1935(3)	-519(2)	5940(2)	46(1)
C(18)	2899(3)	308(2)	5069(2)	39(1)
C(19)	4001(3)	2046(2)	4423(2)	44(1)
C(20)	5243(3)	2447(2)	4507(2)	46(1)
C(21)	6081(3)	3336(2)	3785(2)	43(1)
C(22)	5646(3)	3835(2)	3011(2)	45(1)
C(23)	4480(3)	3446(2)	2900(2)	47(1)
C(24)	3589(3)	2566(2)	3604(2)	41(1)
C(25)	2261(3)	2262(2)	3438(2)	46(1)
C(26)	2394(3)	2312(2)	2485(2)	43(1)
C(27)	3331(3)	1676(2)	2188(2)	42(1)
C(28)	3513(3)	1643(2)	1342(2)	47(1)
C(29)	2756(3)	2298(2)	737(2)	47(1)
C(30)	1845(3)	2959(2)	1001(2)	44(1)
C(31)	1647(3)	2976(2)	1884(2)	40(1)
C(32)	603(3)	3687(2)	2132(2)	47(1)
C(33)	3119(3)	-704(2)	7160(2)	48(1)
C(34)	3446(3)	-282(2)	7809(2)	47(1)
C(35)	2753(3)	-760(2)	8779(2)	45(1)
C(36)	3022(3)	-345(2)	9343(2)	45(1)
C(37)	3990(3)	532(2)	9016(2)	48(1)
C(38)	4650(3)	958(2)	8079(2)	45(1)
C(39)	4382(3)	574(2)	7484(2)	44(1)
F(1)	-639(2)	3193(1)	2712(1)	56(1)
F(2)	1067(2)	4166(1)	2591(1)	48(1)
F(3)	292(2)	4438(1)	1432(1)	49(1)
N(1)	1899(3)	-231(2)	6746(2)	46(1)
N(2)	3158(3)	1202(2)	5173(2)	43(1)
N(3)	908(3)	1142(2)	7448(2)	42(1)
Ni(1)	2086(1)	1258(1)	6294(1)	38(1)
O(1)	-811(2)	-29(2)	8666(1)	49(1)
O(2)	2194(2)	2701(2)	5798(1)	47(1)
O(3)	2642(2)	7595(2)	3806(1)	47(1)

O(4)	3404(2)	129(2)	4363(1)	45(1)
O(5)	1111(2)	2018(2)	4038(1)	45(1)
O(1W)	3035(7)	6043(5)	9572(5)	64(2)
O(2W)	2983(6)	6808(4)	1708(3)	49(1)
O(3W)	4314(7)	5858(5)	1102(4)	48(2)

Table 3. Bond lengths [A] and angles [deg] for No.1.

C(1)-N(1)	1.475(4)
C(1)-C(2)	1.515(4)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-O(1)	1.233(3)
C(2)-N(3)	1.315(4)
C(3)-N(3)	1.402(4)
C(3)-C(4)	1.394(4)
C(3)-C(8)	1.411(4)
C(4)-C(5)	1.361(4)
C(4)-H(4)	0.9300
C(5)-C(6)	1.350(4)
C(5)-H(5)	0.9300
C(6)-C(7)	1.342(4)
C(6)-H(6)	0.9300
C(7)-C(8)	1.428(4)
C(7)-H(7)	0.9300
C(8)-C(9)	1.460(4)
C(9)-O(2)	1.302(3)
C(9)-C(10)	1.460(4)
C(10)-C(11)	1.359(4)
C(10)-C(15)	1.378(4)
C(11)-C(12)	1.379(4)
C(11)-H(11)	0.9300
C(12)-C(13)	1.376(4)
C(12)-H(12)	0.9300
C(13)-O(3)	1.376(3)
C(13)-C(14)	1.403(4)
C(14)-C(15)	1.406(4)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
C(16)-O(3)	1.415(3)
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600

C(16)-H(16C)	0.9600
C(17)-N(1)	1.507(4)
C(17)-C(18)	1.513(4)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-O(4)	1.238(3)
C(18)-N(2)	1.359(4)
C(19)-N(2)	1.395(4)
C(19)-C(20)	1.402(4)
C(19)-C(24)	1.401(4)
C(20)-C(21)	1.411(4)
C(20)-H(20)	0.9300
C(21)-C(22)	1.348(4)
C(21)-H(21)	0.9300
C(22)-C(23)	1.352(4)
C(22)-H(22)	0.9300
C(23)-C(24)	1.415(4)
C(23)-H(23)	0.9300
C(24)-C(25)	1.486(4)
C(25)-O(5)	1.219(3)
C(25)-C(26)	1.495(4)
C(26)-C(27)	1.366(4)
C(26)-C(31)	1.394(4)
C(27)-C(28)	1.358(4)
C(27)-H(27)	0.9300
C(28)-C(29)	1.400(4)
C(28)-H(28)	0.9300
C(29)-C(30)	1.357(4)
C(29)-H(29)	0.9300
C(30)-C(31)	1.407(4)
C(30)-H(30)	0.9300
C(31)-C(32)	1.471(4)
C(32)-F(3)	1.305(3)
C(32)-F(1)	1.322(3)
C(32)-F(2)	1.341(4)
C(33)-C(34)	1.496(4)
C(33)-N(1)	1.512(4)
C(33)-H(33A)	0.9700
C(33)-H(33B)	0.9700
C(34)-C(39)	1.359(4)
C(34)-C(35)	1.422(4)
C(35)-C(36)	1.342(4)
C(35)-H(35)	0.9300
C(36)-C(37)	1.399(4)

C(36)-H(36)	0.9300
C(37)-C(38)	1.371(4)
C(37)-H(37)	0.9300
C(38)-C(39)	1.356(4)
C(38)-H(38)	0.9300
C(39)-H(39)	0.9300
N(1)-Ni(1)	1.902(3)
N(2)-Ni(1)	1.868(2)
N(3)-Ni(1)	1.864(2)
Ni(1)-O(2)	1.839(2)
O(1W)-H(1WA)	0.8500
O(1W)-H(1WB)	0.8500
O(2W)-H(2WA)	0.8499
O(2W)-H(2WC)	0.8500
O(3W)-H(3WA)	0.8500
O(3W)-H(3WB)	0.8500
N(1)-C(1)-C(2)	111.5(3)
N(1)-C(1)-H(1A)	109.3
C(2)-C(1)-H(1A)	109.3
N(1)-C(1)-H(1B)	109.3
C(2)-C(1)-H(1B)	109.3
H(1A)-C(1)-H(1B)	108.0
O(1)-C(2)-N(3)	128.0(3)
O(1)-C(2)-C(1)	118.6(3)
N(3)-C(2)-C(1)	113.4(3)
N(3)-C(3)-C(4)	124.1(3)
N(3)-C(3)-C(8)	119.5(3)
C(4)-C(3)-C(8)	116.4(3)
C(5)-C(4)-C(3)	122.8(3)
C(5)-C(4)-H(4)	118.6
C(3)-C(4)-H(4)	118.6
C(4)-C(5)-C(6)	120.1(3)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(7)-C(6)-C(5)	121.1(3)
C(7)-C(6)-H(6)	119.5
C(5)-C(6)-H(6)	119.5
C(6)-C(7)-C(8)	120.4(3)
C(6)-C(7)-H(7)	119.8
C(8)-C(7)-H(7)	119.8
C(3)-C(8)-C(7)	119.1(3)
C(3)-C(8)-C(9)	123.9(3)
C(7)-C(8)-C(9)	117.0(3)
O(2)-C(9)-C(8)	121.1(3)

O(2)-C(9)-C(10)	114.4(3)
C(8)-C(9)-C(10)	124.2(3)
C(11)-C(10)-C(15)	116.3(3)
C(11)-C(10)-C(9)	123.1(3)
C(15)-C(10)-C(9)	120.6(3)
C(10)-C(11)-C(12)	125.3(3)
C(10)-C(11)-H(11)	117.3
C(12)-C(11)-H(11)	117.3
C(13)-C(12)-C(11)	117.2(3)
C(13)-C(12)-H(12)	121.4
C(11)-C(12)-H(12)	121.4
C(12)-C(13)-O(3)	126.2(2)
C(12)-C(13)-C(14)	121.0(3)
O(3)-C(13)-C(14)	112.7(2)
C(13)-C(14)-C(15)	117.9(3)
C(13)-C(14)-H(14)	121.1
C(15)-C(14)-H(14)	121.1
C(10)-C(15)-C(14)	122.2(3)
C(10)-C(15)-H(15)	118.9
C(14)-C(15)-H(15)	118.9
O(3)-C(16)-H(16A)	109.5
O(3)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
O(3)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
N(1)-C(17)-C(18)	108.0(2)
N(1)-C(17)-H(17A)	110.1
C(18)-C(17)-H(17A)	110.1
N(1)-C(17)-H(17B)	110.1
C(18)-C(17)-H(17B)	110.1
H(17A)-C(17)-H(17B)	108.4
O(4)-C(18)-N(2)	126.1(3)
O(4)-C(18)-C(17)	120.6(3)
N(2)-C(18)-C(17)	113.3(2)
N(2)-C(19)-C(20)	119.7(3)
N(2)-C(19)-C(24)	121.9(3)
C(20)-C(19)-C(24)	118.2(3)
C(19)-C(20)-C(21)	121.6(3)
C(19)-C(20)-H(20)	119.2
C(21)-C(20)-H(20)	119.2
C(22)-C(21)-C(20)	119.2(3)
C(22)-C(21)-H(21)	120.4
C(20)-C(21)-H(21)	120.4

C(21)-C(22)-C(23)	120.4(3)
C(21)-C(22)-H(22)	119.8
C(23)-C(22)-H(22)	119.8
C(22)-C(23)-C(24)	122.8(3)
C(22)-C(23)-H(23)	118.6
C(24)-C(23)-H(23)	118.6
C(19)-C(24)-C(23)	117.7(3)
C(19)-C(24)-C(25)	124.0(3)
C(23)-C(24)-C(25)	118.3(3)
O(5)-C(25)-C(24)	121.9(3)
O(5)-C(25)-C(26)	121.6(3)
C(24)-C(25)-C(26)	116.5(2)
C(27)-C(26)-C(31)	118.7(3)
C(27)-C(26)-C(25)	117.2(3)
C(31)-C(26)-C(25)	124.1(3)
C(28)-C(27)-C(26)	122.0(3)
C(28)-C(27)-H(27)	119.0
C(26)-C(27)-H(27)	119.0
C(27)-C(28)-C(29)	119.7(3)
C(27)-C(28)-H(28)	120.1
C(29)-C(28)-H(28)	120.1
C(30)-C(29)-C(28)	119.7(3)
C(30)-C(29)-H(29)	120.2
C(28)-C(29)-H(29)	120.2
C(29)-C(30)-C(31)	120.1(3)
C(29)-C(30)-H(30)	119.9
C(31)-C(30)-H(30)	119.9
C(26)-C(31)-C(30)	119.6(3)
C(26)-C(31)-C(32)	123.4(3)
C(30)-C(31)-C(32)	116.9(2)
F(3)-C(32)-F(1)	106.5(2)
F(3)-C(32)-F(2)	105.5(2)
F(1)-C(32)-F(2)	103.6(2)
F(3)-C(32)-C(31)	115.2(3)
F(1)-C(32)-C(31)	113.0(3)
F(2)-C(32)-C(31)	112.1(2)
C(34)-C(33)-N(1)	116.0(2)
C(34)-C(33)-H(33A)	108.3
N(1)-C(33)-H(33A)	108.3
C(34)-C(33)-H(33B)	108.3
N(1)-C(33)-H(33B)	108.3
H(33A)-C(33)-H(33B)	107.4
C(39)-C(34)-C(35)	118.8(3)
C(39)-C(34)-C(33)	120.9(3)

C(35)-C(34)-C(33)	120.3(3)
C(36)-C(35)-C(34)	119.2(3)
C(36)-C(35)-H(35)	120.4
C(34)-C(35)-H(35)	120.4
C(35)-C(36)-C(37)	122.3(3)
C(35)-C(36)-H(36)	118.8
C(37)-C(36)-H(36)	118.8
C(38)-C(37)-C(36)	116.4(3)
C(38)-C(37)-H(37)	121.8
C(36)-C(37)-H(37)	121.8
C(39)-C(38)-C(37)	122.9(3)
C(39)-C(38)-H(38)	118.6
C(37)-C(38)-H(38)	118.6
C(38)-C(39)-C(34)	120.3(3)
C(38)-C(39)-H(39)	119.9
C(34)-C(39)-H(39)	119.9
C(1)-N(1)-C(17)	112.6(2)
C(1)-N(1)-C(33)	111.6(2)
C(17)-N(1)-C(33)	109.9(2)
C(1)-N(1)-Ni(1)	104.20(18)
C(17)-N(1)-Ni(1)	107.81(18)
C(33)-N(1)-Ni(1)	110.60(19)
C(18)-N(2)-C(19)	119.9(2)
C(18)-N(2)-Ni(1)	114.77(19)
C(19)-N(2)-Ni(1)	124.59(19)
C(2)-N(3)-C(3)	122.2(2)
C(2)-N(3)-Ni(1)	113.3(2)
C(3)-N(3)-Ni(1)	124.14(19)
O(2)-Ni(1)-N(3)	93.67(10)
O(2)-Ni(1)-N(2)	93.03(9)
N(3)-Ni(1)-N(2)	172.54(11)
O(2)-Ni(1)-N(1)	175.95(11)
N(3)-Ni(1)-N(1)	87.90(11)
N(2)-Ni(1)-N(1)	85.21(10)
C(9)-O(2)-Ni(1)	128.69(19)
C(13)-O(3)-C(16)	117.6(2)
H(1WA)-O(1W)-H(1WB)	109.5
H(2WA)-O(2W)-H(2WC)	109.5
H(3WA)-O(3W)-H(3WB)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for No.1.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	53(2)	53(2)	45(2)	-18(2)	5(1)	-6(2)
C(2)	43(2)	41(2)	38(2)	-10(1)	-1(1)	1(1)
C(3)	40(2)	48(2)	36(2)	-17(1)	-5(1)	2(1)
C(4)	42(2)	46(2)	36(2)	-14(1)	-6(1)	5(1)
C(5)	42(2)	41(2)	36(2)	-14(1)	-10(1)	13(1)
C(6)	43(2)	56(2)	40(2)	-13(2)	-15(1)	-11(1)
C(7)	42(2)	46(2)	36(2)	-5(1)	-14(1)	-1(1)
C(8)	46(2)	45(2)	36(2)	-7(1)	-4(1)	4(1)
C(9)	50(2)	31(1)	36(2)	-11(1)	-2(1)	0(1)
C(10)	53(2)	43(2)	38(2)	-11(1)	-10(1)	-2(1)
C(11)	43(2)	40(2)	31(1)	-12(1)	-8(1)	-8(1)
C(12)	39(2)	40(2)	53(2)	-11(1)	-5(1)	2(1)
C(13)	42(2)	37(2)	33(1)	-7(1)	-11(1)	13(1)
C(14)	52(2)	41(2)	46(2)	-12(1)	2(1)	11(1)
C(15)	58(2)	42(2)	42(2)	-5(2)	4(2)	13(2)
C(16)	42(2)	39(2)	39(2)	0(1)	-18(1)	12(1)
C(17)	45(2)	48(2)	41(2)	-19(1)	-4(1)	-5(1)
C(18)	40(2)	41(1)	40(2)	-19(1)	-16(1)	3(1)
C(19)	47(2)	46(2)	33(1)	-13(1)	-5(1)	-4(1)
C(20)	38(2)	42(2)	50(2)	-11(1)	-13(1)	13(1)
C(21)	35(2)	47(2)	43(2)	-18(1)	-6(1)	-3(1)
C(22)	45(2)	39(2)	48(2)	-11(1)	-14(1)	-14(1)
C(23)	45(2)	45(2)	44(2)	-10(1)	-9(1)	-16(1)
C(24)	35(2)	43(2)	37(2)	-12(1)	-5(1)	-1(1)
C(25)	41(2)	50(2)	39(2)	-14(1)	-5(1)	-6(1)
C(26)	43(2)	41(2)	46(2)	-16(1)	-16(1)	5(1)
C(27)	36(2)	43(2)	46(2)	-14(1)	-13(1)	9(1)
C(28)	42(2)	47(2)	51(2)	-20(2)	-13(1)	17(1)
C(29)	47(2)	44(2)	45(2)	-13(1)	-11(1)	12(1)
C(30)	45(2)	44(2)	42(2)	-15(1)	-13(1)	15(1)
C(31)	45(2)	30(1)	43(2)	-12(1)	-13(1)	1(1)
C(32)	49(2)	45(2)	39(2)	-11(1)	-11(1)	11(1)
C(33)	55(2)	43(2)	37(2)	-10(1)	-8(1)	11(1)
C(34)	43(2)	52(2)	40(2)	-13(1)	-10(1)	7(1)
C(35)	53(2)	36(2)	35(2)	-8(1)	-4(1)	4(1)

C(36)	44(2)	47(2)	40(2)	-16(1)	-9(1)	11(1)
C(37)	50(2)	45(2)	46(2)	-16(2)	-15(1)	13(1)
C(38)	49(2)	46(2)	38(2)	-15(1)	-11(1)	14(1)
C(39)	43(2)	46(2)	37(2)	-10(1)	-14(1)	18(1)
F(1)	51(1)	50(1)	52(1)	-17(1)	5(1)	13(1)
F(2)	49(1)	43(1)	50(1)	-19(1)	-14(1)	18(1)
F(3)	43(1)	49(1)	49(1)	-12(1)	-16(1)	20(1)
N(1)	47(2)	38(1)	44(1)	-14(1)	-4(1)	-4(1)
N(2)	47(1)	34(1)	39(1)	-12(1)	-3(1)	6(1)
N(3)	44(1)	44(1)	34(1)	-13(1)	-8(1)	6(1)
Ni(1)	45(1)	35(1)	34(1)	-17(1)	-6(1)	2(1)
O(1)	43(1)	41(1)	50(1)	-19(1)	12(1)	-14(1)
O(2)	49(1)	39(1)	46(1)	-16(1)	-5(1)	5(1)
O(3)	42(1)	33(1)	45(1)	1(1)	-3(1)	3(1)
O(4)	46(1)	38(1)	42(1)	-14(1)	-1(1)	1(1)
O(5)	35(1)	43(1)	50(1)	-15(1)	-4(1)	-6(1)
O(1W)	42(4)	39(4)	77(5)	-21(4)	35(4)	1(3)
O(2W)	51(3)	53(3)	41(3)	-13(3)	-15(2)	-4(2)
O(3W)	34(4)	64(5)	39(4)	-16(3)	-4(3)	-5(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for No.1.

	x	y	z	U(eq)
H(1A)	508	-1225	7923	65
H(1B)	-257	-552	7167	65
H(4)	239	956	9196	52
H(5)	534	2150	9780	48
H(6)	1259	3849	8813	56
H(7)	1933	4348	7253	53
H(11)	212	4877	6255	46
H(12)	394	6619	5296	58
H(14)	4200	6165	3744	62
H(15)	3880	4390	4738	66
H(16A)	1070	8053	4584	66
H(16B)	1112	8537	3529	66
H(16C)	2234	8958	3872	66
H(17A)	969	-547	5874	55
H(17B)	2309	-1203	6043	55
H(20)	5520	2120	5052	55
H(21)	6923	3575	3842	51

H(22)	6152	4451	2550	54
H(23)	4253	3771	2337	57
H(27)	3859	1251	2577	51
H(28)	4139	1188	1166	56
H(29)	2876	2280	157	57
H(30)	1350	3402	597	53
H(33A)	2890	-1454	7492	58
H(33B)	3985	-597	6655	58
H(35)	2120	-1353	9018	54
H(36)	2548	-652	9974	54
H(37)	4175	811	9413	57
H(38)	5311	1535	7841	54
H(39)	4840	898	6852	53
H(1WA)	3931	6233	9349	96
H(1WB)	2551	6564	9362	96
H(2WA)	3202	7441	1324	74
H(2WC)	2147	6617	1724	74
H(3WA)	4199	5990	570	72
H(3WB)	5191	6005	1045	72

Table 6. Torsion angles [deg] for No.1.

N(1)-C(1)-C(2)-O(1)	-162.9(3)
N(1)-C(1)-C(2)-N(3)	17.8(4)
N(3)-C(3)-C(4)-C(5)	174.8(3)
C(8)-C(3)-C(4)-C(5)	-2.2(4)
C(3)-C(4)-C(5)-C(6)	2.6(4)
C(4)-C(5)-C(6)-C(7)	-3.0(4)
C(5)-C(6)-C(7)-C(8)	3.1(4)
N(3)-C(3)-C(8)-C(7)	-175.0(3)
C(4)-C(3)-C(8)-C(7)	2.2(4)
N(3)-C(3)-C(8)-C(9)	3.6(4)
C(4)-C(3)-C(8)-C(9)	-179.3(3)
C(6)-C(7)-C(8)-C(3)	-2.7(4)
C(6)-C(7)-C(8)-C(9)	178.7(3)
C(3)-C(8)-C(9)-O(2)	-21.5(5)
C(7)-C(8)-C(9)-O(2)	157.0(3)
C(3)-C(8)-C(9)-C(10)	164.7(3)
C(7)-C(8)-C(9)-C(10)	-16.7(4)
O(2)-C(9)-C(10)-C(11)	138.5(3)
C(8)-C(9)-C(10)-C(11)	-47.3(5)
O(2)-C(9)-C(10)-C(15)	-40.9(4)

C(8)-C(9)-C(10)-C(15)	133.2(3)
C(15)-C(10)-C(11)-C(12)	0.6(5)
C(9)-C(10)-C(11)-C(12)	-178.8(3)
C(10)-C(11)-C(12)-C(13)	-0.9(5)
C(11)-C(12)-C(13)-O(3)	-176.4(3)
C(11)-C(12)-C(13)-C(14)	0.0(5)
C(12)-C(13)-C(14)-C(15)	1.0(5)
O(3)-C(13)-C(14)-C(15)	177.8(3)
C(11)-C(10)-C(15)-C(14)	0.5(5)
C(9)-C(10)-C(15)-C(14)	180.0(3)
C(13)-C(14)-C(15)-C(10)	-1.2(5)
N(1)-C(17)-C(18)-O(4)	161.5(3)
N(1)-C(17)-C(18)-N(2)	-16.4(3)
N(2)-C(19)-C(20)-C(21)	-176.5(3)
C(24)-C(19)-C(20)-C(21)	-1.3(4)
C(19)-C(20)-C(21)-C(22)	2.7(5)
C(20)-C(21)-C(22)-C(23)	-4.7(5)
C(21)-C(22)-C(23)-C(24)	5.5(5)
N(2)-C(19)-C(24)-C(23)	176.9(3)
C(20)-C(19)-C(24)-C(23)	1.9(4)
N(2)-C(19)-C(24)-C(25)	-1.7(5)
C(20)-C(19)-C(24)-C(25)	-176.8(3)
C(22)-C(23)-C(24)-C(19)	-4.0(5)
C(22)-C(23)-C(24)-C(25)	174.7(3)
C(19)-C(24)-C(25)-O(5)	42.3(5)
C(23)-C(24)-C(25)-O(5)	-136.3(3)
C(19)-C(24)-C(25)-C(26)	-140.0(3)
C(23)-C(24)-C(25)-C(26)	41.4(4)
O(5)-C(25)-C(26)-C(27)	-120.5(3)
C(24)-C(25)-C(26)-C(27)	61.8(4)
O(5)-C(25)-C(26)-C(31)	60.8(4)
C(24)-C(25)-C(26)-C(31)	-116.9(3)
C(31)-C(26)-C(27)-C(28)	-2.5(5)
C(25)-C(26)-C(27)-C(28)	178.7(3)
C(26)-C(27)-C(28)-C(29)	1.8(5)
C(27)-C(28)-C(29)-C(30)	0.0(5)
C(28)-C(29)-C(30)-C(31)	-0.9(5)
C(27)-C(26)-C(31)-C(30)	1.5(4)
C(25)-C(26)-C(31)-C(30)	-179.7(3)
C(27)-C(26)-C(31)-C(32)	179.4(3)
C(25)-C(26)-C(31)-C(32)	-1.9(5)
C(29)-C(30)-C(31)-C(26)	0.1(5)
C(29)-C(30)-C(31)-C(32)	-177.9(3)
C(26)-C(31)-C(32)-F(3)	162.7(3)

C(30)-C(31)-C(32)-F(3)	-19.4(4)
C(26)-C(31)-C(32)-F(1)	-74.6(4)
C(30)-C(31)-C(32)-F(1)	103.3(3)
C(26)-C(31)-C(32)-F(2)	42.0(4)
C(30)-C(31)-C(32)-F(2)	-140.1(3)
N(1)-C(33)-C(34)-C(39)	-87.9(3)
N(1)-C(33)-C(34)-C(35)	90.6(3)
C(39)-C(34)-C(35)-C(36)	1.0(4)
C(33)-C(34)-C(35)-C(36)	-177.5(3)
C(34)-C(35)-C(36)-C(37)	-1.5(4)
C(35)-C(36)-C(37)-C(38)	0.5(4)
C(36)-C(37)-C(38)-C(39)	1.0(4)
C(37)-C(38)-C(39)-C(34)	-1.4(4)
C(35)-C(34)-C(39)-C(38)	0.4(4)
C(33)-C(34)-C(39)-C(38)	178.9(3)
C(2)-C(1)-N(1)-C(17)	-147.1(3)
C(2)-C(1)-N(1)-C(33)	88.8(3)
C(2)-C(1)-N(1)-Ni(1)	-30.5(3)
C(18)-C(17)-N(1)-C(1)	146.3(3)
C(18)-C(17)-N(1)-C(33)	-88.7(3)
C(18)-C(17)-N(1)-Ni(1)	31.9(3)
C(34)-C(33)-N(1)-C(1)	-68.7(3)
C(34)-C(33)-N(1)-C(17)	165.7(2)
C(34)-C(33)-N(1)-Ni(1)	46.8(3)
O(4)-C(18)-N(2)-C(19)	3.8(4)
C(17)-C(18)-N(2)-C(19)	-178.4(3)
O(4)-C(18)-N(2)-Ni(1)	174.6(2)
C(17)-C(18)-N(2)-Ni(1)	-7.6(3)
C(20)-C(19)-N(2)-C(18)	-122.8(3)
C(24)-C(19)-N(2)-C(18)	62.2(4)
C(20)-C(19)-N(2)-Ni(1)	67.3(4)
C(24)-C(19)-N(2)-Ni(1)	-107.7(3)
O(1)-C(2)-N(3)-C(3)	13.0(5)
C(1)-C(2)-N(3)-C(3)	-167.7(3)
O(1)-C(2)-N(3)-Ni(1)	-173.8(3)
C(1)-C(2)-N(3)-Ni(1)	5.4(3)
C(4)-C(3)-N(3)-C(2)	21.3(4)
C(8)-C(3)-N(3)-C(2)	-161.8(3)
C(4)-C(3)-N(3)-Ni(1)	-151.1(2)
C(8)-C(3)-N(3)-Ni(1)	25.8(4)
C(2)-N(3)-Ni(1)-O(2)	156.5(2)
C(3)-N(3)-Ni(1)-O(2)	-30.6(2)
C(2)-N(3)-Ni(1)-N(1)	-19.8(2)
C(3)-N(3)-Ni(1)-N(1)	153.2(2)

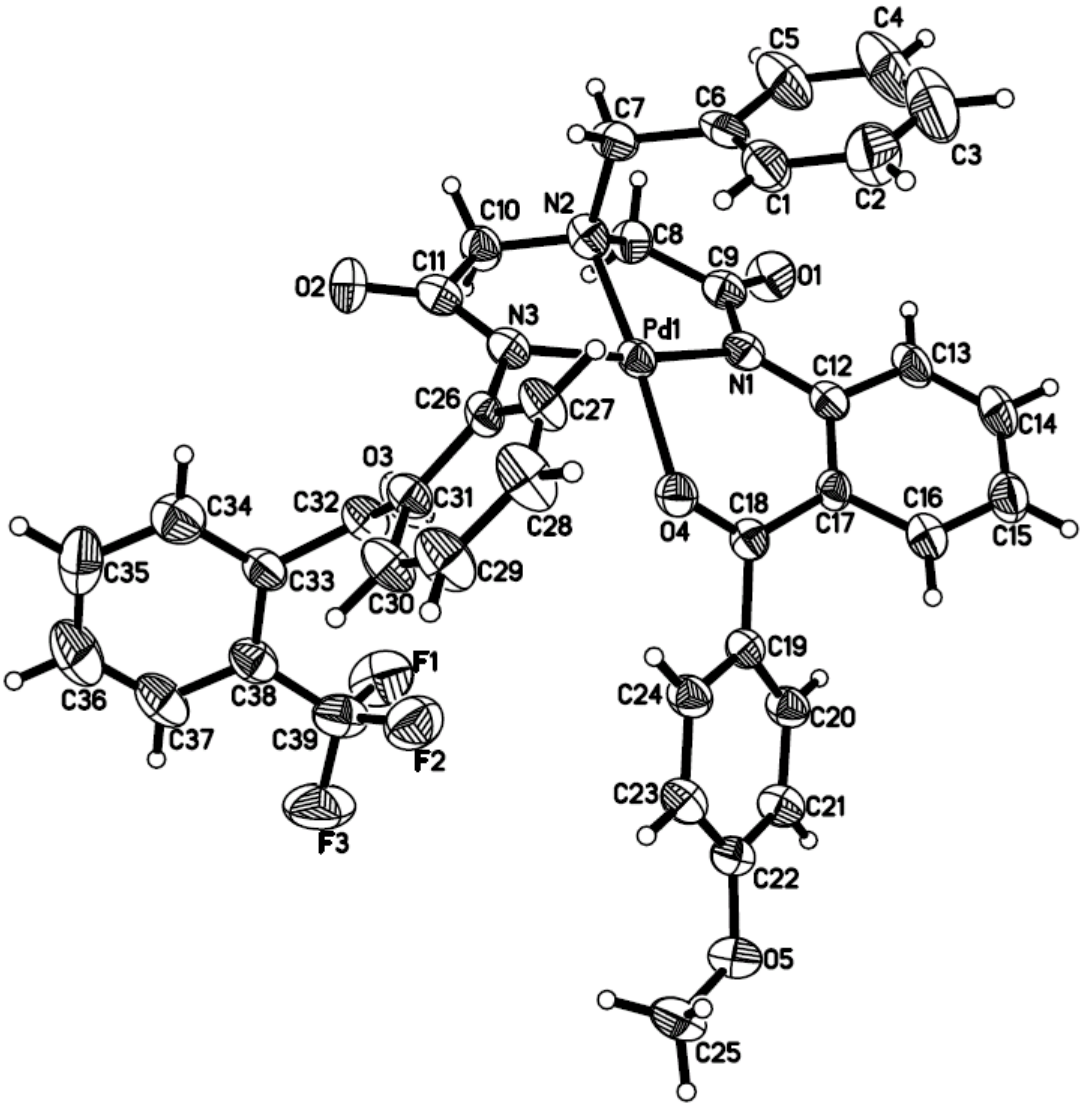
C(18)-N(2)-Ni(1)-O(2)	-154.3(2)
C(19)-N(2)-Ni(1)-O(2)	16.1(2)
C(18)-N(2)-Ni(1)-N(1)	22.1(2)
C(19)-N(2)-Ni(1)-N(1)	-167.5(2)
C(1)-N(1)-Ni(1)-N(3)	27.4(2)
C(17)-N(1)-Ni(1)-N(3)	147.24(19)
C(33)-N(1)-Ni(1)-N(3)	-92.57(19)
C(1)-N(1)-Ni(1)-N(2)	-149.7(2)
C(17)-N(1)-Ni(1)-N(2)	-29.9(2)
C(33)-N(1)-Ni(1)-N(2)	90.28(19)
C(8)-C(9)-O(2)-Ni(1)	8.3(4)
C(10)-C(9)-O(2)-Ni(1)	-177.4(2)
N(3)-Ni(1)-O(2)-C(9)	13.7(3)
N(2)-Ni(1)-O(2)-C(9)	-169.6(3)
C(12)-C(13)-O(3)-C(16)	1.5(4)
C(14)-C(13)-O(3)-C(16)	-175.2(3)

