

Supporting Information

for

From betaines to anionic N-heterocyclic carbenes. Borane, gold, rhodium, and nickel complexes starting from an imidazoliumphenolate and its carbene tautomer

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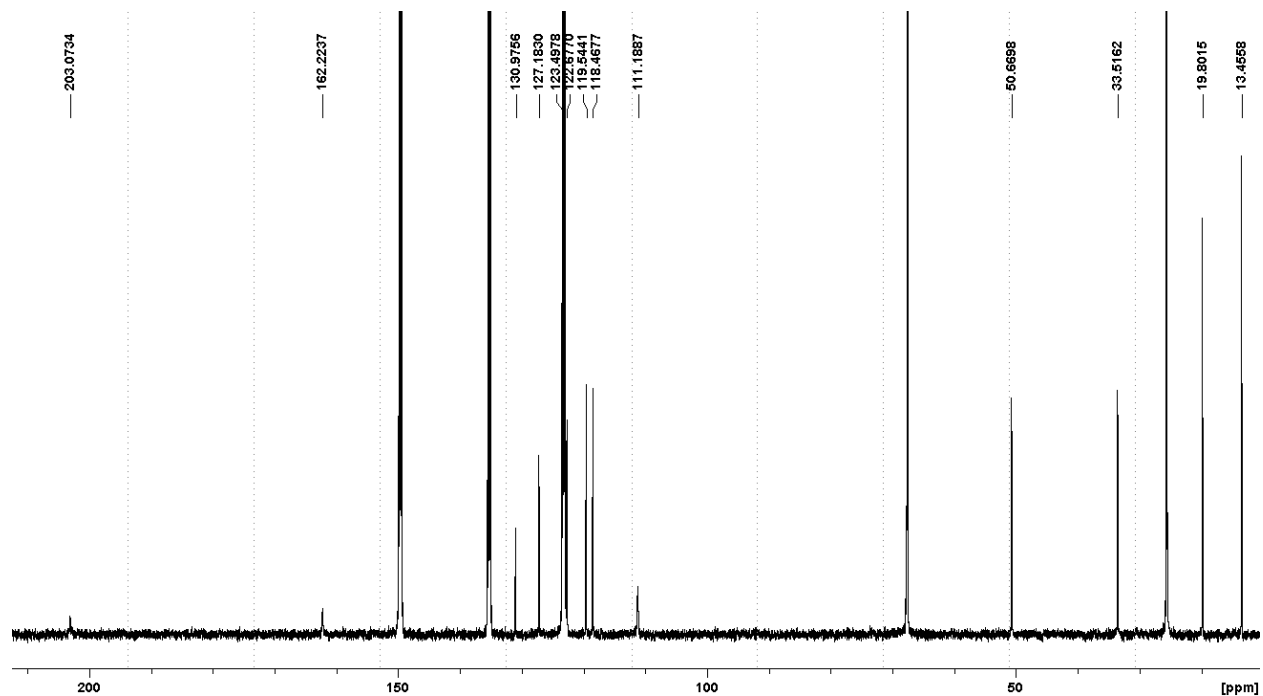
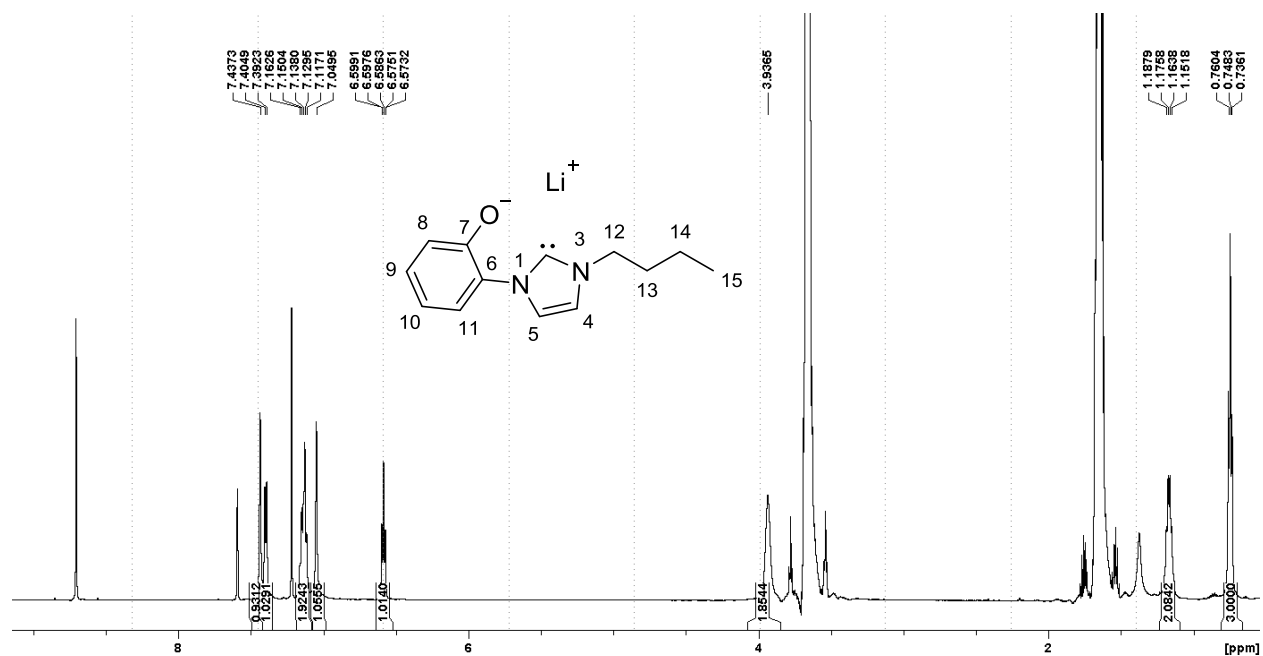
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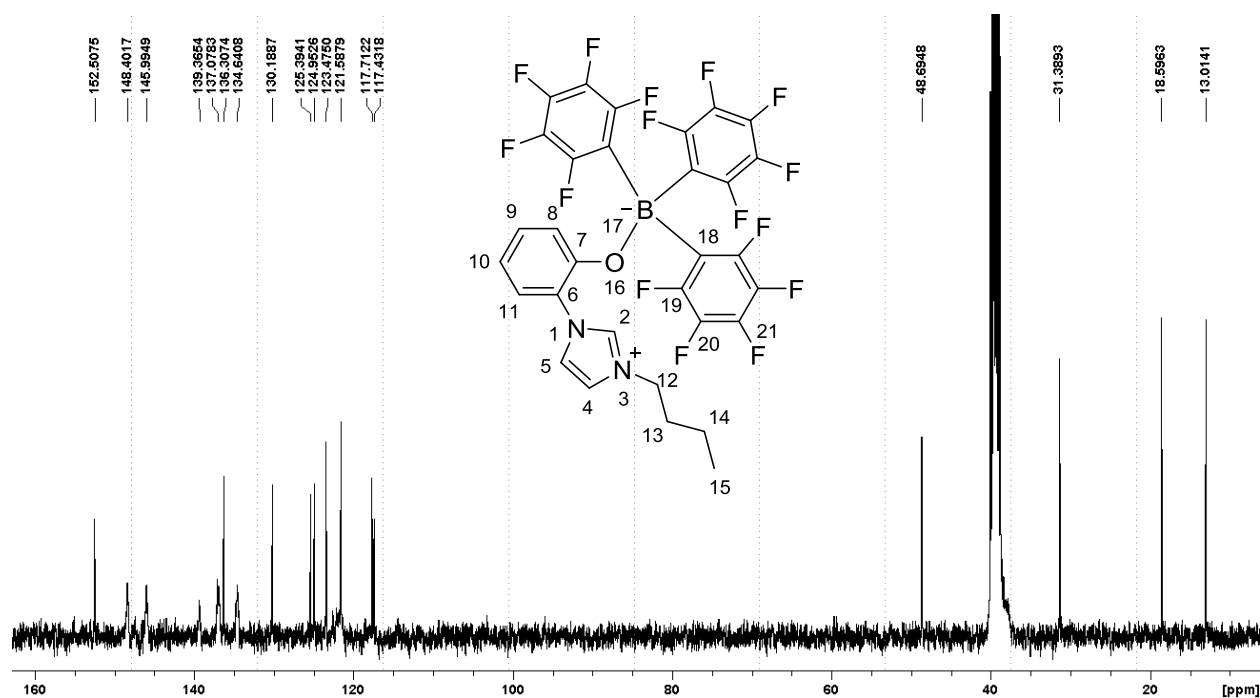
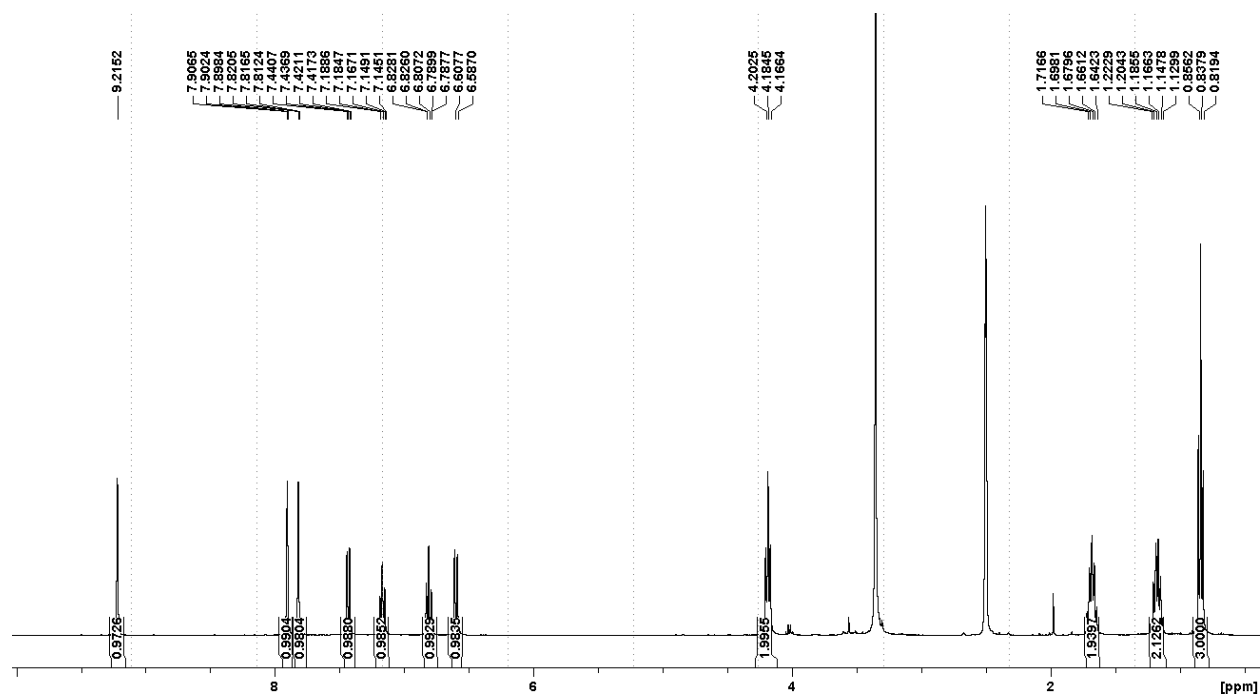
NMR spectra and molecular drawings

Lithium 2-(3-butyl-1*H*-imidazol-2-ylidene-1-yl)phenolate (7)

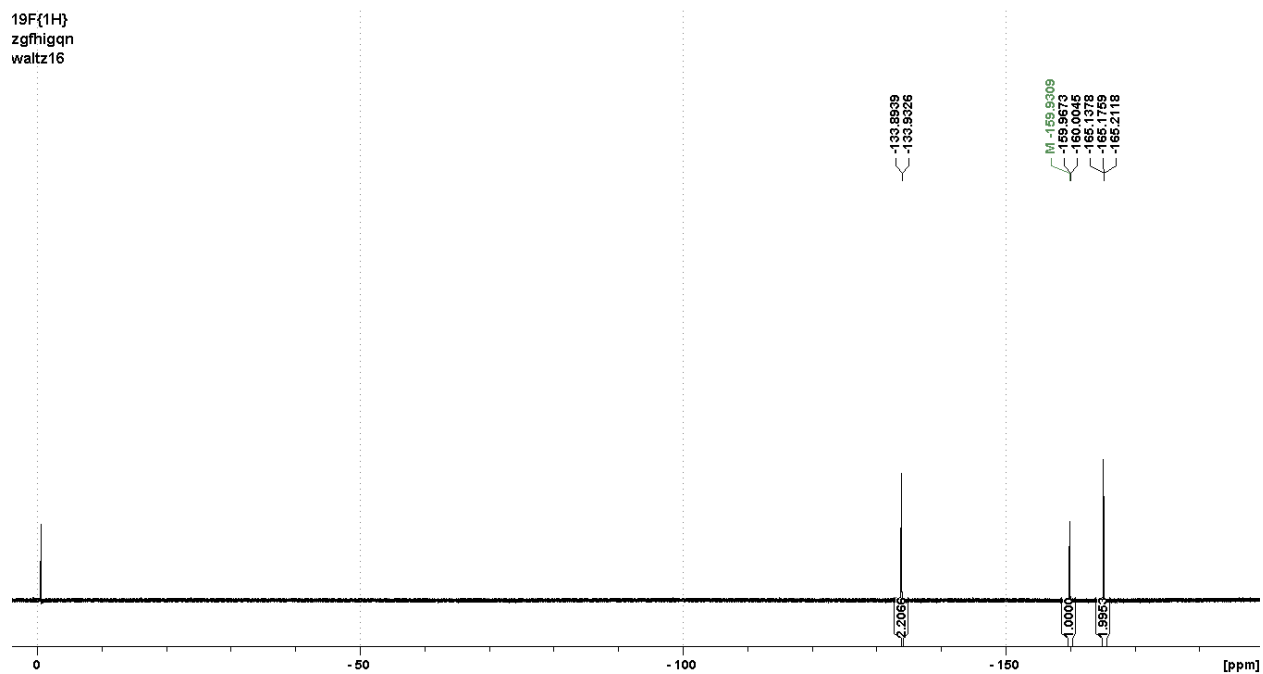
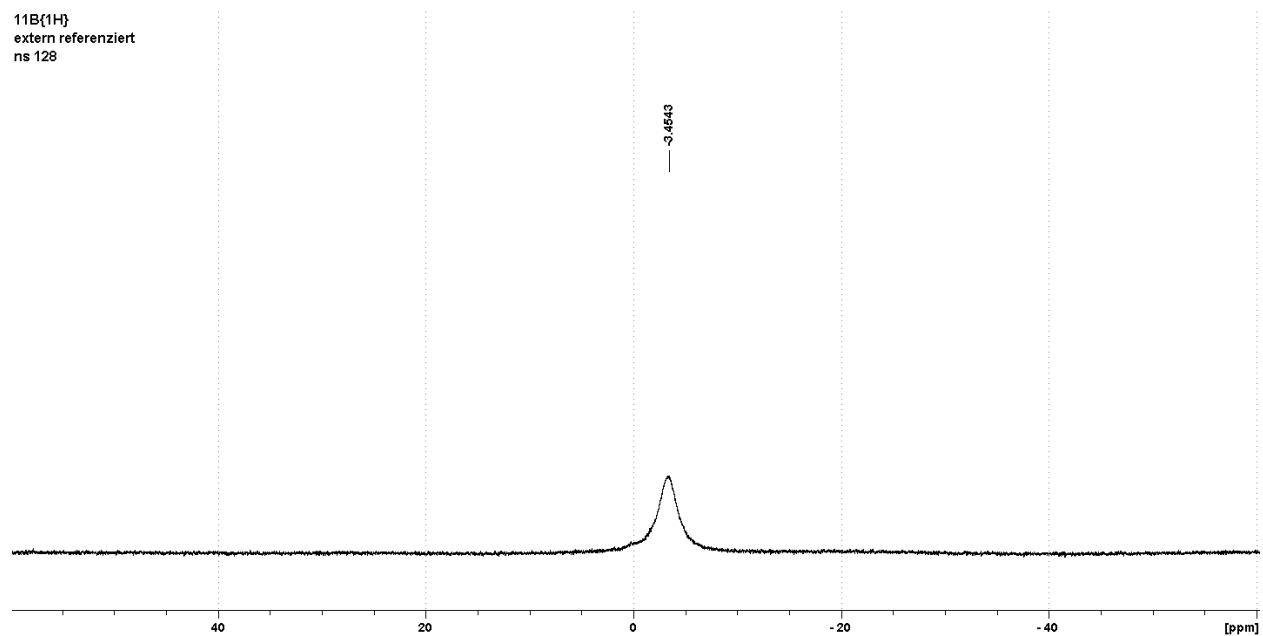


Figures S1/2: ¹H and ¹³C NMR spectra of the lithium salt of the anionic NHC 7.

(2-(3-Butyl-1*H*-imidazolium-1-yl)phenoxy)tris(perfluorophenyl)borate (8)

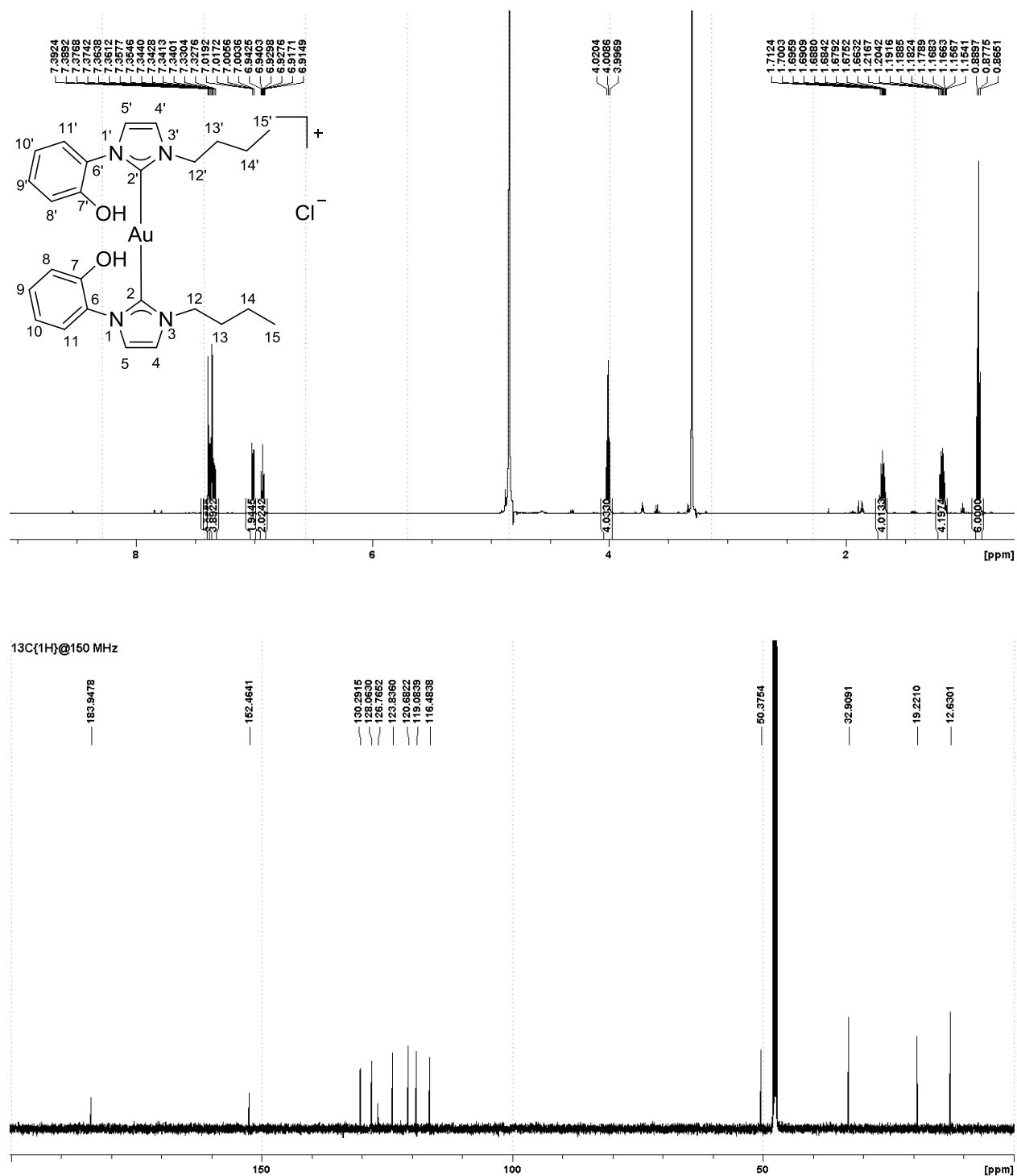


Figures S3/4: ¹H and ¹³C NMR spectra of borane adduct **8**.



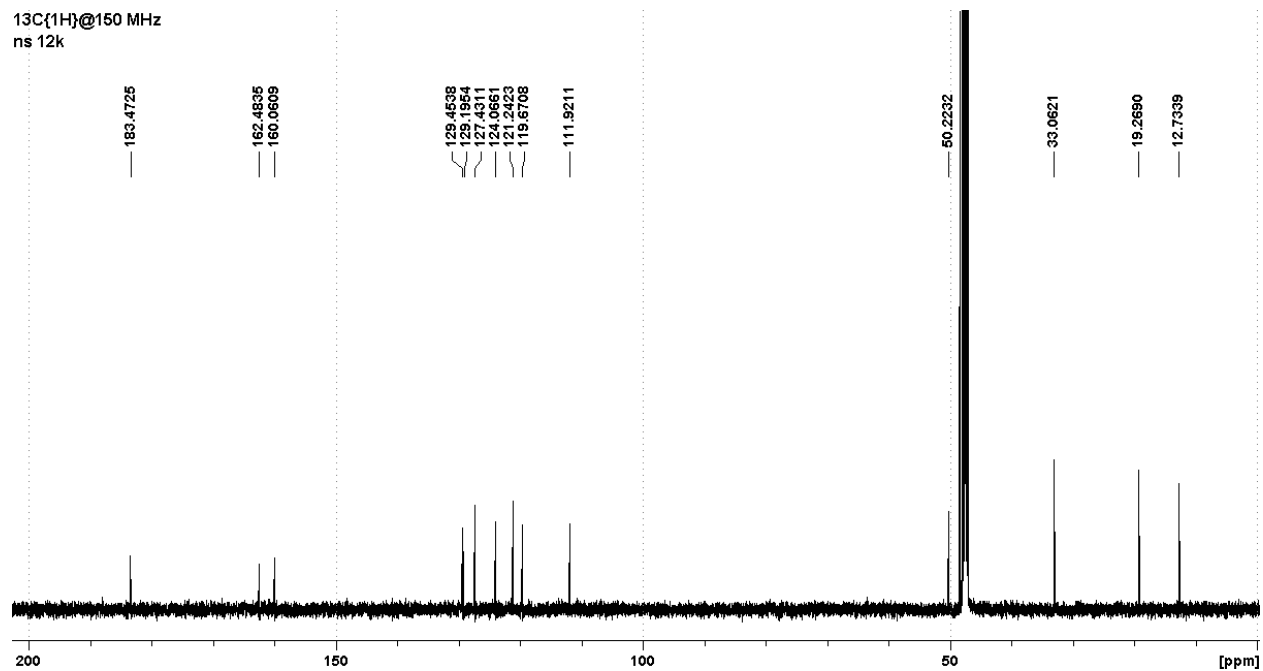
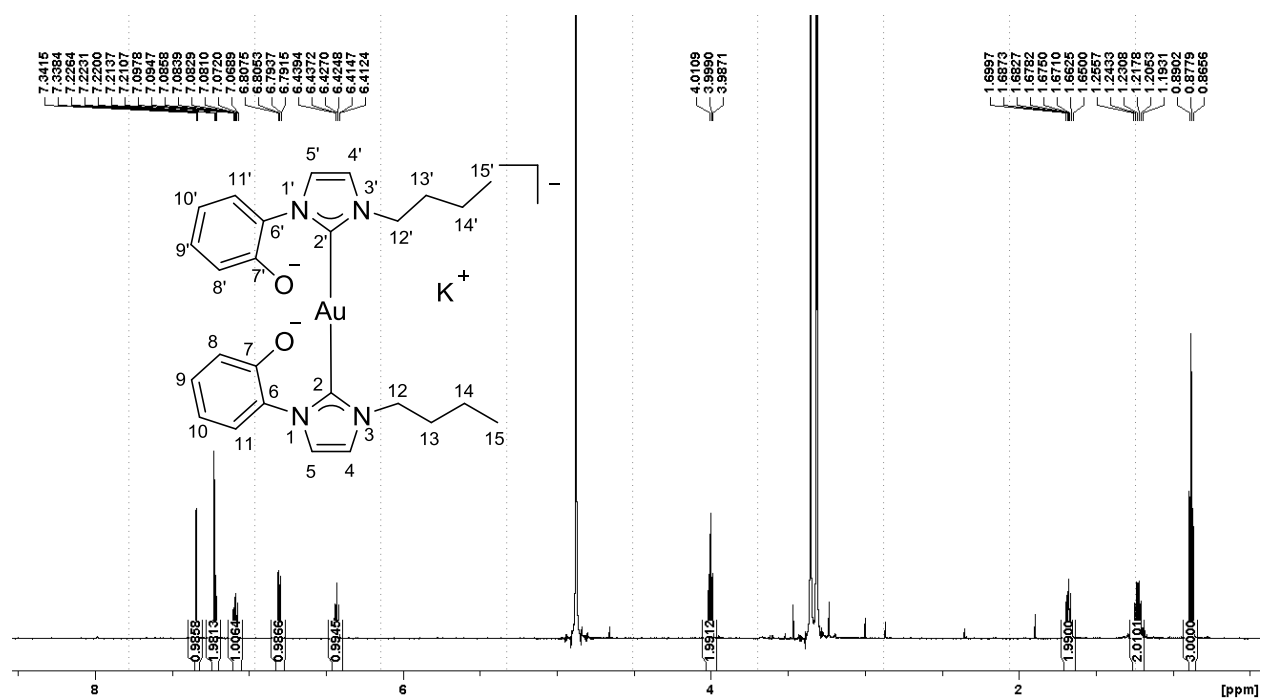
Figures S5/6: ¹¹B and ¹⁹F NMR spectra of borane adduct **8**.

Bis(3-butyl-1-(2-hydroxyphenyl)-1*H*-imidazolium-2-yl)gold monochloride (9)



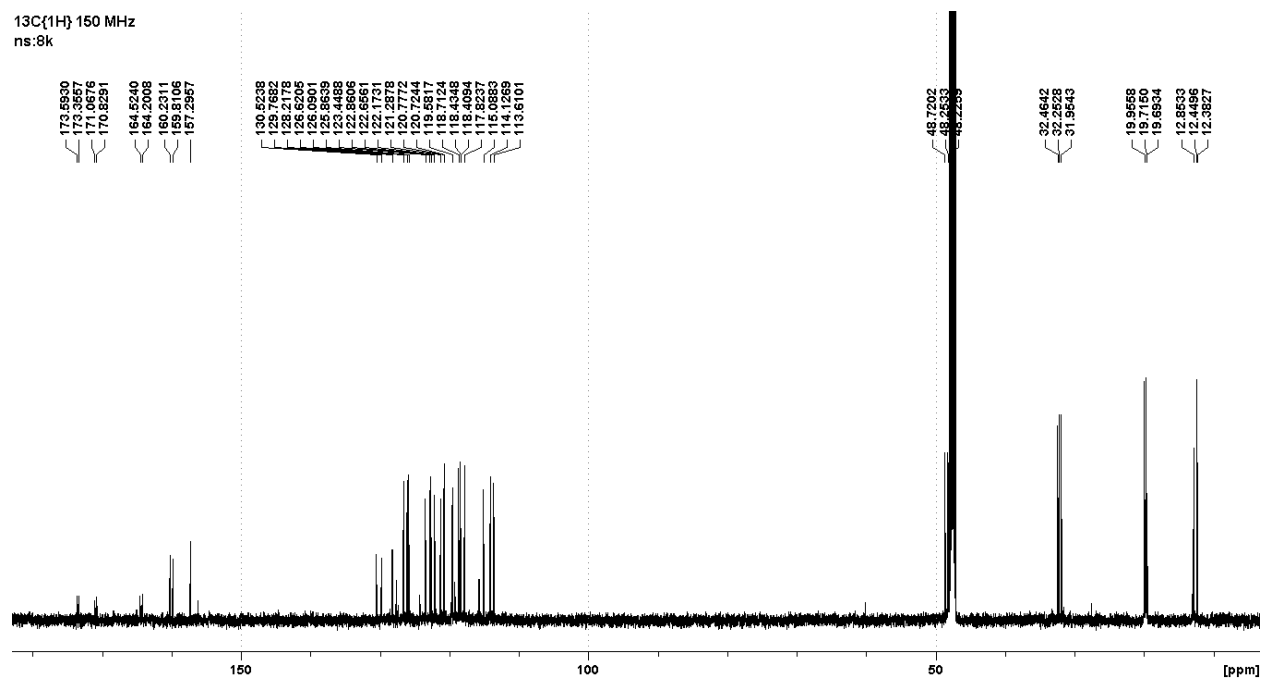
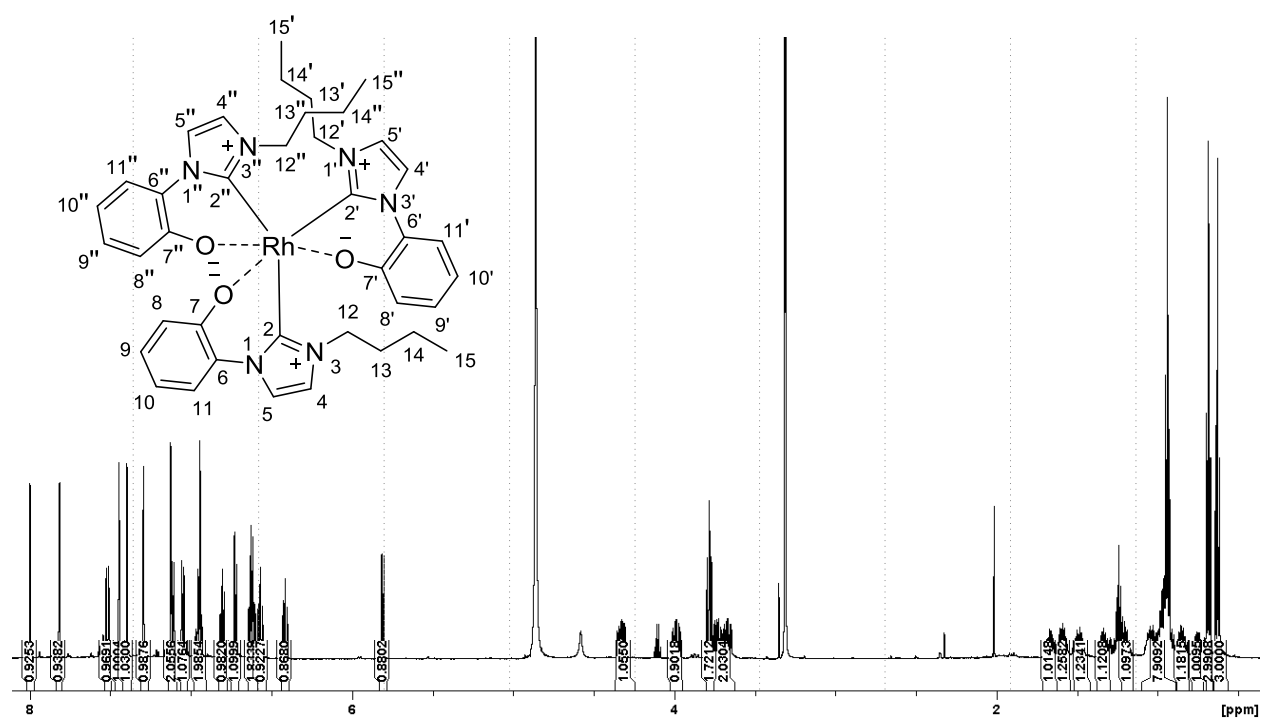
Figures S7/8: ¹H and ¹³C NMR spectra of gold complex 9.

Potassium bis(3-butyl-1-(2-phenolate)-1*H*-imidazolium-2-yl)gold (10)



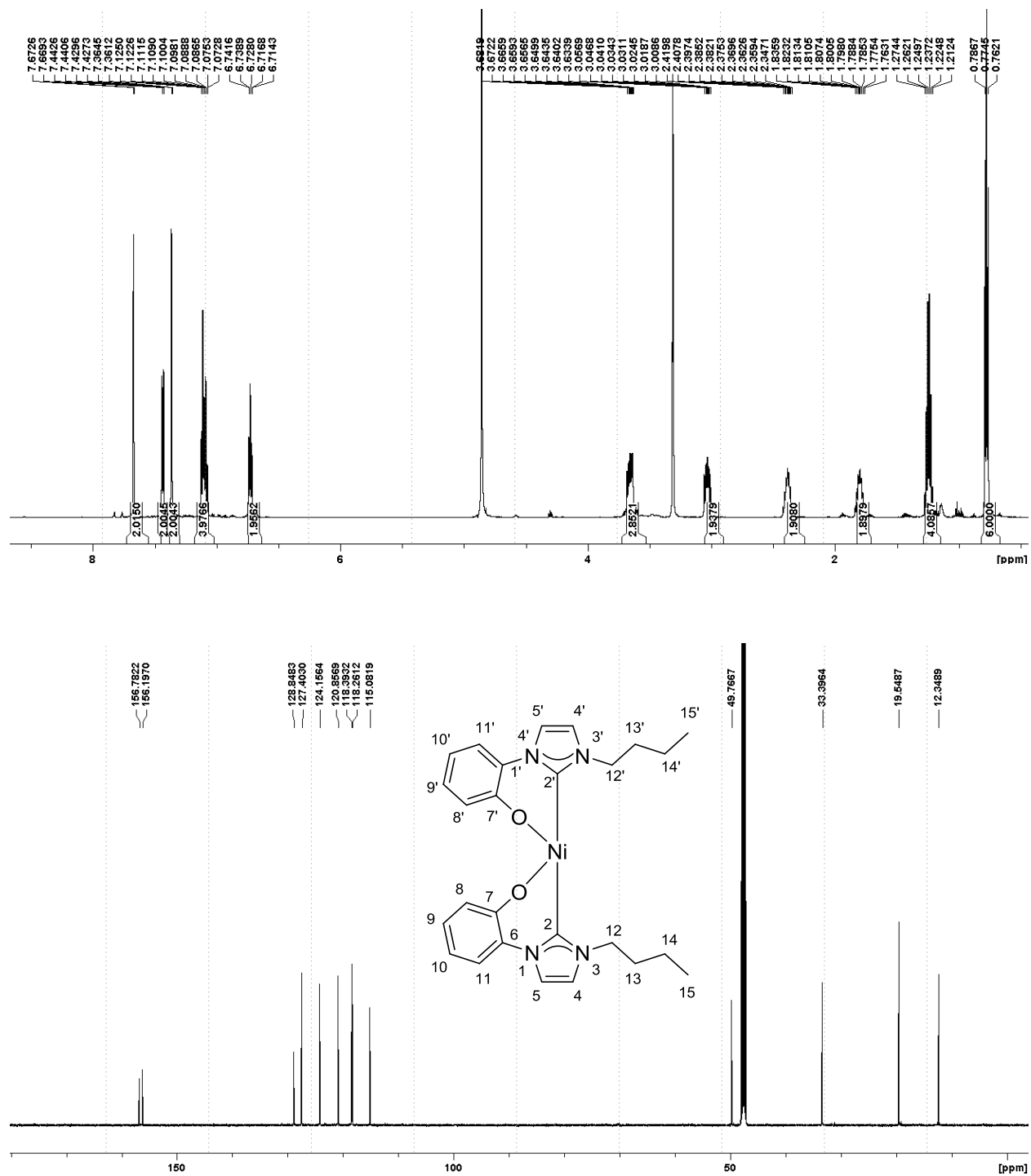
Figures S9/10: ¹H and ¹³C NMR spectra of the anionic gold complex **10**.

Tris(3-butyl-1-(2-oxidophenyl)-1*H*-imidazolium-2-yl)rhodium (11)



Figures S11/12: ¹H and ¹³C NMR spectra of rhodium complex 11.

Bis(3-butyl-1-(2-oxidophenyl)-1H-imidazolium-2-yl)nickel (12)



Figures S13/14: ¹H and ¹³C NMR spectra of nickel complex 12.

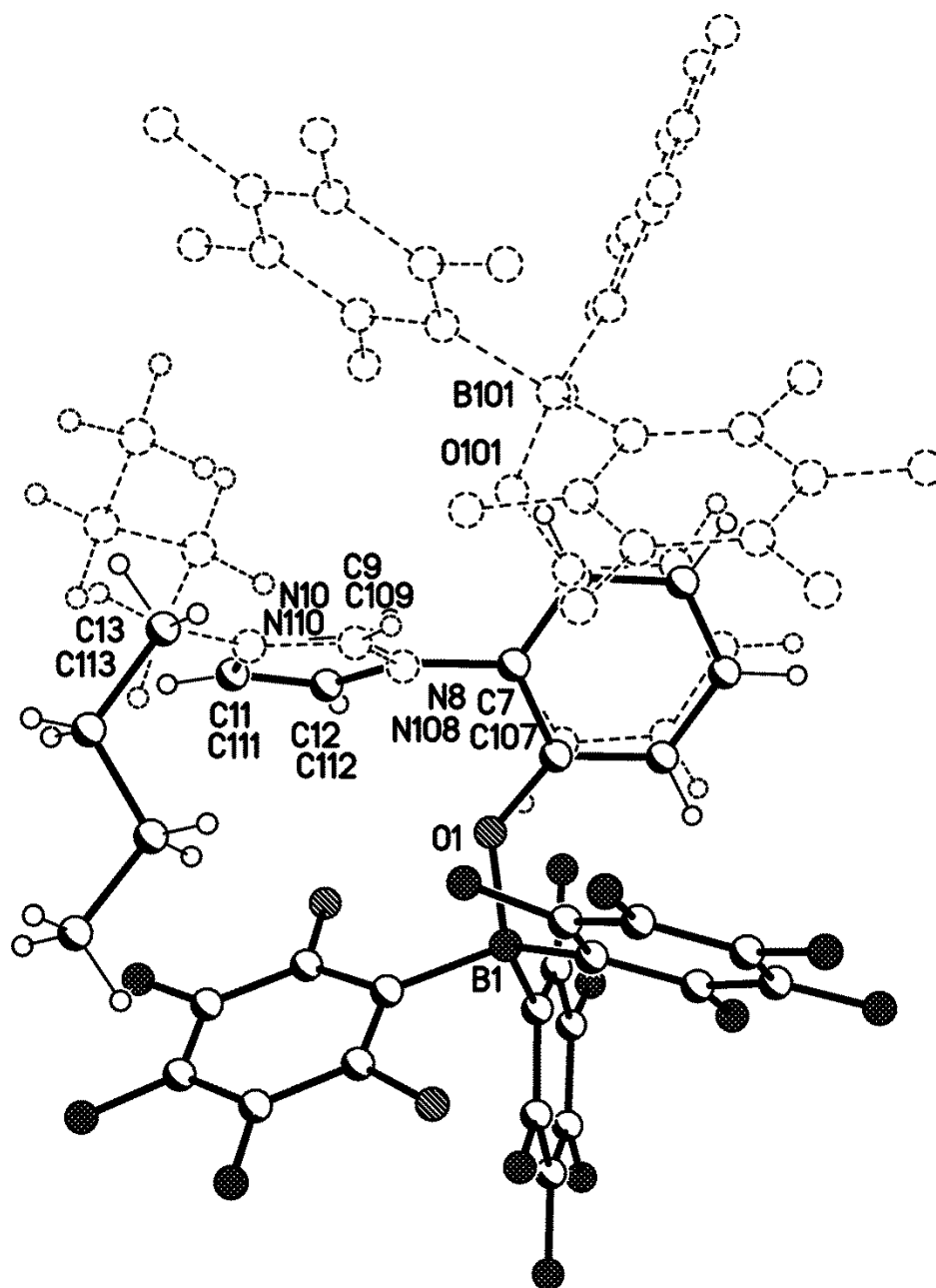


Figure S15: Fit of the two independent molecules of borane adduct **8**

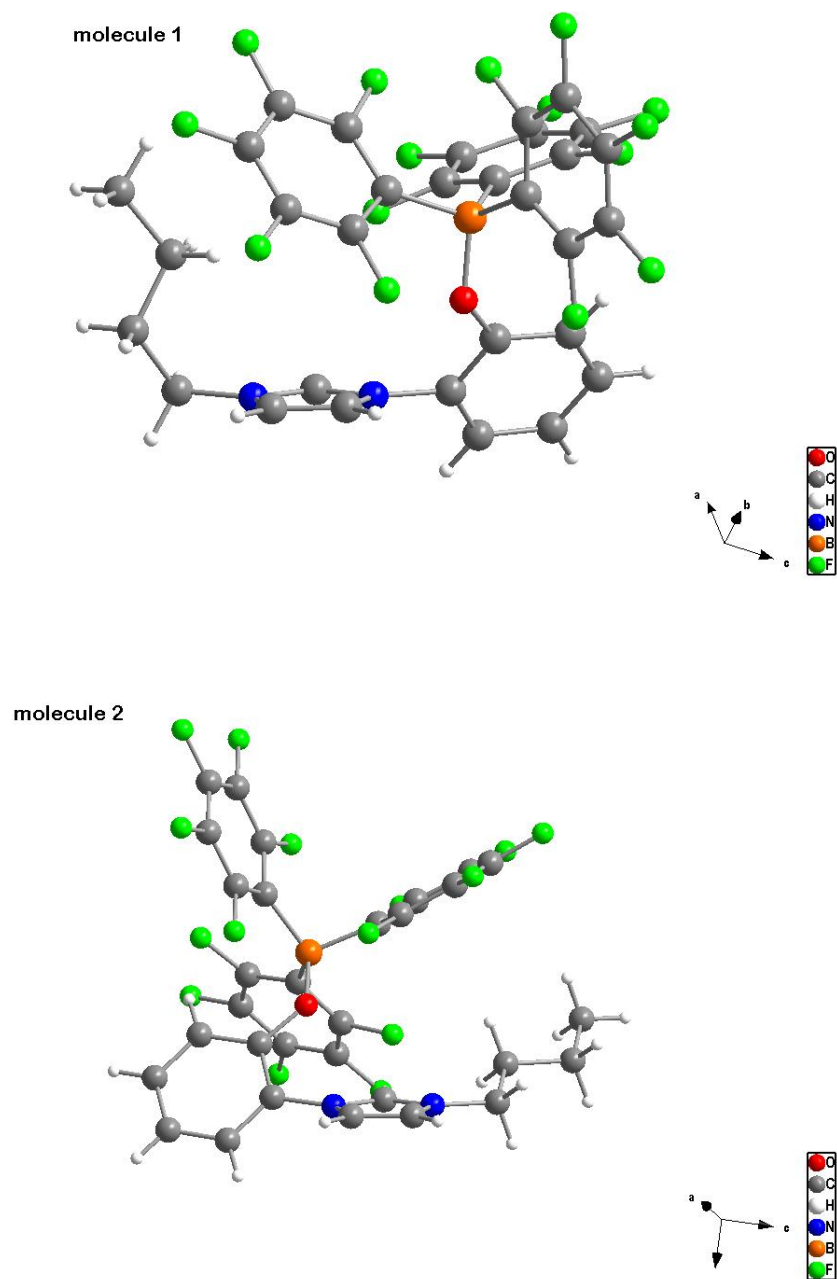


Figure S16: Drawing of the two independent molecules of borane adduct **8**.

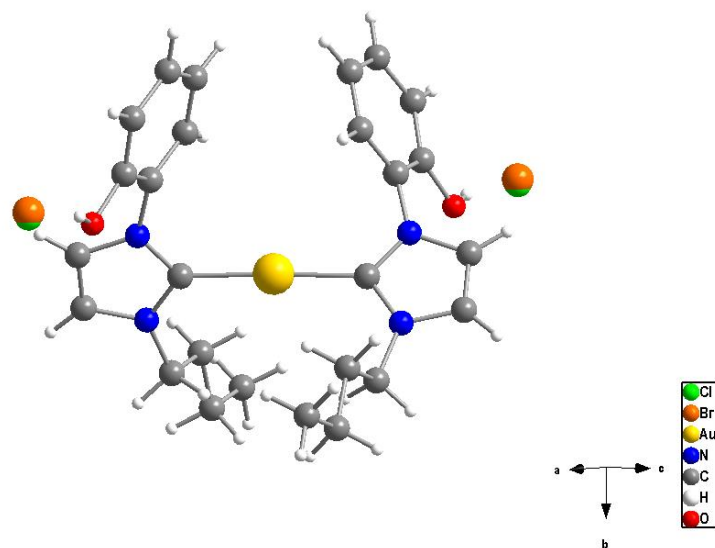


Figure S17: Molecular drawing of gold complex **9**, with disorder of the anion.

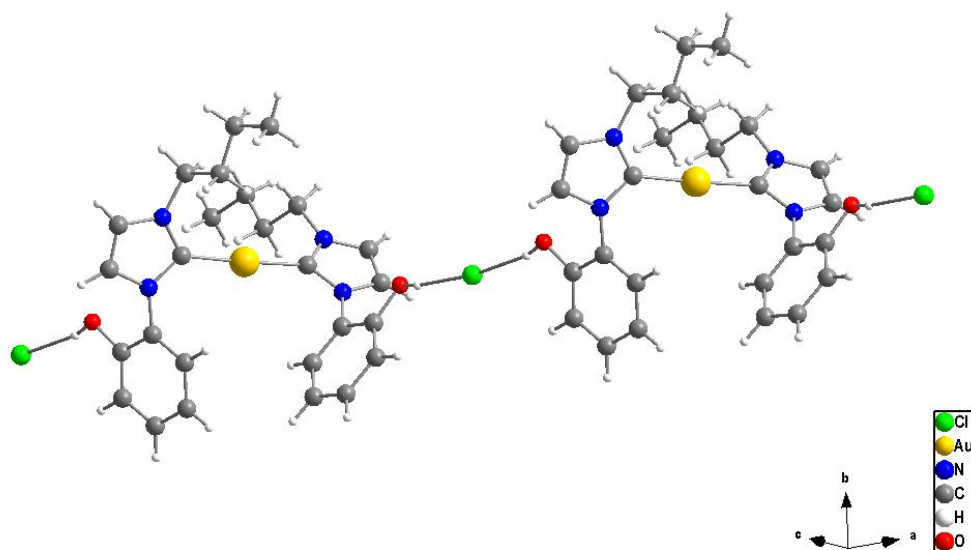


Figure S18: Molecular drawing of the dimer of the coordination polymer of the gold complex **9**; two complexes of **9** are bridged by two hydrogen bonds via the halogen (chloride) counterion.

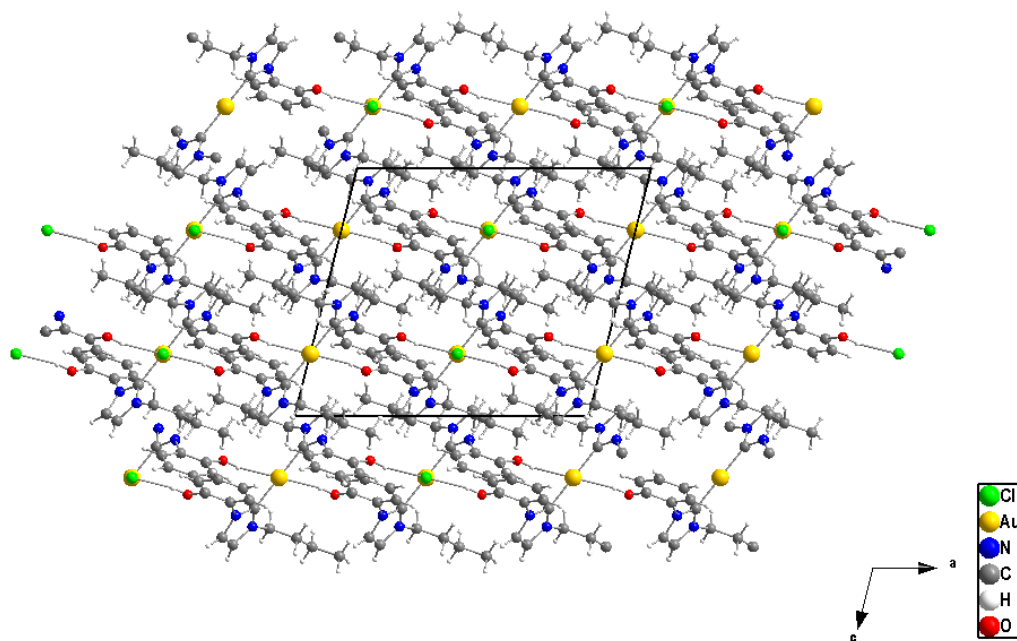


Figure S19: Unit cell of gold complex 9.

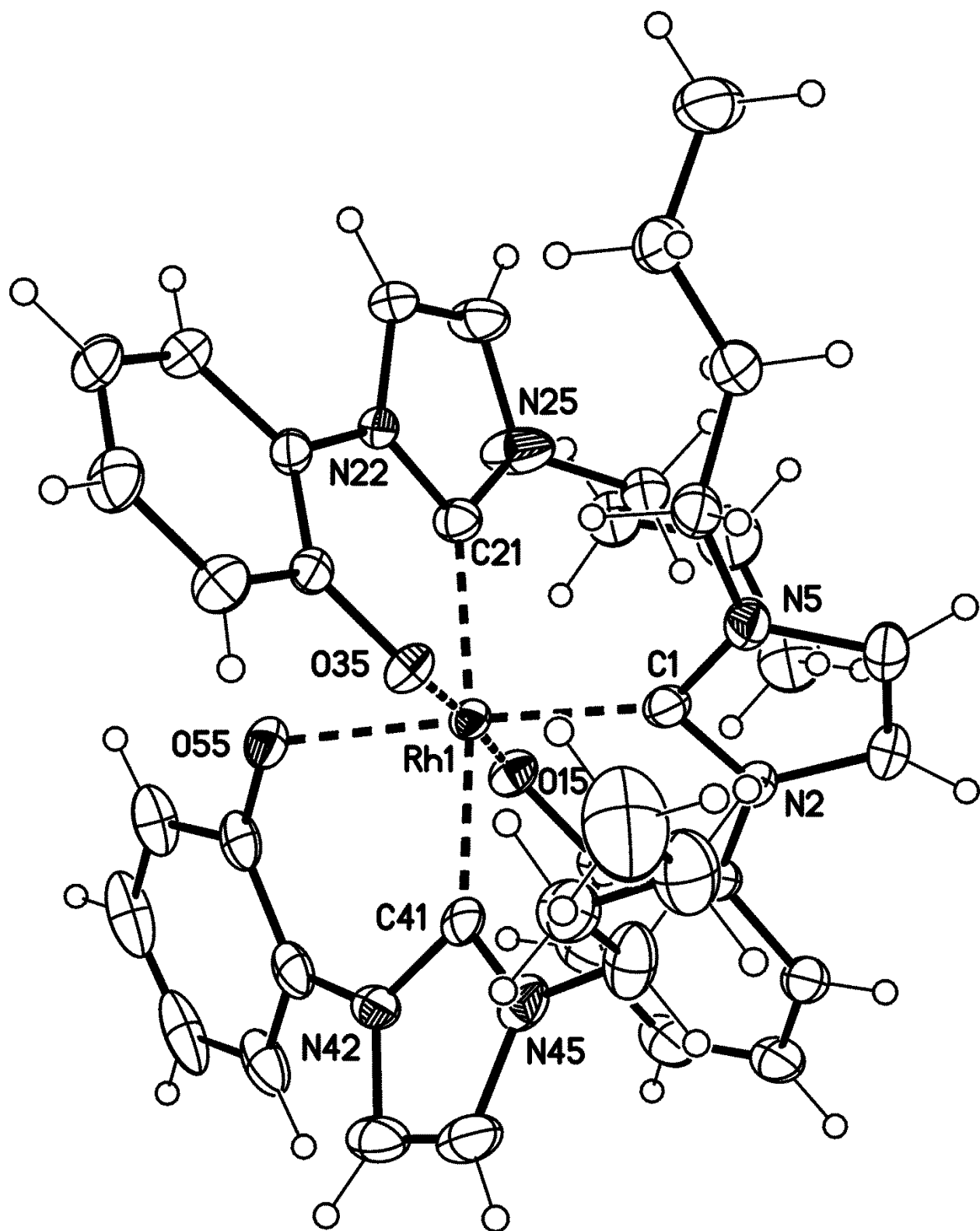


Figure S20: Molecular drawing of the rhodium complex **11** (minor disorder part omitted for clarity, displacement parameters are drawn at 50% probability level).

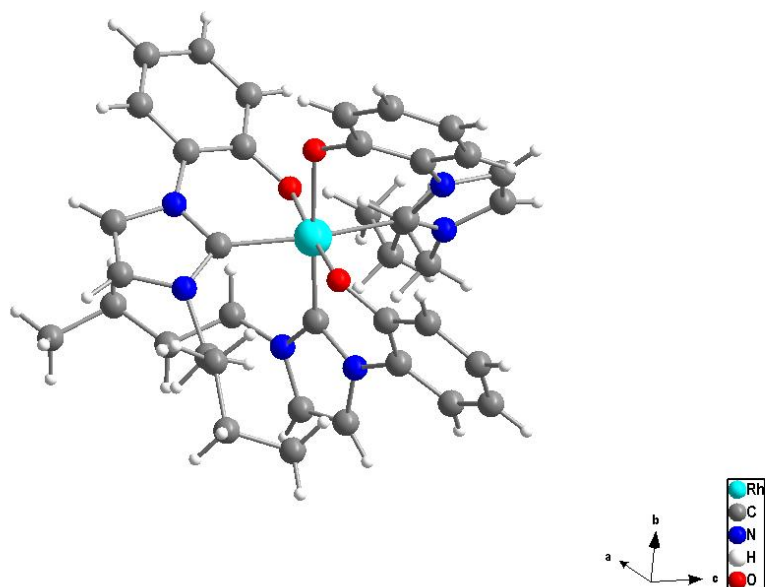


Figure S21: Molecular drawing of the rhodium complex **11**.

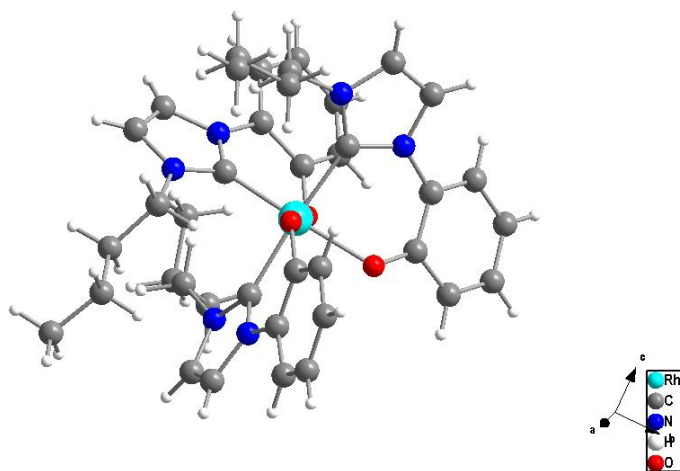


Figure S22: Molecular drawing of the rhodium complex **11**.

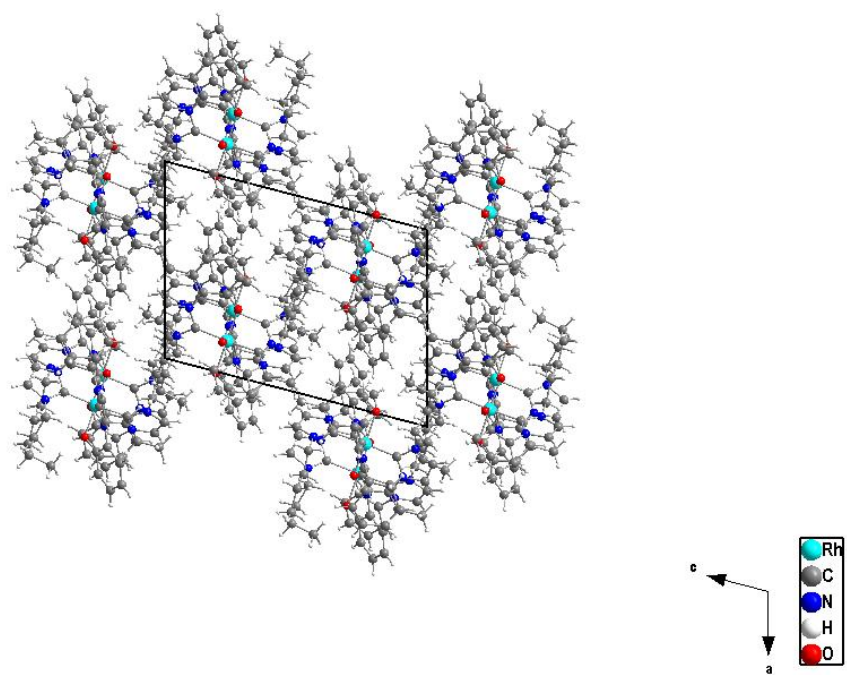


Figure S23: Unit cell of the rhodium complex **11**.

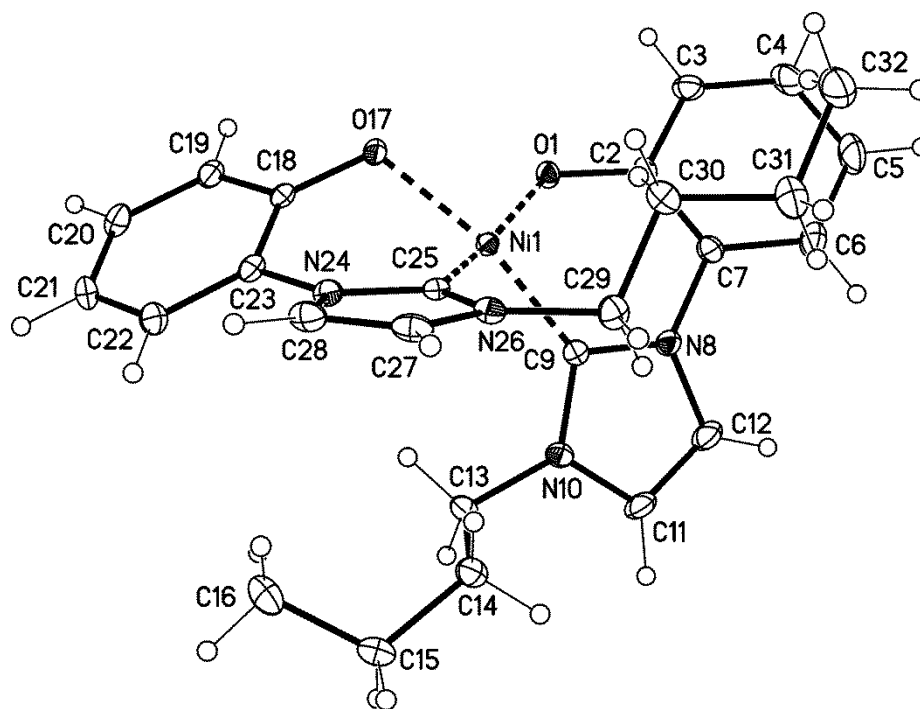


Figure S24: Molecular drawing of one of the crystallographic independent molecules of the nickel complex **12** (minor disorder part omitted for clarity, displacement parameters are drawn at 50% probability level).

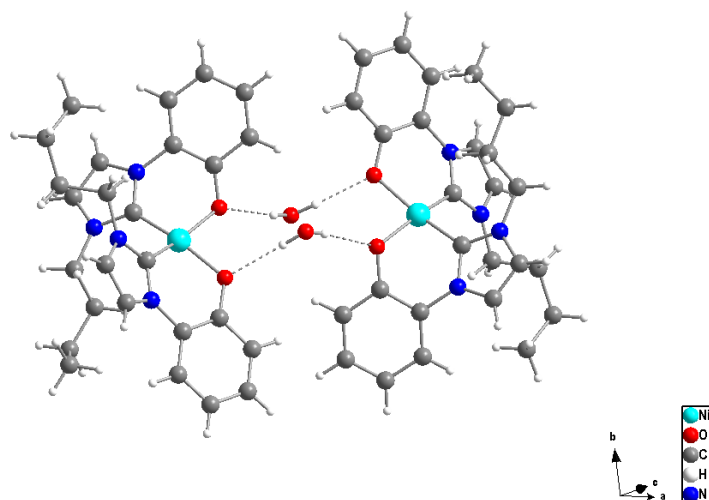


Figure S25: Molecular drawing of the dimeric nickel complex **12**.

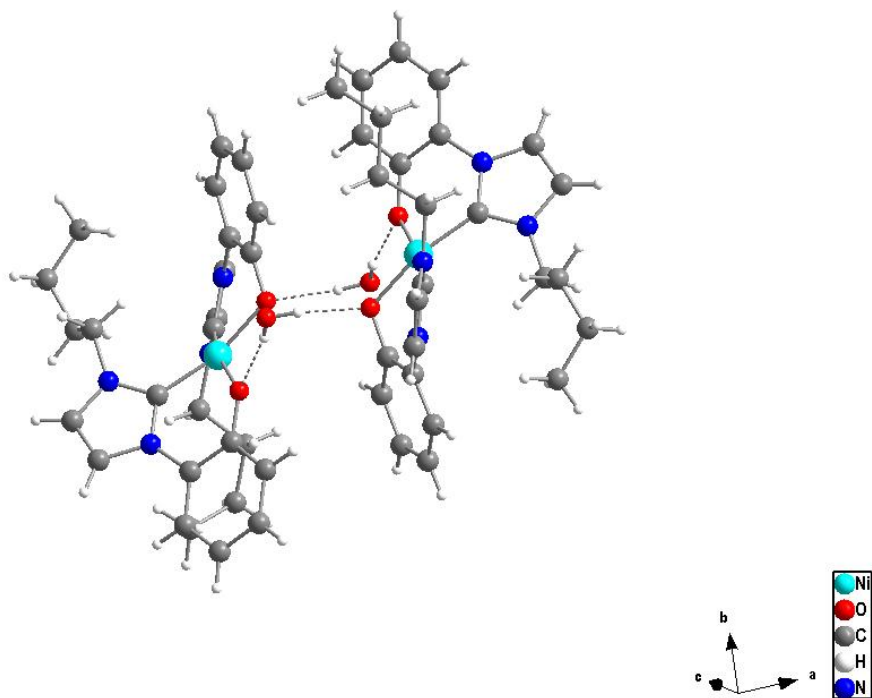


Figure S26: Molecular drawing of nickel complex 12.