Supporting Information for

Ligand effects on the properties of Ni(III) complexes:

aerobically-induced aromatic cyanation at room temperature

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I. Reactivity of (^{R}N3C)Ni complexes

Reaction of [(^{Np}N3C)Ni^{II}(MeCN)$_2$]PF$_6$ (11) with 1 equiv of *t*BuNC in air

To a solution of [(^{Np}N3C)Ni^{II}(MeCN)$_2$]PF$_6$ (**11**) (12.5 mg, 0.019 mmol, 1 equiv) in 1 mL of CD_3CN, *t*BuNC (1.6 mg, 0.019 mmol, 1 equiv) was added. The reaction mixture was stirred for 5 min at RT and then brought out from the glovebox and exposed to air. The red solution turned almost colorless within 5 min. The reaction was monitored by ^{1}H NMR and ESI-MS and the quantitative generation of $^{t\text{Bu}}$N3CCN is observed. The solvent was removed under vacuum, and the solid was washed with Et_2O (3 x 1 mL) and dried under vacuum (isolated yield: 7.6 mg, 99%).

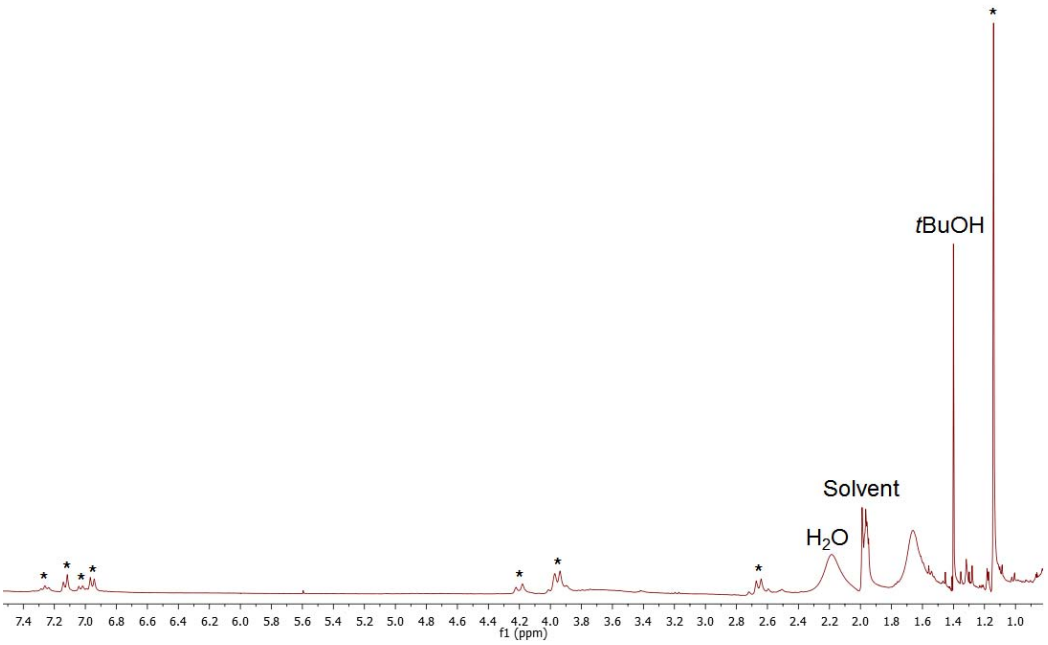

Figure S1. ^{1}H NMR monitoring of the oxidatively induced aromatic cyanation reaction of **11** using air as an oxidant at room temperature and proposed mechanism. The "*" labelled peaks are corresponding to ^{Np}N3CCN.

Reaction of (^{Np}N3C)Ni^{II}Br (10) with 1 equiv of *t*BuNC in air

To a solution of (^{Np}N3C)Ni^{II}Br (**10**) (10.2 mg, 0.020 mmol, 1 equiv) in 1 mL of CD_3CN, *t*BuNC (1.7 mg, 0.020 mmol, 1 equiv) was added. The reaction mixture was stirred for 5 min at RT and then brought out from the glovebox and exposed to air. The red solution turned almost colorless within 5 min. The reaction was monitored by ^{1}H NMR and ESI-MS and generation of $^{t\text{Bu}}$N3CCN is observed. The solvent was removed under vacuum, and the solid was washed with Et_2O (3 x 1 mL) and dried under vacuum (isolated yield: 7.9 mg, 99%).

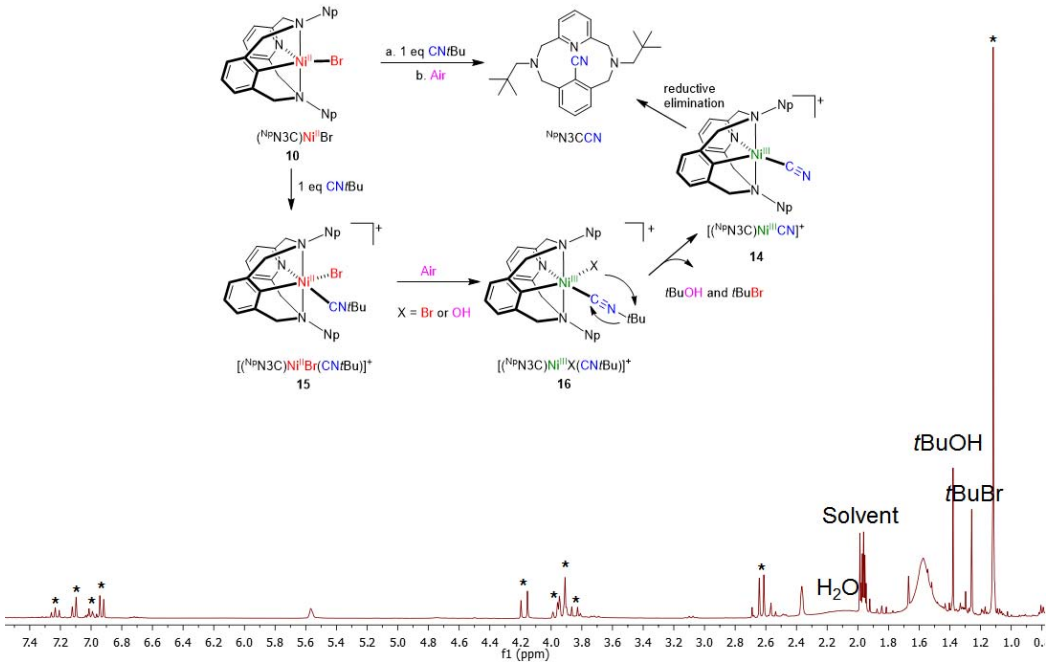

Figure S2. ^{1}H NMR monitoring of the aerobically induced aromatic cyanation reaction of **10** using air as an oxidant at room temperature and proposed mechanism. The "*" labelled peaks are corresponding to ^{Np}N3CCN.

Aerobic aromatic cyanation in one pot

To a solution of ^{Np}N3CBr (15.0 mg, 0.033 mmol, 1 equiv) in 1.5 mL of THF, Ni(COD)$_2$ (9.2 mg, 0.034 mmol, 1 equiv) was added at –35 ^{o}C. The reaction was warmed up and stirred at RT for 3 hours. Then, 1 equiv of *t*BuNC (2.8 mg, 0.033 mmol, 1 equiv) was added, the reaction mixture was stirred for 5 min and then brought out from the glvovebox and stirred in air for 5 min. The solvent was removed under vacuum and the solid was extracted with Et_2O (3 x 1 mL). The solvent was evaporated and the solid was dissolved in $CDCl_3$, followed by addition of 1,3,5-trimethoxybenzene was added as the standard. Analysis of the reaction mixture by ^{1}H NMR reveals the formation of ^{Np}N3CBCN in 50% yield.

Reaction of (^{pOMe}N3C)Ni^{II}Br with 1 equiv of *t*BuNC in air

To a solution of (^{pOMe}N3C)Ni^{II}Br (9.4 mg, 0.018 mmol, 1 equiv) in 1 mL of CD_3CN, CN*t*Bu (1.6 mg, 0.020 mmol, 1 equiv) was added. The reaction mixture was stirred for 5 min at RT and then brought out from the glovebox and exposed to air. The red solution turned almost colorless within 5 min. The reaction was monitored by ^{1}H NMR and ESI-MS and the generation of ^{pOMe}N3CCN was observed (yield: ~65% based on NMR integration).

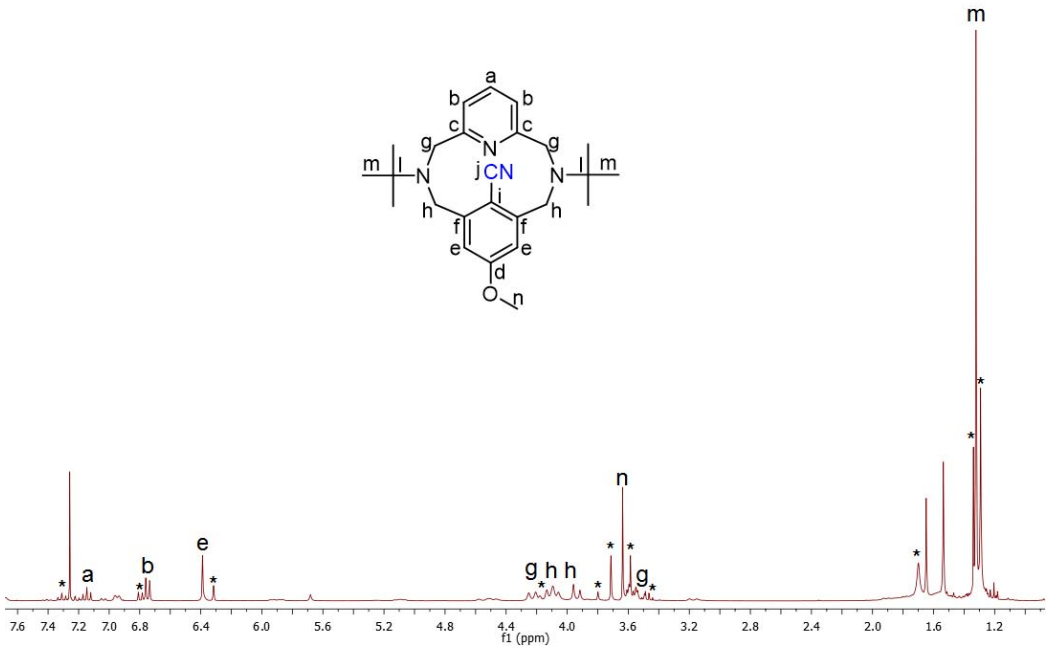

Figure S3. ^{1}H NMR monitoring of the oxidatively induced aromatic cyanation reaction of $^{p\mathrm{OMe}}$N3CNi system using air as an oxidant at room temperature. The "*" labelled peaks are corresponding to unknown ligand side products.

Identification of ^{Np}N3CCN

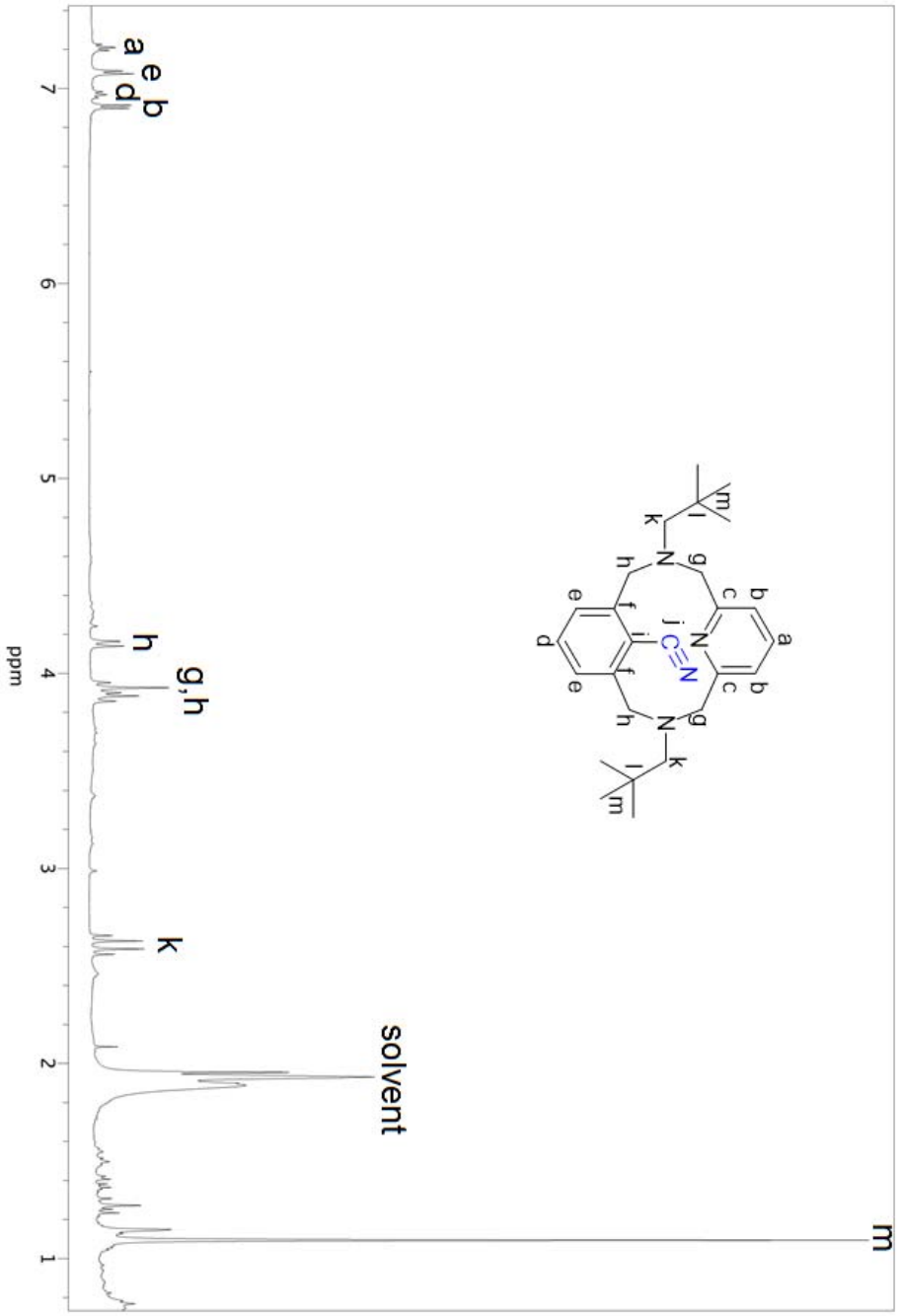

Figure S4. ^{1}H NMR of ^{Np}N3CCN in CD_3CN.

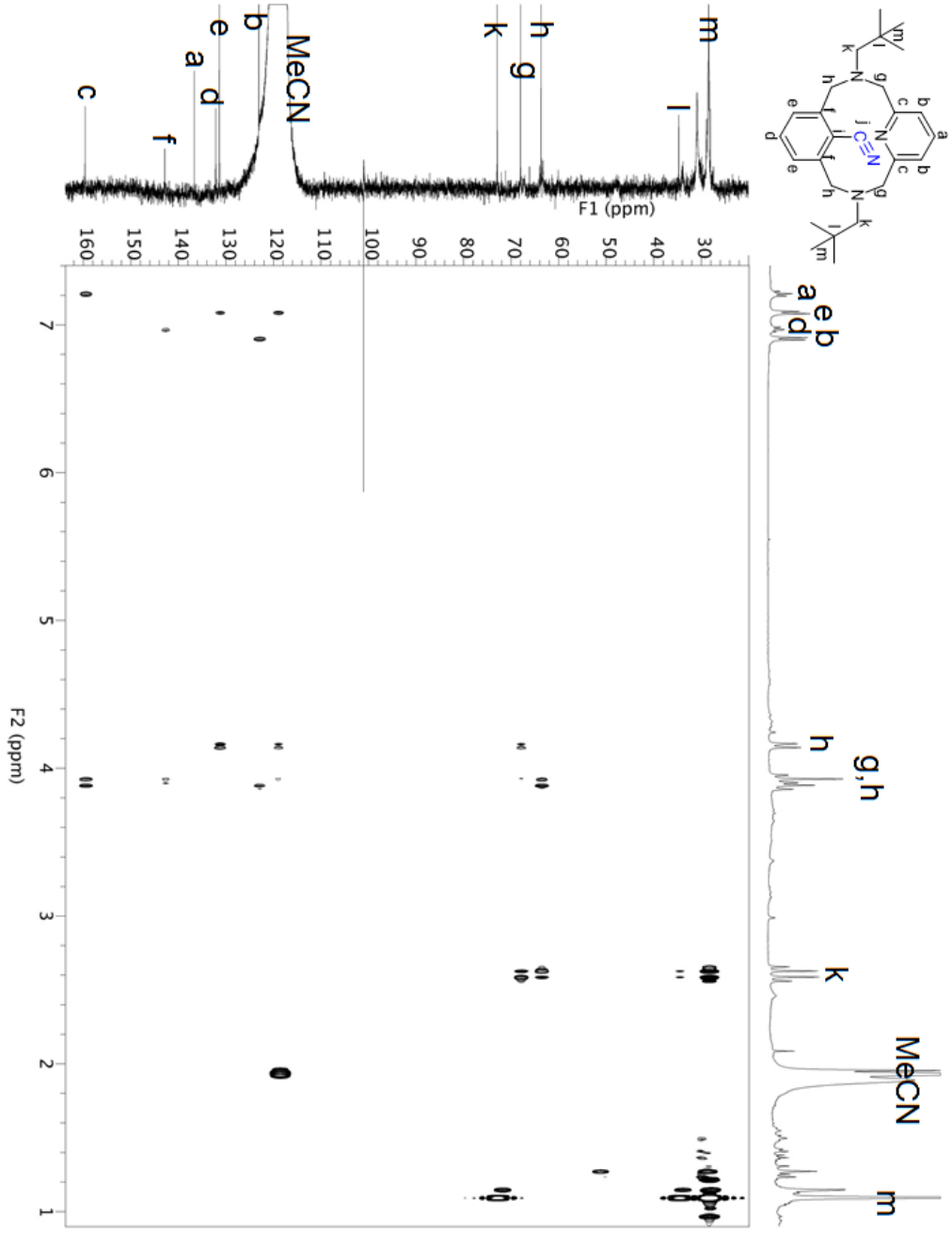

Figure S5. HMBC spectrum of ^{Np}N3CCN in CD_3CN.

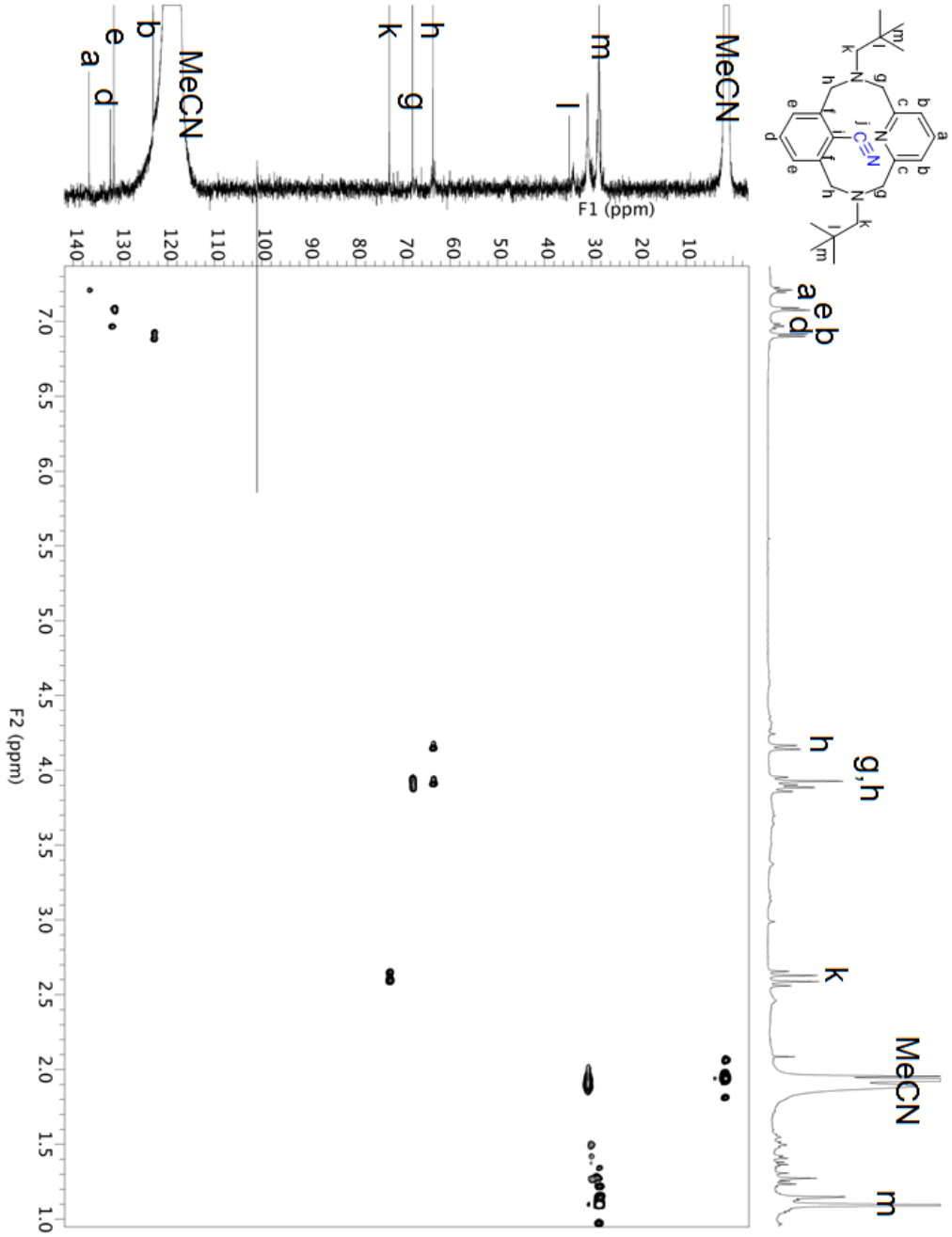

Figure S6. HSQC spectrum of ^{Np}N3CCN in CD_3CN.

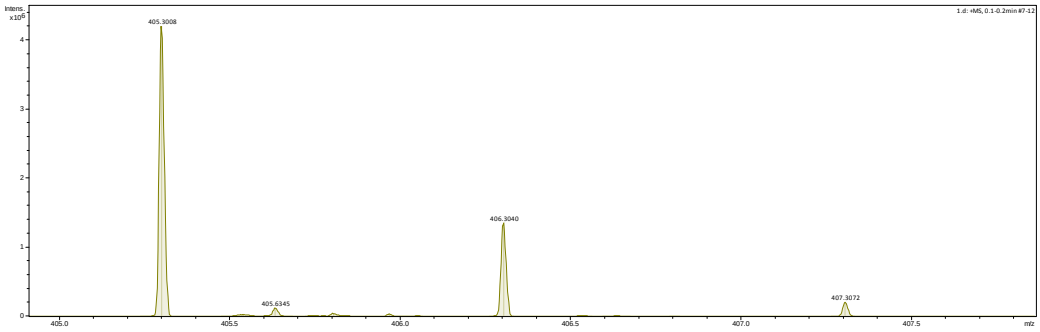

Figure S7. ESI-MS analysis of ^{Np}N3CCN, *m/z* 405.3008 (calcd for $[^{Np}N3CCN{\cdot}H]^+$, $C_{26}H_{37}N_4$: 405.3013).

Identification of ^{pOMe}N3CCN

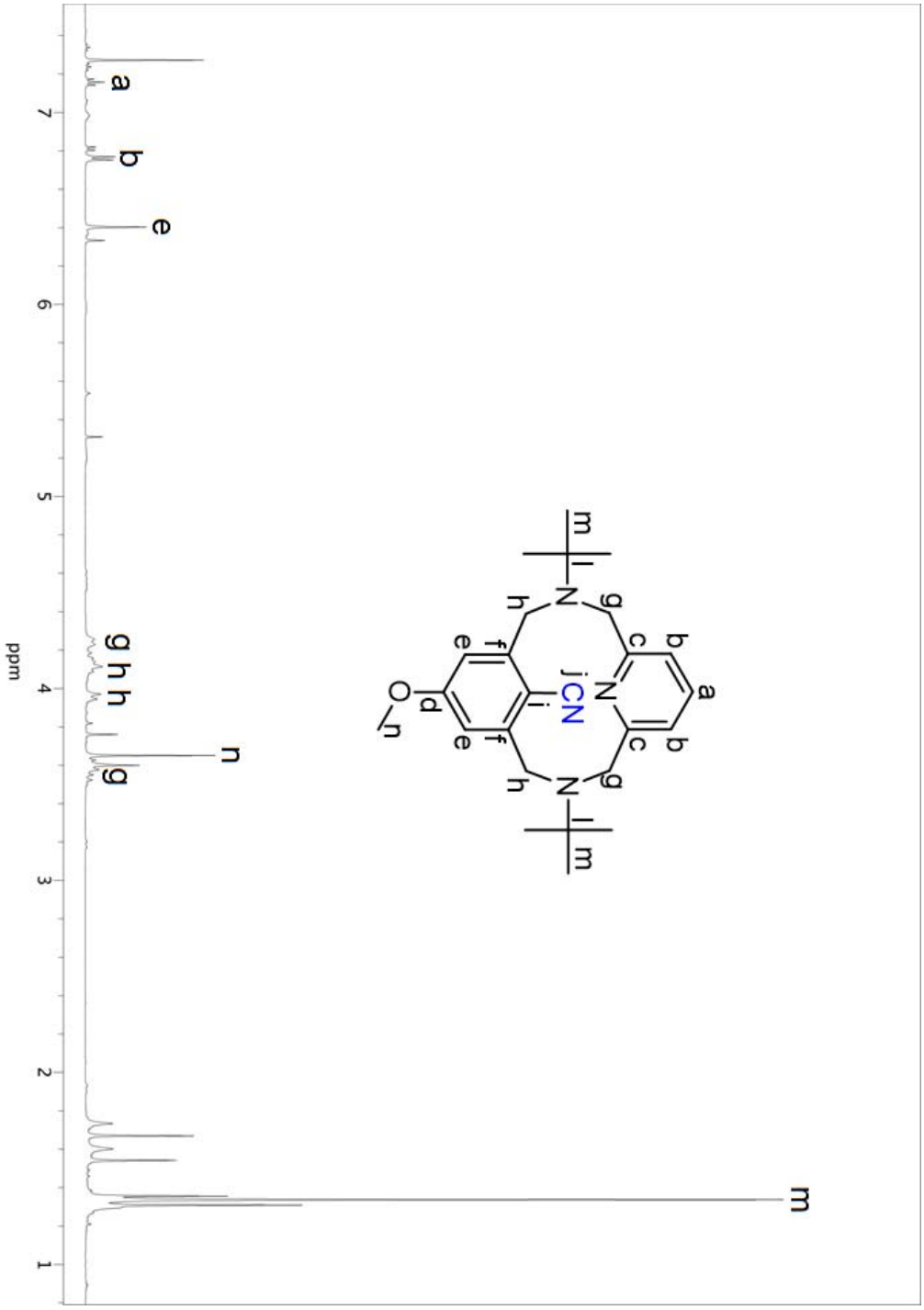

Figure S8. ^{1}H NMR of ^{pOMe}N3CCN in $CDCl_3$.

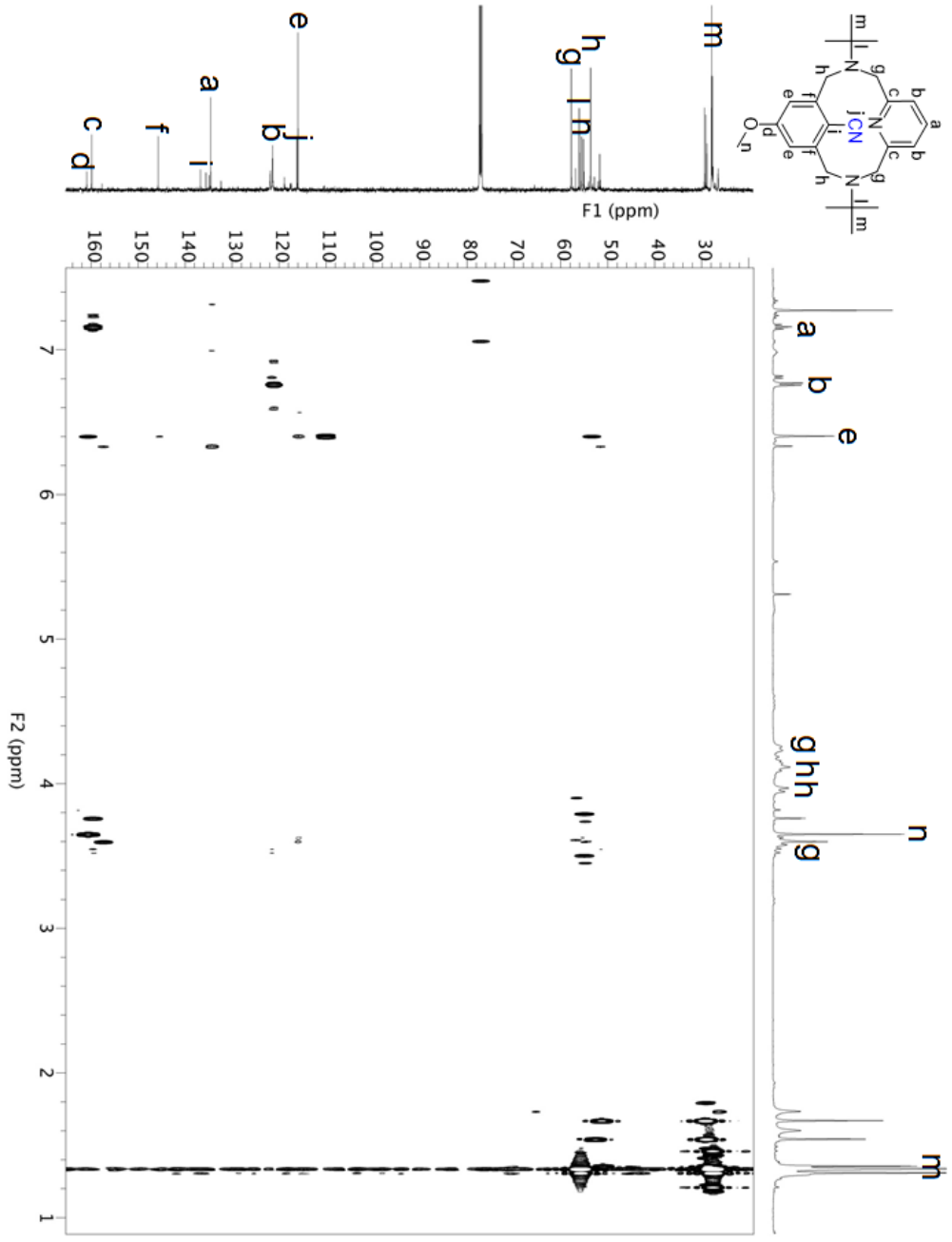

Figure S9. HMBC spectrum of $^{p\mathrm{OMe}}$N3CCN in $CDCl_3$.

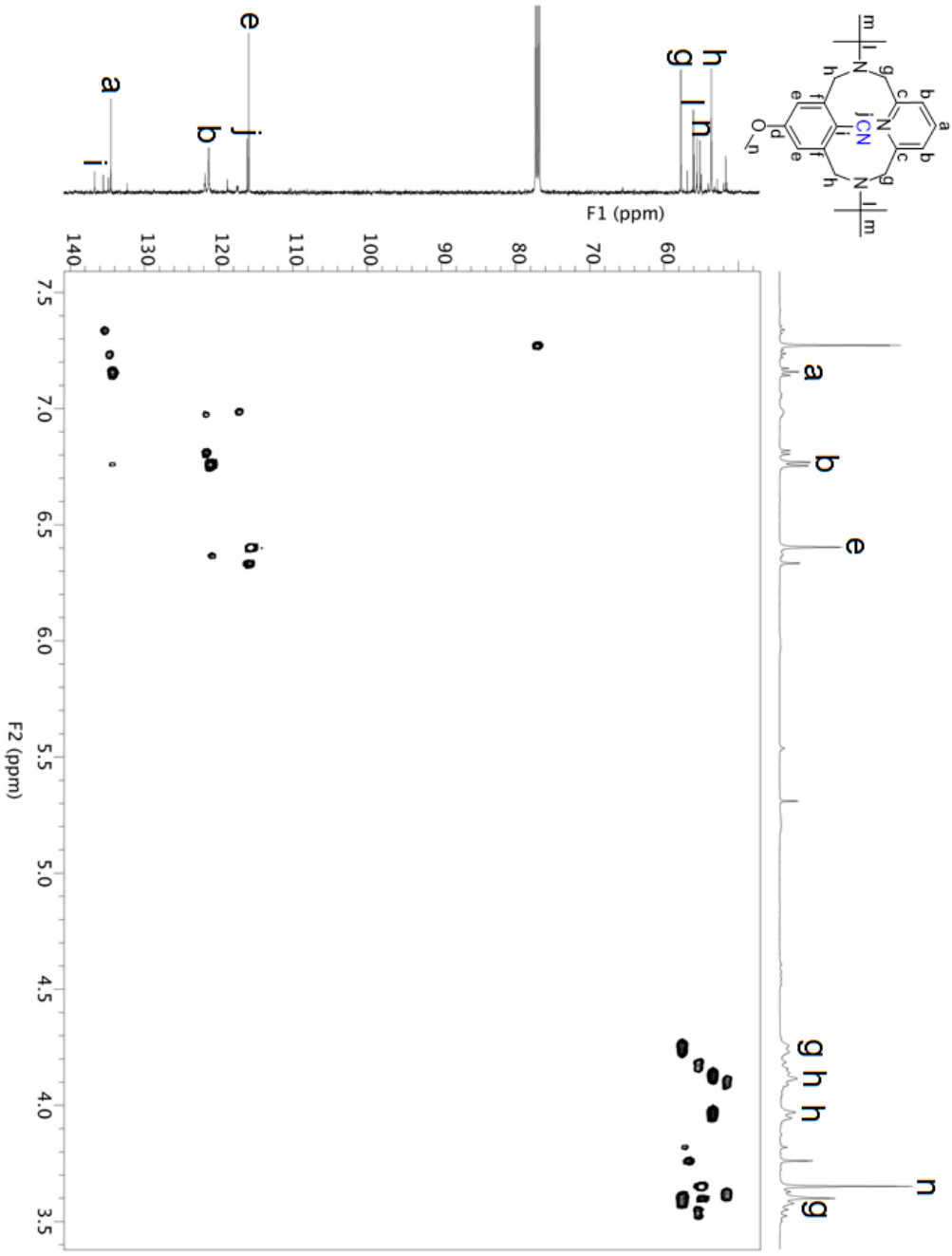

Figure S10. HSQC spectrum of $^{p\text{OMe}}$N3CCN in $CDCl_3$.

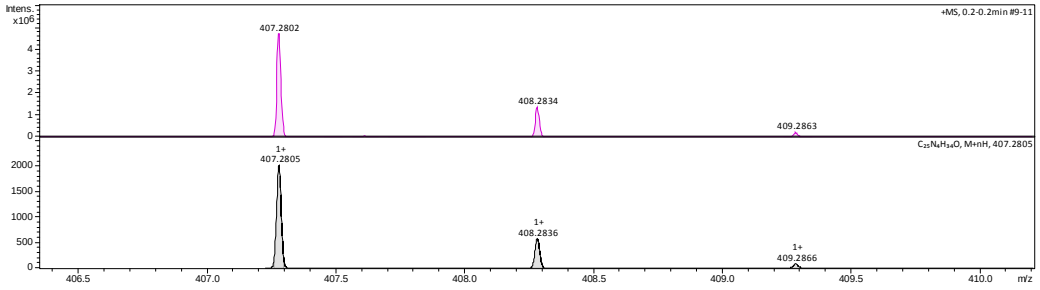

Figure S11. ESI-MS analysis of $^{p\text{OMe}}$N3CCN, *m/z* 407.2802 (calcd for $[^{p\text{OMe}}\text{N3CCN}\cdot\text{H}]^+$, $C_{25}H_{35}N_4O$: 407.2805).

II. Cyclic voltammograms of (^{R}N3C)Ni complexes

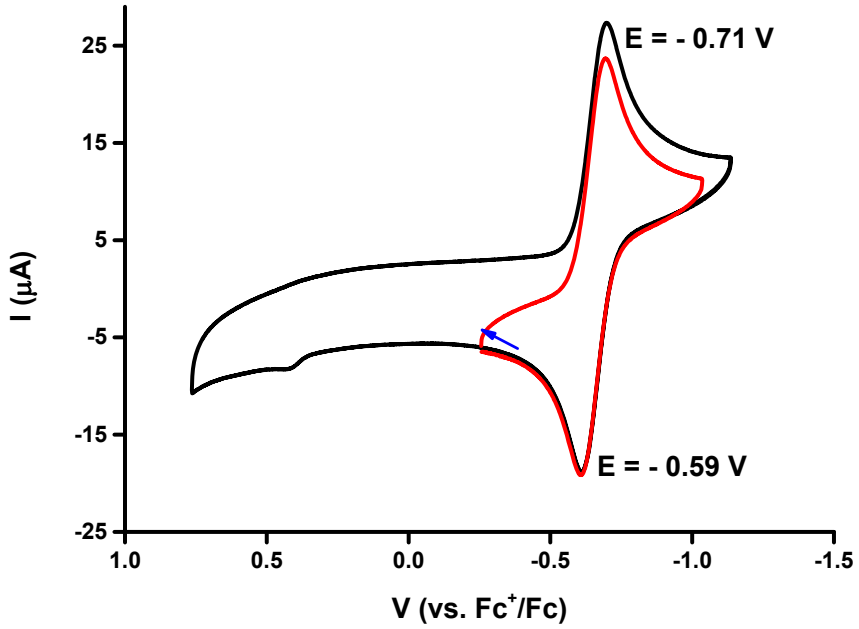

Figure S12. Cyclic voltammograms of **1** in 0.1 M *n*-Bu_4NBF_4/MeCN.

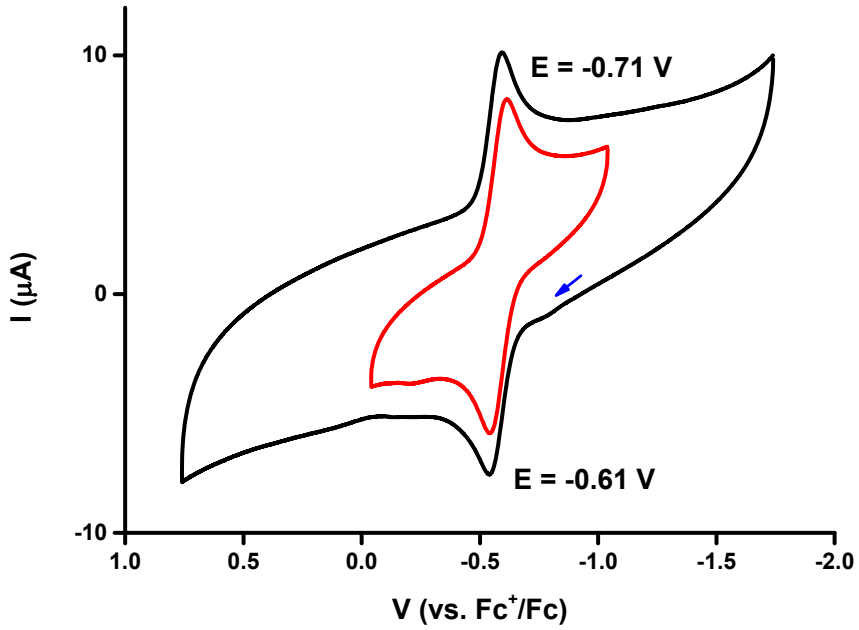

Figure S13. Cyclic voltammograms of **2** in 0.1 M *n*-Bu_4NBF_4/MeCN.

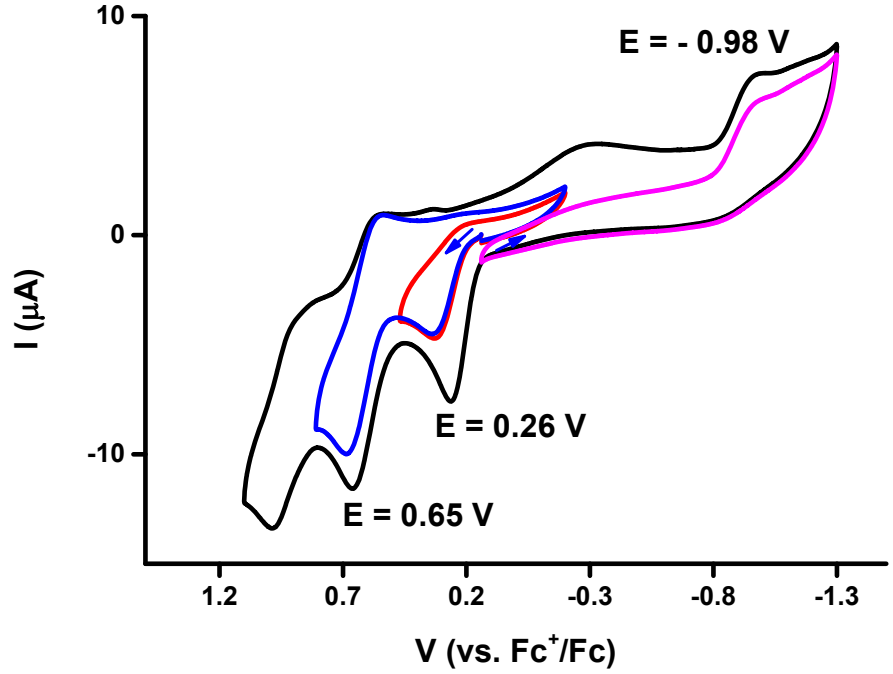

Figure S14. Cyclic voltammograms of **3** in 0.1 M *n*-Bu_4NBF_4/MeCN.

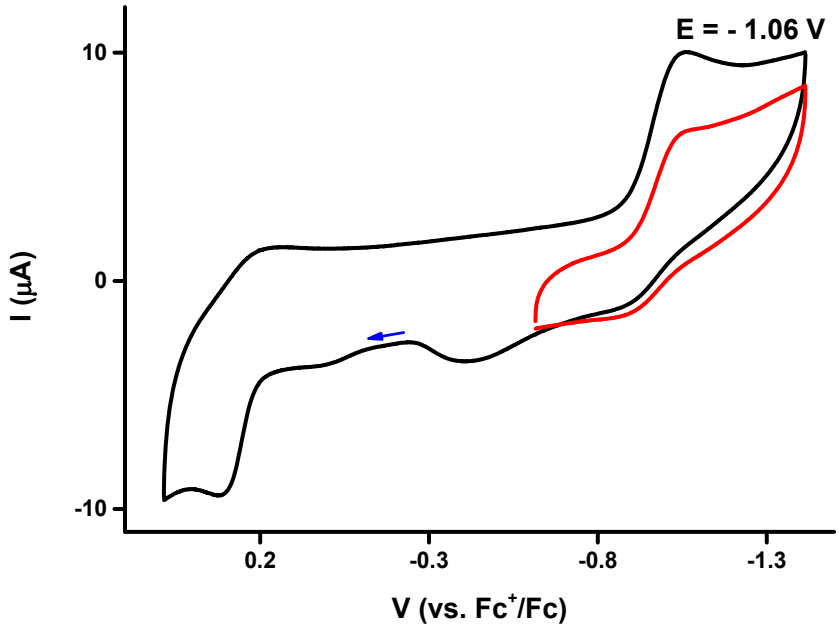

Figure S15. Cyclic voltammograms of **4** in 0.1 M *n*-Bu_4NBF_4/MeCN.

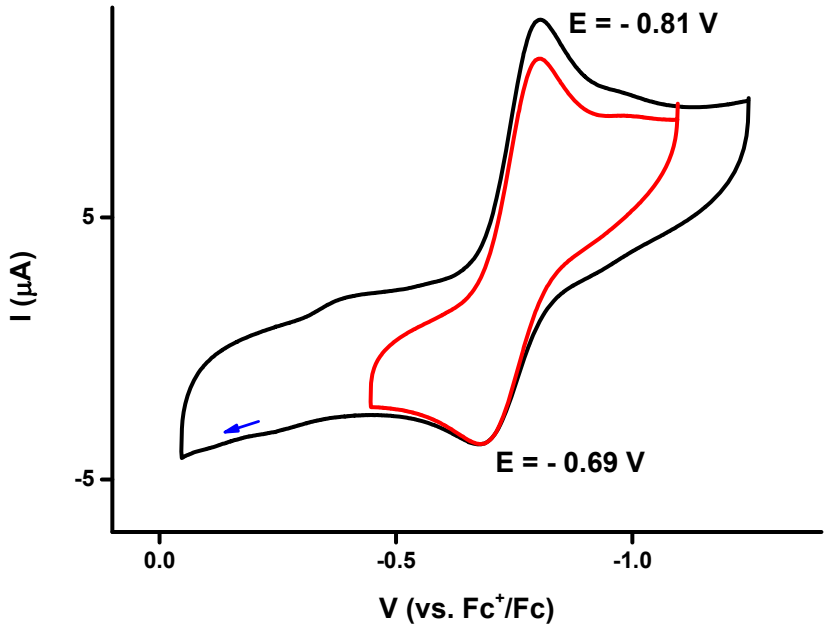

Figure S16. Cyclic voltammograms of **5** in 0.1 M *n*-Bu_4NBF_4/MeCN.

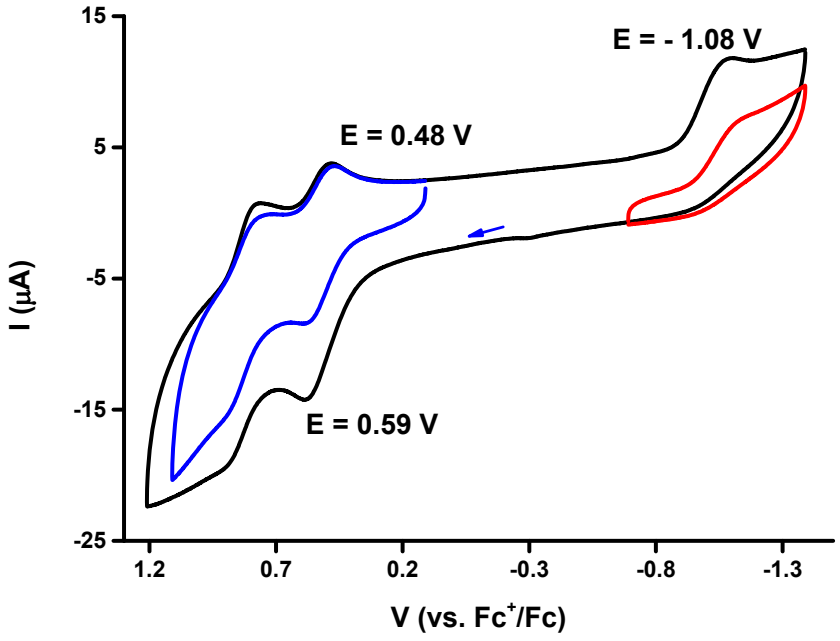

Figure S17. Cyclic voltammograms of **6** in 0.1 M *n*-Bu_4NBF_4/MeCN.

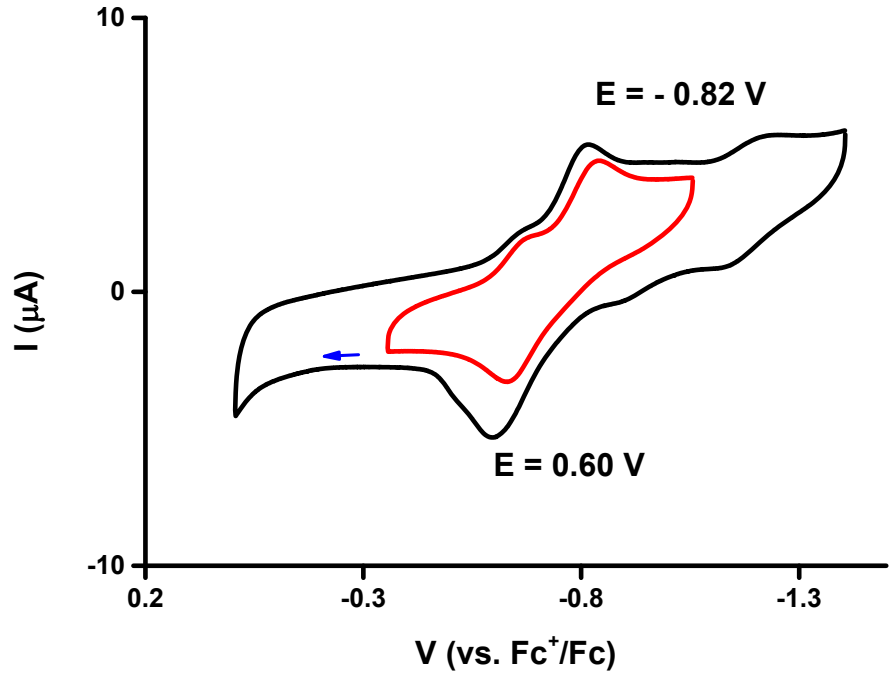

Figure S18. Cyclic voltammograms of **7** in 0.1 M *n*-Bu_4NBF_4/MeCN.

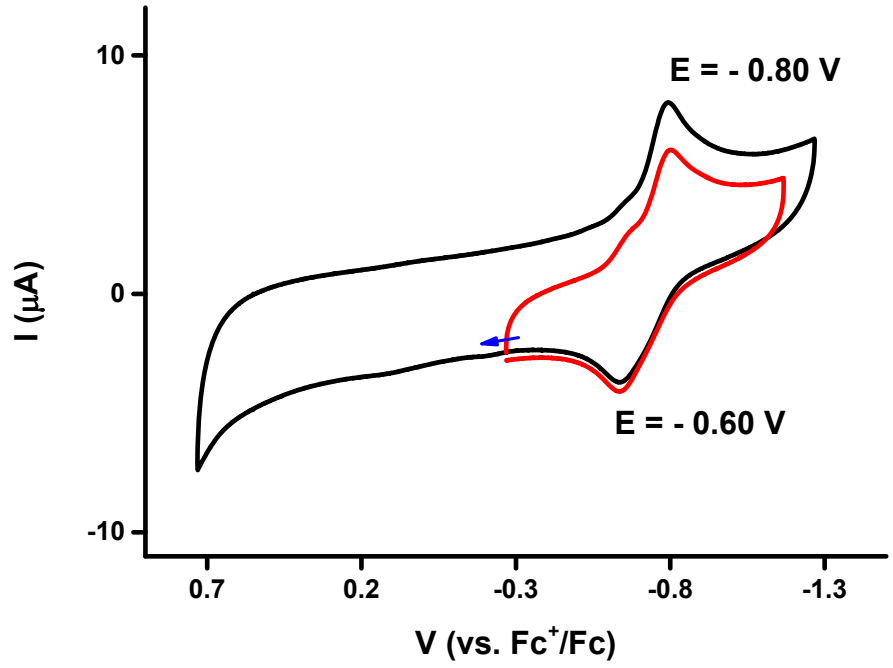

Figure S19. Cyclic voltammograms of **8** in 0.1 M *n*-Bu_4NBF_4/MeCN.

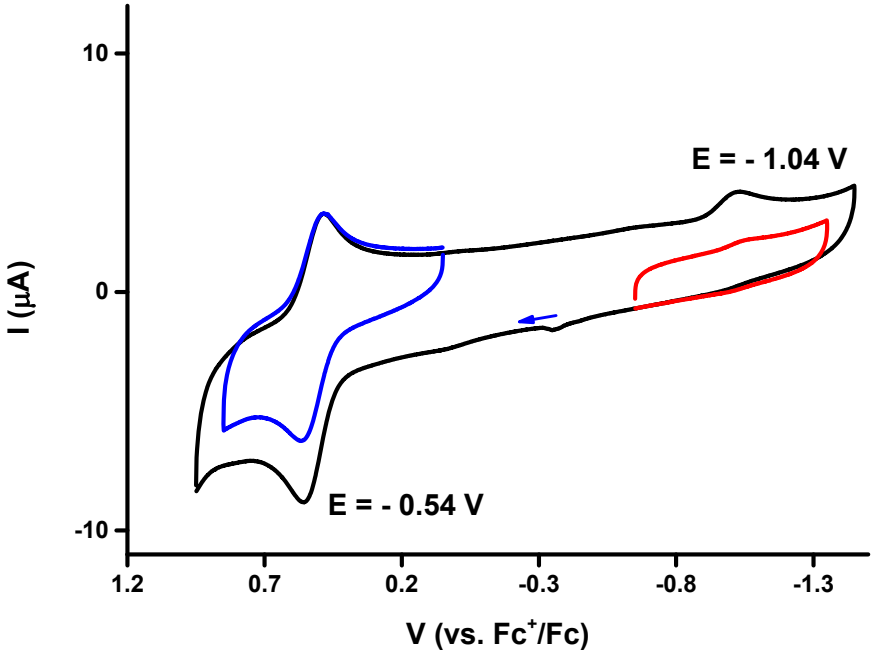

Figure S20. Cyclic voltammograms of **9** in 0.1 M *n*-Bu_4NBF_4/MeCN.

III. UV-vis spectra of (^{R}N3C)Ni complexes

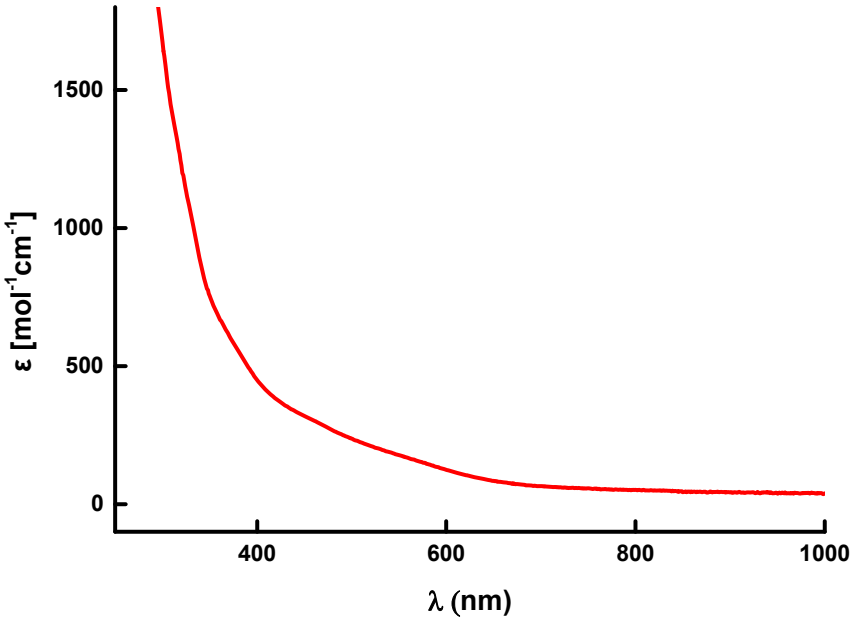

Figure S21. UV-vis spectrum of **3** in MeCN at RT.

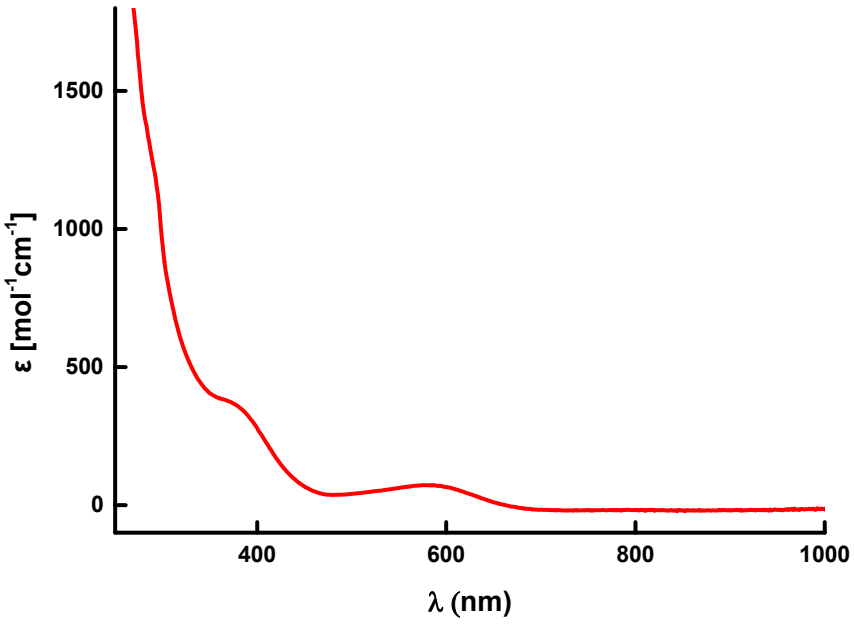

Figure S22. UV-vis spectrum of **7** in MeCN at RT.

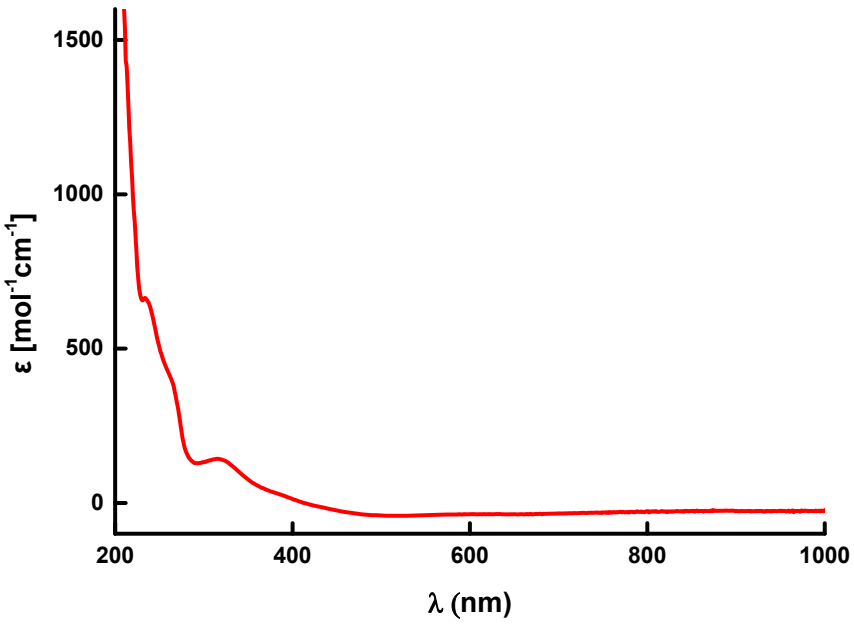

Figure S23. UV-vis spectrum of **8** in MeCN at RT.

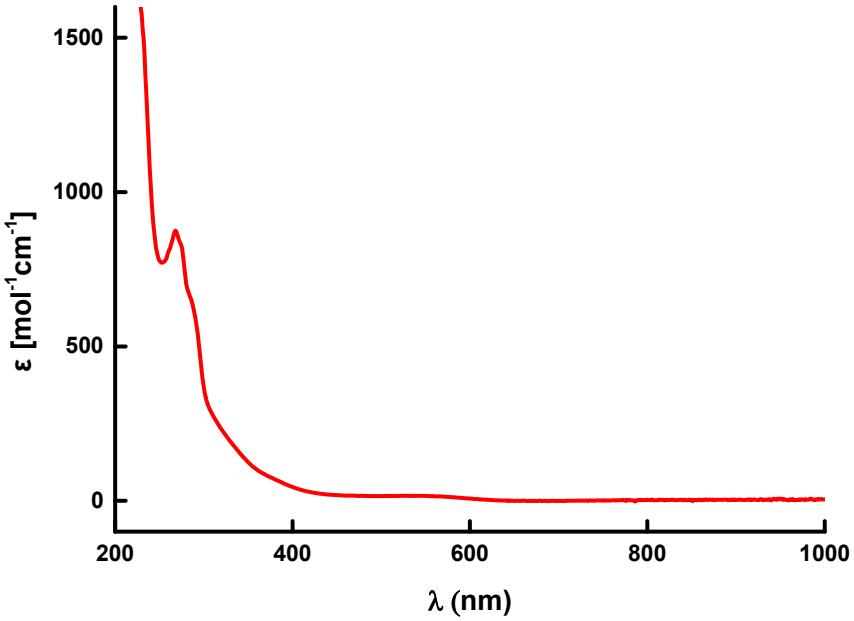

Figure S24. UV-vis spectrum of **9** in MeCN at RT.

IV. Solid state structure determinations

General information

Suitable crystals were mounted on MiTeGen cryoloops in random orientations in a Bruker Kappa Apex-II CCD X-ray diffractometer equipped with an Oxford Cryostream LT device and a fine focus Mo Kα radiation X-ray source (λ = 0.71073 Å). Preliminary unit cell constants were determined with a set of 36 narrow frame scans. Typical data sets consist of combinations of $\bar{w}$ and ϕ scan frames with a typical scan width of 0.5° and a counting time of 15−30 s/frame at a crystal-to-detector distance of 3.5 cm. The collected frames were integrated using an orientation matrix determined from the narrow frame scans. Apex II and SAINT software packages (Bruker Analytical X-Ray, Madison, WI, 2008) were used for data collection and data integration. Analysis of the integrated data did not show any decay. Final cell constants were determined by global refinement of xyz centroids of reflections from the complete data sets. Collected data were corrected for systematic errors using SADABS Bruker Analytical X-Ray, Madison, WI, 2008) based on the Laue symmetry using equivalent reflections. Crystal data and intensity data collection parameters are listed in corresponding tables of each complex. Structure solutions and refinement were carried out using the SHELXTL-PLUS software package. The structures were solved by direct methods and refined successfully. Full matrix least-squares refinements were carried out by minimizing $\Sigma w(Fo^2-Fc^2)^2$. The non-hydrogen atoms were refined anisotropically to convergence. The hydrogen atoms were treated using appropriate riding model.

X-ray structure determination of (^{tBu}N3C)Ni^{III}F$_2$ (3)

Table 1. Crystal data and structure refinement for lm3214. (CCDC 1458980)

Identification code	l3214/lt/zw-121	
Empirical formula	C_{23} H_{36} F_2 N_3 Ni O_2	
Formula weight	483.26	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/n	
Unit cell dimensions	a = 11.2020(7) Å	α= 90°.
	b = 14.3642(9) Å	β= 92.280(3)°.
	c = 13.7494(10) Å	γ = 90°.
Volume	2210.6(3) Å^3	
Z	4	
Density (calculated)	1.452 Mg/m^3	
Absorption coefficient	0.920 mm^{-1}	
F(000)	1028	
Crystal size	0.356 x 0.272 x 0.095 mm^3	
Theta range for data collection	2.051 to 27.840°.	
Index ranges	-14≤h≤13, -18≤k≤13, -18≤l≤18	
Reflections collected	35932	
Independent reflections	5236 [R(int) = 0.0465]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6587	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5236 / 18 / 298	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0357, wR2 = 0.0874	
R indices (all data)	R1 = 0.0477, wR2 = 0.0940	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.761 and -0.580 e.Å^{-3}	

Projection view of **3** with 50% probability ellipsoids- solvent water molecules omitted for clarity:

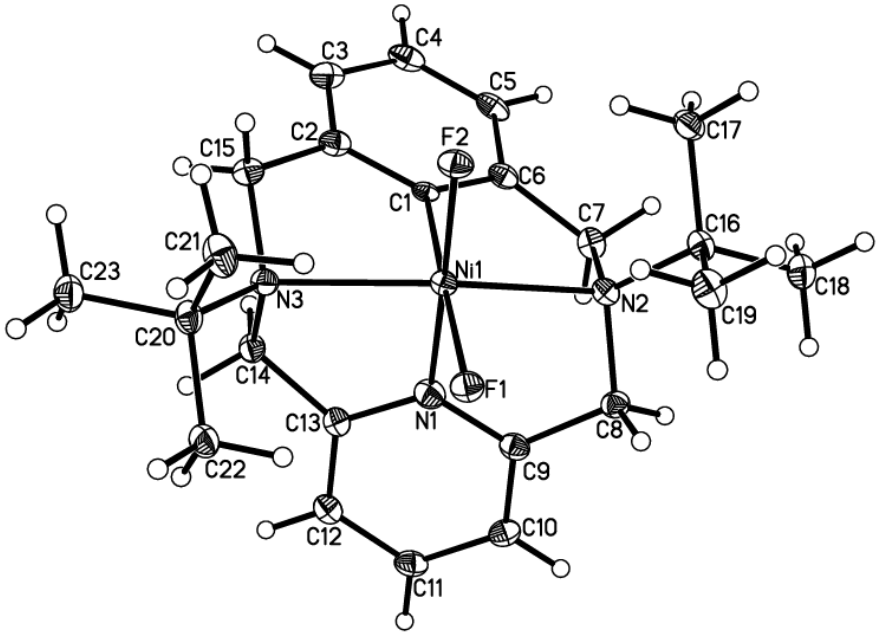

Table 2. Bond lengths [Å] and angles [°] for lm3214.

Ni(1)-C(1)	1.8882(18)
Ni(1)-N(1)	1.8997(18)
Ni(1)-F(2)	1.9123(12)
Ni(1)-F(1)	1.9256(12)
Ni(1)-N(2)	2.2564(17)
Ni(1)-N(3)	2.2827(17)
N(1)-C(13)	1.354(3)
N(1)-C(9)	1.359(3)
N(2)-C(8)	1.492(3)
N(2)-C(7)	1.503(2)
N(2)-C(16)	1.529(2)
N(3)-C(15)	1.487(3)
N(3)-C(14)	1.500(2)
N(3)-C(20)	1.523(3)
C(1)-C(6)	1.364(3)
C(1)-C(2)	1.371(3)
C(2)-C(3)	1.390(3)
C(2)-C(15)	1.506(3)
C(3)-C(4)	1.391(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.393(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.389(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.507(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.504(3)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.390(3)
C(10)-C(11)	1.393(3)
C(10)-H(10)	0.9500
C(11)-C(12)	1.389(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.389(3)

C(12)-H(12)	0.9500
C(13)-C(14)	1.502(3)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.526(3)
C(16)-C(19)	1.527(3)
C(16)-C(18)	1.536(3)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(22)	1.524(3)
C(20)-C(21)	1.526(3)
C(20)-C(23)	1.540(3)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
O(1S)-H(1S1)	0.869(2)
O(1S)-H(1S2)	0.868(2)
O(2S)-H(2S1)	0.869(2)
O(2S)-H(2S2)	0.869(2)

C(1)-Ni(1)-N(1)	89.77(8)
C(1)-Ni(1)-F(2)	91.26(7)
N(1)-Ni(1)-F(2)	178.21(6)

C(1)-Ni(1)-F(1)	178.73(7)
N(1)-Ni(1)-F(1)	89.64(6)
F(2)-Ni(1)-F(1)	89.36(5)
C(1)-Ni(1)-N(2)	82.92(7)
N(1)-Ni(1)-N(2)	79.84(7)
F(2)-Ni(1)-N(2)	101.74(6)
F(1)-Ni(1)-N(2)	95.88(6)
C(1)-Ni(1)-N(3)	79.13(7)
N(1)-Ni(1)-N(3)	81.90(7)
F(2)-Ni(1)-N(3)	96.86(6)
F(1)-Ni(1)-N(3)	101.89(6)
N(2)-Ni(1)-N(3)	154.35(6)
C(13)-N(1)-C(9)	123.21(18)
C(13)-N(1)-Ni(1)	119.41(14)
C(9)-N(1)-Ni(1)	116.70(14)
C(8)-N(2)-C(7)	108.45(15)
C(8)-N(2)-C(16)	112.19(15)
C(7)-N(2)-C(16)	111.51(15)
C(8)-N(2)-Ni(1)	100.57(11)
C(7)-N(2)-Ni(1)	103.96(11)
C(16)-N(2)-Ni(1)	119.15(12)
C(15)-N(3)-C(14)	108.88(15)
C(15)-N(3)-C(20)	112.52(16)
C(14)-N(3)-C(20)	111.45(15)
C(15)-N(3)-Ni(1)	100.67(12)
C(14)-N(3)-Ni(1)	103.16(11)
C(20)-N(3)-Ni(1)	119.13(12)
C(6)-C(1)-C(2)	123.32(18)
C(6)-C(1)-Ni(1)	118.79(15)
C(2)-C(1)-Ni(1)	117.74(15)
C(1)-C(2)-C(3)	118.43(19)
C(1)-C(2)-C(15)	116.55(18)
C(3)-C(2)-C(15)	125.02(19)
C(2)-C(3)-C(4)	119.5(2)
C(2)-C(3)-H(3)	120.3
C(4)-C(3)-H(3)	120.3
C(3)-C(4)-C(5)	120.65(19)
C(3)-C(4)-H(4)	119.7

C(5)-C(4)-H(4)	119.7
C(6)-C(5)-C(4)	119.41(19)
C(6)-C(5)-H(5)	120.3
C(4)-C(5)-H(5)	120.3
C(1)-C(6)-C(5)	118.63(19)
C(1)-C(6)-C(7)	117.22(18)
C(5)-C(6)-C(7)	123.97(19)
N(2)-C(7)-C(6)	112.06(16)
N(2)-C(7)-H(7A)	109.2
C(6)-C(7)-H(7A)	109.2
N(2)-C(7)-H(7B)	109.2
C(6)-C(7)-H(7B)	109.2
H(7A)-C(7)-H(7B)	107.9
N(2)-C(8)-C(9)	110.00(16)
N(2)-C(8)-H(8A)	109.7
C(9)-C(8)-H(8A)	109.7
N(2)-C(8)-H(8B)	109.7
C(9)-C(8)-H(8B)	109.7
H(8A)-C(8)-H(8B)	108.2
N(1)-C(9)-C(10)	119.08(19)
N(1)-C(9)-C(8)	116.72(18)
C(10)-C(9)-C(8)	124.19(19)
C(9)-C(10)-C(11)	118.68(19)
C(9)-C(10)-H(10)	120.7
C(11)-C(10)-H(10)	120.7
C(12)-C(11)-C(10)	120.87(19)
C(12)-C(11)-H(11)	119.6
C(10)-C(11)-H(11)	119.6
C(13)-C(12)-C(11)	119.03(19)
C(13)-C(12)-H(12)	120.5
C(11)-C(12)-H(12)	120.5
N(1)-C(13)-C(12)	118.98(19)
N(1)-C(13)-C(14)	116.29(18)
C(12)-C(13)-C(14)	124.60(18)
N(3)-C(14)-C(13)	112.05(16)
N(3)-C(14)-H(14A)	109.2
C(13)-C(14)-H(14A)	109.2
N(3)-C(14)-H(14B)	109.2

C(13)-C(14)-H(14B)	109.2
H(14A)-C(14)-H(14B)	107.9
N(3)-C(15)-C(2)	108.68(17)
N(3)-C(15)-H(15A)	110.0
C(2)-C(15)-H(15A)	110.0
N(3)-C(15)-H(15B)	110.0
C(2)-C(15)-H(15B)	110.0
H(15A)-C(15)-H(15B)	108.3
C(17)-C(16)-C(19)	108.48(17)
C(17)-C(16)-N(2)	108.79(16)
C(19)-C(16)-N(2)	109.66(16)
C(17)-C(16)-C(18)	108.66(17)
C(19)-C(16)-C(18)	109.74(17)
N(2)-C(16)-C(18)	111.46(16)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
N(3)-C(20)-C(22)	108.49(16)
N(3)-C(20)-C(21)	108.56(16)
C(22)-C(20)-C(21)	108.24(18)
N(3)-C(20)-C(23)	111.86(17)
C(22)-C(20)-C(23)	109.73(17)
C(21)-C(20)-C(23)	109.88(17)

C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(20)-C(23)-H(23A)	109.5
C(20)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(20)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
H(1S1)-O(1S)-H(1S2)	103.7(18)
H(2S1)-O(2S)-H(2S2)	103.7(19)

X-ray structure determination of [(^{pOMe}N3C)Ni^{III}Br(MeCN)]PF_6 (7)

Table 3. Crystal data and structure refinement for lm2016. (CCDC 1458981)

Identification code	l2016/lt/smart/110K/POMeN3CNi(III)Br	
Empirical formula	C_{26} H_{37} Br F_6 N_4 N_i O P	
Formula weight	705.18	
Temperature	111(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P $\bar{1}$	
Unit cell dimensions	a = 10.747(3) Å	α= 106.335(13)°.
	b = 11.639(3) Å	β= 95.317(18)°.
	c = 12.569(4) Å	γ = 95.342(14)°.
Volume	1490.5(8) Å^3	
Z	2	
Density (calculated)	1.571 Mg/m^3	
Absorption coefficient	2.110 mm^{-1}	
F(000)	722	
Crystal size	0.259 x 0.149 x 0.115 mm^3	
Theta range for data collection	1.702 to 28.796°.	
Index ranges	-14≤h≤14, -15≤k≤15, -17≤l≤16	
Reflections collected	21266	
Independent reflections	7532 [R(int) = 0.0498]	
Completeness to theta = 25.242°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6261	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7532 / 0 / 369	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0422, wR2 = 0.1022	
R indices (all data)	R1 = 0.0644, wR2 = 0.1146	
Largest diff. peak and hole	0.921 and -0.485 e.Å^{-3}	

Projection view of **7** with 50% probability ellipsoids:

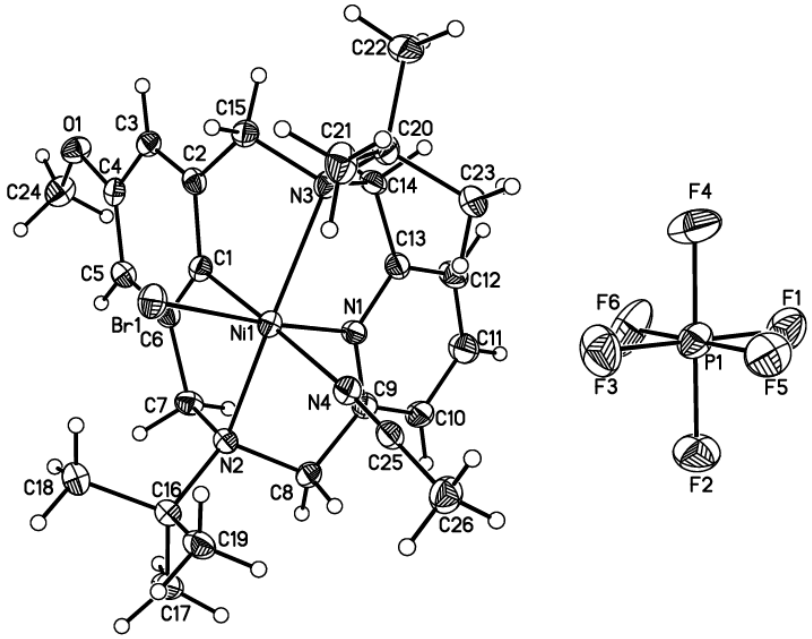

Table 4. Bond lengths [Å] and angles [°] for lm2016.

Br(1)-Ni(1)	2.3987(8)
Ni(1)-C(1)	1.895(3)
Ni(1)-N(1)	1.961(2)
Ni(1)-N(4)	2.006(2)
Ni(1)-N(2)	2.300(2)
Ni(1)-N(3)	2.333(2)
O(1)-C(4)	1.381(3)
O(1)-C(24)	1.433(3)
N(1)-C(9)	1.338(3)
N(1)-C(13)	1.351(3)
N(2)-C(8)	1.493(3)
N(2)-C(7)	1.520(3)
N(2)-C(16)	1.542(3)
N(3)-C(14)	1.495(4)
N(3)-C(15)	1.501(3)
N(3)-C(20)	1.534(3)
N(4)-C(25)	1.140(3)
C(1)-C(6)	1.372(4)
C(1)-C(2)	1.397(4)
C(2)-C(3)	1.391(4)
C(2)-C(15)	1.508(4)
C(3)-C(4)	1.395(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.388(4)
C(5)-C(6)	1.408(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.502(4)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.511(4)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.387(4)
C(10)-C(11)	1.398(4)
C(10)-H(10)	0.9500
C(11)-C(12)	1.384(4)

C(11)-H(11)	0.9500
C(12)-C(13)	1.385(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.502(4)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(19)	1.526(4)
C(16)-C(18)	1.535(4)
C(16)-C(17)	1.537(4)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.528(4)
C(20)-C(23)	1.530(4)
C(20)-C(22)	1.546(4)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(26)	1.459(4)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800

C(26)-H(26C)	0.9800
P(1)-F(6)	1.593(2)
P(1)-F(2)	1.601(2)
P(1)-F(5)	1.602(2)
P(1)-F(4)	1.606(2)
P(1)-F(3)	1.606(2)
P(1)-F(1)	1.610(2)

C(1)-Ni(1)-N(1)	87.85(11)
C(1)-Ni(1)-N(4)	178.18(10)
N(1)-Ni(1)-N(4)	91.89(10)
C(1)-Ni(1)-N(2)	82.61(10)
N(1)-Ni(1)-N(2)	78.47(9)
N(4)-Ni(1)-N(2)	95.58(9)
C(1)-Ni(1)-N(3)	78.79(10)
N(1)-Ni(1)-N(3)	79.69(9)
N(4)-Ni(1)-N(3)	102.93(9)
N(2)-Ni(1)-N(3)	151.70(8)
C(1)-Ni(1)-Br(1)	87.45(8)
N(1)-Ni(1)-Br(1)	174.82(7)
N(4)-Ni(1)-Br(1)	92.87(7)
N(2)-Ni(1)-Br(1)	103.06(6)
N(3)-Ni(1)-Br(1)	97.26(6)
C(4)-O(1)-C(24)	116.6(2)
C(9)-N(1)-C(13)	121.5(2)
C(9)-N(1)-Ni(1)	117.64(18)
C(13)-N(1)-Ni(1)	120.83(19)
C(8)-N(2)-C(7)	108.0(2)
C(8)-N(2)-C(16)	110.2(2)
C(7)-N(2)-C(16)	111.0(2)
C(8)-N(2)-Ni(1)	98.64(15)
C(7)-N(2)-Ni(1)	103.81(15)
C(16)-N(2)-Ni(1)	123.81(16)
C(14)-N(3)-C(15)	108.3(2)
C(14)-N(3)-C(20)	110.2(2)
C(15)-N(3)-C(20)	112.9(2)
C(14)-N(3)-Ni(1)	104.01(15)
C(15)-N(3)-Ni(1)	99.76(15)

C(20)-N(3)-Ni(1)	120.63(16)
C(25)-N(4)-Ni(1)	175.6(2)
C(6)-C(1)-C(2)	123.9(2)
C(6)-C(1)-Ni(1)	118.5(2)
C(2)-C(1)-Ni(1)	117.30(19)
C(3)-C(2)-C(1)	117.7(2)
C(3)-C(2)-C(15)	124.7(2)
C(1)-C(2)-C(15)	117.4(2)
C(2)-C(3)-C(4)	119.5(3)
C(2)-C(3)-H(3)	120.3
C(4)-C(3)-H(3)	120.3
O(1)-C(4)-C(5)	123.7(2)
O(1)-C(4)-C(3)	114.5(2)
C(5)-C(4)-C(3)	121.8(2)
C(4)-C(5)-C(6)	119.2(2)
C(4)-C(5)-H(5)	120.4
C(6)-C(5)-H(5)	120.4
C(1)-C(6)-C(5)	117.8(2)
C(1)-C(6)-C(7)	119.7(2)
C(5)-C(6)-C(7)	122.2(2)
C(6)-C(7)-N(2)	112.0(2)
C(6)-C(7)-H(7A)	109.2
N(2)-C(7)-H(7A)	109.2
C(6)-C(7)-H(7B)	109.2
N(2)-C(7)-H(7B)	109.2
H(7A)-C(7)-H(7B)	107.9
N(2)-C(8)-C(9)	110.1(2)
N(2)-C(8)-H(8A)	109.6
C(9)-C(8)-H(8A)	109.6
N(2)-C(8)-H(8B)	109.6
C(9)-C(8)-H(8B)	109.6
H(8A)-C(8)-H(8B)	108.1
N(1)-C(9)-C(10)	120.9(3)
N(1)-C(9)-C(8)	115.6(2)
C(10)-C(9)-C(8)	123.5(2)
C(9)-C(10)-C(11)	118.4(3)
C(9)-C(10)-H(10)	120.8
C(11)-C(10)-H(10)	120.8

C(12)-C(11)-C(10)	119.8(3)
C(12)-C(11)-H(11)	120.1
C(10)-C(11)-H(11)	120.1
C(11)-C(12)-C(13)	119.3(3)
C(11)-C(12)-H(12)	120.3
C(13)-C(12)-H(12)	120.3
N(1)-C(13)-C(12)	120.0(3)
N(1)-C(13)-C(14)	116.8(2)
C(12)-C(13)-C(14)	122.8(2)
N(3)-C(14)-C(13)	113.8(2)
N(3)-C(14)-H(14A)	108.8
C(13)-C(14)-H(14A)	108.8
N(3)-C(14)-H(14B)	108.8
C(13)-C(14)-H(14B)	108.8
H(14A)-C(14)-H(14B)	107.7
N(3)-C(15)-C(2)	107.0(2)
N(3)-C(15)-H(15A)	110.3
C(2)-C(15)-H(15A)	110.3
N(3)-C(15)-H(15B)	110.3
C(2)-C(15)-H(15B)	110.3
H(15A)-C(15)-H(15B)	108.6
C(19)-C(16)-C(18)	107.8(2)
C(19)-C(16)-C(17)	109.9(2)
C(18)-C(16)-C(17)	109.3(2)
C(19)-C(16)-N(2)	109.4(2)
C(18)-C(16)-N(2)	109.2(2)
C(17)-C(16)-N(2)	111.1(2)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5

H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(21)-C(20)-C(23)	108.1(2)
C(21)-C(20)-N(3)	110.3(2)
C(23)-C(20)-N(3)	108.5(2)
C(21)-C(20)-C(22)	109.1(2)
C(23)-C(20)-C(22)	109.3(2)
N(3)-C(20)-C(22)	111.3(2)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(20)-C(23)-H(23A)	109.5
C(20)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(20)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
O(1)-C(24)-H(24A)	109.5
O(1)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
O(1)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
N(4)-C(25)-C(26)	179.2(3)

C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
F(6)-P(1)-F(2)	89.98(12)
F(6)-P(1)-F(5)	179.06(12)
F(2)-P(1)-F(5)	89.49(10)
F(6)-P(1)-F(4)	90.62(12)
F(2)-P(1)-F(4)	179.36(12)
F(5)-P(1)-F(4)	89.91(11)
F(6)-P(1)-F(3)	90.76(12)
F(2)-P(1)-F(3)	90.68(11)
F(5)-P(1)-F(3)	90.02(11)
F(4)-P(1)-F(3)	89.56(11)
F(6)-P(1)-F(1)	89.73(12)
F(2)-P(1)-F(1)	89.84(11)
F(5)-P(1)-F(1)	89.49(11)
F(4)-P(1)-F(1)	89.91(11)
F(3)-P(1)-F(1)	179.28(12)

X-ray structure determination of [(^{pOMe}N3C)Ni^{III} (MeCN)$_2$](PF$_6$)$_2$ (8)

Table 5. Crystal data and structure refinement for lm11415. (CCDC 1458982)

Identification code	l11415/lt/x8//zw-POMetBuN3CNi(III)	
Empirical formula	C_{30} H_{43} F_{12} N_6 Ni O Sb_2	
Formula weight	1033.91	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.5192(5) Å	α= 90°.
	b = 11.0107(6) Å	β= 90.808(3)°.
	c = 35.5858(18) Å	γ = 90°.
Volume	3729.5(3) Å^3	
Z	4	
Density (calculated)	1.841 Mg/m^3	
Absorption coefficient	2.032 mm^{-1}	
F(000)	2044	
Crystal size	0.273 x 0.175 x 0.105 mm^3	
Theta range for data collection	1.145 to 27.671°.	
Index ranges	-12≤h≤12, -14≤k≤14, -46≤l≤45	
Reflections collected	46378	
Independent reflections	8625 [R(int) = 0.0432]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6637	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8625 / 0 / 489	
Goodness-of-fit on F^2	1.023	
Final R indices [I>2sigma(I)]	R1 = 0.0302, wR2 = 0.0582	
R indices (all data)	R1 = 0.0461, wR2 = 0.0625	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.721 and -0.933 e.Å^{-3}	

Projection view of **8** with 50% probability ellipsoids:

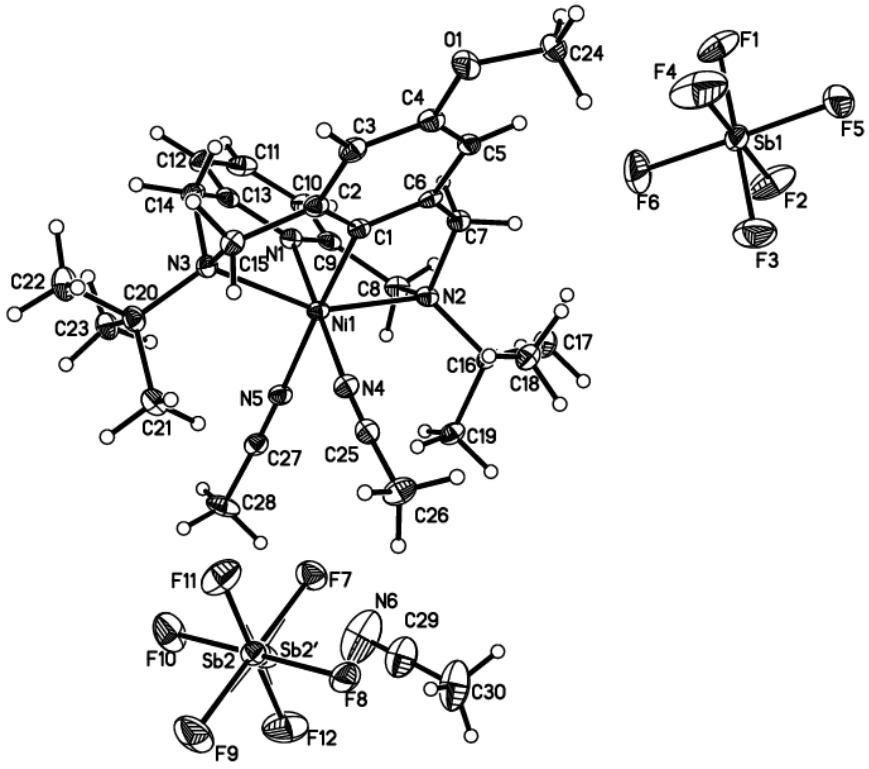

Table 6. Bond lengths [Å] and angles [°] for lm11415.

Sb(1)-F(5)	1.8506(19)
Sb(1)-F(6)	1.856(2)
Sb(1)-F(4)	1.859(2)
Sb(1)-F(2)	1.8607(19)
Sb(1)-F(3)	1.8667(19)
Sb(1)-F(1)	1.8690(18)
Sb(2)-F(11)	1.844(2)
Sb(2)-F(10)	1.859(2)
Sb(2)-F(9)	1.862(3)
Sb(2)-F(12)	1.871(3)
Sb(2)-F(8)	1.878(2)
Sb(2)-F(7)	1.883(2)
Sb(2')-F(12)	1.771(10)
Sb(2')-F(7)	1.808(8)
Sb(2')-F(8)	1.844(7)
Sb(2')-F(10)	1.896(7)
Sb(2')-F(9)	1.943(9)
Sb(2')-F(11)	1.949(11)
Ni(1)-C(1)	1.889(3)
Ni(1)-N(1)	1.912(2)
Ni(1)-N(4)	1.961(2)
Ni(1)-N(5)	2.007(2)
Ni(1)-N(2)	2.237(2)
Ni(1)-N(3)	2.243(2)
O(1)-C(4)	1.362(3)
O(1)-C(24)	1.420(3)
N(1)-C(9)	1.339(4)
N(1)-C(13)	1.342(3)
N(2)-C(8)	1.491(3)
N(2)-C(7)	1.515(3)
N(2)-C(16)	1.537(3)
N(3)-C(14)	1.494(3)
N(3)-C(15)	1.499(3)
N(3)-C(20)	1.522(4)
N(4)-C(25)	1.133(3)
N(5)-C(27)	1.131(4)

C(1)-C(6)	1.372(4)
C(1)-C(2)	1.374(4)
C(2)-C(3)	1.385(4)
C(2)-C(15)	1.508(4)
C(3)-C(4)	1.393(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.392(4)
C(5)-C(6)	1.403(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.488(4)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.512(4)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.375(4)
C(10)-C(11)	1.383(4)
C(10)-H(10)	0.9500
C(11)-C(12)	1.389(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.381(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.492(4)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(19)	1.521(4)
C(16)-C(18)	1.524(4)
C(16)-C(17)	1.529(4)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800

C(19)-H(19C)	0.9800
C(20)-C(21)	1.527(4)
C(20)-C(23)	1.528(4)
C(20)-C(22)	1.532(4)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(26)	1.448(4)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(28)	1.448(4)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
N(6)-C(29)	1.131(4)
C(29)-C(30)	1.452(5)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800

F(5)-Sb(1)-F(6)	178.53(12)
F(5)-Sb(1)-F(4)	90.18(11)
F(6)-Sb(1)-F(4)	90.55(13)
F(5)-Sb(1)-F(2)	89.78(10)
F(6)-Sb(1)-F(2)	89.49(12)
F(4)-Sb(1)-F(2)	179.96(14)
F(5)-Sb(1)-F(3)	91.30(9)
F(6)-Sb(1)-F(3)	89.97(11)

F(4)-Sb(1)-F(3)	90.73(9)
F(2)-Sb(1)-F(3)	89.27(9)
F(5)-Sb(1)-F(1)	89.23(9)
F(6)-Sb(1)-F(1)	89.50(11)
F(4)-Sb(1)-F(1)	89.65(9)
F(2)-Sb(1)-F(1)	90.35(8)
F(3)-Sb(1)-F(1)	179.35(9)
F(11)-Sb(2)-F(10)	92.55(12)
F(11)-Sb(2)-F(9)	90.23(12)
F(10)-Sb(2)-F(9)	90.80(12)
F(11)-Sb(2)-F(12)	179.13(13)
F(10)-Sb(2)-F(12)	88.29(12)
F(9)-Sb(2)-F(12)	89.51(12)
F(11)-Sb(2)-F(8)	90.01(11)
F(10)-Sb(2)-F(8)	177.16(13)
F(9)-Sb(2)-F(8)	90.43(11)
F(12)-Sb(2)-F(8)	89.16(11)
F(11)-Sb(2)-F(7)	89.22(11)
F(10)-Sb(2)-F(7)	90.12(10)
F(9)-Sb(2)-F(7)	178.94(14)
F(12)-Sb(2)-F(7)	91.03(11)
F(8)-Sb(2)-F(7)	88.67(11)
F(12)-Sb(2')-F(7)	96.9(6)
F(12)-Sb(2')-F(8)	93.4(5)
F(7)-Sb(2')-F(8)	92.0(4)
F(12)-Sb(2')-F(10)	90.2(3)
F(7)-Sb(2')-F(10)	91.3(3)
F(8)-Sb(2')-F(10)	174.8(8)
F(12)-Sb(2')-F(9)	90.0(3)
F(7)-Sb(2')-F(9)	173.0(7)
F(8)-Sb(2')-F(9)	89.0(3)
F(10)-Sb(2')-F(9)	87.3(4)
F(12)-Sb(2')-F(11)	174.7(6)
F(7)-Sb(2')-F(11)	88.2(3)
F(8)-Sb(2')-F(11)	87.9(3)
F(10)-Sb(2')-F(11)	88.2(4)
F(9)-Sb(2')-F(11)	84.9(5)
C(1)-Ni(1)-N(1)	89.82(10)

C(1)-Ni(1)-N(4)	88.39(10)
N(1)-Ni(1)-N(4)	177.65(10)
C(1)-Ni(1)-N(5)	178.08(11)
N(1)-Ni(1)-N(5)	91.14(9)
N(4)-Ni(1)-N(5)	90.69(9)
C(1)-Ni(1)-N(2)	82.66(10)
N(1)-Ni(1)-N(2)	78.95(9)
N(4)-Ni(1)-N(2)	102.32(9)
N(5)-Ni(1)-N(2)	95.89(9)
C(1)-Ni(1)-N(3)	79.56(10)
N(1)-Ni(1)-N(3)	82.09(9)
N(4)-Ni(1)-N(3)	96.09(9)
N(5)-Ni(1)-N(3)	102.22(9)
N(2)-Ni(1)-N(3)	153.95(8)
C(4)-O(1)-C(24)	117.2(2)
C(9)-N(1)-C(13)	122.4(2)
C(9)-N(1)-Ni(1)	117.61(18)
C(13)-N(1)-Ni(1)	119.22(18)
C(8)-N(2)-C(7)	108.4(2)
C(8)-N(2)-C(16)	111.9(2)
C(7)-N(2)-C(16)	110.5(2)
C(8)-N(2)-Ni(1)	100.45(16)
C(7)-N(2)-Ni(1)	104.60(16)
C(16)-N(2)-Ni(1)	120.04(16)
C(14)-N(3)-C(15)	108.0(2)
C(14)-N(3)-C(20)	111.6(2)
C(15)-N(3)-C(20)	111.5(2)
C(14)-N(3)-Ni(1)	102.74(16)
C(15)-N(3)-Ni(1)	101.79(15)
C(20)-N(3)-Ni(1)	120.07(17)
C(25)-N(4)-Ni(1)	176.5(2)
C(27)-N(5)-Ni(1)	171.5(2)
C(6)-C(1)-C(2)	125.0(3)
C(6)-C(1)-Ni(1)	118.1(2)
C(2)-C(1)-Ni(1)	116.6(2)
C(1)-C(2)-C(3)	117.4(3)
C(1)-C(2)-C(15)	117.1(2)
C(3)-C(2)-C(15)	125.4(3)

C(2)-C(3)-C(4)	119.5(3)
C(2)-C(3)-H(3)	120.2
C(4)-C(3)-H(3)	120.2
O(1)-C(4)-C(5)	123.6(3)
O(1)-C(4)-C(3)	114.7(3)
C(5)-C(4)-C(3)	121.7(3)
C(4)-C(5)-C(6)	118.9(3)
C(4)-C(5)-H(5)	120.6
C(6)-C(5)-H(5)	120.6
C(1)-C(6)-C(5)	117.3(3)
C(1)-C(6)-C(7)	117.9(2)
C(5)-C(6)-C(7)	124.7(3)
C(6)-C(7)-N(2)	110.5(2)
C(6)-C(7)-H(7A)	109.6
N(2)-C(7)-H(7A)	109.6
C(6)-C(7)-H(7B)	109.6
N(2)-C(7)-H(7B)	109.6
H(7A)-C(7)-H(7B)	108.1
N(2)-C(8)-C(9)	109.8(2)
N(2)-C(8)-H(8A)	109.7
C(9)-C(8)-H(8A)	109.7
N(2)-C(8)-H(8B)	109.7
C(9)-C(8)-H(8B)	109.7
H(8A)-C(8)-H(8B)	108.2
N(1)-C(9)-C(10)	120.3(3)
N(1)-C(9)-C(8)	115.3(2)
C(10)-C(9)-C(8)	124.4(3)
C(9)-C(10)-C(11)	118.5(3)
C(9)-C(10)-H(10)	120.7
C(11)-C(10)-H(10)	120.7
C(10)-C(11)-C(12)	120.4(3)
C(10)-C(11)-H(11)	119.8
C(12)-C(11)-H(11)	119.8
C(13)-C(12)-C(11)	118.7(3)
C(13)-C(12)-H(12)	120.7
C(11)-C(12)-H(12)	120.7
N(1)-C(13)-C(12)	119.6(3)
N(1)-C(13)-C(14)	115.0(2)

C(12)-C(13)-C(14)	125.3(3)
C(13)-C(14)-N(3)	113.0(2)
C(13)-C(14)-H(14A)	109.0
N(3)-C(14)-H(14A)	109.0
C(13)-C(14)-H(14B)	109.0
N(3)-C(14)-H(14B)	109.0
H(14A)-C(14)-H(14B)	107.8
N(3)-C(15)-C(2)	107.8(2)
N(3)-C(15)-H(15A)	110.1
C(2)-C(15)-H(15A)	110.1
N(3)-C(15)-H(15B)	110.1
C(2)-C(15)-H(15B)	110.1
H(15A)-C(15)-H(15B)	108.5
C(19)-C(16)-C(18)	109.5(2)
C(19)-C(16)-C(17)	109.3(2)
C(18)-C(16)-C(17)	108.5(2)
C(19)-C(16)-N(2)	109.6(2)
C(18)-C(16)-N(2)	108.6(2)
C(17)-C(16)-N(2)	111.2(2)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
N(3)-C(20)-C(21)	110.2(2)

N(3)-C(20)-C(23)	108.6(2)
C(21)-C(20)-C(23)	109.3(2)
N(3)-C(20)-C(22)	111.5(2)
C(21)-C(20)-C(22)	108.0(2)
C(23)-C(20)-C(22)	109.4(2)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(20)-C(23)-H(23A)	109.5
C(20)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(20)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
O(1)-C(24)-H(24A)	109.5
O(1)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
O(1)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
N(4)-C(25)-C(26)	177.2(3)
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
N(5)-C(27)-C(28)	177.3(3)
C(27)-C(28)-H(28A)	109.5

C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
N(6)-C(29)-C(30)	178.9(5)
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5