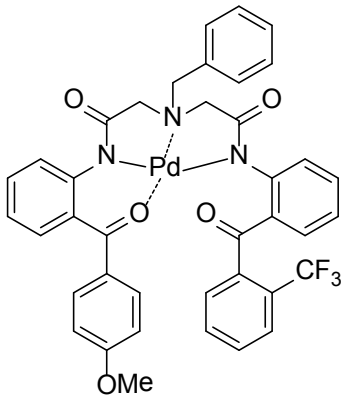
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for No.1 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

ORTEP drawing of compound 14. (CCDC number 951883)





Pd-o-CF3-p-OMe

Table 1. Crystal data and structure refinement for complex **14**.

Identification code	Pd-o-CF3-p-OMe
Empirical formula	$C_{39}\ H_{30}\ F_3\ N_3\ O_5\ Pd$
Formula weight	784.06
Temperature	293(2) K
Wavelength	1.54186 Å
Crystal system	Orthorhombic
Space group	*P b c a*
Unit cell dimensions	*a* = 10.9428(2) Å.
	b = 23.9074(4) Å.
	c = 26.1834(5) Å.
Volume	6849.9(2) $Å^3$
Z	8
Density (calculated)	1.521 Mg/m^3
Absorption coefficient	4.935 mm^{-1}
F(000)	3184
Crystal size	0.09 x 0.02 x 0.02 mm^3
Theta range for data collection	4.75 to 68.17°.
Index ranges	-13<=h<=13, -28<=k<=28, -31<=l<=31
Reflections collected	74634
Independent reflections	6252 [R(int) = 0.0564]
Completeness to theta = 68.17°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9077 and 0.7593
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6252 / 0 / 461
Goodness-of-fit on F^2	1.109
Final R indices [I>2sigma(I)]	R1 = 0.0584, wR2 = 0.1344
R indices (all data)	R1 = 0.0997, wR2 = 0.1883
Extinction coefficient	0.00023(4)
Largest diff. peak and hole	1.308 and -1.081 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Pd-o-CF3-p-OMe. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6722(9)	124(4)	6399(3)	79(3)
C(2)	7473(13)	-35(6)	6800(5)	116(4)
C(3)	7193(17)	133(6)	7286(5)	136(6)
C(4)	6174(18)	445(5)	7379(4)	137(6)
C(5)	5410(12)	601(4)	6973(3)	96(3)
C(25)	13682(9)	1948(4)	3802(3)	78(3)

C(6)	5697(9)	451(3)	6482(3)	64(2)
C(7)	4884(8)	602(3)	6040(3)	63(2)
C(8)	5138(7)	1641(3)	6094(3)	63(2)
C(9)	6297(8)	1789(3)	6382(3)	61(2)
C(10)	4584(7)	1155(4)	5265(3)	62(2)
C(11)	5187(7)	814(3)	4846(3)	57(2)
C(12)	8506(7)	1631(3)	6384(3)	53(2)
C(13)	8660(9)	1716(3)	6910(3)	67(2)
C(14)	9807(9)	1748(4)	7123(3)	72(2)
C(15)	10849(9)	1689(4)	6829(3)	75(2)
C(16)	10717(8)	1610(3)	6310(3)	62(2)
C(17)	9554(7)	1587(3)	6070(2)	49(2)
C(18)	9535(7)	1502(3)	5515(2)	49(2)
C(19)	10541(6)	1703(3)	5187(2)	49(2)
C(20)	11216(7)	2186(3)	5293(3)	59(2)
C(21)	12134(7)	2355(3)	4973(3)	62(2)
C(22)	12424(7)	2053(3)	4541(3)	57(2)
C(23)	11738(7)	1577(3)	4420(3)	63(2)
C(24)	10804(7)	1413(3)	4734(3)	59(2)
C(26)	7155(7)	464(3)	4573(2)	48(2)
C(27)	7842(8)	13(3)	4724(3)	64(2)
C(28)	8673(10)	-235(4)	4394(3)	84(3)
C(29)	8800(9)	-40(4)	3901(3)	83(3)
C(30)	8121(8)	416(3)	3745(3)	70(2)
C(31)	7319(7)	686(3)	4074(3)	53(2)
C(32)	6786(7)	1222(3)	3914(3)	59(2)
C(33)	6555(8)	1312(3)	3354(3)	60(2)
C(34)	5697(9)	986(4)	3113(4)	81(3)
C(35)	5384(11)	1088(5)	2603(4)	107(4)
C(36)	5967(13)	1519(6)	2347(4)	112(4)
C(37)	6823(11)	1838(5)	2582(4)	89(3)
C(38)	7119(8)	1746(4)	3079(3)	66(2)
C(39)	8097(9)	2088(4)	3317(4)	83(3)
O(1)	6225(6)	2100(3)	6754(2)	83(2)
O(2)	4589(5)	668(2)	4467(2)	70(2)
O(3)	6541(7)	1599(2)	4213(2)	83(2)
O(4)	8713(5)	1239(2)	5288(2)	59(1)
O(5)	13390(5)	2234(2)	4265(2)	70(2)
N(1)	7337(6)	1579(3)	6173(2)	55(2)
N(2)	5266(6)	1125(2)	5761(2)	57(2)
N(3)	6371(6)	717(2)	4937(2)	53(1)
F(1)	7701(6)	2471(3)	3655(3)	114(2)
F(2)	8916(5)	1780(3)	3572(2)	105(2)
F(3)	8740(6)	2379(3)	2977(3)	134(3)

Pd(1)	7014(1)	1134(1)	5549(1)	49(1)

Table 3. Bond lengths [Å] and angles [°] for Pd-o-CF3-p-OMe.

C(1)-C(6)	1.385(12)
C(1)-C(2)	1.387(14)
C(1)-H(1)	0.9300
C(2)-C(3)	1.370(18)
C(2)-H(2)	0.9300
C(3)-C(4)	1.36(2)
C(3)-H(3)	0.9300
C(4)-C(5)	1.404(16)
C(4)-H(4)	0.9300
C(5)-C(6)	1.369(11)
C(5)-H(5)	0.9300
C(25)-O(5)	1.428(9)
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(6)-C(7)	1.504(11)
C(7)-N(2)	1.507(9)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-N(2)	1.517(9)
C(8)-C(9)	1.518(11)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-O(1)	1.227(8)
C(9)-N(1)	1.359(9)
C(10)-N(2)	1.498(9)
C(10)-C(11)	1.521(10)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-O(2)	1.239(9)
C(11)-N(3)	1.337(9)
C(12)-N(1)	1.399(9)
C(12)-C(13)	1.403(9)
C(12)-C(17)	1.415(10)
C(13)-C(14)	1.375(12)
C(13)-H(13)	0.9300
C(14)-C(15)	1.383(12)
C(14)-H(14)	0.9300
C(15)-C(16)	1.378(10)

C(15)-H(15)	0.9300
C(16)-C(17)	1.421(10)
C(16)-H(16)	0.9300
C(17)-C(18)	1.466(8)
C(18)-O(4)	1.248(8)
C(18)-C(19)	1.478(9)
C(19)-C(20)	1.399(10)
C(19)-C(24)	1.402(9)
C(20)-C(21)	1.369(10)
C(20)-H(20)	0.9300
C(21)-C(22)	1.378(10)
C(21)-H(21)	0.9300
C(22)-O(5)	1.352(9)
C(22)-C(23)	1.400(11)
C(23)-C(24)	1.369(10)
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(26)-C(27)	1.373(10)
C(26)-N(3)	1.418(8)
C(26)-C(31)	1.421(9)
C(27)-C(28)	1.388(11)
C(27)-H(27)	0.9300
C(28)-C(29)	1.380(11)
C(28)-H(28)	0.9300
C(29)-C(30)	1.380(11)
C(29)-H(29)	0.9300
C(30)-C(31)	1.390(10)
C(30)-H(30)	0.9300
C(31)-C(32)	1.470(10)
C(32)-O(3)	1.222(8)
C(32)-C(33)	1.503(10)
C(33)-C(34)	1.374(12)
C(33)-C(38)	1.404(11)
C(34)-C(35)	1.402(13)
C(34)-H(34)	0.9300
C(35)-C(36)	1.384(16)
C(35)-H(35)	0.9300
C(36)-C(37)	1.355(16)
C(36)-H(36)	0.9300
C(37)-C(38)	1.361(12)
C(37)-H(37)	0.9300
C(38)-C(39)	1.484(13)
C(39)-F(3)	1.331(10)
C(39)-F(2)	1.339(10)

C(39)-F(1)	1.346(11)
O(4)-Pd(1)	1.996(5)
N(1)-Pd(1)	1.983(6)
N(2)-Pd(1)	1.992(7)
N(3)-Pd(1)	2.012(6)
C(6)-C(1)-C(2)	121.0(10)
C(6)-C(1)-H(1)	119.5
C(2)-C(1)-H(1)	119.5
C(3)-C(2)-C(1)	119.4(14)
C(3)-C(2)-H(2)	120.3
C(1)-C(2)-H(2)	120.3
C(4)-C(3)-C(2)	120.7(13)
C(4)-C(3)-H(3)	119.7
C(2)-C(3)-H(3)	119.7
C(3)-C(4)-C(5)	119.8(12)
C(3)-C(4)-H(4)	120.1
C(5)-C(4)-H(4)	120.1
C(6)-C(5)-C(4)	120.4(12)
C(6)-C(5)-H(5)	119.8
C(4)-C(5)-H(5)	119.8
O(5)-C(25)-H(25A)	109.5
O(5)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
O(5)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(5)-C(6)-C(1)	118.8(9)
C(5)-C(6)-C(7)	121.6(9)
C(1)-C(6)-C(7)	119.5(7)
C(6)-C(7)-N(2)	114.1(6)
C(6)-C(7)-H(7A)	108.7
N(2)-C(7)-H(7A)	108.7
C(6)-C(7)-H(7B)	108.7
N(2)-C(7)-H(7B)	108.7
H(7A)-C(7)-H(7B)	107.6
N(2)-C(8)-C(9)	113.5(6)
N(2)-C(8)-H(8A)	108.9
C(9)-C(8)-H(8A)	108.9
N(2)-C(8)-H(8B)	108.9
C(9)-C(8)-H(8B)	108.9
H(8A)-C(8)-H(8B)	107.7
O(1)-C(9)-N(1)	126.7(8)
O(1)-C(9)-C(8)	118.8(7)
N(1)-C(9)-C(8)	114.4(6)

N(2)-C(10)-C(11)	112.5(6)
N(2)-C(10)-H(10A)	109.1
C(11)-C(10)-H(10A)	109.1
N(2)-C(10)-H(10B)	109.1
C(11)-C(10)-H(10B)	109.1
H(10A)-C(10)-H(10B)	107.8
O(2)-C(11)-N(3)	127.4(7)
O(2)-C(11)-C(10)	120.0(7)
N(3)-C(11)-C(10)	112.6(7)
N(1)-C(12)-C(13)	120.7(7)
N(1)-C(12)-C(17)	120.3(6)
C(13)-C(12)-C(17)	118.9(7)
C(14)-C(13)-C(12)	121.0(8)
C(14)-C(13)-H(13)	119.5
C(12)-C(13)-H(13)	119.5
C(13)-C(14)-C(15)	121.5(7)
C(13)-C(14)-H(14)	119.3
C(15)-C(14)-H(14)	119.3
C(16)-C(15)-C(14)	118.4(8)
C(16)-C(15)-H(15)	120.8
C(14)-C(15)-H(15)	120.8
C(15)-C(16)-C(17)	122.4(8)
C(15)-C(16)-H(16)	118.8
C(17)-C(16)-H(16)	118.8
C(12)-C(17)-C(16)	117.7(6)
C(12)-C(17)-C(18)	125.0(6)
C(16)-C(17)-C(18)	117.2(7)
O(4)-C(18)-C(17)	123.6(6)
O(4)-C(18)-C(19)	115.0(6)
C(17)-C(18)-C(19)	121.4(6)
C(20)-C(19)-C(24)	117.8(7)
C(20)-C(19)-C(18)	123.2(6)
C(24)-C(19)-C(18)	119.0(6)
C(21)-C(20)-C(19)	120.7(7)
C(21)-C(20)-H(20)	119.6
C(19)-C(20)-H(20)	119.6
C(20)-C(21)-C(22)	121.0(7)
C(20)-C(21)-H(21)	119.5
C(22)-C(21)-H(21)	119.5
O(5)-C(22)-C(21)	116.8(7)
O(5)-C(22)-C(23)	124.0(7)
C(21)-C(22)-C(23)	119.2(7)
C(24)-C(23)-C(22)	119.8(7)
C(24)-C(23)-H(23)	120.1

C(22)-C(23)-H(23)	120.1
C(23)-C(24)-C(19)	121.3(7)
C(23)-C(24)-H(24)	119.3
C(19)-C(24)-H(24)	119.3
C(27)-C(26)-N(3)	118.2(6)
C(27)-C(26)-C(31)	119.2(6)
N(3)-C(26)-C(31)	122.4(6)
C(26)-C(27)-C(28)	121.1(7)
C(26)-C(27)-H(27)	119.5
C(28)-C(27)-H(27)	119.5
C(29)-C(28)-C(27)	120.2(8)
C(29)-C(28)-H(28)	119.9
C(27)-C(28)-H(28)	119.9
C(28)-C(29)-C(30)	119.3(8)
C(28)-C(29)-H(29)	120.3
C(30)-C(29)-H(29)	120.3
C(29)-C(30)-C(31)	121.6(7)
C(29)-C(30)-H(30)	119.2
C(31)-C(30)-H(30)	119.2
C(30)-C(31)-C(26)	118.5(7)
C(30)-C(31)-C(32)	118.7(6)
C(26)-C(31)-C(32)	122.5(6)
O(3)-C(32)-C(31)	123.2(7)
O(3)-C(32)-C(33)	118.8(7)
C(31)-C(32)-C(33)	118.0(6)
C(34)-C(33)-C(38)	119.0(8)
C(34)-C(33)-C(32)	118.8(7)
C(38)-C(33)-C(32)	122.1(7)
C(33)-C(34)-C(35)	120.4(9)
C(33)-C(34)-H(34)	119.8
C(35)-C(34)-H(34)	119.8
C(36)-C(35)-C(34)	118.5(11)
C(36)-C(35)-H(35)	120.7
C(34)-C(35)-H(35)	120.7
C(37)-C(36)-C(35)	121.3(10)
C(37)-C(36)-H(36)	119.4
C(35)-C(36)-H(36)	119.4
C(36)-C(37)-C(38)	120.5(10)
C(36)-C(37)-H(37)	119.8
C(38)-C(37)-H(37)	119.8
C(37)-C(38)-C(33)	120.4(9)
C(37)-C(38)-C(39)	118.9(9)
C(33)-C(38)-C(39)	120.6(8)
F(3)-C(39)-F(2)	105.5(8)

