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ELECTRONIC SUPPLEMENTARY INFORMATION

Evaluation of an External Initiating Ni(II) Diimine Catalyst for Electron-Deficient π-Conjugated Polymers

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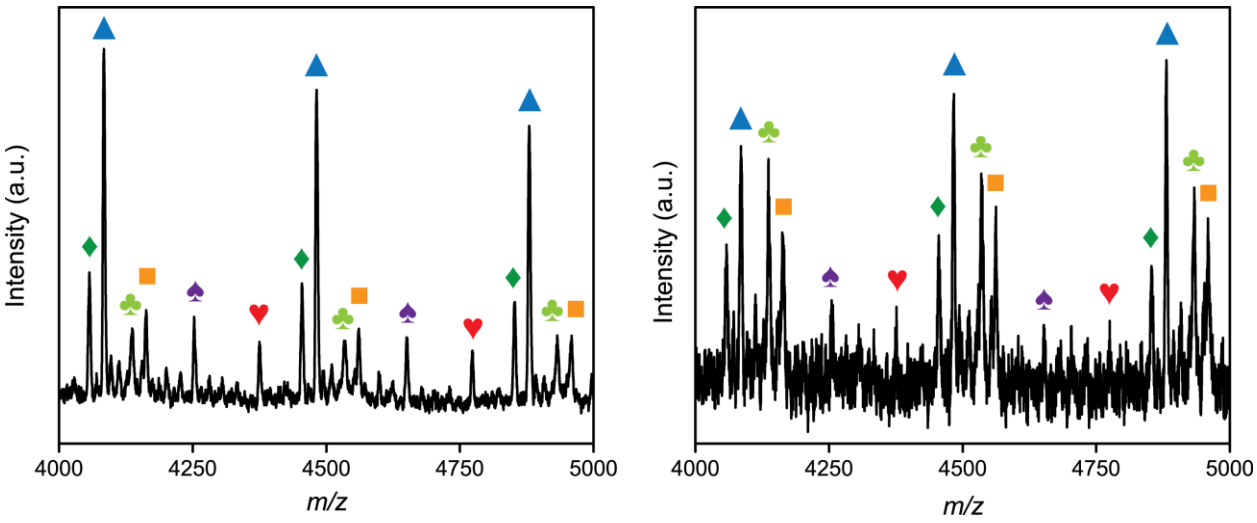

Figure S1. MALDI-ToF spectra of poly(BTz) prepared at 4% (left) and 2% (right) catalyst loading. End-group distributions: ▲ = OMePh/H, ■ = OMePh/Br, ♦ = Br/H, ♣ = Br/Br, ♥ = H/H, ♠ = Br/Br – $C_{20}H_{41}$.

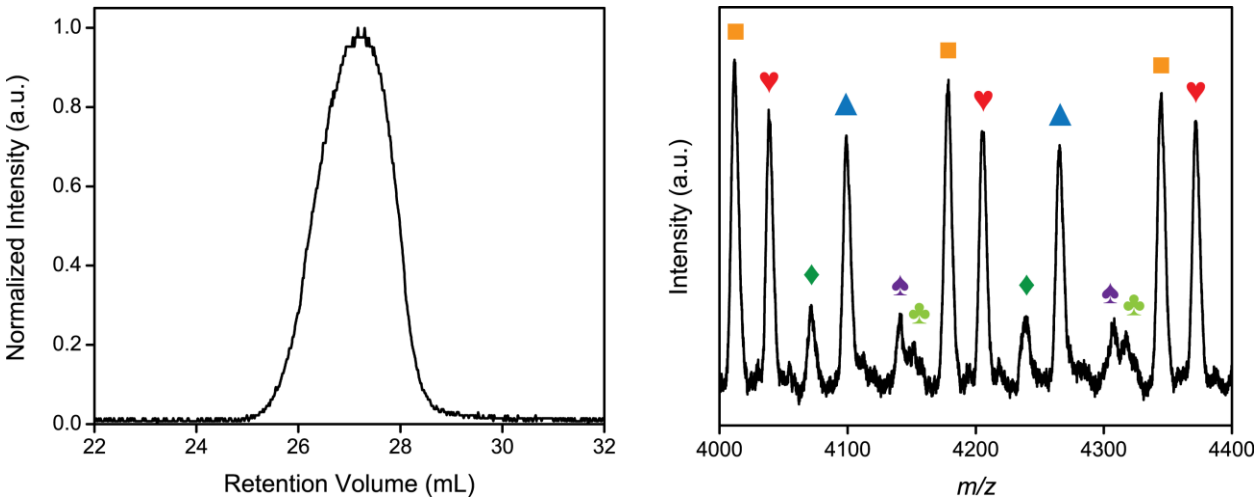

Figure S2. Left: GPC elution curve for P3HT prepared at 8% catalyst loading of Ni(MesAn)OMePhBr. Right: MALDI-ToF spectrum of P3HT prepared at 8% catalyst loading. End-group distributions: ▲ = OMePh/H (21.9%), ■ = OMePh/Br (30.6%), ♦ = Br/H (6.9%), ♣ = Br/Br (4.4%), ♥ = OMePh/OMePh (30.2%), ♠ = mod(*m/z*) = 150 (5.7%).

Table S1. Crystal data and structure refinement for Ni(MesAn)OMePhBr.

Identification code	d16139_a	
Empirical formula	C41 H43 Br N2 Ni O2	
Formula weight	734.39	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 10.2766(16) Å	a= 90°.
	b = 16.387(3) Å	b= 92.547(5)°.
	c = 21.498(3) Å	g = 90°.
Volume	3616.7(10) $Å^3$	
Z	4	
Density (calculated)	1.349 Mg/m^3	
Absorption coefficient	1.678 mm^{-1}	
F(000)	1528	
Crystal size	0.120 x 0.040 x 0.040 mm^3	
Theta range for data collection	1.563 to 27.519°.	
Index ranges	-13<=h<=13, -21<=k<=21, -27<=l<=24	
Reflections collected	56322	
Independent reflections	8307 [R(int) = 0.1475]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6524	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8307 / 5 / 441
Goodness-of-fit on F^2	0.992
Final R indices [I>2sigma(I)]	R1 = 0.0491, wR2 = 0.1006
R indices (all data)	R1 = 0.1391, wR2 = 0.1315
Extinction coefficient	n/a
Largest diff. peak and hole	0.897 and -0.561 e.$Å^{-3}$

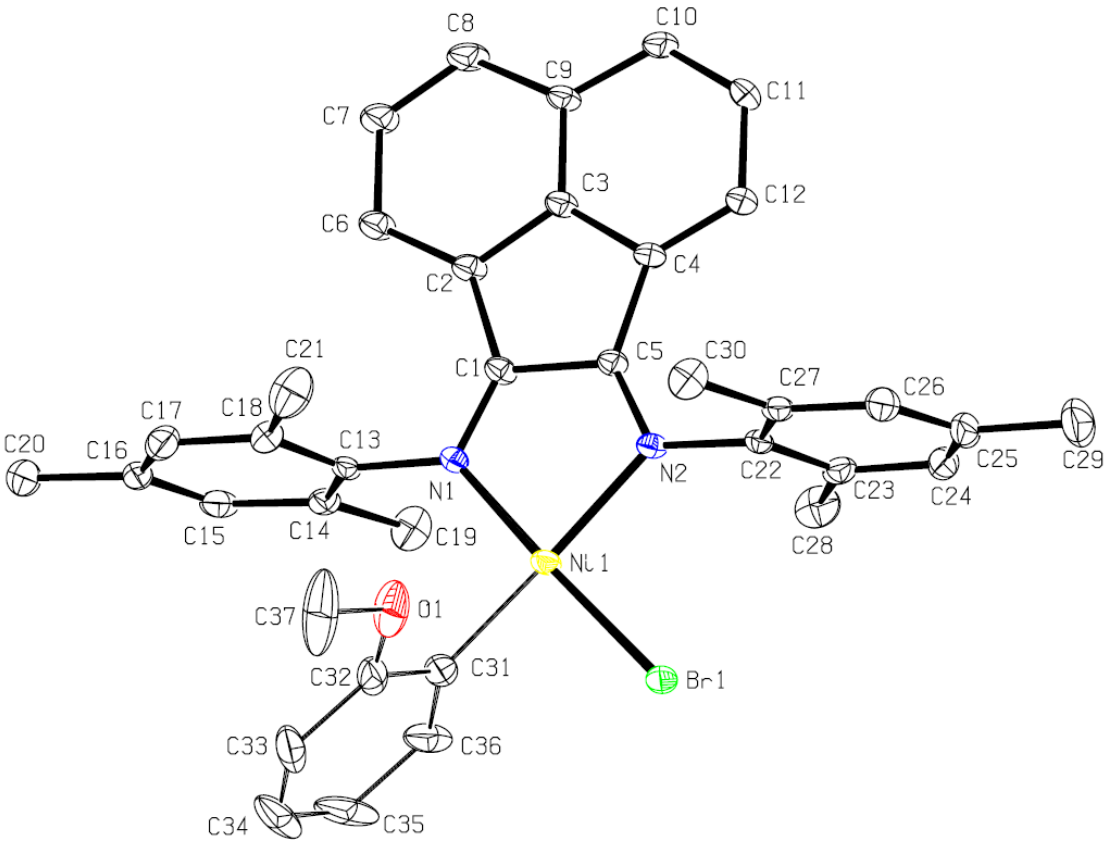

Figure S3. Thermal ellipsoid plot of Ni(MesAn)OMePhBr with atom labels. H atoms, solvent of crystallization, and disorder in the *o*-methoxyphenyl ligand are not shown.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Ni(MesAn)OMePhBr. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	8600(1)	2112(1)	7178(1)	24(1)
Br(1)	10431(1)	1531(1)	7634(1)	28(1)
N(1)	7056(3)	2564(2)	6757(1)	22(1)
N(2)	9114(3)	1865(2)	6311(2)	22(1)
C(1)	7091(4)	2508(3)	6158(2)	24(1)
C(2)	6226(4)	2755(3)	5629(2)	26(1)
C(3)	6874(4)	2496(3)	5091(2)	25(1)
C(4)	8091(4)	2110(3)	5222(2)	25(1)
C(5)	8247(4)	2108(2)	5906(2)	22(1)
C(6)	5061(4)	3170(3)	5560(2)	34(1)
C(7)	4544(4)	3302(3)	4945(2)	40(1)
C(8)	5148(4)	3045(3)	4424(2)	37(1)
C(9)	6365(4)	2631(3)	4481(2)	27(1)
C(10)	7150(4)	2360(3)	3998(2)	31(1)
C(11)	8337(5)	2000(3)	4126(2)	33(1)
C(12)	8829(4)	1863(3)	4742(2)	30(1)
C(13)	5927(4)	2942(3)	7004(2)	23(1)
C(14)	4867(4)	2454(3)	7137(2)	27(1)
C(15)	3757(4)	2840(3)	7347(2)	36(1)
C(16)	3691(5)	3673(3)	7431(2)	36(1)

C(17)	4768(5)	4139(3)	7295(2)	40(1)
C(18)	5899(4)	3786(3)	7071(2)	32(1)
C(19)	4885(4)	1551(3)	7025(2)	43(1)
C(20)	2468(5)	4079(4)	7654(2)	57(2)
C(21)	7006(5)	4319(3)	6879(3)	57(2)
C(22)	10284(4)	1501(3)	6092(2)	23(1)
C(23)	10331(4)	663(3)	6013(2)	30(1)
C(24)	11471(5)	328(3)	5785(2)	40(1)
C(25)	12521(5)	808(3)	5653(2)	42(1)
C(26)	12439(4)	1634(3)	5751(2)	38(1)
C(27)	11326(4)	2003(3)	5970(2)	27(1)
C(28)	9195(5)	128(3)	6153(2)	48(1)
C(29)	13754(5)	438(4)	5406(3)	69(2)
C(30)	11243(4)	2912(3)	6068(2)	40(1)
C(31)	7971(5)	2326(3)	7986(2)	33(2)
C(32)	8253(5)	3087(3)	8244(2)	44(2)
C(33)	7772(6)	3299(4)	8816(2)	78(4)
C(34)	7009(6)	2749(5)	9131(2)	95(5)
C(35)	6726(5)	1988(5)	8873(2)	84(4)
C(36)	7207(5)	1777(3)	8301(2)	50(2)
C(37)	9326(9)	4385(5)	8171(6)	106(4)
O(1)	9047(5)	3595(3)	7917(3)	56(2)
C(31A)	8212(14)	2569(8)	7965(5)	16(4)
C(32A)	8772(13)	3297(8)	8173(5)	26(5)

C(33A)	8428(13)	3631(6)	8736(5)	40(5)
C(34A)	7523(13)	3237(7)	9093(5)	33(5)
C(35A)	6963(12)	2509(6)	8885(5)	23(4)
C(36A)	7307(13)	2175(6)	8322(5)	16(4)
O(1A)	6857(11)	1433(6)	8106(5)	30(3)
C(37A)	5854(14)	1044(10)	8440(7)	43(5)
O(1S)	1005(17)	5421(9)	5984(8)	441(14)
C(1S)	1131(7)	5786(4)	5353(3)	78(2)
C(2S)	2123(11)	5376(6)	5004(5)	154(5)
C(3S)	2611(10)	4811(6)	5449(6)	149(5)
C(4S)	2397(16)	5184(6)	6040(4)	181(7)

Table S3. Bond lengths [Å] and angles [°] for Ni(MesAn)OMePhBr.

Ni(1)-C(31A)	1.908(8)
Ni(1)-C(31)	1.912(3)
Ni(1)-N(1)	1.938(3)
Ni(1)-N(2)	2.003(3)
Ni(1)-Br(1)	2.2899(7)
N(1)-C(1)	1.292(5)
N(1)-C(13)	1.439(5)
N(2)-C(5)	1.281(5)
N(2)-C(22)	1.439(5)
C(1)-C(2)	1.470(5)
C(1)-C(5)	1.481(6)
C(2)-C(6)	1.379(6)
C(2)-C(3)	1.424(6)
C(3)-C(9)	1.407(5)
C(3)-C(4)	1.418(6)
C(4)-C(12)	1.368(6)
C(4)-C(5)	1.471(5)
C(6)-C(7)	1.420(6)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.371(6)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.424(6)
C(8)-H(8A)	0.9500

C(9)-C(10)	1.413(6)
C(10)-C(11)	1.372(6)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.414(6)
C(11)-H(11A)	0.9500
C(12)-H(12A)	0.9500
C(13)-C(18)	1.390(6)
C(13)-C(14)	1.391(6)
C(14)-C(15)	1.396(6)
C(14)-C(19)	1.499(6)
C(15)-C(16)	1.379(7)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.386(7)
C(16)-C(20)	1.518(6)
C(17)-C(18)	1.403(6)
C(17)-H(17A)	0.9500
C(18)-C(21)	1.506(7)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800

C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(27)	1.384(6)
C(22)-C(23)	1.385(6)
C(23)-C(24)	1.401(6)
C(23)-C(28)	1.501(6)
C(24)-C(25)	1.375(7)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.373(7)
C(25)-C(29)	1.522(7)
C(26)-C(27)	1.394(6)
C(26)-H(26A)	0.9500
C(27)-C(30)	1.507(6)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(32)	1.3900
C(31)-C(36)	1.3900

C(32)-O(1)	1.379(7)
C(32)-C(33)	1.3900
C(33)-C(34)	1.3900
C(33)-H(33A)	0.9500
C(34)-C(35)	1.3900
C(34)-H(34A)	0.9500
C(35)-C(36)	1.3900
C(35)-H(35A)	0.9500
C(36)-H(36A)	0.9500
C(37)-O(1)	1.431(8)
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(31A)-C(32A)	1.3900
C(31A)-C(36A)	1.3900
C(32A)-C(33A)	1.3900
C(32A)-H(32A)	0.9500
C(33A)-C(34A)	1.3900
C(33A)-H(33B)	0.9500
C(34A)-C(35A)	1.3900
C(34A)-H(34B)	0.9500
C(35A)-C(36A)	1.3900
C(35A)-H(35B)	0.9500
C(36A)-O(1A)	1.373(9)

O(1A)-C(37A)	1.432(11)
C(37A)-H(37D)	0.9800
C(37A)-H(37E)	0.9800
C(37A)-H(37F)	0.9800
O(1S)-C(4S)	1.482(14)
O(1S)-C(1S)	1.494(13)
C(1S)-C(2S)	1.458(9)
C(1S)-H(1SA)	0.9900
C(1S)-H(1SB)	0.9900
C(2S)-C(3S)	1.409(12)
C(2S)-H(2SA)	0.9900
C(2S)-H(2SB)	0.9900
C(3S)-C(4S)	1.437(9)
C(3S)-H(3SA)	0.9900
C(3S)-H(3SB)	0.9900
C(4S)-H(4SC)	0.9900
C(4S)-H(4SA)	0.9900

C(31A)-Ni(1)-N(1)	93.8(5)
C(31)-Ni(1)-N(1)	93.0(2)
C(31A)-Ni(1)-N(2)	168.3(4)
C(31)-Ni(1)-N(2)	175.5(2)
N(1)-Ni(1)-N(2)	83.47(13)
C(31A)-Ni(1)-Br(1)	89.1(5)
C(31)-Ni(1)-Br(1)	89.56(18)

N(1)-Ni(1)-Br(1)	177.02(10)
N(2)-Ni(1)-Br(1)	93.92(10)
C(1)-N(1)-C(13)	117.2(3)
C(1)-N(1)-Ni(1)	112.3(3)
C(13)-N(1)-Ni(1)	130.4(2)
C(5)-N(2)-C(22)	118.2(3)
C(5)-N(2)-Ni(1)	111.4(3)
C(22)-N(2)-Ni(1)	130.3(2)
N(1)-C(1)-C(2)	135.2(4)
N(1)-C(1)-C(5)	117.1(3)
C(2)-C(1)-C(5)	107.7(3)
C(6)-C(2)-C(3)	119.7(4)
C(6)-C(2)-C(1)	135.3(4)
C(3)-C(2)-C(1)	105.0(3)
C(9)-C(3)-C(4)	122.9(4)
C(9)-C(3)-C(2)	122.8(4)
C(4)-C(3)-C(2)	114.3(3)
C(12)-C(4)-C(3)	119.7(4)
C(12)-C(4)-C(5)	135.5(4)
C(3)-C(4)-C(5)	104.8(3)
N(2)-C(5)-C(4)	136.1(4)
N(2)-C(5)-C(1)	115.7(3)
C(4)-C(5)-C(1)	108.2(3)
C(2)-C(6)-C(7)	117.5(4)

C(2)-C(6)-H(6A)	121.2
C(7)-C(6)-H(6A)	121.2
C(8)-C(7)-C(6)	123.3(4)
C(8)-C(7)-H(7A)	118.3
C(6)-C(7)-H(7A)	118.3
C(7)-C(8)-C(9)	120.3(4)
C(7)-C(8)-H(8A)	119.8
C(9)-C(8)-H(8A)	119.8
C(3)-C(9)-C(10)	115.8(4)
C(3)-C(9)-C(8)	116.3(4)
C(10)-C(9)-C(8)	127.9(4)
C(11)-C(10)-C(9)	121.3(4)
C(11)-C(10)-H(10A)	119.4
C(9)-C(10)-H(10A)	119.4
C(10)-C(11)-C(12)	122.2(4)
C(10)-C(11)-H(11A)	118.9
C(12)-C(11)-H(11A)	118.9
C(4)-C(12)-C(11)	118.2(4)
C(4)-C(12)-H(12A)	120.9
C(11)-C(12)-H(12A)	120.9
C(18)-C(13)-C(14)	122.1(4)
C(18)-C(13)-N(1)	119.1(4)
C(14)-C(13)-N(1)	118.7(4)
C(13)-C(14)-C(15)	117.6(4)

C(13)-C(14)-C(19)	121.3(4)
C(15)-C(14)-C(19)	121.0(4)
C(16)-C(15)-C(14)	122.5(4)
C(16)-C(15)-H(15A)	118.8
C(14)-C(15)-H(15A)	118.8
C(15)-C(16)-C(17)	118.2(4)
C(15)-C(16)-C(20)	121.5(5)
C(17)-C(16)-C(20)	120.3(5)
C(16)-C(17)-C(18)	121.8(4)
C(16)-C(17)-H(17A)	119.1
C(18)-C(17)-H(17A)	119.1
C(13)-C(18)-C(17)	117.8(4)
C(13)-C(18)-C(21)	122.0(4)
C(17)-C(18)-C(21)	120.1(4)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5

H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(27)-C(22)-C(23)	122.3(4)
C(27)-C(22)-N(2)	118.7(4)
C(23)-C(22)-N(2)	119.0(4)
C(22)-C(23)-C(24)	117.7(4)
C(22)-C(23)-C(28)	121.5(4)
C(24)-C(23)-C(28)	120.7(4)
C(25)-C(24)-C(23)	121.6(5)
C(25)-C(24)-H(24A)	119.2
C(23)-C(24)-H(24A)	119.2
C(26)-C(25)-C(24)	118.5(4)
C(26)-C(25)-C(29)	120.3(5)
C(24)-C(25)-C(29)	121.2(5)
C(25)-C(26)-C(27)	122.4(5)
C(25)-C(26)-H(26A)	118.8
C(27)-C(26)-H(26A)	118.8
C(22)-C(27)-C(26)	117.4(4)

C(22)-C(27)-C(30)	120.8(4)
C(26)-C(27)-C(30)	121.8(4)
C(23)-C(28)-H(28A)	109.5
C(23)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(23)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(25)-C(29)-H(29A)	109.5
C(25)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(25)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(27)-C(30)-H(30A)	109.5
C(27)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(27)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-C(36)	120.0
C(32)-C(31)-Ni(1)	117.0(3)
C(36)-C(31)-Ni(1)	122.9(3)
O(1)-C(32)-C(31)	117.1(4)

O(1)-C(32)-C(33)	122.9(4)
C(31)-C(32)-C(33)	120.0
C(34)-C(33)-C(32)	120.0
C(34)-C(33)-H(33A)	120.0
C(32)-C(33)-H(33A)	120.0
C(33)-C(34)-C(35)	120.0
C(33)-C(34)-H(34A)	120.0
C(35)-C(34)-H(34A)	120.0
C(36)-C(35)-C(34)	120.0
C(36)-C(35)-H(35A)	120.0
C(34)-C(35)-H(35A)	120.0
C(35)-C(36)-C(31)	120.0
C(35)-C(36)-H(36A)	120.0
C(31)-C(36)-H(36A)	120.0
O(1)-C(37)-H(37A)	109.5
O(1)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
O(1)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(32)-O(1)-C(37)	117.6(7)
C(32A)-C(31A)-C(36A)	120.0
C(32A)-C(31A)-Ni(1)	121.4(6)
C(36A)-C(31A)-Ni(1)	118.5(6)

C(33A)-C(32A)-C(31A) 120.0

C(33A)-C(32A)-H(32A) 120.0

C(31A)-C(32A)-H(32A) 120.0

C(34A)-C(33A)-C(32A) 120.0

C(34A)-C(33A)-H(33B) 120.0

C(32A)-C(33A)-H(33B) 120.0

C(33A)-C(34A)-C(35A) 120.0

C(33A)-C(34A)-H(34B) 120.0

C(35A)-C(34A)-H(34B) 120.0

C(34A)-C(35A)-C(36A) 120.0

C(34A)-C(35A)-H(35B) 120.0

C(36A)-C(35A)-H(35B) 120.0

O(1A)-C(36A)-C(35A) 123.2(9)

O(1A)-C(36A)-C(31A) 116.7(9)

C(35A)-C(36A)-C(31A) 120.0

C(36A)-O(1A)-C(37A) 117.7(12)

O(1A)-C(37A)-H(37D) 109.5

O(1A)-C(37A)-H(37E) 109.5

H(37D)-C(37A)-H(37E) 109.5

O(1A)-C(37A)-H(37F) 109.5

H(37D)-C(37A)-H(37F) 109.5

H(37E)-C(37A)-H(37F) 109.5

C(4S)-O(1S)-C(1S) 93.2(11)

C(2S)-C(1S)-O(1S) 112.0(9)

C(2S)-C(1S)-H(1SA)	109.2
O(1S)-C(1S)-H(1SA)	109.2
C(2S)-C(1S)-H(1SB)	109.2
O(1S)-C(1S)-H(1SB)	109.2
H(1SA)-C(1S)-H(1SB)	107.9
C(3S)-C(2S)-C(1S)	100.9(7)
C(3S)-C(2S)-H(2SA)	111.6
C(1S)-C(2S)-H(2SA)	111.6
C(3S)-C(2S)-H(2SB)	111.6
C(1S)-C(2S)-H(2SB)	111.6
H(2SA)-C(2S)-H(2SB)	109.4
C(2S)-C(3S)-C(4S)	104.9(8)
C(2S)-C(3S)-H(3SA)	110.8
C(4S)-C(3S)-H(3SA)	110.8
C(2S)-C(3S)-H(3SB)	110.8
C(4S)-C(3S)-H(3SB)	110.8
H(3SA)-C(3S)-H(3SB)	108.8
C(3S)-C(4S)-O(1S)	103.0(9)
C(3S)-C(4S)-H(4SC)	111.2
O(1S)-C(4S)-H(4SC)	111.2
C(3S)-C(4S)-H(4SA)	111.2
O(1S)-C(4S)-H(4SA)	111.2
H(4SC)-C(4S)-H(4SA)	109.1

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Ni(MesAn)OMePhBr. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	23(1)	34(1)	15(1)	0(1)	-2(1)	2(1)
Br(1)	28(1)	36(1)	20(1)	-2(1)	-5(1)	5(1)
N(1)	24(2)	24(2)	17(2)	1(1)	4(2)	-1(2)
N(2)	19(2)	28(2)	18(2)	3(2)	0(2)	-3(2)
C(1)	20(2)	33(3)	19(2)	-2(2)	0(2)	-4(2)
C(2)	17(2)	42(3)	20(2)	3(2)	-2(2)	-4(2)
C(3)	25(2)	33(2)	18(2)	0(2)	-1(2)	-2(2)
C(4)	27(2)	29(2)	17(2)	0(2)	-3(2)	-1(2)
C(5)	22(2)	27(2)	18(2)	-1(2)	-2(2)	-2(2)
C(6)	22(3)	56(3)	23(2)	5(2)	1(2)	2(2)
C(7)	25(3)	70(4)	26(3)	6(2)	-5(2)	11(2)
C(8)	31(3)	55(3)	23(2)	4(2)	-12(2)	-2(2)
C(9)	28(3)	36(3)	16(2)	0(2)	-2(2)	-2(2)
C(10)	38(3)	37(3)	19(2)	1(2)	-7(2)	4(2)
C(11)	44(3)	37(3)	20(2)	-6(2)	4(2)	6(2)
C(12)	37(3)	34(3)	20(2)	-1(2)	-1(2)	6(2)
C(13)	19(2)	37(3)	13(2)	1(2)	-1(2)	5(2)
C(14)	20(2)	40(3)	20(2)	2(2)	-6(2)	4(2)
C(15)	25(3)	58(4)	24(2)	12(2)	1(2)	3(2)
C(16)	33(3)	55(4)	21(2)	2(2)	-2(2)	21(2)

C(17)	52(3)	33(3)	35(3)	-4(2)	-9(2)	13(2)
C(18)	31(3)	34(3)	32(3)	3(2)	-2(2)	6(2)
C(19)	29(3)	39(3)	61(3)	3(3)	2(2)	-7(2)
C(20)	47(3)	87(5)	38(3)	8(3)	6(3)	37(3)
C(21)	51(4)	36(3)	84(4)	3(3)	0(3)	-3(3)
C(22)	23(2)	30(2)	15(2)	1(2)	0(2)	3(2)
C(23)	35(3)	29(3)	23(2)	1(2)	-8(2)	4(2)
C(24)	55(4)	38(3)	25(2)	-10(2)	-9(2)	19(3)
C(25)	35(3)	63(4)	29(3)	-5(2)	-1(2)	23(3)
C(26)	23(3)	59(4)	33(3)	6(2)	4(2)	9(2)
C(27)	26(3)	36(3)	19(2)	5(2)	-1(2)	4(2)
C(28)	60(4)	30(3)	53(3)	-2(2)	-8(3)	-9(3)
C(29)	55(4)	103(5)	50(4)	-18(3)	2(3)	40(4)
C(30)	31(3)	37(3)	53(3)	5(2)	3(2)	-6(2)
C(31)	26(4)	45(5)	27(4)	-2(3)	-4(3)	6(4)
C(32)	33(5)	64(6)	33(4)	-12(4)	-8(4)	23(4)
C(33)	63(7)	131(10)	36(5)	-34(5)	-16(5)	65(7)
C(34)	45(6)	220(16)	20(5)	-18(7)	-9(4)	62(8)
C(35)	22(4)	201(14)	27(5)	37(6)	-5(4)	9(6)
C(36)	27(5)	92(9)	30(5)	22(5)	0(4)	2(5)
C(37)	71(7)	60(7)	186(12)	-71(7)	1(7)	13(5)
O(1)	52(3)	34(3)	81(4)	-29(3)	-10(3)	5(3)
O(1S)	450(20)	303(17)	590(30)	226(19)	210(20)	159(17)
C(1S)	76(5)	68(5)	88(5)	11(4)	-15(4)	-26(4)

C(2S)	209(12)	131(9)	128(9)	-59(8)	82(9)	-71(9)
C(3S)	134(9)	97(8)	224(14)	62(9)	89(9)	44(7)
C(4S)	370(20)	96(8)	73(6)	-10(5)	-51(9)	-105(11)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Ni(MesAn)OMePhBr.

	x	y	z	U(eq)
H(6A)	4621	3359	5912	41
H(7A)	3738	3583	4892	48
H(8A)	4754	3145	4023	44
H(10A)	6850	2430	3577	38
H(11A)	8845	1836	3790	40
H(12A)	9649	1608	4821	36
H(15A)	3020	2517	7434	43
H(17A)	4739	4713	7355	48
H(19A)	4149	1297	7226	64
H(19B)	5703	1322	7200	64
H(19C)	4816	1444	6576	64
H(20A)	1742	3692	7625	86
H(20B)	2259	4557	7394	86
H(20C)	2615	4252	8088	86
H(21A)	6907	4867	7054	86
H(21B)	6998	4354	6424	86
H(21C)	7835	4083	7035	86
H(24A)	11519	-244	5721	48
H(26A)	13167	1967	5666	46
H(28A)	9470	-444	6154	72
H(28B)	8496	209	5833	72

H(28C)	8877	272	6562	72
H(29A)	13551	-95	5219	104
H(29B)	14406	370	5749	104
H(29C)	14100	800	5090	104
H(30A)	12094	3160	6003	60
H(30B)	10987	3024	6493	60
H(30C)	10593	3144	5770	60
H(33A)	7966	3819	8992	93
H(34A)	6680	2893	9522	115
H(35A)	6204	1612	9088	101
H(36A)	7014	1257	8125	60
H(37A)	9930	4672	7907	159
H(37B)	9724	4327	8592	159
H(37C)	8517	4698	8190	159
H(32A)	9391	3567	7929	31
H(33B)	8811	4129	8878	48
H(34B)	7288	3465	9478	39
H(35B)	6345	2239	9129	28
H(37D)	5584	541	8225	65
H(37E)	5105	1412	8461	65
H(37F)	6186	913	8863	65
H(1SA)	283	5750	5118	93
H(1SB)	1359	6371	5398	93
H(2SA)	1740	5099	4629	184

H(2SB)	2807	5760	4878	184
H(3SA)	3551	4711	5399	179
H(3SB)	2140	4285	5409	179
H(4SC)	2962	5668	6109	218
H(4SA)	2560	4794	6386	218

Table S6. Torsion angles [°] for Ni(MesAn)OMePhBr.

C(13)-N(1)-C(1)-C(2)	1.0(7)
Ni(1)-N(1)-C(1)-C(2)	-178.7(4)
C(13)-N(1)-C(1)-C(5)	-179.2(3)
Ni(1)-N(1)-C(1)-C(5)	1.1(5)
N(1)-C(1)-C(2)-C(6)	2.8(9)
C(5)-C(1)-C(2)-C(6)	-177.0(5)
N(1)-C(1)-C(2)-C(3)	-179.8(5)
C(5)-C(1)-C(2)-C(3)	0.4(4)
C(6)-C(2)-C(3)-C(9)	-1.2(6)
C(1)-C(2)-C(3)-C(9)	-179.1(4)
C(6)-C(2)-C(3)-C(4)	177.2(4)
C(1)-C(2)-C(3)-C(4)	-0.7(5)
C(9)-C(3)-C(4)-C(12)	1.0(6)
C(2)-C(3)-C(4)-C(12)	-177.4(4)
C(9)-C(3)-C(4)-C(5)	179.1(4)
C(2)-C(3)-C(4)-C(5)	0.7(5)
C(22)-N(2)-C(5)-C(4)	1.0(7)
Ni(1)-N(2)-C(5)-C(4)	178.7(4)
C(22)-N(2)-C(5)-C(1)	-177.5(3)
Ni(1)-N(2)-C(5)-C(1)	0.2(4)
C(12)-C(4)-C(5)-N(2)	-1.3(9)
C(3)-C(4)-C(5)-N(2)	-179.0(5)
C(12)-C(4)-C(5)-C(1)	177.3(5)

C(3)-C(4)-C(5)-C(1)	-0.4(5)
N(1)-C(1)-C(5)-N(2)	-0.9(6)
C(2)-C(1)-C(5)-N(2)	179.0(4)
N(1)-C(1)-C(5)-C(4)	-179.9(4)
C(2)-C(1)-C(5)-C(4)	0.0(5)
C(3)-C(2)-C(6)-C(7)	1.4(6)
C(1)-C(2)-C(6)-C(7)	178.6(5)
C(2)-C(6)-C(7)-C(8)	-0.5(7)
C(6)-C(7)-C(8)-C(9)	-0.7(8)
C(4)-C(3)-C(9)-C(10)	-0.4(6)
C(2)-C(3)-C(9)-C(10)	177.9(4)
C(4)-C(3)-C(9)-C(8)	-178.3(4)
C(2)-C(3)-C(9)-C(8)	-0.1(6)
C(7)-C(8)-C(9)-C(3)	1.0(7)
C(7)-C(8)-C(9)-C(10)	-176.7(5)
C(3)-C(9)-C(10)-C(11)	-0.7(6)
C(8)-C(9)-C(10)-C(11)	176.9(5)
C(9)-C(10)-C(11)-C(12)	1.3(7)
C(3)-C(4)-C(12)-C(11)	-0.5(6)
C(5)-C(4)-C(12)-C(11)	-177.9(5)
C(10)-C(11)-C(12)-C(4)	-0.6(7)
C(1)-N(1)-C(13)-C(18)	-86.5(5)
Ni(1)-N(1)-C(13)-C(18)	93.2(4)
C(1)-N(1)-C(13)-C(14)	90.0(5)

Ni(1)-N(1)-C(13)-C(14)	-90.4(4)
C(18)-C(13)-C(14)-C(15)	-0.4(6)
N(1)-C(13)-C(14)-C(15)	-176.8(3)
C(18)-C(13)-C(14)-C(19)	176.2(4)
N(1)-C(13)-C(14)-C(19)	-0.1(6)
C(13)-C(14)-C(15)-C(16)	-0.8(6)
C(19)-C(14)-C(15)-C(16)	-177.5(4)
C(14)-C(15)-C(16)-C(17)	0.8(6)
C(14)-C(15)-C(16)-C(20)	179.5(4)
C(15)-C(16)-C(17)-C(18)	0.6(6)
C(20)-C(16)-C(17)-C(18)	-178.1(4)
C(14)-C(13)-C(18)-C(17)	1.7(6)
N(1)-C(13)-C(18)-C(17)	178.0(3)
C(14)-C(13)-C(18)-C(21)	-175.1(4)
N(1)-C(13)-C(18)-C(21)	1.2(6)
C(16)-C(17)-C(18)-C(13)	-1.8(6)
C(16)-C(17)-C(18)-C(21)	175.1(4)
C(5)-N(2)-C(22)-C(27)	88.5(5)
Ni(1)-N(2)-C(22)-C(27)	-88.6(4)
C(5)-N(2)-C(22)-C(23)	-91.6(5)
Ni(1)-N(2)-C(22)-C(23)	91.2(4)
C(27)-C(22)-C(23)-C(24)	-1.6(6)
N(2)-C(22)-C(23)-C(24)	178.5(3)
C(27)-C(22)-C(23)-C(28)	179.5(4)

N(2)-C(22)-C(23)-C(28)	-0.4(6)
C(22)-C(23)-C(24)-C(25)	1.0(6)
C(28)-C(23)-C(24)-C(25)	179.9(4)
C(23)-C(24)-C(25)-C(26)	0.2(7)
C(23)-C(24)-C(25)-C(29)	-179.9(4)
C(24)-C(25)-C(26)-C(27)	-0.9(7)
C(29)-C(25)-C(26)-C(27)	179.2(4)
C(23)-C(22)-C(27)-C(26)	1.0(6)
N(2)-C(22)-C(27)-C(26)	-179.1(3)
C(23)-C(22)-C(27)-C(30)	-179.5(4)
N(2)-C(22)-C(27)-C(30)	0.4(6)
C(25)-C(26)-C(27)-C(22)	0.3(6)
C(25)-C(26)-C(27)-C(30)	-179.2(4)
C(36)-C(31)-C(32)-O(1)	178.2(5)
Ni(1)-C(31)-C(32)-O(1)	-5.0(4)
C(36)-C(31)-C(32)-C(33)	0.0
Ni(1)-C(31)-C(32)-C(33)	176.9(4)
O(1)-C(32)-C(33)-C(34)	-178.0(5)
C(31)-C(32)-C(33)-C(34)	0.0
C(32)-C(33)-C(34)-C(35)	0.0
C(33)-C(34)-C(35)-C(36)	0.0
C(34)-C(35)-C(36)-C(31)	0.0
C(32)-C(31)-C(36)-C(35)	0.0
Ni(1)-C(31)-C(36)-C(35)	-176.7(4)

C(31)-C(32)-O(1)-C(37)	178.9(6)
C(33)-C(32)-O(1)-C(37)	-3.0(8)
C(36A)-C(31A)-C(32A)-C(33A)	0.0
Ni(1)-C(31A)-C(32A)-C(33A)	177.3(11)
C(31A)-C(32A)-C(33A)-C(34A)	0.0
C(32A)-C(33A)-C(34A)-C(35A)	0.0
C(33A)-C(34A)-C(35A)-C(36A)	0.0
C(34A)-C(35A)-C(36A)-O(1A)	175.7(14)
C(34A)-C(35A)-C(36A)-C(31A)	0.0
C(32A)-C(31A)-C(36A)-O(1A)	-176.0(13)
Ni(1)-C(31A)-C(36A)-O(1A)	6.6(12)
C(32A)-C(31A)-C(36A)-C(35A)	0.0
Ni(1)-C(31A)-C(36A)-C(35A)	-177.4(11)
C(35A)-C(36A)-O(1A)-C(37A)	8.7(18)
C(31A)-C(36A)-O(1A)-C(37A)	-175.5(11)
C(4S)-O(1S)-C(1S)-C(2S)	30.9(13)
O(1S)-C(1S)-C(2S)-C(3S)	-3.3(14)
C(1S)-C(2S)-C(3S)-C(4S)	-27.8(12)
C(2S)-C(3S)-C(4S)-O(1S)	50.6(12)
C(1S)-O(1S)-C(4S)-C(3S)	-46.7(12)

Symmetry transformations used to generate equivalent atoms: