

Supporting Information

for

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

Ming Liu¹, Jan C. Namyslo¹, Martin Nieger², Mika Polamo² and Andreas Schmidt*¹

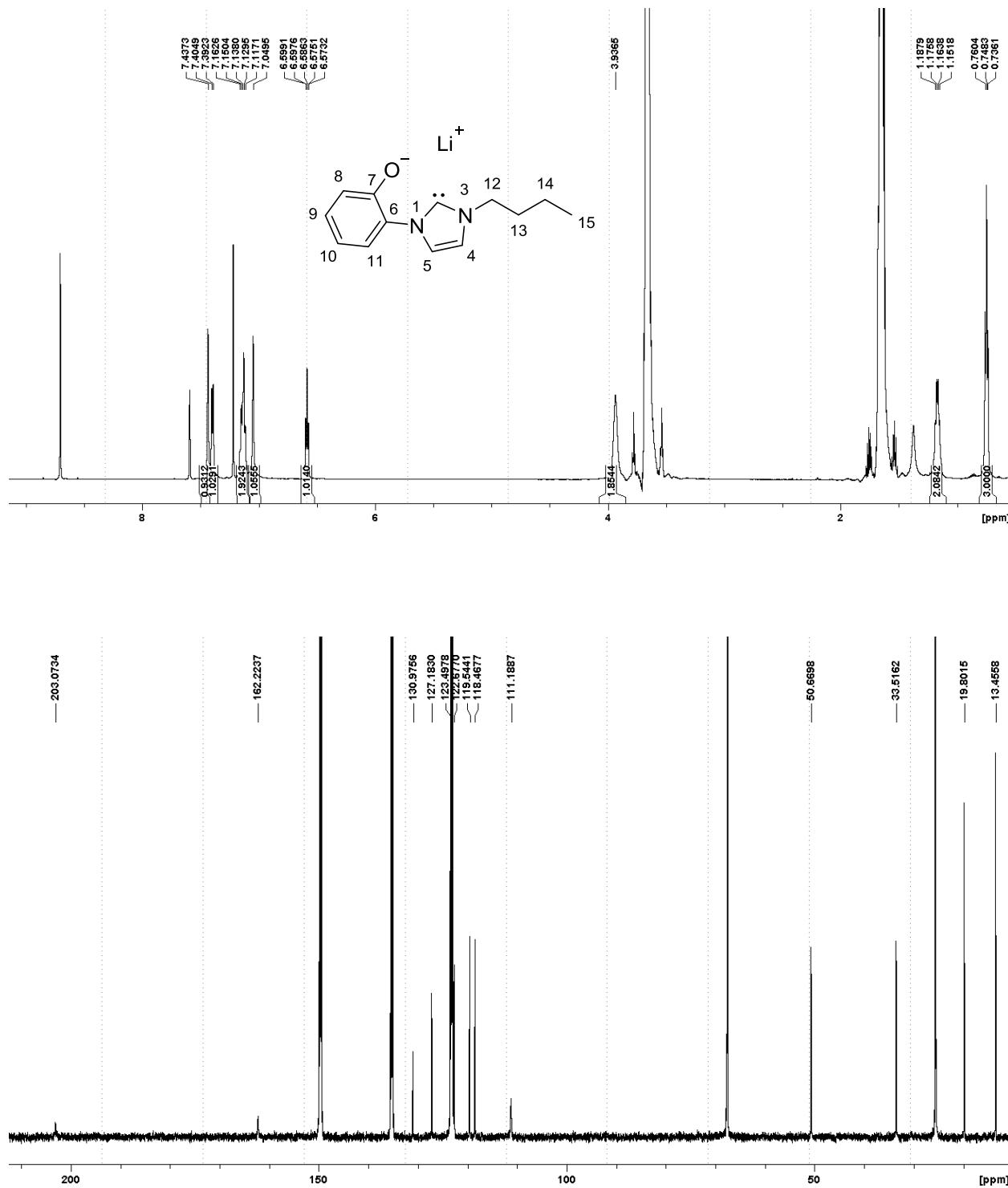
Address: ¹Clausthal University of Technology, Institute of Organic Chemistry, Leibnizstrasse 6, D-38678 Clausthal-Zellerfeld, Germany and ²University of Helsinki, Department of Chemistry, P.O. Box 55, FIN-00014 Helsinki, Finland