F(3)-C(39)-F(1)	104.8(9)
F(2)-C(39)-F(1)	105.1(9)
F(3)-C(39)-C(38)	112.9(9)
F(2)-C(39)-C(38)	112.9(8)
F(1)-C(39)-C(38)	114.8(8)
C(18)-O(4)-Pd(1)	124.8(4)
C(22)-O(5)-C(25)	118.5(6)
C(9)-N(1)-C(12)	125.0(6)
C(9)-N(1)-Pd(1)	112.4(5)
C(12)-N(1)-Pd(1)	122.4(5)
C(10)-N(2)-C(7)	108.8(6)
C(10)-N(2)-C(8)	114.3(6)
C(7)-N(2)-C(8)	111.7(6)
C(10)-N(2)-Pd(1)	103.7(4)
C(7)-N(2)-Pd(1)	114.2(5)
C(8)-N(2)-Pd(1)	103.9(5)
C(11)-N(3)-C(26)	122.6(6)
C(11)-N(3)-Pd(1)	113.4(5)
C(26)-N(3)-Pd(1)	122.3(5)
N(1)-Pd(1)-N(2)	87.0(2)
N(1)-Pd(1)-O(4)	92.8(2)
N(2)-Pd(1)-O(4)	172.3(2)
N(1)-Pd(1)-N(3)	169.7(2)
N(2)-Pd(1)-N(3)	83.1(2)
O(4)-Pd(1)-N(3)	96.7(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for Pd-o-CF3-p-OMe. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	100(7)	77(6)	61(5)	12(5)	-5(5)	-7(5)
C(2)	119(9)	119(10)	110(9)	24(8)	-25(8)	-13(8)
C(3)	220(18)	99(10)	88(9)	19(8)	-57(11)	-22(11)
C(4)	270(20)	91(9)	53(6)	-1(6)	-20(9)	-4(11)
C(5)	160(10)	76(6)	52(5)	2(4)	10(6)	6(7)
C(25)	87(7)	88(6)	60(5)	9(5)	25(5)	7(5)
C(6)	94(6)	54(4)	44(4)	5(3)	15(4)	-21(4)
C(7)	76(5)	59(5)	53(4)	1(4)	11(4)	-12(4)
C(8)	70(5)	59(5)	59(4)	-12(4)	1(4)	-3(4)
C(9)	71(5)	59(5)	52(4)	-1(4)	11(4)	0(4)

C(10)	61(5)	76(5)	49(4)	-6(4)	3(3)	7(4)
C(11)	64(5)	55(4)	51(4)	3(3)	12(4)	4(4)
C(12)	67(5)	49(4)	42(4)	2(3)	1(3)	-4(4)
C(13)	91(6)	76(5)	34(3)	-2(4)	0(4)	-6(5)
C(14)	103(7)	74(6)	39(4)	-4(4)	-13(4)	1(5)
C(15)	86(6)	86(6)	54(5)	3(4)	-17(5)	-6(5)
C(16)	75(5)	62(5)	49(4)	2(4)	-5(4)	1(4)
C(17)	59(4)	52(4)	36(3)	-7(3)	-8(3)	-7(3)
C(18)	60(4)	41(3)	46(4)	-4(3)	-4(3)	-5(3)
C(19)	53(4)	51(4)	43(3)	-2(3)	1(3)	1(3)
C(20)	70(5)	58(4)	50(4)	-6(3)	6(4)	-6(4)
C(21)	74(5)	50(4)	62(4)	0(4)	7(4)	-4(4)
C(22)	58(4)	58(4)	54(4)	5(3)	7(4)	-1(4)
C(23)	74(5)	66(5)	49(4)	-2(4)	7(4)	3(4)
C(24)	68(5)	61(5)	47(4)	-7(3)	6(4)	-8(4)
C(26)	65(5)	44(4)	35(3)	-13(3)	-2(3)	-3(3)
C(27)	86(6)	63(5)	44(4)	12(4)	2(4)	14(4)
C(28)	122(8)	70(6)	59(5)	2(4)	8(5)	39(6)
C(29)	111(8)	78(6)	61(5)	1(4)	15(5)	35(6)
C(30)	101(7)	64(5)	44(4)	-3(4)	15(4)	16(5)
C(31)	70(5)	47(4)	43(4)	-5(3)	8(3)	3(3)
C(32)	71(5)	53(4)	53(4)	-4(3)	10(4)	13(4)
C(33)	75(5)	60(4)	45(4)	1(3)	9(4)	-6(4)
C(34)	96(7)	67(6)	80(6)	-2(5)	9(5)	-7(5)
C(35)	103(9)	132(10)	86(8)	-17(7)	-36(7)	5(8)
C(36)	143(11)	127(10)	66(6)	23(7)	-13(7)	30(9)
C(37)	119(9)	89(7)	61(6)	25(5)	7(6)	18(6)
C(38)	75(6)	64(5)	60(5)	13(4)	6(4)	12(4)
C(39)	76(6)	83(6)	89(7)	22(6)	17(5)	6(5)
O(1)	93(4)	92(4)	63(3)	-46(3)	14(3)	-3(3)
O(2)	75(4)	77(4)	56(3)	-12(3)	-20(3)	-1(3)
O(3)	137(6)	51(3)	60(3)	0(3)	14(4)	22(3)
O(4)	68(3)	62(3)	46(3)	-11(2)	0(2)	-9(3)
O(5)	72(3)	67(3)	71(3)	2(3)	19(3)	-6(3)
N(1)	60(4)	57(4)	47(3)	1(3)	9(3)	4(3)
N(2)	77(4)	45(3)	49(3)	-9(3)	1(3)	3(3)
N(3)	59(4)	54(3)	44(3)	0(3)	7(3)	2(3)
F(1)	112(5)	86(4)	144(5)	-26(4)	17(4)	-6(4)
F(2)	79(4)	113(5)	122(5)	15(4)	-1(3)	1(3)
F(3)	121(5)	132(6)	148(6)	47(5)	35(5)	-34(4)
Pd(1)	59(1)	50(1)	37(1)	-4(1)	4(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Pd-o-CF3-p-OMe.

	x	y	z	U(eq)
H(1)	6909	9	6069	95
H(2)	8160	-254	6739	139
H(3)	7704	34	7555	163
H(4)	5986	554	7711	164
H(5)	4706	807	7037	115
H(25A)	14382	2121	3646	118
H(25B)	13000	1969	3572	118
H(25C)	13862	1564	3875	118
H(7A)	4057	652	6165	76
H(7B)	4876	293	5800	76
H(8A)	4485	1579	6338	75
H(8B)	4905	1955	5881	75
H(10A)	4533	1543	5158	75
H(10B)	3758	1020	5317	75
H(13)	7976	1750	7119	80
H(14)	9884	1812	7472	86
H(15)	11620	1702	6977	90
H(16)	11414	1571	6111	74
H(20)	11039	2394	5583	71
H(21)	12569	2679	5048	74
H(23)	11916	1372	4128	76
H(24)	10334	1104	4646	71
H(27)	7750	-128	5053	77
H(28)	9145	-535	4506	100
H(29)	9338	-213	3676	100
H(30)	8202	545	3412	84
H(34)	5322	695	3290	97
H(35)	4797	871	2439	128
H(36)	5767	1591	2008	134
H(37)	7211	2122	2401	107

Table 6. Torsion angles [°] for Pd-o-CF3-p-OMe.

C(6)-C(1)-C(2)-C(3)	0.1(17)
C(1)-C(2)-C(3)-C(4)	1(2)
C(2)-C(3)-C(4)-C(5)	-1(2)
C(3)-C(4)-C(5)-C(6)	-1.3(19)

C(4)-C(5)-C(6)-C(1)	2.8(15)
C(4)-C(5)-C(6)-C(7)	178.8(9)
C(2)-C(1)-C(6)-C(5)	-2.2(14)
C(2)-C(1)-C(6)-C(7)	-178.3(9)
C(5)-C(6)-C(7)-N(2)	96.5(9)
C(1)-C(6)-C(7)-N(2)	-87.5(9)
N(2)-C(8)-C(9)-O(1)	-161.5(7)
N(2)-C(8)-C(9)-N(1)	22.0(9)
N(2)-C(10)-C(11)-O(2)	159.9(7)
N(2)-C(10)-C(11)-N(3)	-21.5(9)
N(1)-C(12)-C(13)-C(14)	177.9(7)
C(17)-C(12)-C(13)-C(14)	-0.9(12)
C(12)-C(13)-C(14)-C(15)	-1.2(13)
C(13)-C(14)-C(15)-C(16)	1.7(13)
C(14)-C(15)-C(16)-C(17)	-0.1(13)
N(1)-C(12)-C(17)-C(16)	-176.4(7)
C(13)-C(12)-C(17)-C(16)	2.4(10)
N(1)-C(12)-C(17)-C(18)	1.5(11)
C(13)-C(12)-C(17)-C(18)	-179.6(7)
C(15)-C(16)-C(17)-C(12)	-1.9(11)
C(15)-C(16)-C(17)-C(18)	180.0(7)
C(12)-C(17)-C(18)-O(4)	-30.6(11)
C(16)-C(17)-C(18)-O(4)	147.3(7)
C(12)-C(17)-C(18)-C(19)	152.4(7)
C(16)-C(17)-C(18)-C(19)	-29.7(10)
O(4)-C(18)-C(19)-C(20)	150.3(7)
C(17)-C(18)-C(19)-C(20)	-32.4(10)
O(4)-C(18)-C(19)-C(24)	-26.7(10)
C(17)-C(18)-C(19)-C(24)	150.5(7)
C(24)-C(19)-C(20)-C(21)	-2.5(11)
C(18)-C(19)-C(20)-C(21)	-179.6(7)
C(19)-C(20)-C(21)-C(22)	-0.5(12)
C(20)-C(21)-C(22)-O(5)	-176.3(7)
C(20)-C(21)-C(22)-C(23)	2.3(12)
O(5)-C(22)-C(23)-C(24)	177.5(7)
C(21)-C(22)-C(23)-C(24)	-0.9(12)
C(22)-C(23)-C(24)-C(19)	-2.1(12)
C(20)-C(19)-C(24)-C(23)	3.8(11)
C(18)-C(19)-C(24)-C(23)	-179.0(7)
N(3)-C(26)-C(27)-C(28)	-176.7(8)
C(31)-C(26)-C(27)-C(28)	-1.4(12)
C(26)-C(27)-C(28)-C(29)	-1.5(15)
C(27)-C(28)-C(29)-C(30)	2.0(16)
C(28)-C(29)-C(30)-C(31)	0.6(15)

C(29)-C(30)-C(31)-C(26)	-3.5(13)
C(29)-C(30)-C(31)-C(32)	169.6(8)
C(27)-C(26)-C(31)-C(30)	3.9(11)
N(3)-C(26)-C(31)-C(30)	179.0(7)
C(27)-C(26)-C(31)-C(32)	-169.0(7)
N(3)-C(26)-C(31)-C(32)	6.1(11)
C(30)-C(31)-C(32)-O(3)	-147.0(9)
C(26)-C(31)-C(32)-O(3)	25.8(13)
C(30)-C(31)-C(32)-C(33)	32.0(11)
C(26)-C(31)-C(32)-C(33)	-155.2(7)
O(3)-C(32)-C(33)-C(34)	-115.4(10)
C(31)-C(32)-C(33)-C(34)	65.6(11)
O(3)-C(32)-C(33)-C(38)	59.7(12)
C(31)-C(32)-C(33)-C(38)	-119.3(9)
C(38)-C(33)-C(34)-C(35)	-0.5(14)
C(32)-C(33)-C(34)-C(35)	174.7(9)
C(33)-C(34)-C(35)-C(36)	0.7(17)
C(34)-C(35)-C(36)-C(37)	0.0(19)
C(35)-C(36)-C(37)-C(38)	-0.9(18)
C(36)-C(37)-C(38)-C(33)	1.1(15)
C(36)-C(37)-C(38)-C(39)	177.5(10)
C(34)-C(33)-C(38)-C(37)	-0.4(13)
C(32)-C(33)-C(38)-C(37)	-175.4(8)
C(34)-C(33)-C(38)-C(39)	-176.7(8)
C(32)-C(33)-C(38)-C(39)	8.2(12)
C(37)-C(38)-C(39)-F(3)	-12.3(13)
C(33)-C(38)-C(39)-F(3)	164.1(8)
C(37)-C(38)-C(39)-F(2)	-131.9(9)
C(33)-C(38)-C(39)-F(2)	44.5(12)
C(37)-C(38)-C(39)-F(1)	107.7(10)
C(33)-C(38)-C(39)-F(1)	-75.9(11)
C(17)-C(18)-O(4)-Pd(1)	24.3(10)
C(19)-C(18)-O(4)-Pd(1)	-158.6(5)
C(21)-C(22)-O(5)-C(25)	-177.0(7)
C(23)-C(22)-O(5)-C(25)	4.6(12)
O(1)-C(9)-N(1)-C(12)	7.8(12)
C(8)-C(9)-N(1)-C(12)	-176.0(7)
O(1)-C(9)-N(1)-Pd(1)	-176.5(7)
C(8)-C(9)-N(1)-Pd(1)	-0.3(8)
C(13)-C(12)-N(1)-C(9)	24.3(11)
C(17)-C(12)-N(1)-C(9)	-156.9(7)
C(13)-C(12)-N(1)-Pd(1)	-151.1(6)
C(17)-C(12)-N(1)-Pd(1)	27.8(9)
C(11)-C(10)-N(2)-C(7)	-83.6(8)

C(11)-C(10)-N(2)-C(8)	150.8(7)
C(11)-C(10)-N(2)-Pd(1)	38.3(7)
C(6)-C(7)-N(2)-C(10)	166.8(6)
C(6)-C(7)-N(2)-C(8)	-66.1(9)
C(6)-C(7)-N(2)-Pd(1)	51.5(7)
C(9)-C(8)-N(2)-C(10)	-143.4(7)
C(9)-C(8)-N(2)-C(7)	92.5(8)
C(9)-C(8)-N(2)-Pd(1)	-31.1(7)
O(2)-C(11)-N(3)-C(26)	5.9(12)
C(10)-C(11)-N(3)-C(26)	-172.5(6)
O(2)-C(11)-N(3)-Pd(1)	171.1(6)
C(10)-C(11)-N(3)-Pd(1)	-7.4(8)
C(27)-C(26)-N(3)-C(11)	-128.6(8)
C(31)-C(26)-N(3)-C(11)	56.2(10)
C(27)-C(26)-N(3)-Pd(1)	67.5(8)
C(31)-C(26)-N(3)-Pd(1)	-107.6(7)
C(9)-N(1)-Pd(1)-N(2)	-14.9(5)
C(12)-N(1)-Pd(1)-N(2)	161.0(5)
C(9)-N(1)-Pd(1)-O(4)	157.4(5)
C(12)-N(1)-Pd(1)-O(4)	-26.7(5)
C(9)-N(1)-Pd(1)-N(3)	0.7(16)
C(12)-N(1)-Pd(1)-N(3)	176.5(11)
C(10)-N(2)-Pd(1)-N(1)	144.4(5)
C(7)-N(2)-Pd(1)-N(1)	-97.3(5)
C(8)-N(2)-Pd(1)-N(1)	24.6(5)
C(10)-N(2)-Pd(1)-O(4)	56.4(17)
C(7)-N(2)-Pd(1)-O(4)	174.6(14)
C(8)-N(2)-Pd(1)-O(4)	-63.5(17)
C(10)-N(2)-Pd(1)-N(3)	-32.8(4)
C(7)-N(2)-Pd(1)-N(3)	85.4(5)
C(8)-N(2)-Pd(1)-N(3)	-152.7(5)
C(18)-O(4)-Pd(1)-N(1)	1.3(6)
C(18)-O(4)-Pd(1)-N(2)	88.9(16)
C(18)-O(4)-Pd(1)-N(3)	177.2(6)
C(11)-N(3)-Pd(1)-N(1)	8.7(16)
C(26)-N(3)-Pd(1)-N(1)	173.9(11)
C(11)-N(3)-Pd(1)-N(2)	24.3(5)
C(26)-N(3)-Pd(1)-N(2)	-170.5(5)
C(11)-N(3)-Pd(1)-O(4)	-147.9(5)
C(26)-N(3)-Pd(1)-O(4)	17.3(5)

Symmetry transformations used to generate equivalent atoms: