Bifunctional Colorimetric Chemosensing of Fluoride and Cyanide Ions by Nickel-POCOP Pincer Receptors

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Supporting Information

Table S1 Crystallographic data for the neutral bromo complex of **1**.

Empirical formula	$C_{30}H_{23}Br_{0.69}Cl_{0.31}NiO_3P_2$
Mol. Weight / g mol^{-1}	618.14
Crystal size / mm^3	0.201 x 0.164 x 0.156
Crystal system	Monoclinic
Space group	$P2_1/n$
a / Å	16.4872(4)
b / Å	10.6284(2)
c / Å	16.6583(4)
α / °	90
β / °	118.3130(8)
γ / °	90
Volume / Å^3	2569.87(10)
Z	4
Density / g cm^{-3}	1.598
Temperature / *K*	100(2)
Absorption Coeff. / mm^{-1}	2.013
Θ range / °	2.367 to 27.443
Index ranges	-20<=h<=21, -13<=k<=13, -21<=l<=21
Reflections collected	23685
Absorption corrrection	Multi-scan
Max. & min. transmission	0.7456, 0.6542
Data / restraints / param.	5861 / 3 / 341
Goodness-of-fit on F^2	1.037
Final *R* indices [I > 2 s (I)]	R1 = 0.0297, wR2 = 0.0675
R indices (all data)	R1 = 0.0380, wR2 = 0.0708
Larg. diff. peak/hole / eÅ^{-3}	0.533 and -0.295

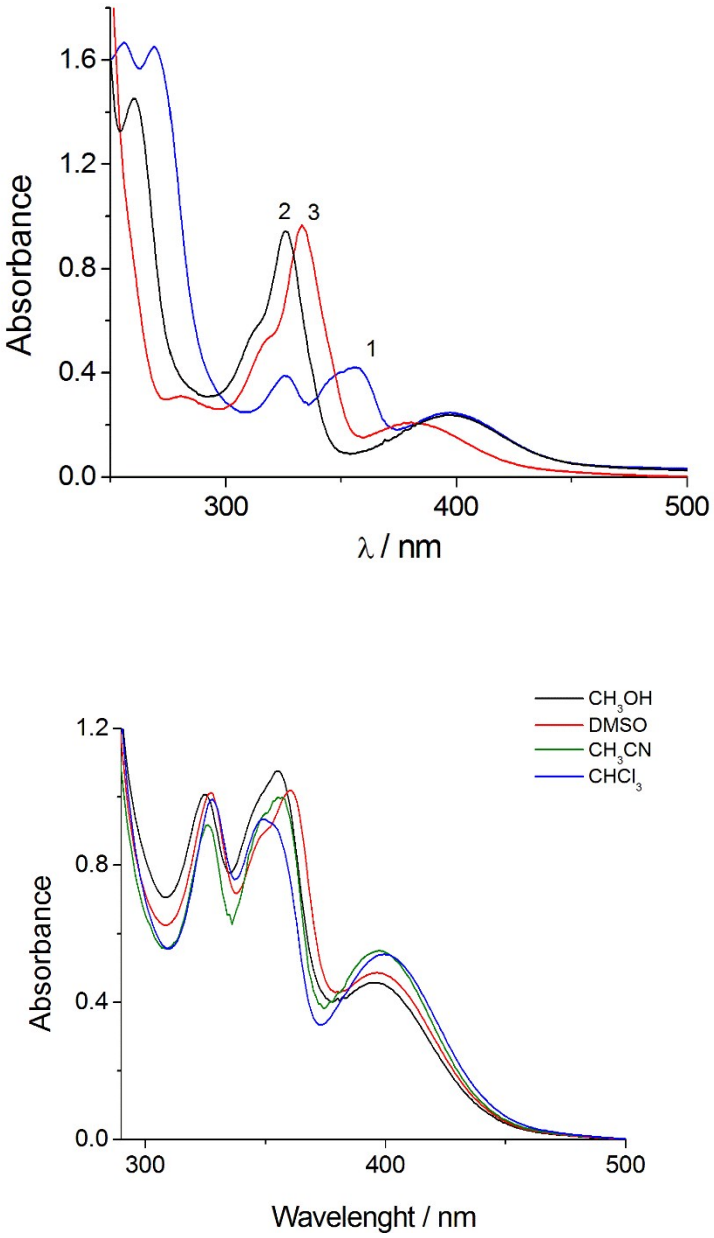

Figure S1. UV-vis absorption spectra of **1**-**3** (50 μM) in CH_3CN (top) and spectrophotometric spectra of **1** in several organic solvents at 20 °C (bottom).

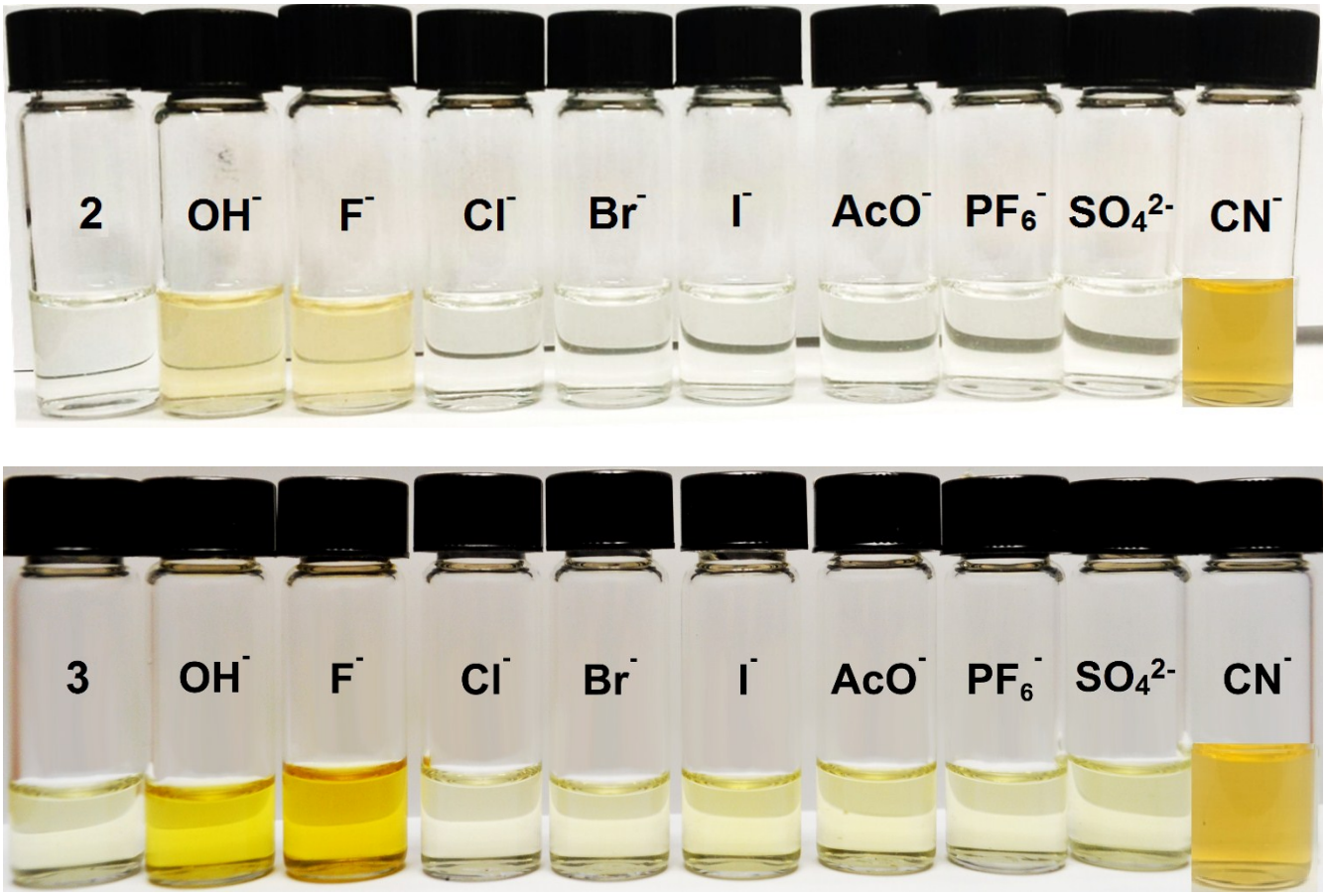

Figure S2. Color change of **1** and **2** (50 μM) in CH_3CN (containing 20 % v/v H_2O) solutions with the addition of 3.0 equiv. of sodium salts of various anions. **2** and **3** = neutral chloro-complex,

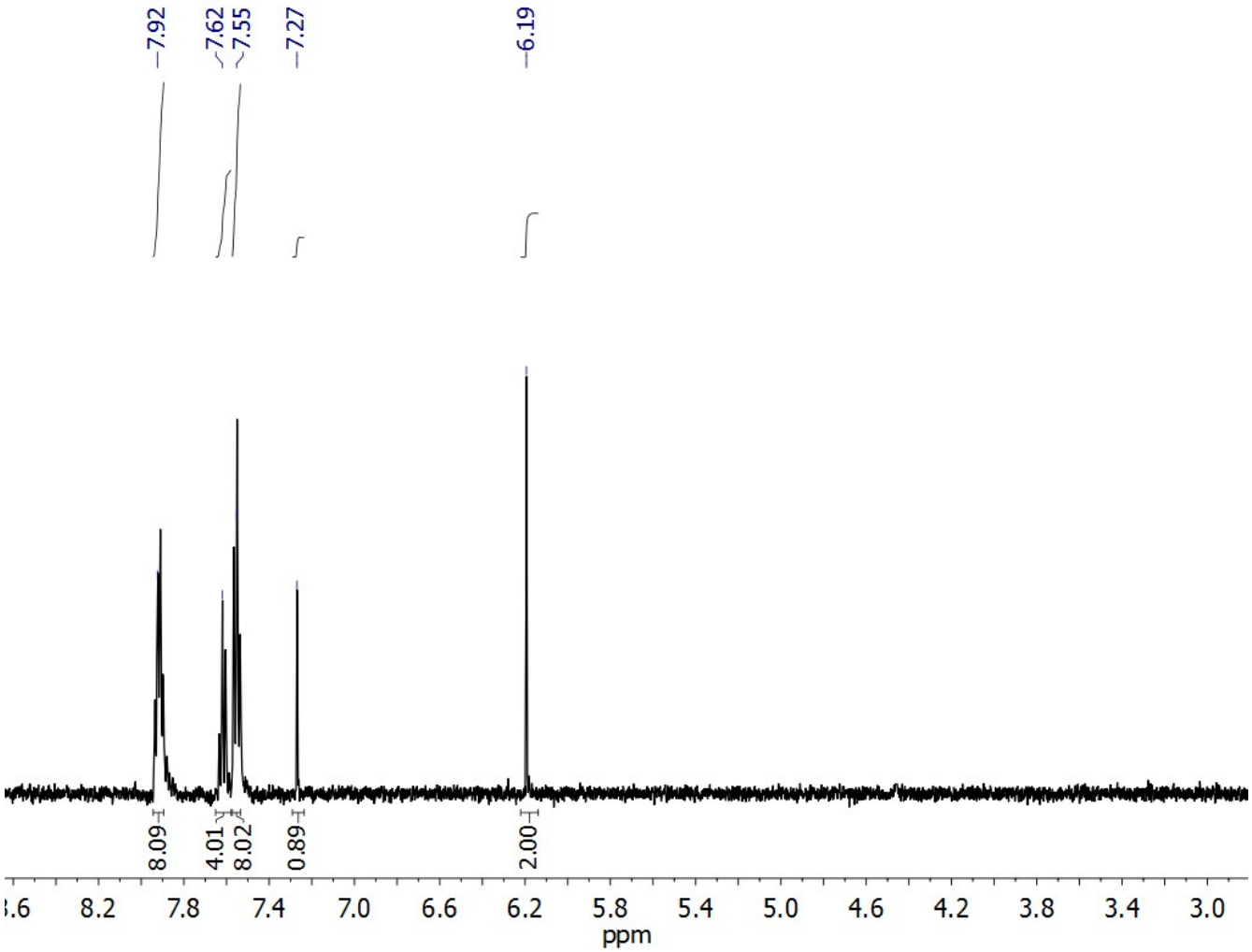

Figure S3. ^{1}H NMR spectrum in CD_3CN of **1.**

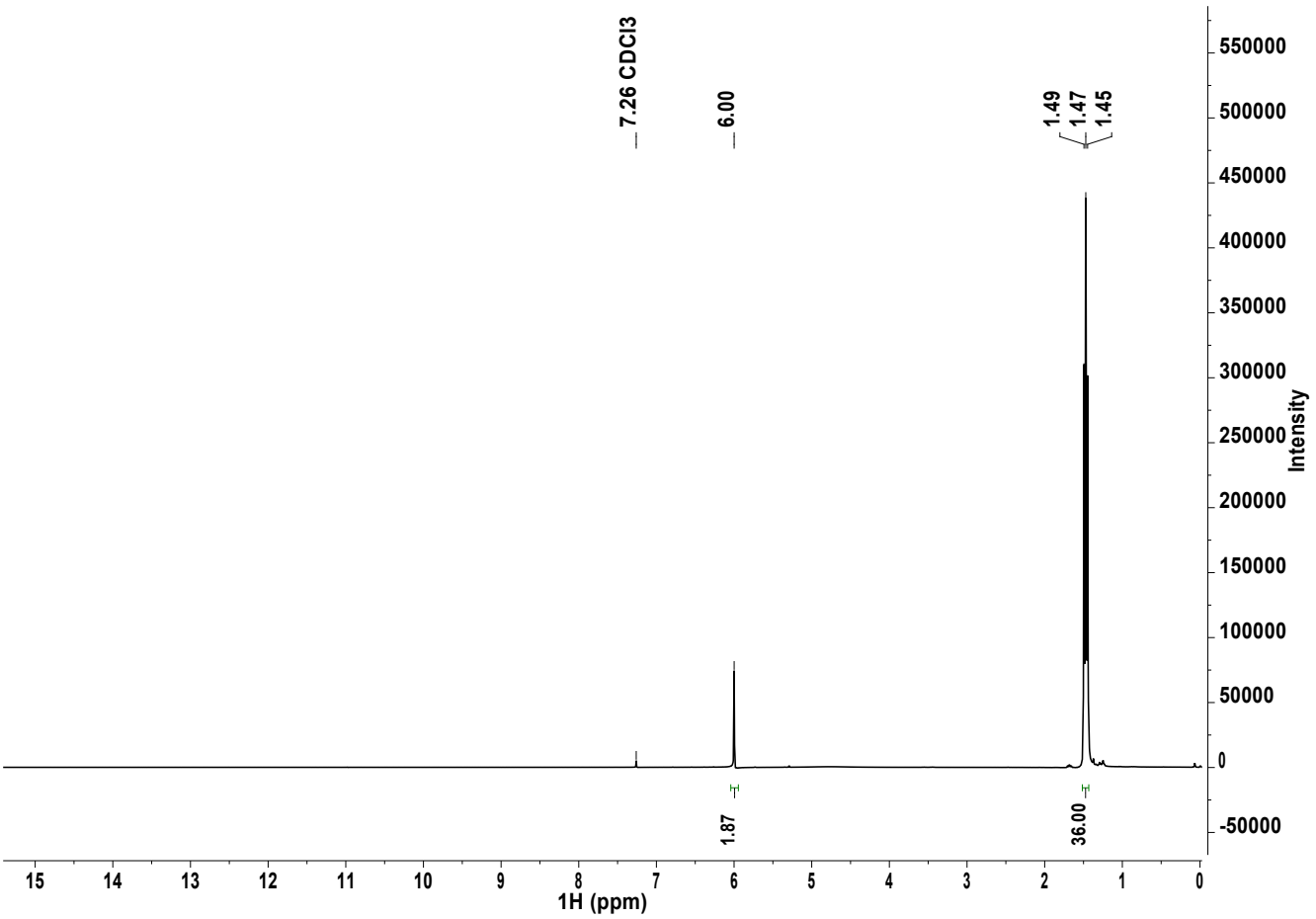

Figure S4. ^{1}H NMR spectrum in CD_3CN of **2.**

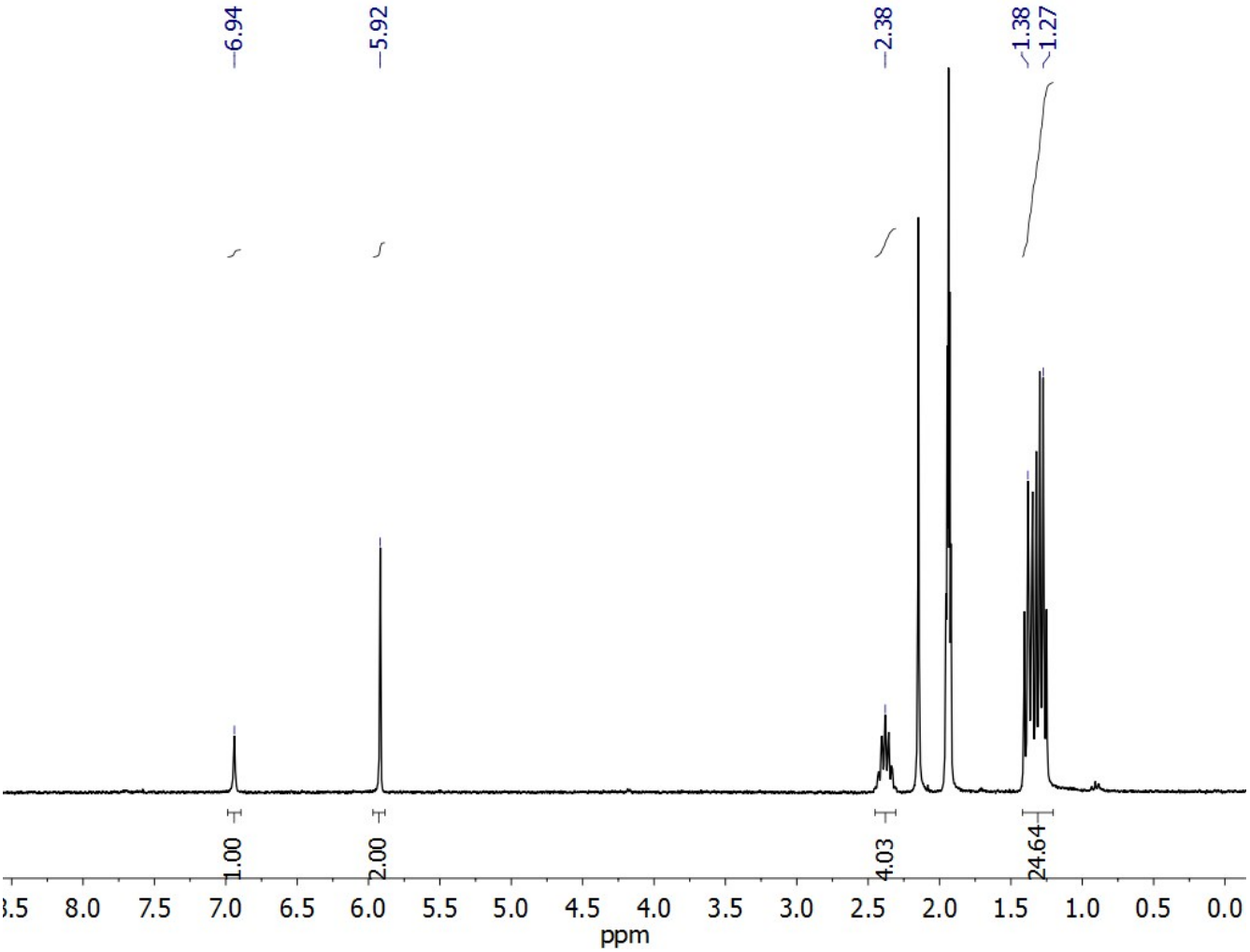

Figure S5. ^{1}H NMR spectrum in CD_3CN of **3.**

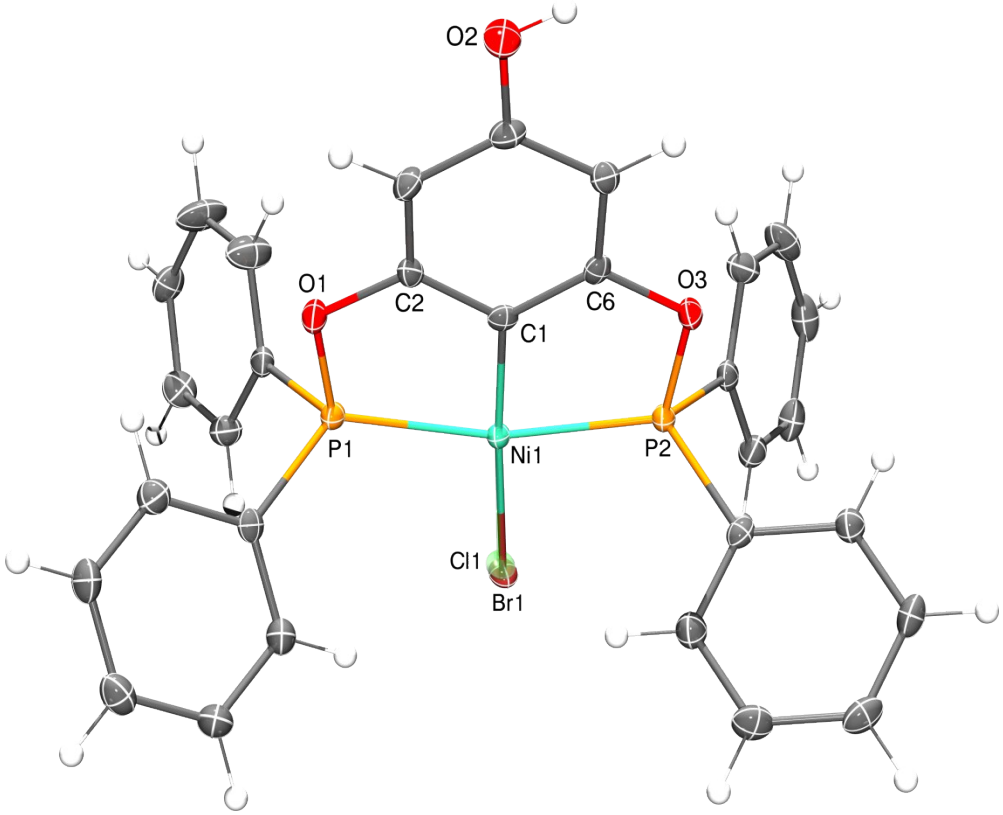

Figure S6. ORTEP diagram at 50% of probability for neutral complex **1**. Two complexes (bromo complex 68.6(2)% and chloro complex 31.4(2) %) are found in the unit cell. The chlorine atom is shown in phantom for clarity.

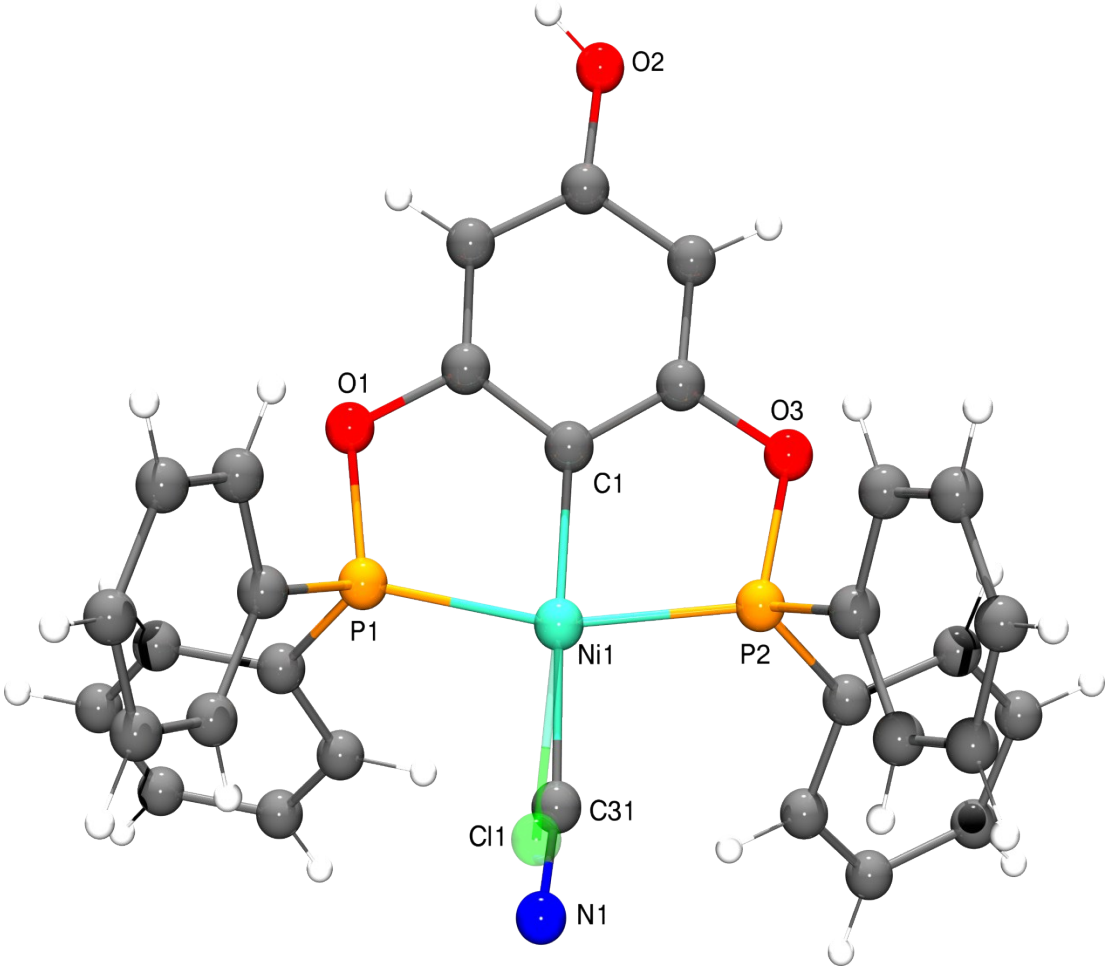

Figure S7. ORTEP diagram at 50% of probability for cyanide complex **1**.CN. Two complexes (chloro complex 83(1)% and cyanide complex 17(1) %) are found in the unit cell, the chlorine atom is shown in phantom for clarity.

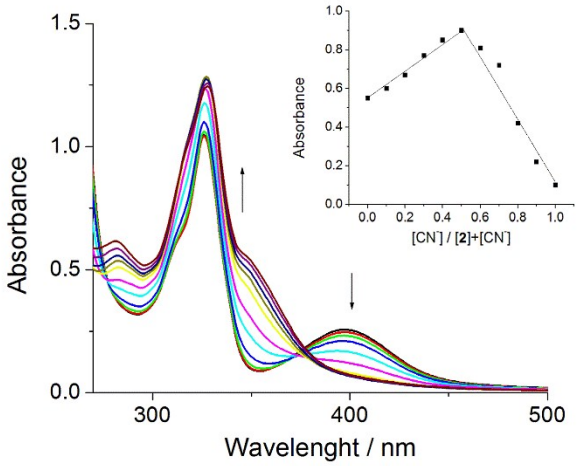

Figure S8. UV-vis spectra changes of **2** (50 μM) in CH_3CN observed upon the addition of 0-2.0 equiv. of NaCN.

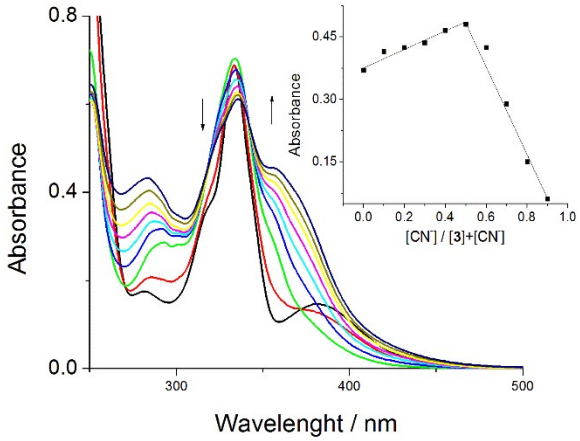

Figure S9. UV-vis spectra changes of **3** (50 μM) in CH_3CN observed upon the addition of 0-2.0 equiv. of NaCN.

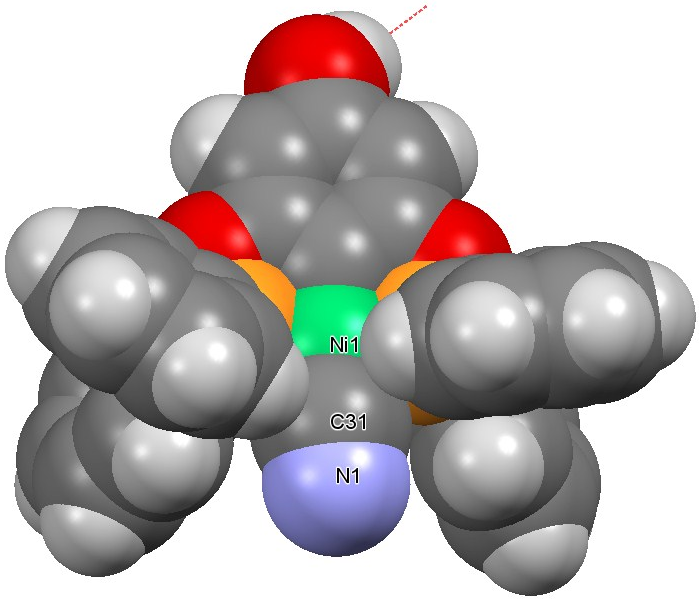

Figure S10. Spacefill model for cyanide complex **1**.CN.

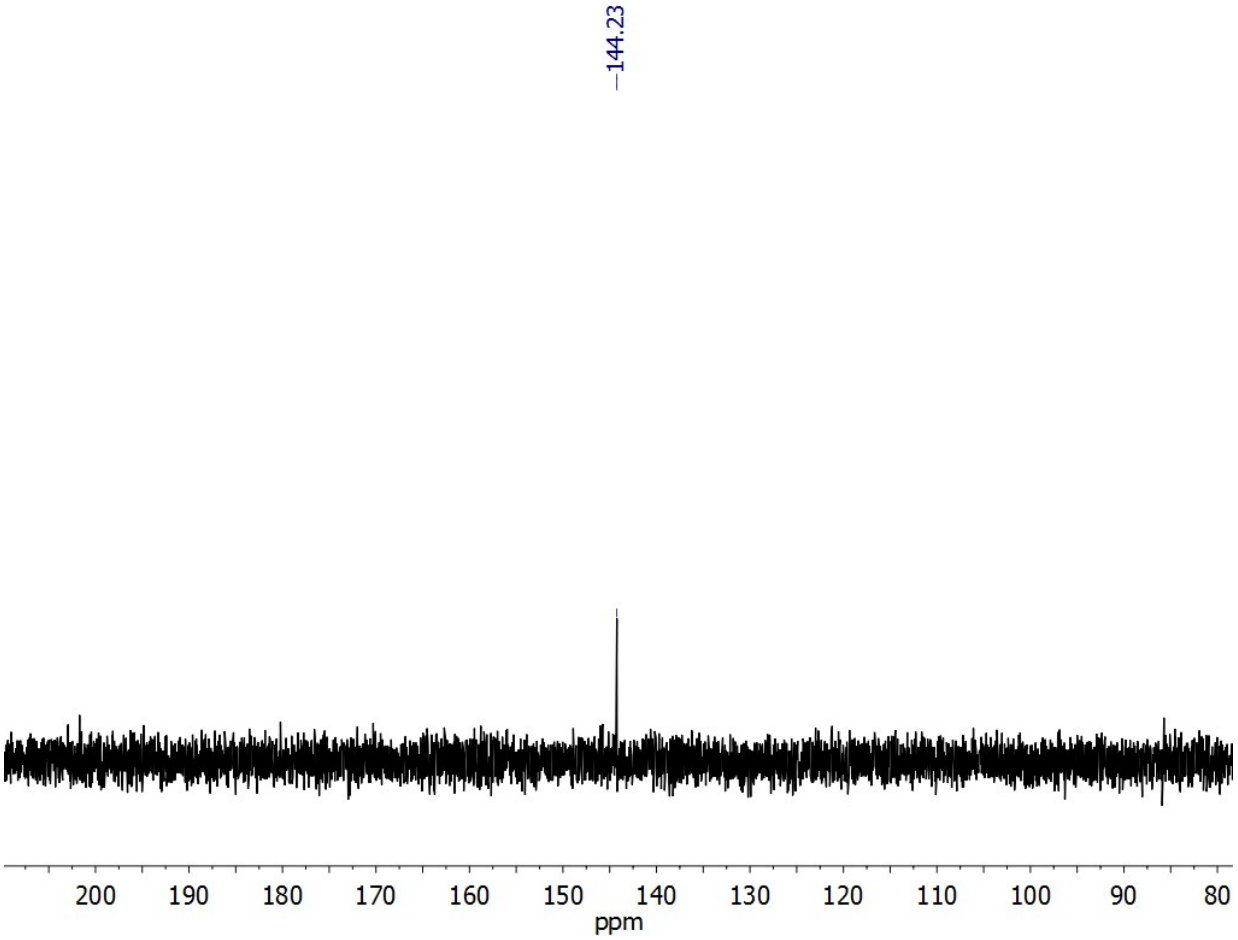

Figure S11. ^{31}P NMR (121.65 MHz) spectrum in CD_3CN of **1**-Br.

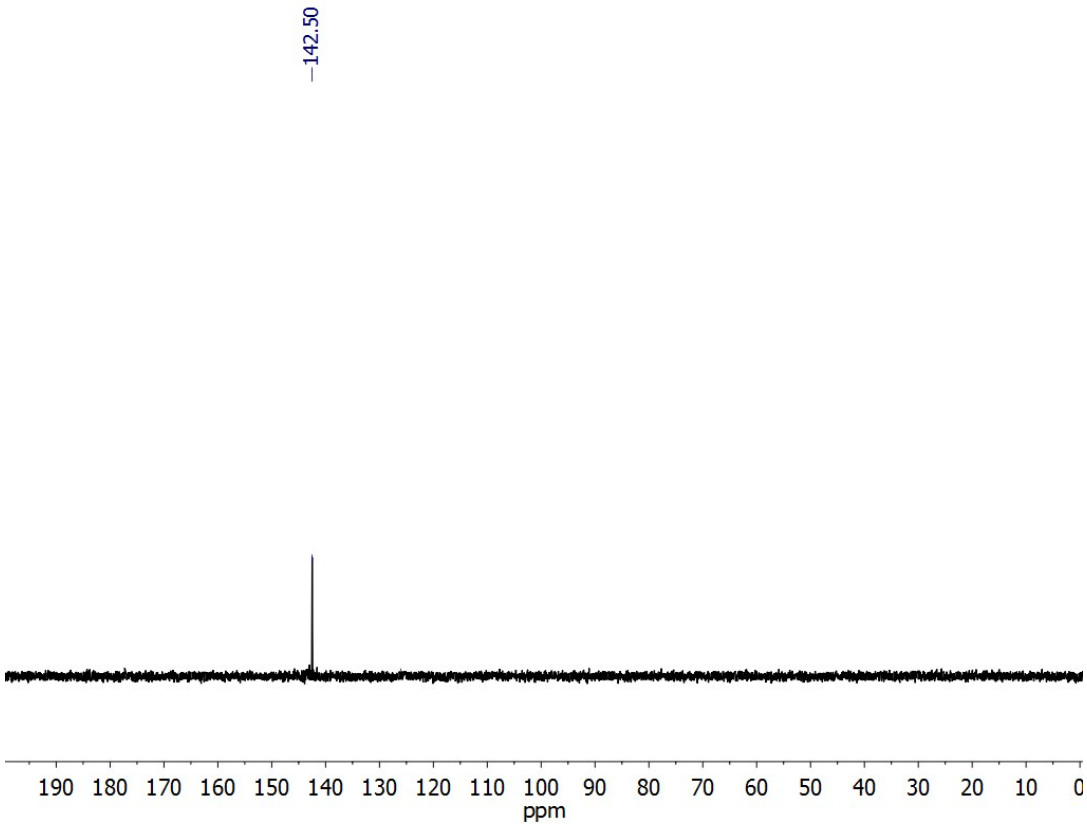

Figure S12. ^{31}P NMR (121.65 MHz) spectrum in CD_3CN of **1**-CN.

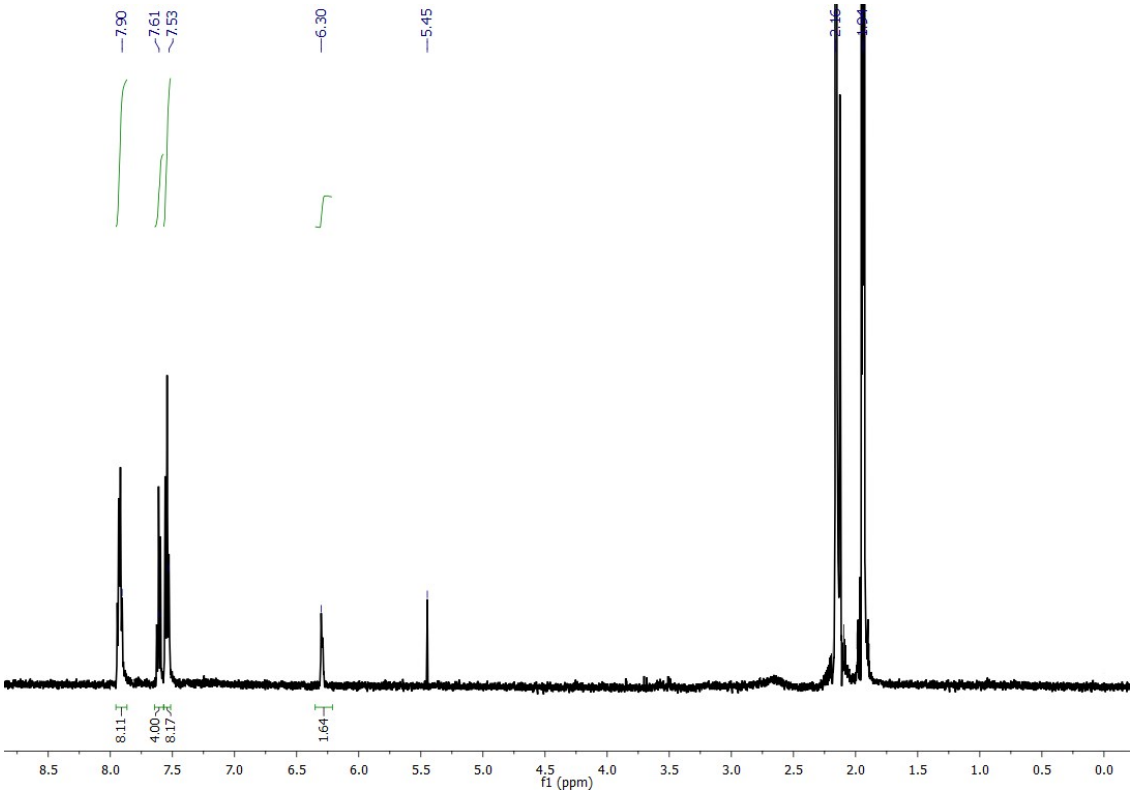

Figure S13. ^{1}H NMR spectrum in CD_3CN of **1**-Br.

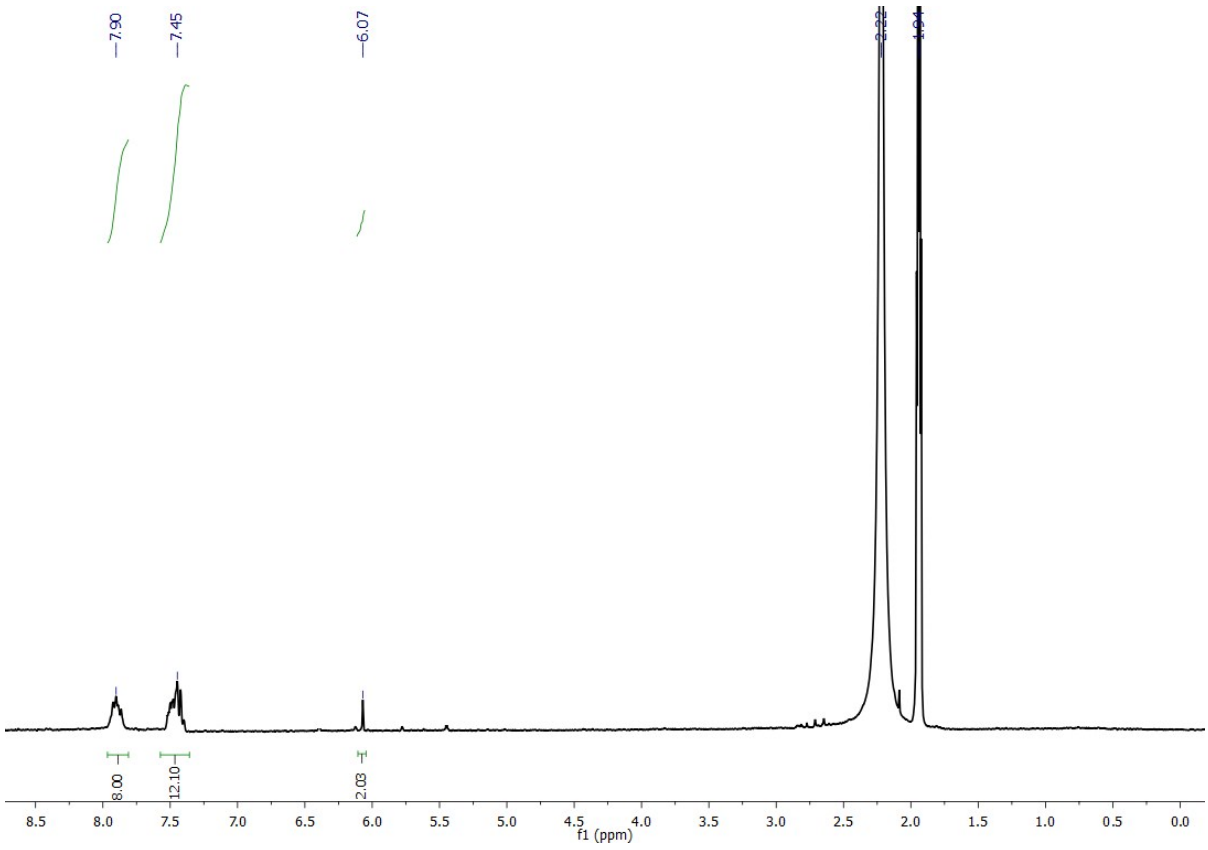

Figure S14. ^{1}H NMR spectrum in CD_3CN of **1**-CN.