Email: Andreas Schmidt - schmidt@ioc.tu-clausthal.de

*Corresponding author

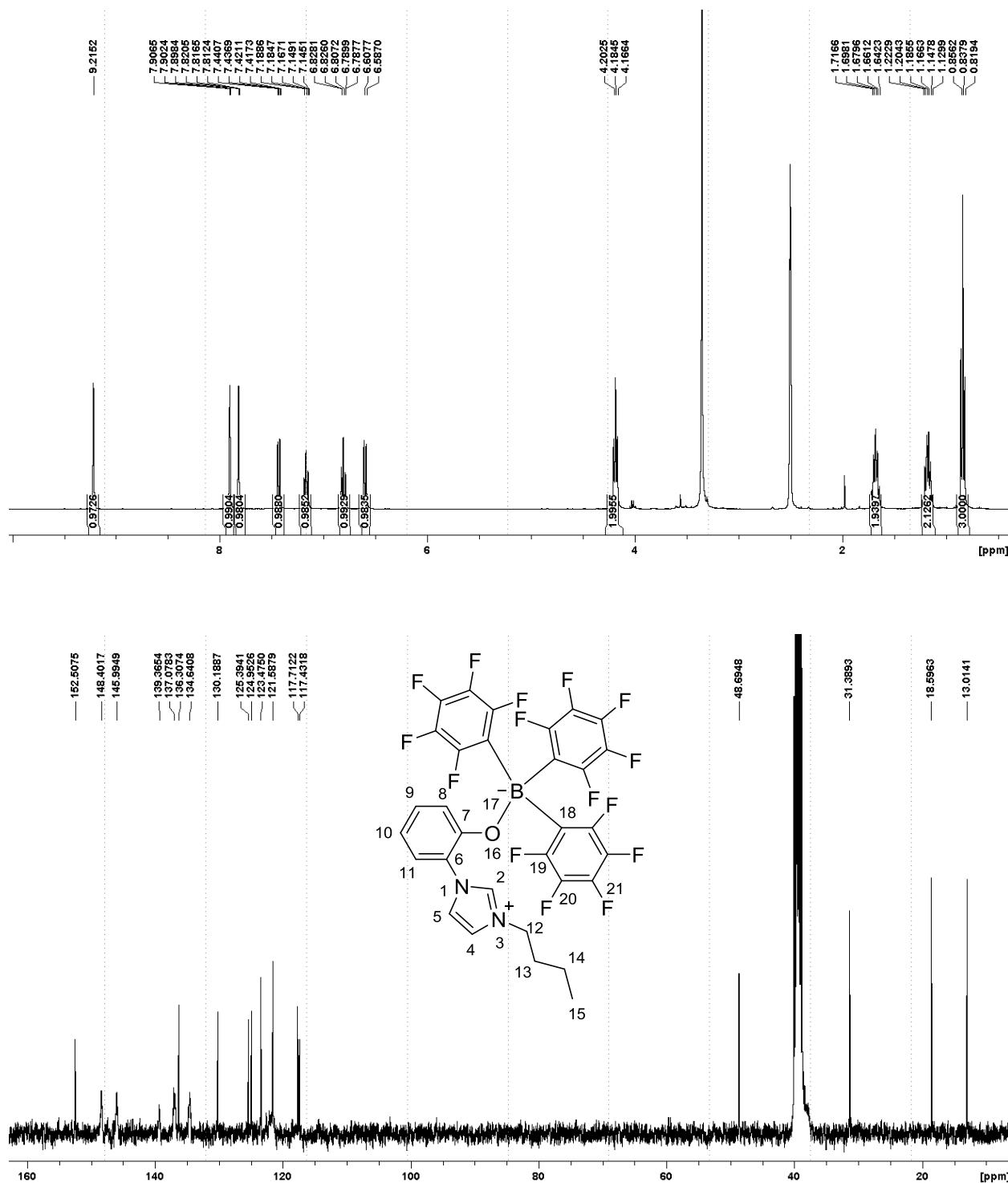
NMR spectra and molecular drawings

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

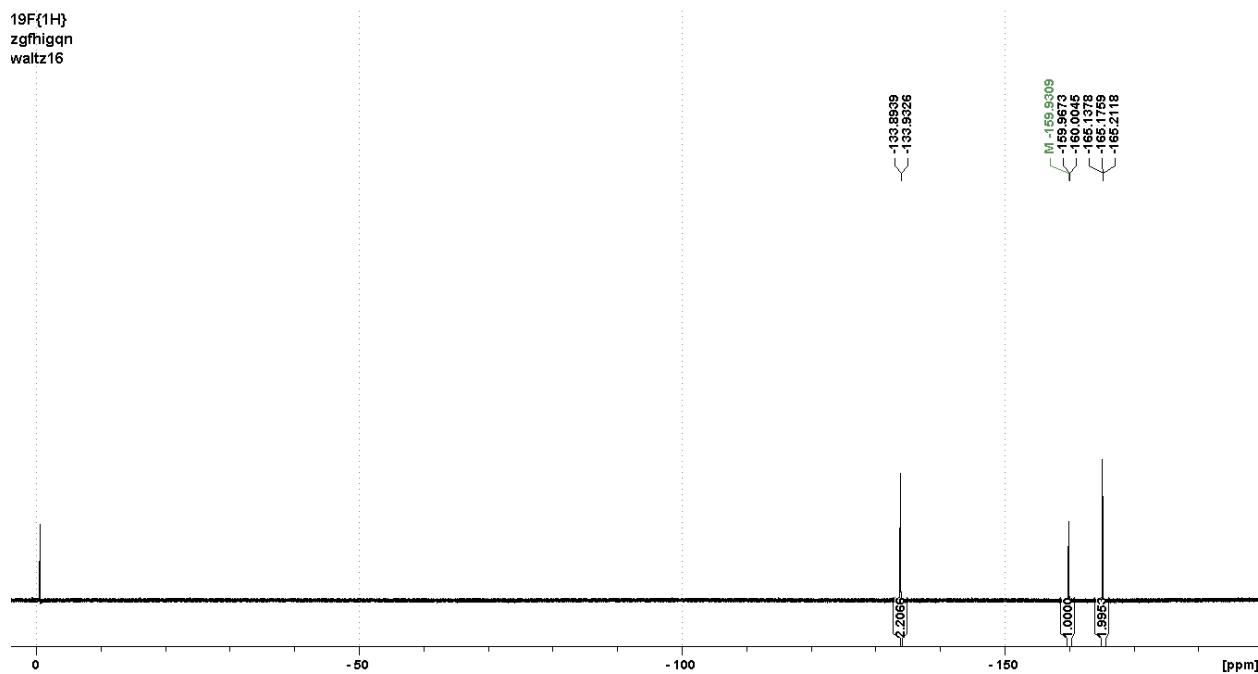
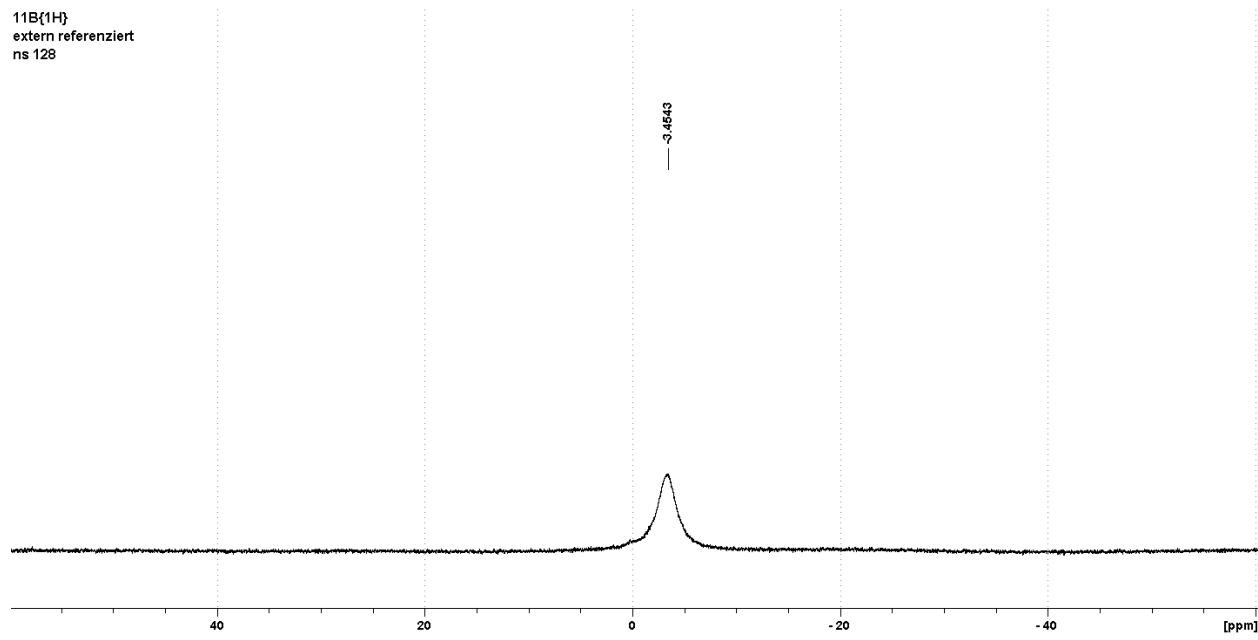


Figures S1/2: ¹H and ¹³C NMR spectra of the lithium salt of the anionic NHC 7.

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

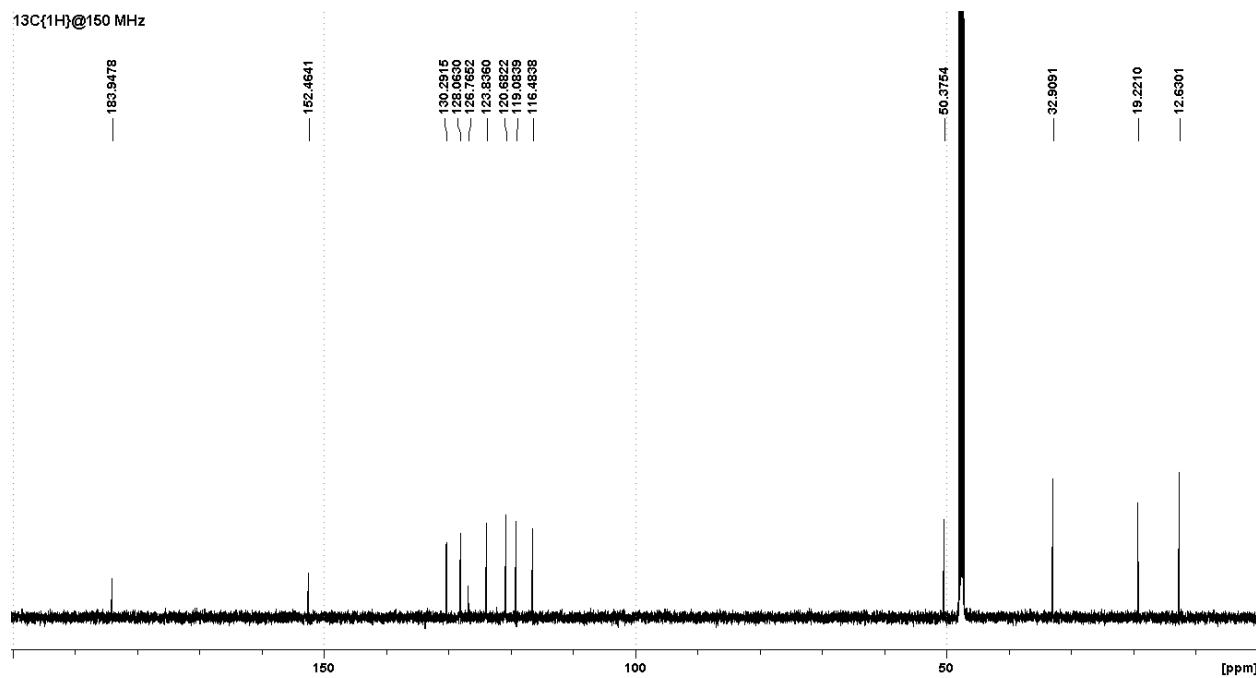
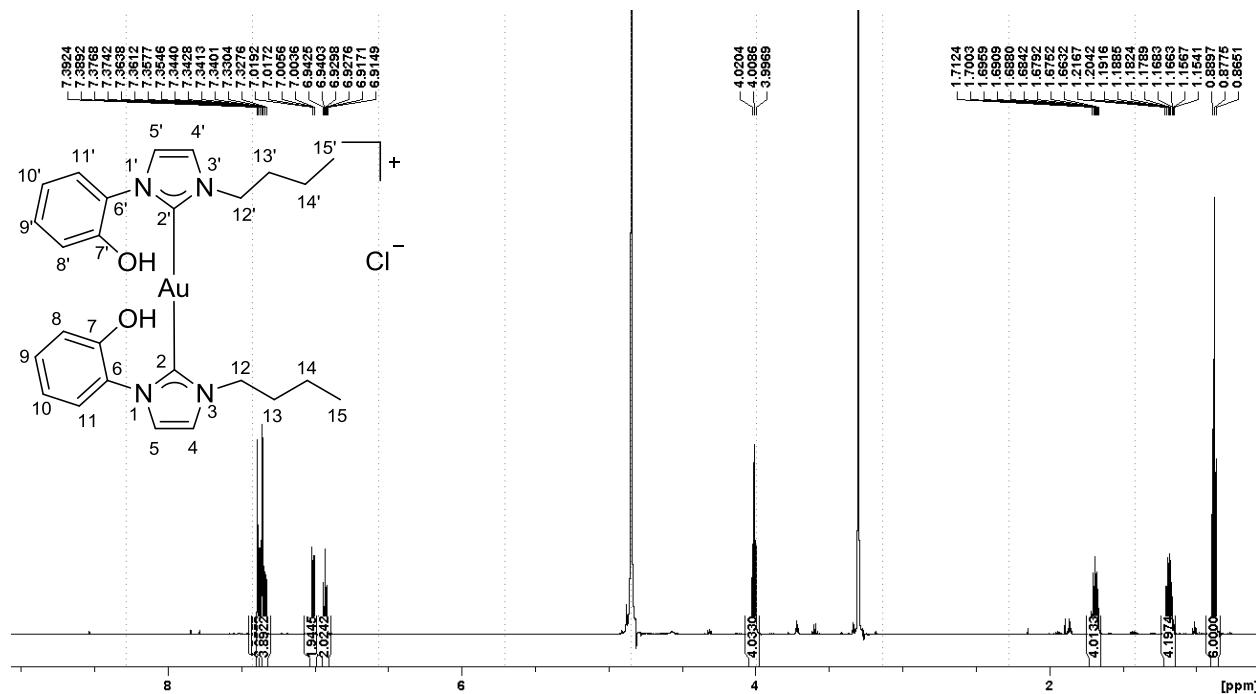


Figures S3/4: ^1H and ^{13}C NMR spectra of borane adduct **8**.



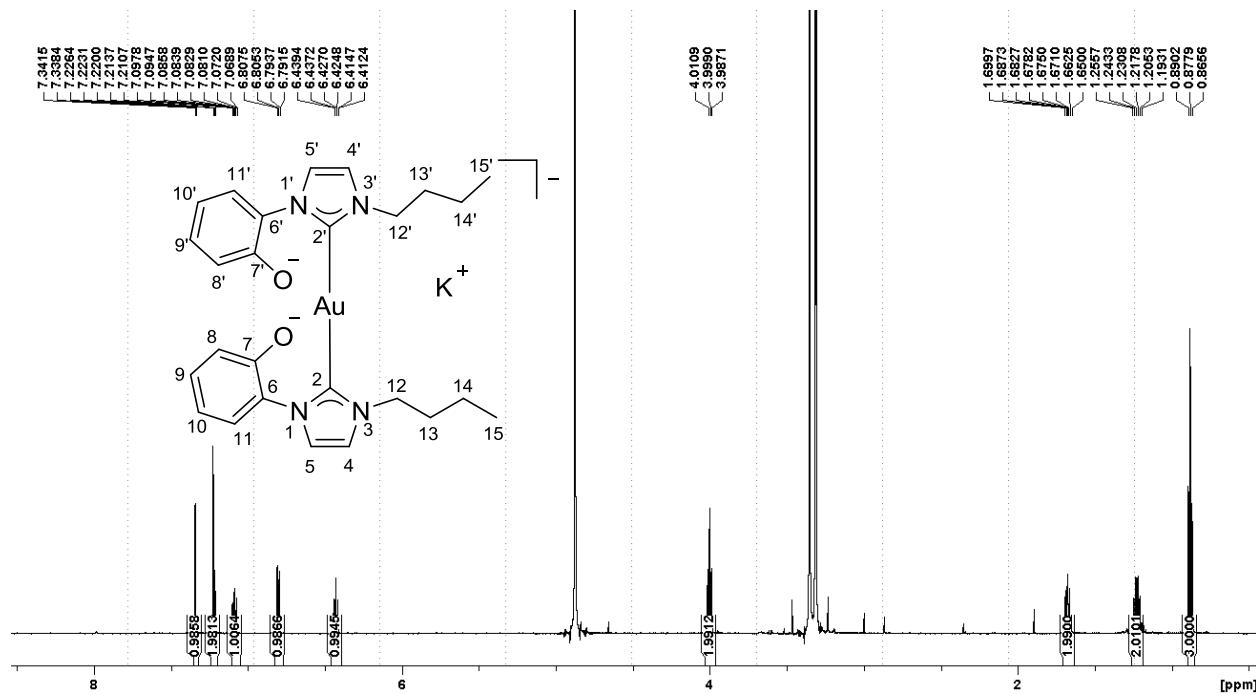
Figures S5/6: ^{11}B and ^{19}F NMR spectra of borane adduct **8**.

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

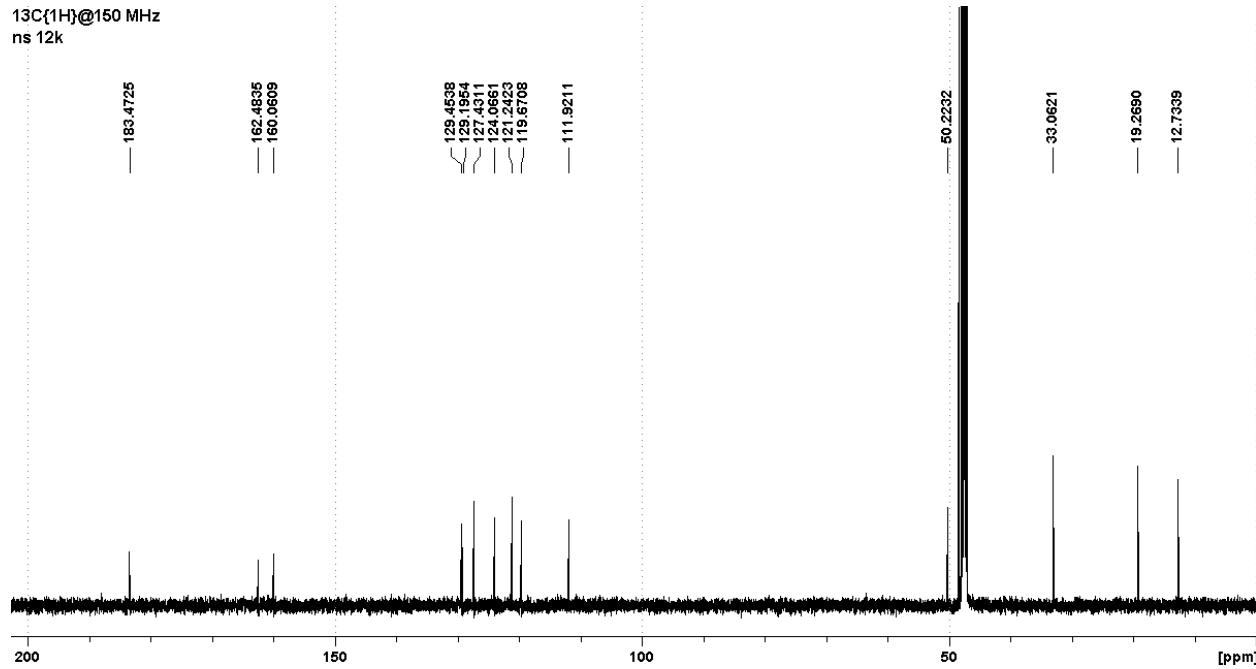


Figures S7/8: ^1H and ^{13}C NMR spectra of gold complex 9.

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

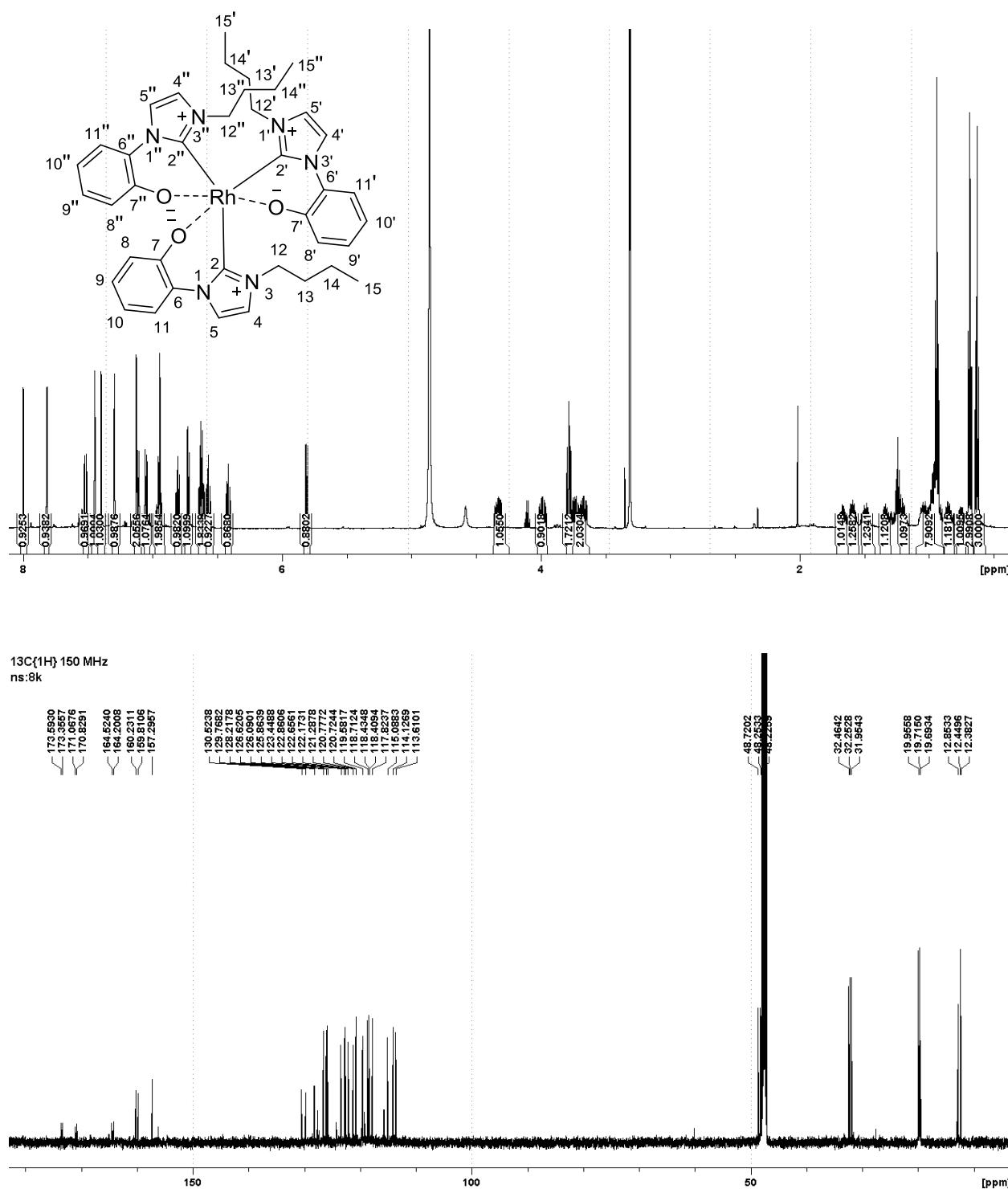


$^{13}\text{C}\{\text{H}\}$ @150 MHz
ns 12k



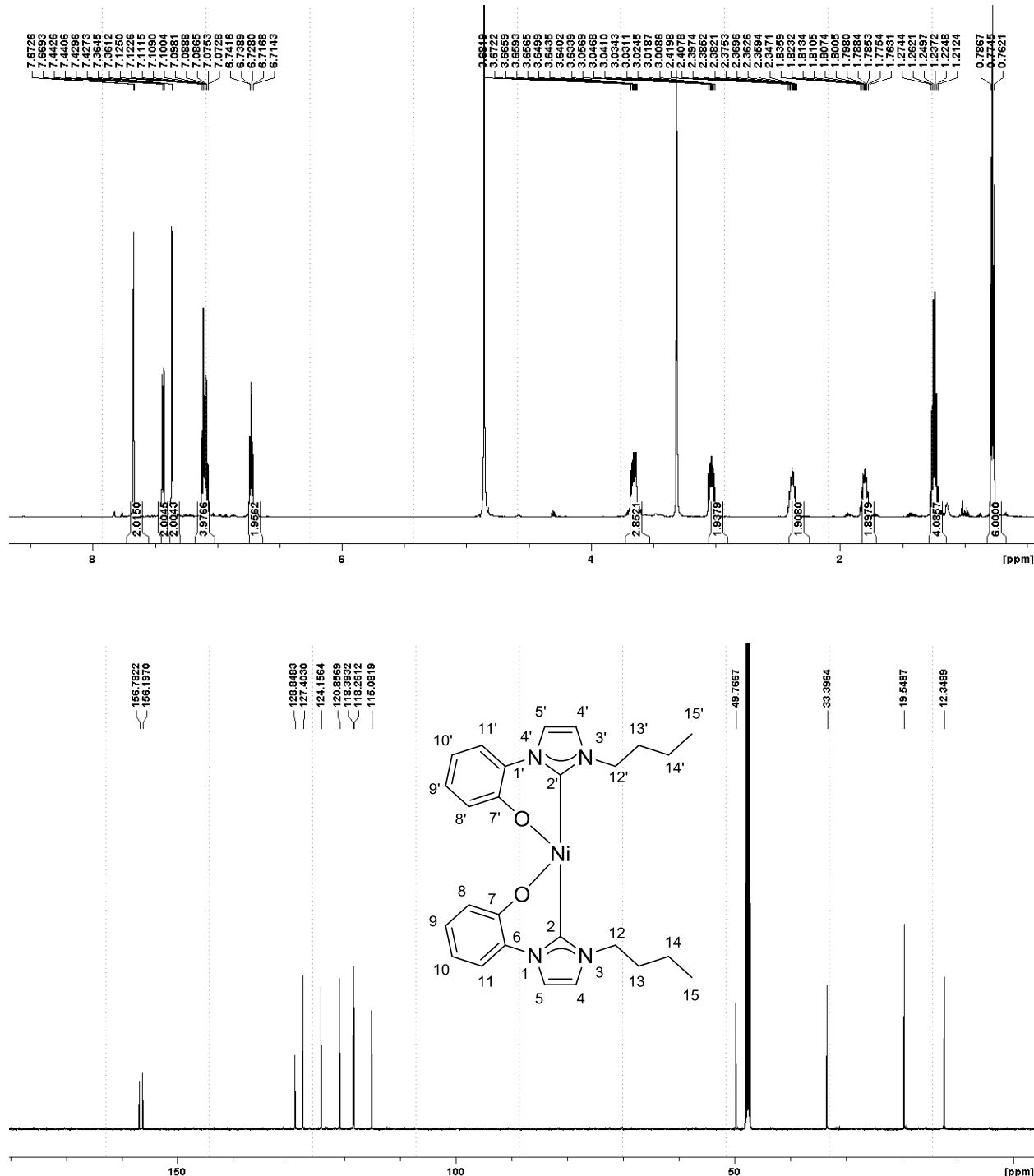
Figures S9/10: ^1H and ^{13}C NMR spectra of the anionic gold complex **10**.

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



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

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



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

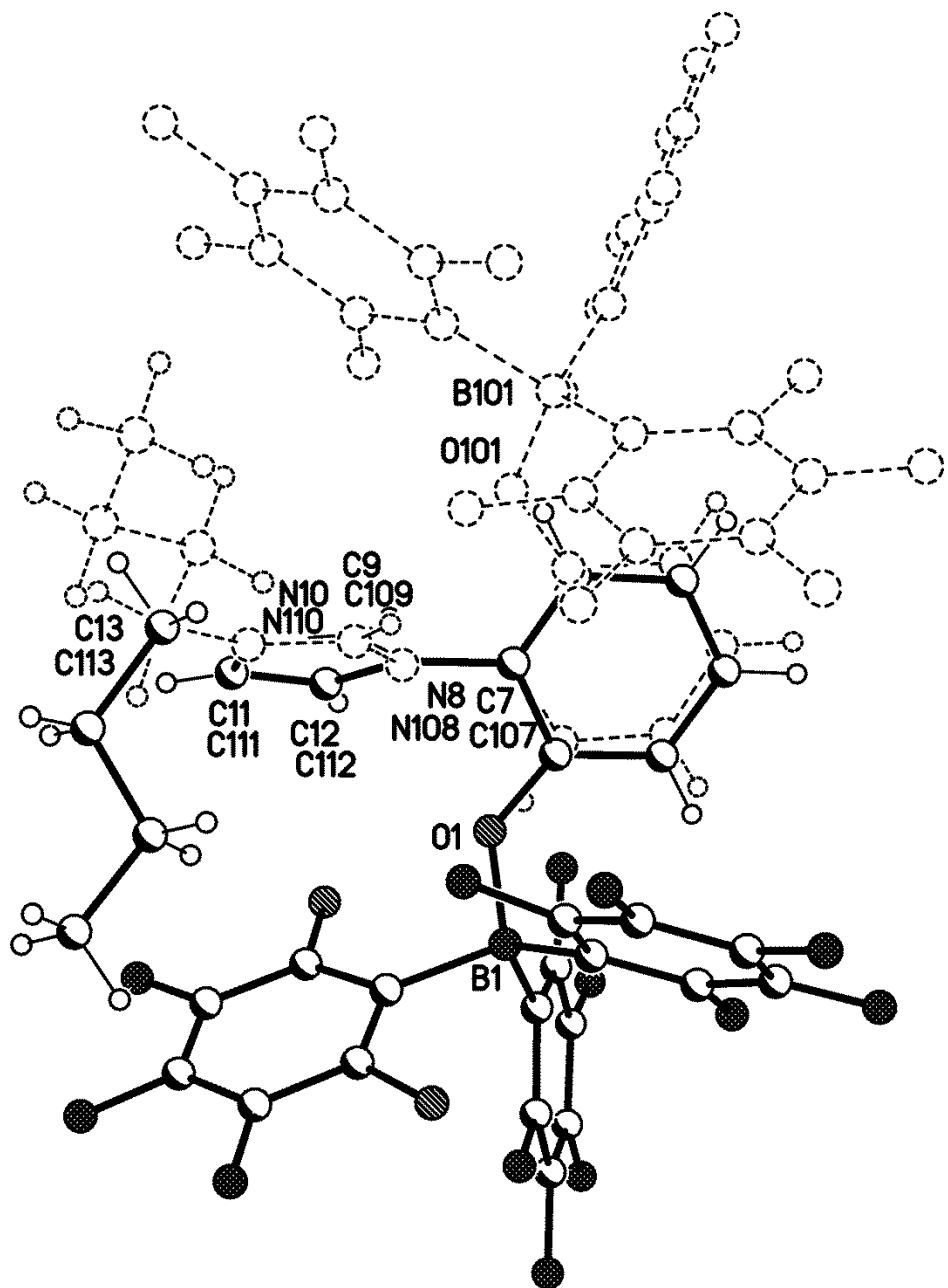


Figure S15: Fit of the two independent molecules of borane adduct **8**

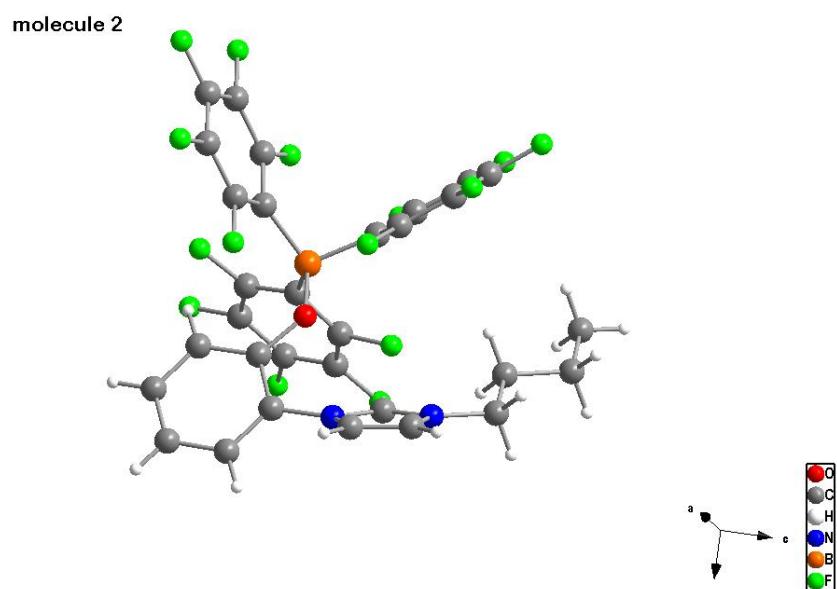
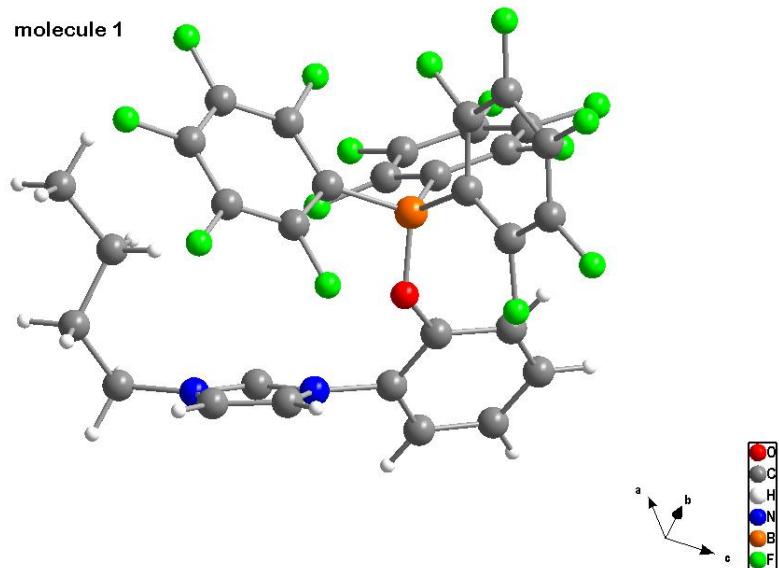


Figure S16: Drawing of the two independent molecules of borane adduct **8**.

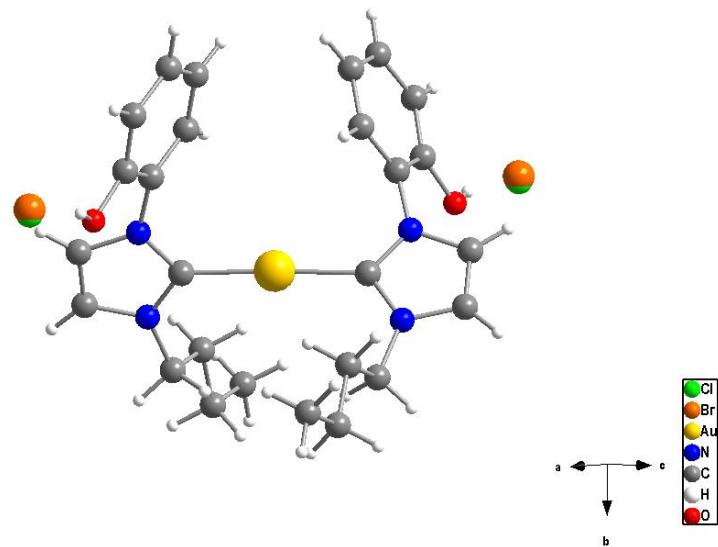


Figure S17: Molecular drawing of gold complex **9**, with disorder of the anion.

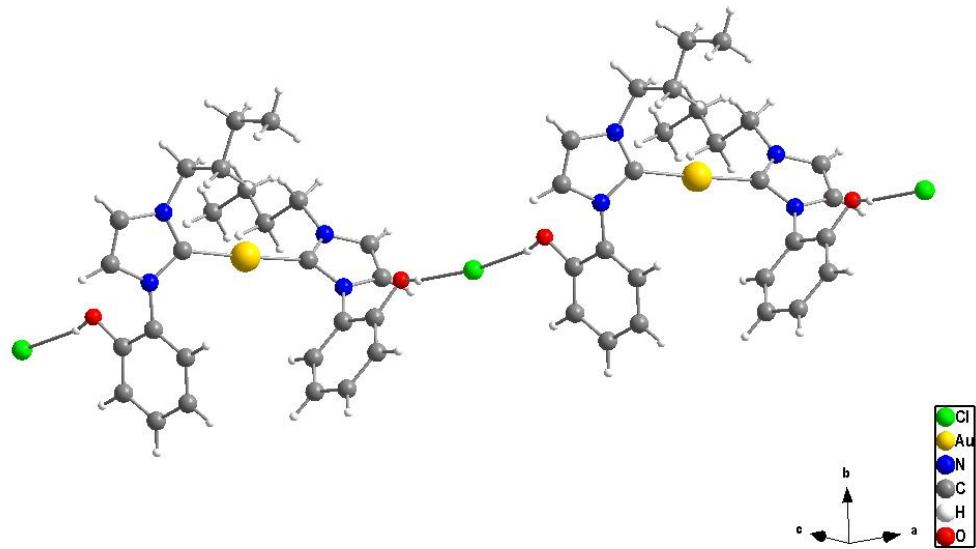


Figure S18: Molecular drawing of the dimer of the coordination polymer of the gold complex **9**; two complexes of **9** are bridged by two hydrogen bonds via the halogen (chloride) counterion.

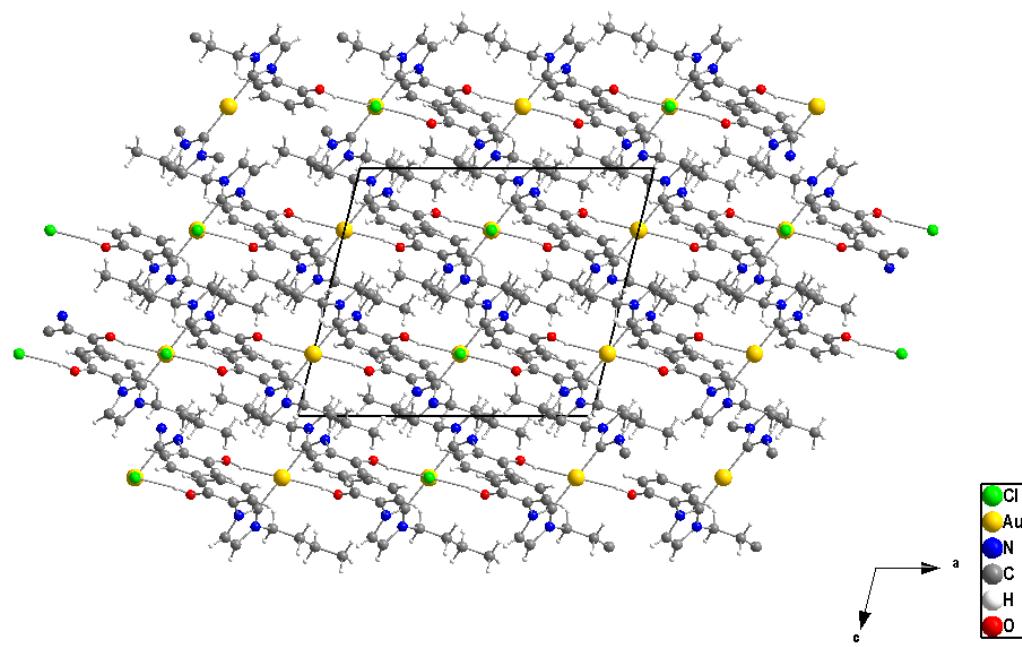


Figure S19: Unit cell of gold complex 9.

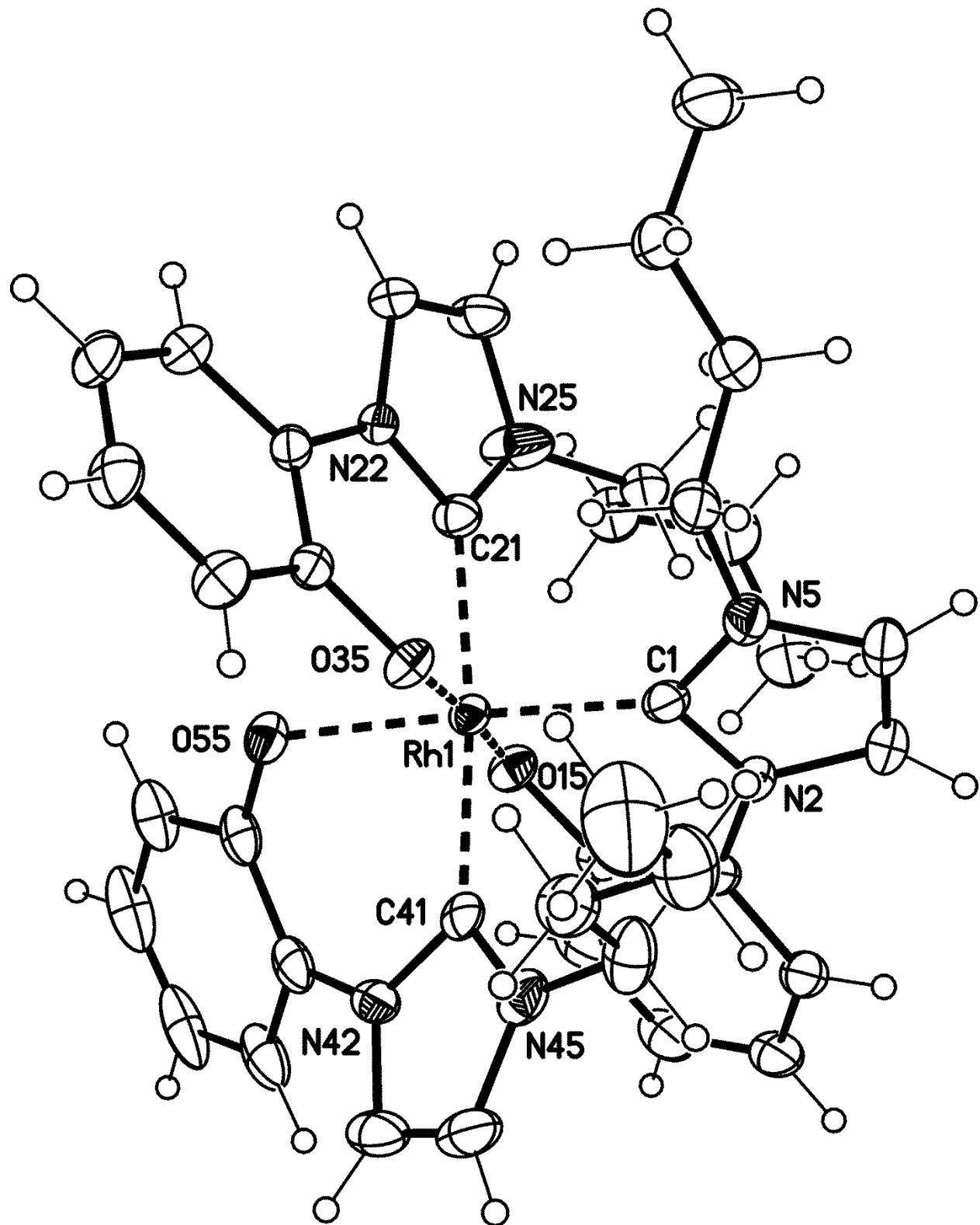


Figure S20: Molecular drawing of the rhodium complex 11 (minor disorder part omitted for clarity, displacement parameters are drawn at 50% probability level).

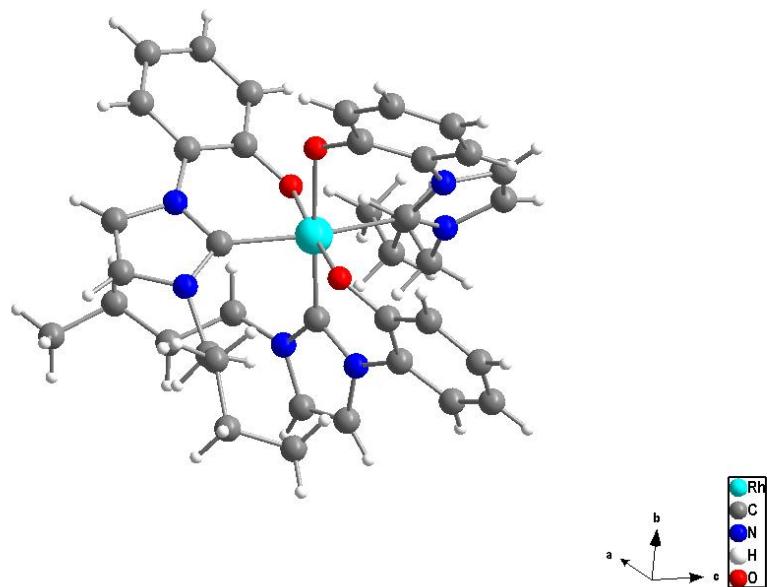


Figure S21: Molecular drawing of the rhodium complex 11.

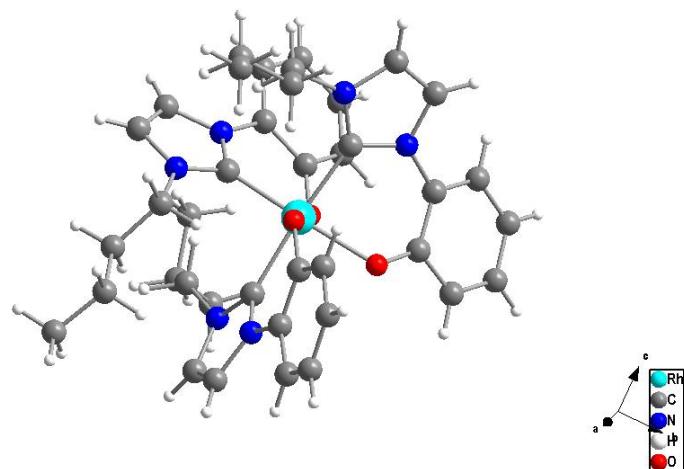


Figure S22: Molecular drawing of the rhodium complex 11.

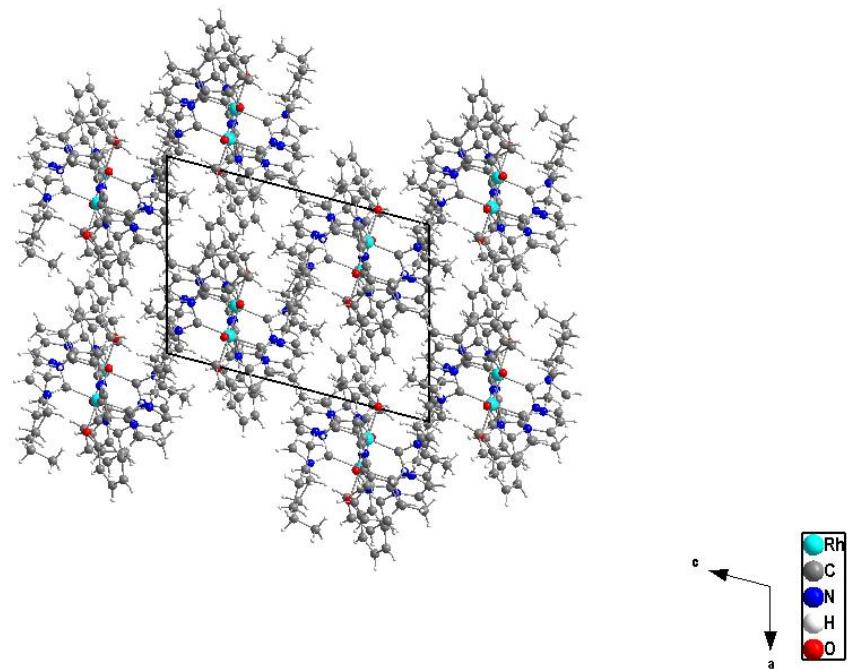


Figure S23: Unit cell of the rhodium complex 11.

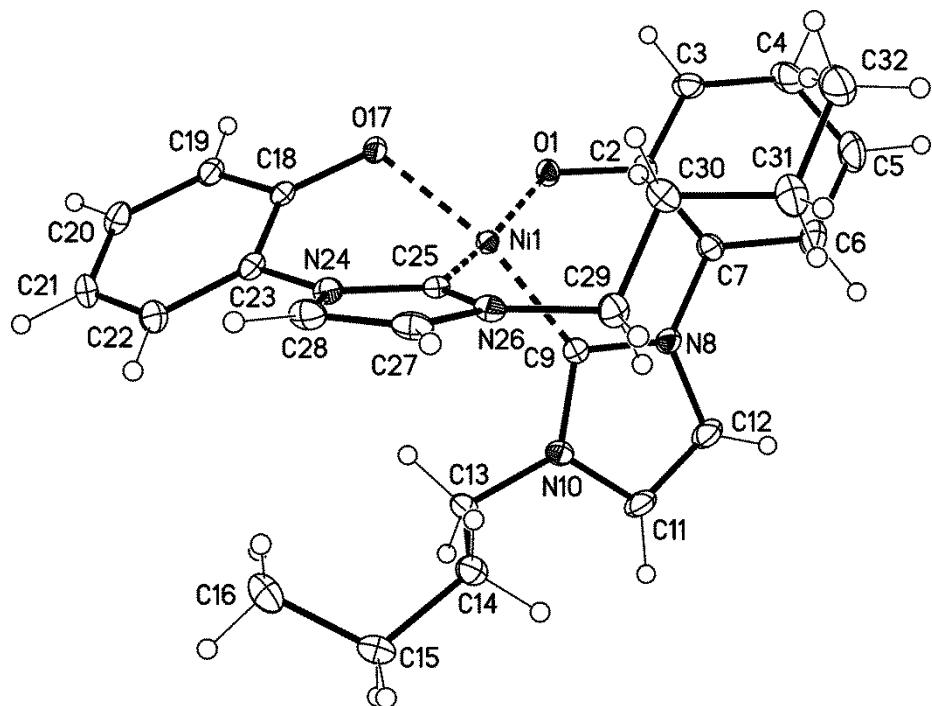


Figure S24: Molecular drawing of one of the crystallographic independent molecules of the nickel complex **12** (minor disorder part omitted for clarity, displacement parameters are drawn at 50% probability level).

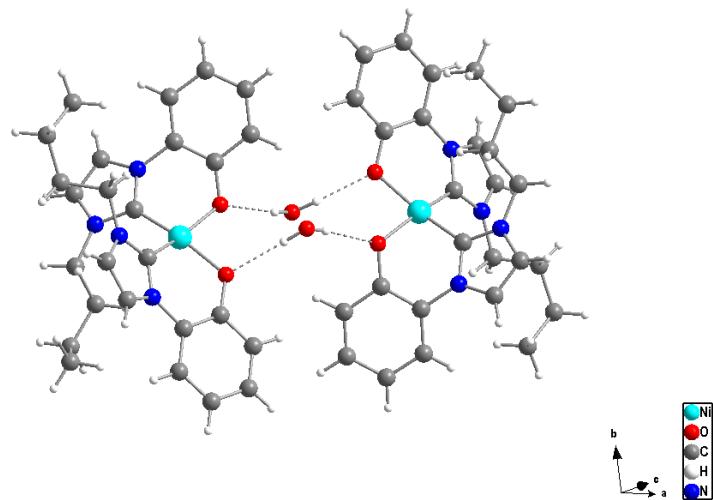


Figure S25: Molecular drawing of the dimeric nickel complex **12**.

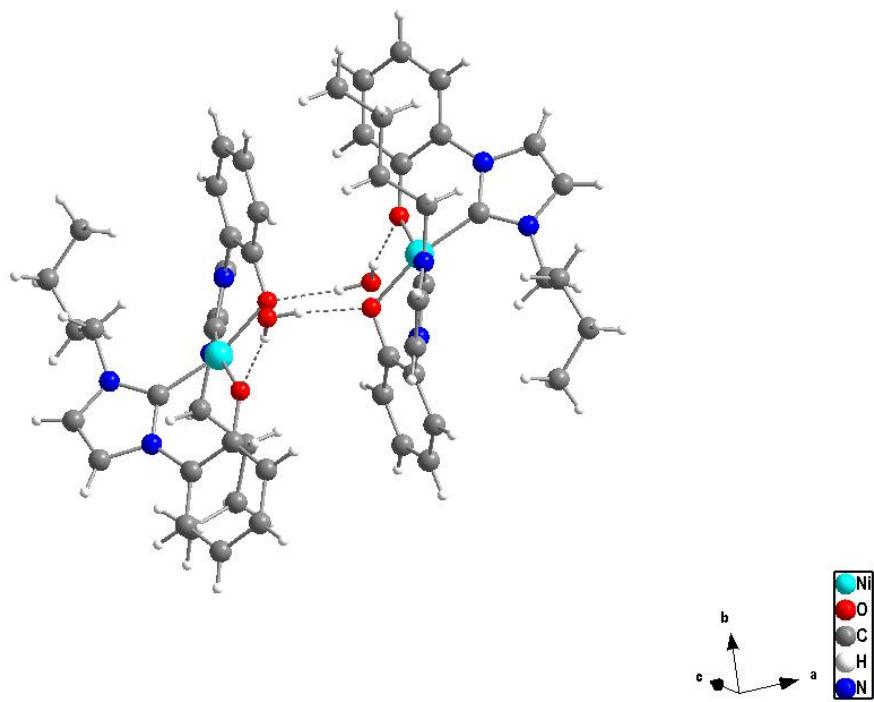


Figure S26: Molecular drawing of nickel complex **12**.